Lecture Notes on Superconductivity
(A Work in Progress)

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June 23, 2019

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Chapter 0

References

No one book contains all the relevant material. Here I list several resources, arranged by topic. My personal favorites are marked with a diamond ($\diamond$).

0.1 General Texts

- $\diamond$ P. G. De Gennes, *Superconductivity of Metals and Alloys* (Westview Press, 1999)
- $\diamond$ M. Tinkham, *Introduction to Superconductivity (2nd Edition)* (Dover, 2004)
- $\diamond$ A. A. Abrikosov, *Fundamentals of the Theory of Metals* (North-Holland, 1988)
- $\diamond$ J. R. Schrieffer, *Theory of Superconductivity* (Perseus Books, 1999)
- T. Tsuneto, *Superconductivity and Superfluidity* (Cambridge, 1999)
- J. B. Ketterson and S. N. Song, *Superconductivity* (Cambridge, 1999)
- J. F. Annett, *Superconductivity, Superfluids, and Condensates* (Oxford, 2004)
- M. Crisan, *Theory of Superconductivity* (World Scientific, 1989)
- L.-P. Levy, *Magnetism and Superconductivity* (Springer, 2000)

0.2 Organic Superconductors

- ◇ T. Ishiguro, K. Yamaji, and G. Saito, *Organic Superconductors* (2nd Edition) (Springer, 1998)

0.3 Unconventional Superconductors

- ◇ V. P. Mineev and K. Samokhin *Introduction to Unconventional Superconductivity* (CRC Press, 1989)
- M. Yu Kagan, *Modern Trends in Superconductivity and Superfluidity* (Springer, 2013)
- G. Goll, *Unconventional Superconductors : Experimental Investigation of the Order Parameter Symmetry* (Springer, 2010)
- E. Bauer and M. Sigrist, *Non-Centrosymmetric Superconductors : Introduction and Overview* (Springer, 2012)

0.4 Superconducting Devices

- ◇ K. Likharev, *Dynamics of Josephson Junctions and Circuits* (CRC Press, 1986)
- S. T. Ruggiero and D. A. Rudman, *Superconducting Devices* (Academic Press, 1990)

Chapter 1

Phenomenological Theories of Superconductivity

1.1 Basic Phenomenology of Superconductors

The superconducting state is a phase of matter, as is ferromagnetism, metallicity, *etc.* The phenomenon was discovered in the Spring of 1911 by the Dutch physicist H. Kamerlingh Onnes, who observed an abrupt vanishing of the resistivity of solid mercury at $T = 4.15\,\mathrm{K}$[1]. Under ambient pressure, there are 33 elemental superconductors[2], all of which have a metallic phase at higher temperatures, and hundreds of compounds and alloys which exhibit the phenomenon. A timeline of superconductors and their critical temperatures is provided in Fig. 1.1. The related phenomenon of superfluidity was first discovered in liquid helium below $T = 2.17\,\mathrm{K}$, at atmospheric pressure, independently in 1937 by P. Kapitza (Moscow) and by J. F. Allen and A. D. Misener (Cambridge). At some level, a superconductor may be considered as a charged superfluid – we will elaborate on this statement later on. Here we recite the basic phenomenology of superconductors:

- *Vanishing electrical resistance* : The DC electrical resistance at zero magnetic field vanishes in the superconducting state. This is established in some materials to better than one part in 10^{15} of the normal state resistance. Above the critical temperature T_c, the DC resistivity at $H = 0$ is finite. The AC resistivity remains zero up to a critical frequency, $\omega_c = 2\Delta/\hbar$, where Δ is the gap in the electronic excitation spectrum. The frequency threshold is 2Δ because the superconducting condensate is made up of electron *pairs*, so breaking a pair results in two *quasiparticles*, each with energy Δ or greater. For *weak coupling* superconductors, which are described by the famous BCS theory (1957), there is a relation between the gap energy and the superconducting transition temperature, $2\Delta_0 = 3.5\, k_B T_c$, which we derive when we study the BCS model. The gap $\Delta(T)$ is temperature-dependent and vanishes at T_c.

- *Flux expulsion* : In 1933 it was descovered by Meissner and Ochsenfeld that magnetic fields in superconducting tin and lead to not penetrate into the bulk of a superconductor, but rather are confined to a surface layer of thickness λ, called the *London penetration depth*. Typically λ in on the scale of tens to hundreds of nanometers.

  It is important to appreciate the difference between a superconductor and a perfect metal. If we set $\sigma = \infty$ then from $\boldsymbol{j} = \sigma \boldsymbol{E}$ we must have $\boldsymbol{E} = 0$, hence Faraday's law $\boldsymbol{\nabla} \times \boldsymbol{E} = -c^{-1}\partial_t \boldsymbol{B}$ yields $\partial_t \boldsymbol{B} = 0$, which

[1] Coincidentally, this just below the temperature at which helium liquefies under atmospheric pressure.
[2] An additional 23 elements are superconducting under high pressure.

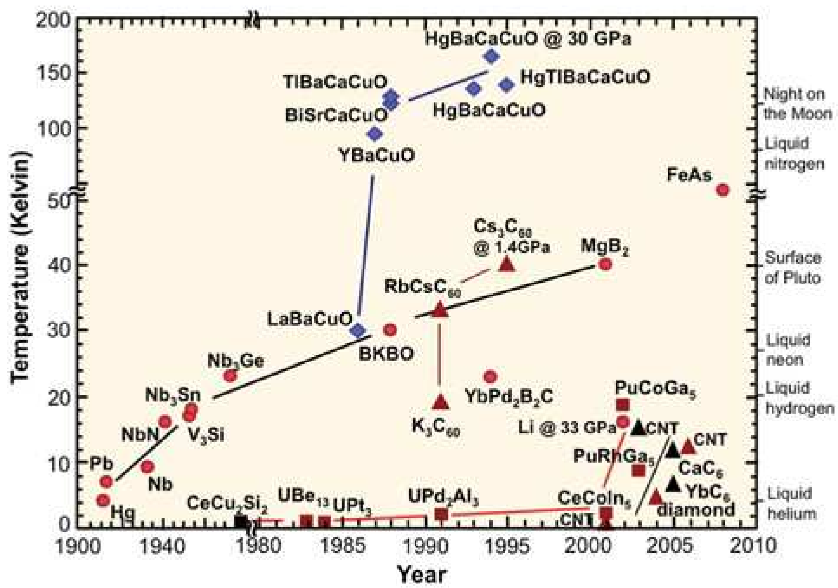

Figure 1.1: Timeline of superconductors and their transition temperatures (from Wikipedia).

says that $\boldsymbol{B}$ remains *constant* in a perfect metal. Yet Meissner and Ochsenfeld found that below T_c the flux was *expelled* from the bulk of the superconductor. If, however, the superconducting sample is not simply connected, *i.e.* if it has holes, such as in the case of a superconducting ring, then in the Meissner phase flux may be trapped in the holes. Such trapped flux is quantized in integer units of the superconducting fluxoid $\phi_L = hc/2e = 2.07 \times 10^{-7}\,\mathrm{G\,cm}^2$ (see Fig. 1.2).

- *Critical field(s)* : The Meissner state exists for $T < T_c$ only when the applied magnetic field H is smaller than the *critical field* $H_c(T)$, with
$$H_c(T) \simeq H_c(0)\left(1 - \frac{T^2}{T_c^2}\right) \quad . \tag{1.1}$$
In so-called type-I superconductors, the system goes normal[3] for $H > H_c(T)$. For most elemental type-I materials (*e.g.*, Hg, Pb, Nb, Sn) one has $H_c(0) \leq 1\,\mathrm{kG}$. In type-II materials, there are two critical fields, $H_{c1}(T)$ and $H_{c2}(T)$. For $H < H_{c1}$, we have flux expulsion, and the system is in the Meissner phase. For $H > H_{c2}$, we have uniform flux penetration and the system is normal. For $H_{c1} < H < H_{c2}$, the system in a *mixed state* in which quantized vortices of flux ϕ_L penetrate the system (see Fig. 1.3). There is a depletion of what we shall describe as the superconducting order parameter $\Psi(\boldsymbol{r})$ in the vortex cores over a length scale ξ, which is the *coherence length* of the superconductor. The upper critical field is set by the condition that the vortex cores start to overlap: $H_{c2} = \phi_L/2\pi\xi^2$. The vortex cores can be pinned by disorder. Vortices also interact with each other out to a distance λ, and at low temperatures in the absence of disorder the vortices order into a (typically triangular) *Abrikosov vortex lattice* (see Fig. 1.4). Typically one has $H_{c2} = \sqrt{2}\kappa\, H_{c1}$, where $\kappa = \lambda/\xi$ is a ratio of the two fundamental length scales. Type-II materials exist when $H_{c2} > H_{c1}$, *i.e.* when $\kappa > \frac{1}{\sqrt{2}}$. Type-II behavior tends to occur in superconducting alloys, such as Nb-Sn.

- *Persistent currents* : We have already mentioned that a metallic ring in the presence of an external magnetic field may enclosed a quantized trapped flux $n\phi_L$ when cooled below its superconducting transition temperature. If the field is now decreased to zero, the trapped flux remains, and is generated by a *persistent current* which flows around the ring. In thick rings, such currents have been demonstrated to exist undiminished for years, and may be stable for astronomically long times.

[3]Here and henceforth, "normal" is an abbreviation for "normal metal".

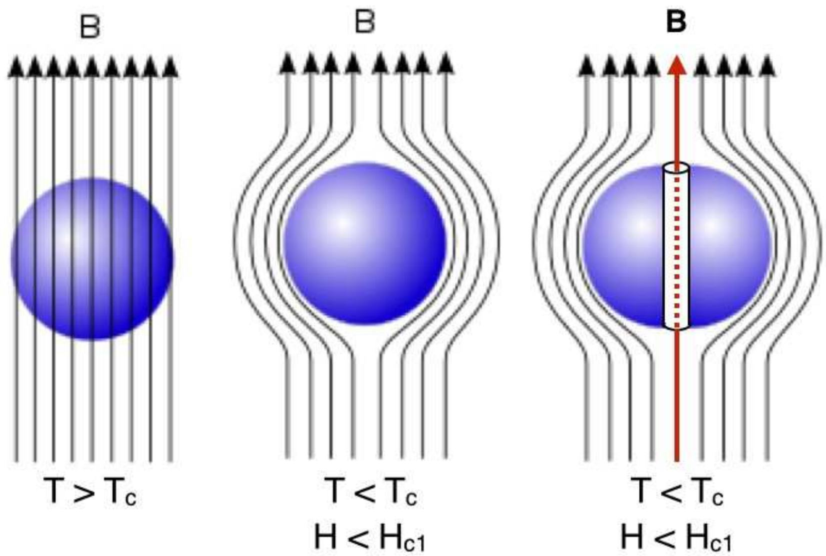

Figure 1.2: Flux expulsion from a superconductor in the Meissner state. In the right panel, quantized trapped flux penetrates a hole in the sample.

- *Specific heat jump* : The heat capacity of metals behaves as $c_V \equiv C_V/V = \frac{\pi^2}{3}\, k_\text{B}^2 T g(\varepsilon_\text{F})$, where $g(\varepsilon_\text{F})$ is the density of states at the Fermi level. In a superconductor, once one subtracts the low temperature phonon contribution $c_V^\text{phonon} = AT^3$, one is left for $T < T_\text{c}$ with an electronic contribution behaving as $c_V^\text{elec} \propto e^{-\Delta/k_\text{B}T}$. There is also a jump in the specific heat at $T = T_\text{c}$, the magnitude of which is generally about three times the normal specific heat just above T_c. This jump is consistent with a second order transition with critical exponent $\alpha = 0$.
- *Tunneling and Josephson effect* : The energy gap in superconductors can be measured by electron tunneling between a superconductor and a normal metal, or between two superconductors separated by an insulating layer. In the case of a weak link between two superconductors, current can flow at zero bias voltage, a situation known as the *Josephson effect*.

1.2 Thermodynamics of Superconductors

The differential free energy density of a magnetic material is given by

$$df = -s\, dT + \frac{1}{4\pi}\, \boldsymbol{H} \cdot d\boldsymbol{B} \quad , \tag{1.2}$$

which says that $f = f(T, \boldsymbol{B})$. Here s is the entropy density, and $\boldsymbol{B}$ the magnetic field. The quantity $\boldsymbol{H}$ is called the *magnetizing field* and is thermodynamically conjugate to $\boldsymbol{B}$:

$$s = -\left(\frac{\partial f}{\partial T}\right)_{\boldsymbol{B}} \quad , \quad \boldsymbol{H} = 4\pi \left(\frac{\partial f}{\partial \boldsymbol{B}}\right)_T \quad . \tag{1.3}$$

In the Ampère-Maxwell equation, $\nabla \times \boldsymbol{H} = 4\pi c^{-1} \boldsymbol{j}_\text{ext} + c^{-1} \partial_t \boldsymbol{D}$, the sources of $\boldsymbol{H}$ appear on the RHS[4]. Usually $c^{-1}\partial_t \boldsymbol{D}$ is negligible, in which $\boldsymbol{H}$ is generated by external sources such as magnetic solenoids. The magnetic field

[4]Throughout these notes, RHS/LHS will be used to abbreviate "right/left hand side".

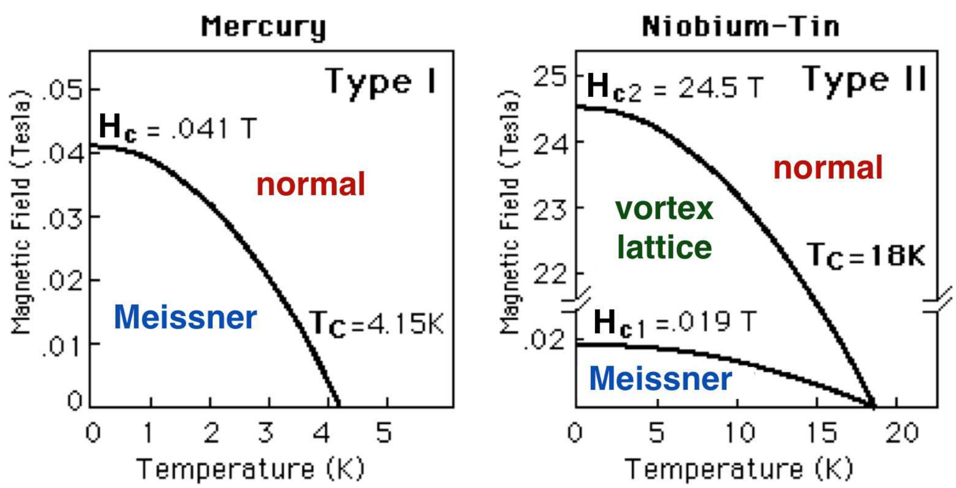

Figure 1.3: Phase diagrams for type I and type II superconductors in the (T, H) plane.

$\boldsymbol{B}$ is given by $\boldsymbol{B} = \boldsymbol{H} + 4\pi\boldsymbol{M} \equiv \mu\boldsymbol{H}$, where $\boldsymbol{M}$ is the magnetization density. We therefore have no direct control over $\boldsymbol{B}$, and it is necessary to discuss the thermodynamics in terms of the Gibbs free energy density, $g(T, \boldsymbol{H})$:

$$\begin{aligned} g(T,\boldsymbol{H}) &= f(T,\boldsymbol{B}) - \frac{1}{4\pi}\boldsymbol{B}\cdot\boldsymbol{H} \\ dg &= -s\,dT - \frac{1}{4\pi}\,\boldsymbol{B}\cdot d\boldsymbol{H} \quad . \end{aligned} \tag{1.4}$$

Thus,

$$s = -\left(\frac{\partial g}{\partial T}\right)_{\boldsymbol{H}} \quad , \quad \boldsymbol{B} = -4\pi\left(\frac{\partial g}{\partial \boldsymbol{H}}\right)_T \quad . \tag{1.5}$$

Assuming a bulk sample which is isotropic, we then have

$$g(T,H) = g(T,0) - \frac{1}{4\pi}\int\limits_0^H dH'\,B(H') \quad . \tag{1.6}$$

In a normal metal, $\mu \approx 1$ (cgs units), which means $B \approx H$, which yields

$$g_{\rm n}(T,H) = g_{\rm n}(T,0) - \frac{H^2}{8\pi} \quad . \tag{1.7}$$

In the Meissner phase of a superconductor, $B = 0$, so

$$g_{\rm s}(T,H) = g_{\rm s}(T,0) \quad . \tag{1.8}$$

For a type-I material, the free energies cross at $H = H_{\rm c}$, so

$$g_{\rm s}(T,0) = g_{\rm n}(T,0) - \frac{H_{\rm c}^2}{8\pi} \quad , \tag{1.9}$$

which says that there is a negative *condensation energy density* $-\frac{H_{\rm c}^2(T)}{8\pi}$ which stabilizes the superconducting phase. We call $H_{\rm c}$ the *thermodynamic critical field*. We may now write

$$g_{\rm s}(T,H) - g_{\rm n}(T,H) = \frac{1}{8\pi}\Big(H^2 - H_{\rm c}^2(T)\Big) \quad , \tag{1.10}$$

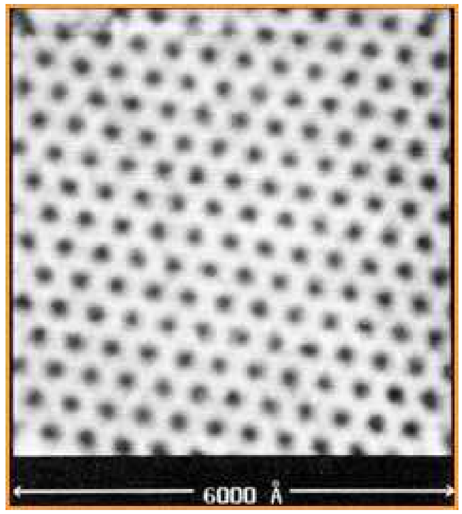

Figure 1.4: STM image of a vortex lattice in $NbSe_2$ at $H = 1\,\mathrm{T}$ and $T = 1.8\,\mathrm{K}$. From H. F. Hess *et al.*, *Phys. Rev. Lett.* **62**, 214 (1989).

so the superconductor is the equilibrium state for $H < H_c$. Taking the derivative with respect to temperature, the entropy difference is given by

$$s_s(T,H) - s_n(T,H) = \frac{1}{4\pi}\,H_c(T)\,\frac{dH_c(T)}{dT} < 0 \quad , \tag{1.11}$$

since $H_c(T)$ is a decreasing function of temperature. Note that the entropy difference is independent of the external magnetizing field H. As we see from Fig. 1.3, the derivative $H_c'(T)$ changes discontinuously at $T = T_c$. The latent heat $\ell = T\,\Delta s$ vanishes because $H_c(T_c)$ itself vanishes, but the specific heat is discontinuous:

$$c_s(T_c, H=0) - c_n(T_c, H=0) = \frac{T_c}{4\pi}\left(\frac{dH_c(T)}{dT}\right)^2_{T_c} \quad , \tag{1.12}$$

and from the phenomenological relation of Eqn. 1.1, we have $H_c'(T_c) = -2H_c(0)/T_c$, hence

$$\Delta c \equiv c_s(T_c, H=0) - c_n(T_c, H=0) = \frac{H_c^2(0)}{\pi T_c} \quad . \tag{1.13}$$

We can appeal to Eqn. 1.11 to compute the difference $\Delta c(T,H)$ for general $T < T_c$:

$$\Delta c(T,H) = \frac{T}{8\pi}\,\frac{d^2}{dT^2}\,H_c^2(T) \quad . \tag{1.14}$$

With the approximation of Eqn. 1.1, we obtain

$$c_s(T,H) - c_n(T,H) \simeq \frac{T H_c^2(0)}{2\pi T_c^2}\left\{3\left(\frac{T}{T_c}\right)^2 - 1\right\} \quad . \tag{1.15}$$

In the limit $T \to 0$, we expect $c_s(T)$ to vanish exponentially as $e^{-\Delta/k_B T}$, hence we have $\Delta c(T \to 0) = -\gamma T$, where γ is the coefficient of the linear T term in the metallic specific heat. Thus, we expect $\gamma \simeq H_c^2(0)/2\pi T_c^2$. Note also

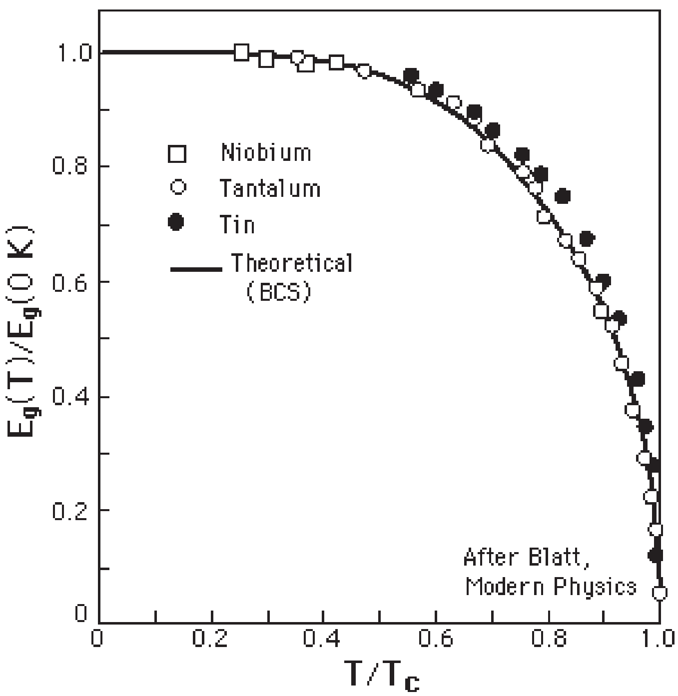

Figure 1.5: Dimensionless energy gap $\Delta(T)/\Delta_0$ in niobium, tantalum, and tin. The solid curve is the prediction from BCS theory, derived in chapter 3 below.

that this also predicts the ratio $\Delta c(T_c, 0)/c_n(T_c, 0) = 2$. In fact, within BCS theory, as we shall later show, this ratio is approximately 1.43. BCS also yields the low temperature form

$$H_c(T) = H_c(0) \left\{ 1 - \alpha \left(\frac{T}{T_c} \right)^2 + \mathcal{O}\big(e^{-\Delta/k_B T}\big) \right\} \tag{1.16}$$

with $\alpha \simeq 1.07$. Thus, $H_c^{BCS}(0) = \big(2\pi\gamma T_c^2/\alpha\big)^{1/2}$.

1.3 London Theory

Fritz and Heinz London in 1935 proposed a two fluid model for the macroscopic behavior of superconductors. The two fluids are: (i) the normal fluid, with electron number density n_n, which has finite resistivity, and (ii) the superfluid, with electron number density n_s, and which moves with zero resistance. The associated velocities are v_n and v_s, respectively. Thus, the total number density and current density are

$$\begin{aligned} n &= n_n + n_s \\ \boldsymbol{j} &= \boldsymbol{j}_n + \boldsymbol{j}_s = -e\big(n_n \boldsymbol{v}_n + n_s \boldsymbol{v}_s\big) \quad . \end{aligned} \tag{1.17}$$

The normal fluid is dissipative, hence $\boldsymbol{j}_n = \sigma_n \boldsymbol{E}$, but the superfluid obeys $F = m\boldsymbol{a}$, *i.e.*

$$m\,\frac{d\boldsymbol{v}_s}{dt} = -e\boldsymbol{E} \quad \Rightarrow \quad \frac{d\boldsymbol{j}_s}{dt} = \frac{n_s e^2}{m}\,\boldsymbol{E} \quad . \tag{1.18}$$

In the presence of an external magnetic field, the superflow satisfies

$$\begin{aligned}\frac{d\boldsymbol{v}_{\rm s}}{dt} &= -\frac{e}{m}\big(\boldsymbol{E} + c^{-1}\boldsymbol{v}_{\rm s}\times\boldsymbol{B}\big)\\ &= \frac{\partial \boldsymbol{v}_{\rm s}}{\partial t} + (\boldsymbol{v}_{\rm s}\cdot\boldsymbol{\nabla})\boldsymbol{v}_{\rm s} = \frac{\partial \boldsymbol{v}_{\rm s}}{\partial t} + \boldsymbol{\nabla}\big(\tfrac{1}{2}\boldsymbol{v}_{\rm s}^2\big) - \boldsymbol{v}_{\rm s}\times(\boldsymbol{\nabla}\times\boldsymbol{v}_{\rm s}) \quad .\end{aligned} \tag{1.19}$$

We then have

$$\frac{\partial \boldsymbol{v}_{\rm s}}{\partial t} + \frac{e}{m}\,\boldsymbol{E} + \boldsymbol{\nabla}\big(\tfrac{1}{2}\boldsymbol{v}_{\rm s}^2\big) = \boldsymbol{v}_{\rm s}\times\bigg(\boldsymbol{\nabla}\times\boldsymbol{v}_{\rm s} - \frac{e\boldsymbol{B}}{mc}\bigg) \quad . \tag{1.20}$$

Taking the curl, and invoking Faraday's law $\boldsymbol{\nabla}\times\boldsymbol{E} = -c^{-1}\partial_t\boldsymbol{B}$, we obtain

$$\frac{\partial}{\partial t}\bigg(\boldsymbol{\nabla}\times\boldsymbol{v}_{\rm s} - \frac{e\boldsymbol{B}}{mc}\bigg) = \boldsymbol{\nabla}\times\bigg\{\boldsymbol{v}_{\rm s}\times\bigg(\boldsymbol{\nabla}\times\boldsymbol{v}_{\rm s} - \frac{e\boldsymbol{B}}{mc}\bigg)\bigg\} \quad , \tag{1.21}$$

which may be written as

$$\frac{\partial \boldsymbol{Q}}{\partial t} = \boldsymbol{\nabla}\times(\boldsymbol{v}_{\rm s}\times\boldsymbol{Q}) \quad , \tag{1.22}$$

where

$$\boldsymbol{Q} \equiv \boldsymbol{\nabla}\times\boldsymbol{v}_{\rm s} - \frac{e\boldsymbol{B}}{mc} \quad . \tag{1.23}$$

Eqn. 1.22 says that if $\boldsymbol{Q} = 0$, it remains zero for all time. Assumption: the equilibrium state has $\boldsymbol{Q} = 0$. Thus,

$$\boldsymbol{\nabla}\times\boldsymbol{v}_{\rm s} = \frac{e\boldsymbol{B}}{mc} \quad\Rightarrow\quad \boldsymbol{\nabla}\times\boldsymbol{j}_{\rm s} = -\frac{n_{\rm s}e^2}{mc}\,\boldsymbol{B} \quad . \tag{1.24}$$

This equation implies the Meissner effect, for upon taking the curl of the last of Maxwell's equations (and assuming a steady state so $\dot{\boldsymbol{E}} = \dot{\boldsymbol{D}} = 0$),

$$-\nabla^2\boldsymbol{B} = \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{B}) = \frac{4\pi}{c}\,\boldsymbol{\nabla}\times\boldsymbol{j} = -\frac{4\pi n_{\rm s}e^2}{mc^2}\,\boldsymbol{B} \quad\Rightarrow\quad \nabla^2\boldsymbol{B} = \lambda_{\rm L}^{-2}\boldsymbol{B} \quad , \tag{1.25}$$

where $\lambda_{\rm L} = \sqrt{mc^2/4\pi n_{\rm s}e^2}$ is the *London penetration depth*. The magnetic field can only penetrate up to a distance on the order of $\lambda_{\rm L}$ inside the superconductor.

Note that

$$\boldsymbol{\nabla}\times\boldsymbol{j}_{\rm s} = -\frac{c}{4\pi\lambda_{\rm L}^2}\,\boldsymbol{B} \tag{1.26}$$

and the definition $\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}$ licenses us to write

$$\boldsymbol{j}_{\rm s} = -\frac{c}{4\pi\lambda_{\rm L}^2}\,\boldsymbol{A} \quad , \tag{1.27}$$

provided an appropriate gauge choice for $\boldsymbol{A}$ is taken. Since $\boldsymbol{\nabla}\cdot\boldsymbol{j}_{\rm s} = 0$ in steady state, we conclude $\boldsymbol{\nabla}\cdot\boldsymbol{A} = 0$ is the proper gauge. This is called the Coulomb gauge. Note, however, that this still allows for the little gauge transformation $\boldsymbol{A}\to\boldsymbol{A}+\boldsymbol{\nabla}\chi$, provided $\nabla^2\chi = 0$. Consider now an isolated body which is simply connected, *i.e.* any closed loop drawn within the body is continuously contractable to a point. The normal component of the superfluid at the boundary, $\boldsymbol{J}_{{\rm s},\perp}$ must vanish, hence $\boldsymbol{A}_\perp = 0$ as well. Therefore $\nabla_\perp\chi$ must also vanish everywhere on the boundary, which says that χ is determined up to a global constant.

If the superconductor is multiply connected, though, the condition $\nabla_\perp\chi = 0$ allows for non-constant solutions for χ. The line integral of $\boldsymbol{A}$ around a closed loop surrounding a hole $\mathcal{D}$ in the superconductor is, by Stokes' theorem, the magnetic flux through the loop:

$$\oint\limits_{\partial\mathcal{D}} d\boldsymbol{l}\cdot\boldsymbol{A} = \int\limits_{\mathcal{D}} dS\;\hat{\boldsymbol{n}}\cdot\boldsymbol{B} = \Phi_{\mathcal{D}} \quad . \tag{1.28}$$

On the other hand, within the interior of the superconductor, since $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A} = 0$, we can write $\boldsymbol{A} = \boldsymbol{\nabla}\chi$, which says that the trapped flux $\Phi_{\mathcal{D}}$ is given by $\Phi_{\mathcal{D}} = \Delta\chi$, then change in the gauge function as one proceeds counterclockwise around the loop. F. London argued that if the gauge transformation $\boldsymbol{A} \to \boldsymbol{A} + \boldsymbol{\nabla}\chi$ is associated with a quantum mechanical wavefunction associated with a charge e object, then the flux $\Phi_{\mathcal{D}}$ will be quantized in units of the Dirac quantum $\phi_0 = hc/e = 4.137 \times 10^{-7}\,\mathrm{G\,cm}^2$. The argument is simple. The transformation of the wavefunction $\Psi \to \Psi\, e^{-i\alpha}$ is cancelled by the replacement $\boldsymbol{A} \to \boldsymbol{A} + (\hbar c/e)\boldsymbol{\nabla}\alpha$. Thus, we have $\chi = \alpha\phi_0/2\pi$, and single-valuedness requires $\Delta\alpha = 2\pi n$ around a loop, hence $\Phi_{\mathcal{D}} = \Delta\chi = n\phi_0$.

The above argument is almost correct. The final piece was put in place by Lars Onsager in 1953. Onsager pointed out that if the particles described by the superconducting wavefunction Ψ were of charge $e^* = 2e$, then, *mutatis mutandis*, one would conclude the quantization condition is $\Phi_{\mathcal{D}} = n\phi_{\mathrm{L}}$, where $\phi_{\mathrm{L}} = hc/2e$ is the London flux quantum, which is half the size of the Dirac flux quantum. This suggestion was confirmed in subsequent experiments by Deaver and Fairbank, and by Doll and Näbauer, both in 1961.

De Gennes' derivation of London Theory

De Gennes writes the total free energy of the superconductor as

$$\begin{aligned} F &= \int\! d^3\!x\; f_{\mathrm{s}} + E_{\mathrm{kinetic}} + E_{\mathrm{field}} \\ E_{\mathrm{kinetic}} &= \int\! d^3\!x\; \tfrac{1}{2} m n_{\mathrm{s}} \boldsymbol{v}_{\mathrm{s}}^2(\boldsymbol{x}) = \int\! d^3\!x\; \frac{m}{2n_{\mathrm{s}}e^2}\, \boldsymbol{j}_{\mathrm{s}}^2(\boldsymbol{x}) \\ E_{\mathrm{field}} &= \int\! d^3\!x\; \frac{\boldsymbol{B}^2(\boldsymbol{x})}{8\pi} \quad . \end{aligned} \tag{1.29}$$

But under steady state conditions $\boldsymbol{\nabla} \times \boldsymbol{B} = 4\pi c^{-1}\boldsymbol{j}_{\mathrm{s}}$, so

$$F = \int\! d^3\!x \left\{ f_s + \frac{\boldsymbol{B}^2}{8\pi} + \lambda_{\mathrm{L}}^2\, \frac{(\boldsymbol{\nabla} \times \boldsymbol{B})^2}{8\pi} \right\} \quad . \tag{1.30}$$

Taking the functional variation and setting it to zero,

$$4\pi\, \frac{\delta F}{\delta \boldsymbol{B}} = \boldsymbol{B} + \lambda_{\mathrm{L}}^2\, \boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \boldsymbol{B}) = \boldsymbol{B} - \lambda_{\mathrm{L}}^2\, \nabla^2 \boldsymbol{B} = 0 \quad . \tag{1.31}$$

Pippard's nonlocal extension

The London equation $\boldsymbol{j}_{\mathrm{s}}(\boldsymbol{x}) = -c\boldsymbol{A}(\boldsymbol{x})/4\pi\lambda_{\mathrm{L}}^2$ says that the supercurrent is perfectly yoked to the vector potential, and on arbitrarily small length scales. This is unrealistic. A. B. Pippard undertook a phenomenological generalization of the (phenomenological) London equation, writing[5]

$$\begin{aligned} j_{\mathrm{s}}^\alpha(\boldsymbol{x}) &= -\frac{c}{4\pi\lambda_{\mathrm{L}}^2} \int\! d^3\!r\; K^{\alpha\beta}(\boldsymbol{r})\, A_\beta(\boldsymbol{x}+\boldsymbol{r}) \\ &= -\frac{c}{4\pi\lambda_{\mathrm{L}}^2} \cdot \frac{3}{4\pi\xi} \int\! d^3\!r\; \frac{e^{-r/\xi}}{r^2}\, \hat{r}^\alpha\, \hat{r}^\beta\, A_\beta(\boldsymbol{x}+\boldsymbol{r}) \quad . \end{aligned} \tag{1.32}$$

[5]See A. B. Pippard, *Proc. Roy. Soc. Lond.* **A216**, 547 (1953).

Note that the kernel $K^{\alpha\beta}(\boldsymbol{r}) = 3\,e^{-r/\xi}\,\hat{r}^\alpha\hat{r}^\beta/4\pi\xi r^2$ is normalized so that

$$\int\! d^3\!r\; K^{\alpha\beta}(\boldsymbol{r}) = \frac{3}{4\pi\xi}\int\! d^3\!r\;\frac{e^{-r/\xi}}{r^2}\,\hat{r}^\alpha\,\hat{r}^\beta = \overbrace{\frac{1}{\xi}\int\limits_0^\infty\! dr\; e^{-r/\xi}}^{1}\cdot\overbrace{3\!\int\!\frac{d\hat{\boldsymbol{r}}}{4\pi}\,\hat{r}^\alpha\,\hat{r}^\beta}^{\delta^{\alpha\beta}} = \delta^{\alpha\beta} \quad . \tag{1.33}$$

The exponential factor means that $K^{\alpha\beta}(\boldsymbol{r})$ is negligible for $r \gg \xi$. If the vector potential is constant on the scale ξ, then we may pull $A_\beta(\boldsymbol{x})$ out of the integral in Eqn. 1.33, in which case we recover the original London equation. Invoking continuity in the steady state, $\boldsymbol{\nabla}\!\cdot\!\boldsymbol{j} = 0$ requires

$$\frac{3}{4\pi\xi^2}\int\! d^3\!r\;\frac{e^{-r/\xi}}{r^2}\;\hat{\boldsymbol{r}}\cdot\boldsymbol{A}(\boldsymbol{x}+\boldsymbol{r}) = 0 \quad , \tag{1.34}$$

which is to be regarded as a gauge condition on the vector potential. One can show that this condition is equivalent to $\boldsymbol{\nabla}\!\cdot\!\boldsymbol{A} = 0$, the original Coulomb gauge.

In disordered superconductors, Pippard took

$$K^{\alpha\beta}(\boldsymbol{r}) = \frac{3}{4\pi\xi_0}\,\frac{e^{-r/\xi}}{r^2}\,\hat{r}^\alpha\,\hat{r}^\beta \quad , \tag{1.35}$$

with

$$\frac{1}{\xi} = \frac{1}{\xi_0} + \frac{1}{a\,\ell} \quad , \tag{1.36}$$

where ℓ is the metallic elastic mean free path, and a is a dimensionless constant on the order of unity. Note that $\int\! d^3\!r\; K^{\alpha\beta}(\boldsymbol{r}) = (\xi/\xi_0)\,\delta^{\alpha\beta}$. Thus, for $\lambda_{\rm L} \gg \xi$, one obtains an effective penetration depth $\lambda = (\xi_0/\xi)^{1/2}\lambda_{\rm L}$, where $\lambda_{\rm L} = \sqrt{mc^2/4\pi n_{\rm s} e^2}$. In the opposite limit, where $\lambda_{\rm L} \ll \xi$, Pippard found $\lambda = (3/4\pi^2)^{1/6}\big(\xi_0\lambda_{\rm L}^2\big)^{1/3}$. For strongly type-I superconductors, $\xi \gg \lambda_{\rm L}$. Since $\boldsymbol{j}_{\rm s}(\boldsymbol{x})$ is averaging the vector potential over a region of size $\xi \gg \lambda_{\rm L}$, the screening currents near the surface of the superconductor are weaker, which means the magnetic field penetrates deeper than $\lambda_{\rm L}$. The physical penetration depth is λ, where, according to Pippard, $\lambda/\lambda_{\rm L} \propto \big(\xi_0/\lambda_{\rm L}\big)^{1/3} \gg 1$.

1.4 Ginzburg-Landau Theory

The basic idea behind Ginzburg-Landau theory is to write the free energy as a simple functional of the *order parameter(s)* of a thermodynamic system and their derivatives. In ^{4}He, the order parameter $\Psi(\boldsymbol{x}) = \langle\psi(\boldsymbol{x})\rangle$ is the quantum and thermal average of the field operator $\psi(\boldsymbol{x})$ which destroys a helium atom at position $\boldsymbol{x}$. When Ψ is nonzero, we have Bose condensation with condensate density $n_0 = |\Psi|^2$. Above the lambda transition, one has $n_0(T > T_\lambda) = 0$.

In an s-wave superconductor, the order parameter field is given by

$$\Psi(\boldsymbol{x}) \propto \big\langle \psi_\uparrow(\boldsymbol{x})\,\psi_\downarrow(\boldsymbol{x})\big\rangle \quad , \tag{1.37}$$

where $\psi_\sigma(\boldsymbol{x})$ destroys a conduction band electron of spin σ at position $\boldsymbol{x}$. Owing to the anticommuting nature of the fermion operators, the fermion field $\psi_\sigma(\boldsymbol{x})$ itself cannot condense, and it is only the *pair field* $\Psi(\boldsymbol{x})$ (and other products involving an even number of fermion field operators) which can take a nonzero value.

1.4.1 Landau theory for superconductors

The superconducting order parameter $\Psi(\boldsymbol{x})$ is thus a complex scalar, as in a superfluid. As we shall see, the difference is that the superconductor is *charged*. In the absence of magnetic fields, the Landau free energy density is approximated as

$$f = a\,|\Psi|^2 + \tfrac{1}{2}b\,|\Psi|^4 \quad . \tag{1.38}$$

The coefficients a and b are real and temperature-dependent but otherwise constant in a spatially homogeneous system. The sign of a is negotiable, but $b > 0$ is necessary for thermodynamic stability. The free energy has an $\mathrm{O}(2)$ symmetry, *i.e.* it is invariant under the substitution $\Psi \to \Psi\, e^{i\alpha}$. For $a < 0$ the free energy is minimized by writing

$$\Psi = \sqrt{-\frac{a}{b}}\; e^{i\phi} \quad , \tag{1.39}$$

where ϕ, the phase of the superconductor, is a constant. The system spontaneously breaks the $\mathrm{O}(2)$ symmetry and chooses a direction in Ψ space in which to point.

In our formulation here, the free energy of the normal state, *i.e.* when $\Psi = 0$, is $f_{\rm n} = 0$ at all temperatures, and that of the superconducting state is $f_{\rm s} = -a^2/2b$. From thermodynamic considerations, therefore, we have

$$f_{\rm s}(T) - f_{\rm n}(T) = -\frac{H_{\rm c}^2(T)}{8\pi} \qquad \Rightarrow \qquad \frac{a^2(T)}{b(T)} = \frac{H_{\rm c}^2(T)}{4\pi} \quad . \tag{1.40}$$

Furthermore, from London theory we have that $\lambda_{\rm L}^2 = mc^2/4\pi n_{\rm s} e^2$, and if we normalize the order parameter according to

$$\big|\Psi\big|^2 = \frac{n_{\rm s}}{n} \quad , \tag{1.41}$$

where $n_{\rm s}$ is the number density of superconducting electrons and n the total number density of conduction band electrons, then

$$\frac{\lambda_{\rm L}^2(0)}{\lambda_{\rm L}^2(T)} = \big|\Psi(T)\big|^2 = -\frac{a(T)}{b(T)} \quad . \tag{1.42}$$

Here we have taken $n_{\rm s}(T=0) = n$, so $|\Psi(0)|^2 = 1$. Putting this all together, we find

$$a(T) = -\frac{H_{\rm c}^2(T)}{4\pi}\cdot\frac{\lambda_{\rm L}^2(T)}{\lambda_{\rm L}^2(0)} \qquad , \qquad b(T) = \frac{H_{\rm c}^2(T)}{4\pi}\cdot\frac{\lambda_{\rm L}^4(T)}{\lambda_{\rm L}^4(0)} \tag{1.43}$$

Close to the transition, $H_{\rm c}(T)$ vanishes in proportion to $\lambda_{\rm L}^{-2}(T)$, so $a(T_{\rm c}) = 0$ while $b(T_{\rm c}) > 0$ remains finite at $T_{\rm c}$. Later on below, we shall relate the penetration depth $\lambda_{\rm L}$ to a stiffness parameter in the Ginzburg-Landau theory.

We may now compute the specific heat discontinuity from $c = -T\,\frac{\partial^2 f}{\partial T^2}$. It is left as an exercise to the reader to show

$$\Delta c = c_{\rm s}(T_{\rm c}) - c_{\rm n}(T_{\rm c}) = \frac{T_{\rm c}\,\big[a'(T_{\rm c})\big]^2}{b(T_{\rm c})} \quad , \tag{1.44}$$

where $a'(T) = da/dT$. Of course, $c_n(T)$ isn't zero! Rather, here we are accounting only for the specific heat due to that part of the free energy associated with the condensate. The Ginzburg-Landau description completely ignores the metal, and doesn't describe the physics of the normal state Fermi surface, which gives rise to $c_{\rm n} = \gamma T$. The discontinuity Δc is a mean field result. It works extremely well for superconductors, where, as we shall see, the Ginzburg criterion is satisfied down to extremely small temperature variations relative to $T_{\rm c}$. In ^{4}He, one sees an cusp-like behavior with an apparent weak divergence at the lambda transition. Recall that in the language of critical phenomena, $c(T) \propto |T - T_{\rm c}|^{-\alpha}$. For the $\mathrm{O}(2)$ model in $d = 3$ dimensions, the exponent α is very close to zero, which is close to the mean field value $\alpha = 0$. The order parameter exponent is $\beta = \frac{1}{2}$ at the mean field level; the exact value is closer to $\frac{1}{3}$. One has, for $T < T_c$,

$$\big|\Psi(T < T_c)\big| = \sqrt{-\frac{a(T)}{b(T)}} = \sqrt{\frac{a'(T_c)}{b(T_c)}}\,(T_c - T)^{1/2} + \ldots \quad . \tag{1.45}$$

1.4.2 Ginzburg-Landau Theory

The Landau free energy is minimized by setting $|\Psi|^2 = -a/b$ for $a < 0$. The phase of Ψ is therefore free to vary, and indeed free to vary independently everywhere in space. Phase fluctuations should cost energy, so we posit an augmented free energy functional,

$$F\big[\Psi,\Psi^*\big] = \int\! d^d\!x\,\Big\{a\,\big|\Psi(\boldsymbol{x})\big|^2 + \tfrac{1}{2}\,b\,\big|\Psi(\boldsymbol{x})\big|^4 + K\,\big|\boldsymbol{\nabla}\Psi(\boldsymbol{x})\big|^2 + \ldots\Big\} \quad . \tag{1.46}$$

Here K is a stiffness with respect to spatial variation of the order parameter $\Psi(\boldsymbol{x})$. From K and a, we can form a length scale, $\xi = \sqrt{K/|a|}$, known as the *coherence length*. This functional in fact is very useful in discussing properties of neutral superfluids, such as ^{4}He, but superconductors are *charged*, and we have instead

$$F\big[\Psi,\Psi^*,\boldsymbol{A}\big] = \int\! d^d\!x\,\Big\{a\,\big|\Psi(\boldsymbol{x})\big|^2 + \tfrac{1}{2}\,b\,\big|\Psi(\boldsymbol{x})\big|^4 + K\,\Big|\big(\boldsymbol{\nabla} + \tfrac{ie^*}{\hbar c}\,\boldsymbol{A}\big)\Psi(\boldsymbol{x})\Big|^2 + \tfrac{1}{8\pi}\,(\boldsymbol{\nabla}\times\boldsymbol{A})^2 + \ldots\Big\} \quad . \tag{1.47}$$

Here $q = -e^* = -2e$ is the *charge* of the condensate. We assume $\boldsymbol{E} = 0$, so $\boldsymbol{A}$ is not time-dependent.

Under a local transformation $\Psi(\boldsymbol{x}) \to \Psi(\boldsymbol{x})\,e^{i\alpha(\boldsymbol{x})}$, we have

$$\big(\boldsymbol{\nabla} + \tfrac{ie^*}{\hbar c}\,\boldsymbol{A}\big)\big(\Psi\,e^{i\alpha}\big) = e^{i\alpha}\big(\boldsymbol{\nabla} + i\boldsymbol{\nabla}\alpha + \tfrac{ie^*}{\hbar c}\boldsymbol{A}\big)\,\Psi \quad , \tag{1.48}$$

which, upon making the gauge transformation $\boldsymbol{A} \to \boldsymbol{A} - \frac{\hbar c}{e^*}\,\boldsymbol{\nabla}\alpha$, reverts to its original form. Thus, the free energy is unchanged upon replacing $\Psi \to \Psi e^{i\alpha}$ and $\boldsymbol{A} \to \boldsymbol{A} - \frac{\hbar c}{e^*}\,\boldsymbol{\nabla}\alpha$. Since gauge transformations result in no physical consequences, we conclude that the *longitudinal* phase fluctuations of a charged order parameter do not really exist. More on this later when we discuss the Anderson-Higgs mechanism.

1.4.3 Equations of motion

Varying the free energy in Eqn. 1.47 with respect to Ψ^* and $\boldsymbol{A}$, respectively, yields

$$\begin{aligned} 0 &= \frac{\delta F}{\delta\Psi^*} = a\,\Psi + b\,|\Psi|^2\,\Psi - K\,\big(\boldsymbol{\nabla} + \tfrac{ie^*}{\hbar c}\,\boldsymbol{A}\big)^2\,\Psi \\ 0 &= \frac{\delta F}{\delta\boldsymbol{A}} = \frac{2Ke^*}{\hbar c}\left[\frac{1}{2i}\big(\Psi^*\boldsymbol{\nabla}\Psi - \Psi\boldsymbol{\nabla}\Psi^*\big) + \frac{e^*}{\hbar c}\,|\Psi|^2\boldsymbol{A}\right] + \frac{1}{4\pi}\,\boldsymbol{\nabla}\times\boldsymbol{B} \quad . \end{aligned} \tag{1.49}$$

The second of these equations is the Ampère-Maxwell law, $\boldsymbol{\nabla}\times\boldsymbol{B} = 4\pi c^{-1}\boldsymbol{j}$, with

$$\boldsymbol{j} = -\frac{2Ke^*}{\hbar^2}\left[\frac{\hbar}{2i}\big(\Psi^*\boldsymbol{\nabla}\Psi - \Psi\boldsymbol{\nabla}\Psi^*\big) + \frac{e^*}{c}\,|\Psi|^2\boldsymbol{A}\right] \quad . \tag{1.50}$$

If we set Ψ to be constant, we obtain $\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{B}) + \lambda_L^{-2}\boldsymbol{B} = 0$, with

$$\lambda_L^{-2} = 8\pi K\left(\frac{e^*}{\hbar c}\right)^2|\Psi|^2 \quad . \tag{1.51}$$

Thus we recover the relation $\lambda_{\rm L}^{-2} \propto |\Psi|^2$. Note that $|\Psi|^2 = |a|/b$ in the ordered phase, hence

$$\lambda_{\rm L}^{-1} = \left[\frac{8\pi a^2}{b} \cdot \frac{K}{|a|}\right]^{1/2} \frac{e^*}{\hbar c} = \frac{\sqrt{2}\, e^*}{\hbar c} H_{\rm c}\, \xi \quad , \tag{1.52}$$

which says

$$H_{\rm c} = \frac{\phi_{\rm L}}{\sqrt{8}\,\pi\,\xi\lambda_{\rm L}} \quad . \tag{1.53}$$

At a superconductor-vacuum interface, we should have

$$\hat{\boldsymbol{n}} \cdot \left(\frac{\hbar}{i}\boldsymbol{\nabla} + \frac{e^*}{c}\boldsymbol{A}\right)\Psi\big|_{\partial\Omega} = 0 \quad , \tag{1.54}$$

where Ω denotes the superconducting region and $\hat{\boldsymbol{n}}$ the surface normal. This guarantees $\hat{\boldsymbol{n}} \cdot \boldsymbol{j}\big|_{\partial\Omega} = 0$, since

$$\boldsymbol{j} = -\frac{2Ke^*}{\hbar^2}\,\mathsf{Re}\left(\frac{\hbar}{i}\,\Psi^*\boldsymbol{\nabla}\Psi + \frac{e^*}{c}\,|\Psi|^2\boldsymbol{A}\right) \quad . \tag{1.55}$$

Note that $\hat{\boldsymbol{n}} \cdot \boldsymbol{j} = 0$ also holds if

$$\hat{\boldsymbol{n}} \cdot \left(\frac{\hbar}{i}\boldsymbol{\nabla} + \frac{e^*}{c}\boldsymbol{A}\right)\Psi\big|_{\partial\Omega} = ir\Psi \quad , \tag{1.56}$$

with r a real constant. This boundary condition is appropriate at a junction with a normal metal.

1.4.4 Critical current

Consider the case where $\Psi = \Psi_0$. The free energy density is

$$f = a\,|\Psi_0|^2 + \tfrac{1}{2}\,b\,|\Psi_0|^4 + K\left(\frac{e^*}{\hbar c}\right)^2 \boldsymbol{A}^2\,|\Psi_0|^2 \quad . \tag{1.57}$$

If $a > 0$ then f is minimized for $\Psi_0 = 0$. What happens for $a < 0$, *i.e.* when $T < T_{\rm c}$. Minimizing with respect to $|\Psi_0|$, we find

$$|\Psi_0|^2 = \frac{|a| - K(e^*/\hbar c)^2\boldsymbol{A}^2}{b} \quad . \tag{1.58}$$

The current density is then

$$\boldsymbol{j} = -2cK\left(\frac{e^*}{\hbar c}\right)^2\left(\frac{|a| - K(e^*/\hbar c)^2\boldsymbol{A}^2}{b}\right)\boldsymbol{A} \quad . \tag{1.59}$$

Taking the magnitude and extremizing with respect to $A = |\boldsymbol{A}|$, we obtain the *critical current density* $j_{\rm c}$:

$$A^2 = \frac{|a|}{3K(e^*/\hbar c)^2} \quad \Rightarrow \quad j_{\rm c} = \frac{4}{3\sqrt{3}}\,\frac{c\,K^{1/2}\,|a|^{3/2}}{b} \quad . \tag{1.60}$$

Physically, what is happening is this. When the kinetic energy density in the superflow exceeds the condensation energy density $H_{\rm c}^2/8\pi = a^2/2b$, the system goes normal. Note that $j_{\rm c}(T) \propto (T_{\rm c} - T)^{3/2}$.

Should we feel bad about using a gauge-covariant variable like $\boldsymbol{A}$ in the above analysis? Not really, because when we write $\boldsymbol{A}$, what we really mean is the gauge-*invariant* combination $\boldsymbol{A} + \frac{\hbar c}{e^*}\boldsymbol{\nabla}\varphi$, where $\varphi = \mathsf{arg}(\Psi)$ is the phase of the order parameter.

London limit

In the so-called *London limit*, we write $\Psi = \sqrt{n_0}\, e^{i\varphi}$, with n_0 constant. Then

$$\boldsymbol{j} = -\frac{2Ke^* n_0}{\hbar}\Big(\boldsymbol{\nabla}\varphi + \frac{e^*}{\hbar c}\boldsymbol{A}\Big) = -\frac{c}{4\pi\lambda_{\rm L}^2}\Big(\frac{\phi_{\rm L}}{2\pi}\,\boldsymbol{\nabla}\varphi + \boldsymbol{A}\Big) \quad . \tag{1.61}$$

Thus,

$$\begin{aligned}\boldsymbol{\nabla}\times\boldsymbol{j} &= \frac{c}{4\pi}\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{B})\\ &= -\frac{c}{4\pi\lambda_{\rm L}^2}\,\boldsymbol{B} - \frac{c}{4\pi\lambda_{\rm L}^2}\,\frac{\phi_{\rm L}}{2\pi}\,\boldsymbol{\nabla}\times\boldsymbol{\nabla}\varphi \quad ,\end{aligned} \tag{1.62}$$

which says

$$\lambda_{\rm L}^2\,\nabla^2\boldsymbol{B} = \boldsymbol{B} + \frac{\phi_{\rm L}}{2\pi}\,\boldsymbol{\nabla}\times\boldsymbol{\nabla}\varphi \quad . \tag{1.63}$$

If we assume $\boldsymbol{B} = B\hat{\boldsymbol{z}}$ and the phase field φ has singular vortex lines of topological index $n_i \in \mathbb{Z}$ located at position $\boldsymbol{\rho}_i$ in the (x,y) plane, we have

$$\lambda_{\rm L}^2\,\nabla^2 B = B + \phi_{\rm L}\sum_i n_i\,\delta\big(\boldsymbol{\rho}-\boldsymbol{\rho}_i\big) \quad . \tag{1.64}$$

Taking the Fourier transform, we solve for $\hat{B}(\boldsymbol{q})$, where $\boldsymbol{k} = (\boldsymbol{q}, k_z)$:

$$\hat{B}(\boldsymbol{q}) = -\frac{\phi_{\rm L}}{1+\boldsymbol{q}^2\lambda_{\rm L}^2}\sum_i n_i\, e^{-i\boldsymbol{q}\cdot\boldsymbol{\rho}_i} \quad , \tag{1.65}$$

whence

$$B(\boldsymbol{\rho}) = -\frac{\phi_{\rm L}}{2\pi\lambda_{\rm L}^2}\sum_i n_i\, K_0\bigg(\frac{|\boldsymbol{\rho}-\boldsymbol{\rho}_i|}{\lambda_{\rm L}}\bigg) \quad , \tag{1.66}$$

where $K_0(z)$ is the MacDonald function, whose asymptotic behaviors are given by

$$K_0(z) \sim \begin{cases} -\mathrm{C} - \ln(z/2) & (z\to 0)\\ (\pi/2z)^{1/2}\exp(-z) & (z\to\infty) \end{cases} \quad , \tag{1.67}$$

where $\mathrm{C} = 0.57721566\ldots$ is the Euler-Mascheroni constant. The logarithmic divergence as $\rho \to 0$ is an artifact of the London limit. Physically, the divergence should be cut off when $|\boldsymbol{\rho}-\boldsymbol{\rho}_i| \sim \xi$. The current density for a single vortex at the origin is

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{nc}{4\pi}\,\boldsymbol{\nabla}\times\boldsymbol{B} = -\frac{c}{4\pi\lambda_{\rm L}}\cdot\frac{\phi_{\rm L}}{2\pi\lambda_{\rm L}^2}\,K_1\big(\rho/\lambda_{\rm L}\big)\,\hat{\boldsymbol{\varphi}} \quad , \tag{1.68}$$

where $n\in\mathbb{Z}$ is the vorticity, and $K_1(z) = -K_0'(z)$ behaves as z^{-1} as $z\to 0$ and $\exp(-z)/\sqrt{2\pi z}$ as $z\to\infty$. Note the $i^{\rm th}$ vortex carries magnetic flux $n_i\,\phi_{\rm L}$.

1.4.5 Ginzburg criterion

Consider fluctuations in $\Psi(\boldsymbol{x})$ above $T_{\rm c}$. If $|\Psi| \ll 1$, we may neglect quartic terms and write

$$F = \int\! d^dx\,\Big(a\,|\Psi|^2 + K\,|\boldsymbol{\nabla}\Psi|^2\Big) = \sum_{\boldsymbol{k}}\big(a+K\boldsymbol{k}^2\big)|\hat{\Psi}(\boldsymbol{k})|^2 \quad , \tag{1.69}$$

where we have expanded

$$\Psi(\boldsymbol{x}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} \hat{\Psi}(\boldsymbol{k})\, e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \quad . \tag{1.70}$$

The Helmholtz free energy $A(T)$ is given by

$$e^{-A/k_\mathrm{B}T} = \int D[\Psi,\Psi^*]\, e^{-F/T} = \prod_{\boldsymbol{k}} \left(\frac{\pi k_\mathrm{B} T}{a + K\boldsymbol{k}^2}\right) \quad , \tag{1.71}$$

which is to say

$$A(T) = k_\mathrm{B} T \sum_{\boldsymbol{k}} \ln\!\left(\frac{\pi k_\mathrm{B} T}{a + K\boldsymbol{k}^2}\right) \quad . \tag{1.72}$$

We write $a(T) = \alpha t$ with $t = (T - T_\mathrm{c})/T_\mathrm{c}$ the reduced temperature. We now compute the singular contribution to the specific heat $C_V = -TA''(T)$, which only requires we differentiate with respect to T as it appears in $a(T)$. Dividing by $N_\mathrm{s} k_\mathrm{B}$, where $N_\mathrm{s} = V/\mathsf{a}^d$ is the number of lattice sites, we obtain the dimensionless heat capacity per unit cell,

$$c = \frac{\alpha^2 \mathsf{a}^d}{K^2} \int^{\Lambda\xi} \frac{d^d k}{(2\pi)^d}\, \frac{1}{(\xi^{-2} + \boldsymbol{k}^2)^2} \quad , \tag{1.73}$$

where $\Lambda \sim \mathsf{a}^{-1}$ is an ultraviolet cutoff on the order of the inverse lattice spacing, and $\xi = (K/a)^{1/2} \propto |t|^{-1/2}$. We define $R_* \equiv (K/\alpha)^{1/2}$, in which case $\xi = R_*\,|t|^{-1/2}$, and

$$c = R_*^{-4}\, \mathsf{a}^d\, \xi^{4-d} \int^{\Lambda\xi} \frac{d^d \bar{q}}{(2\pi)^d}\, \frac{1}{(1 + \bar{q}^2)^2} \,, \tag{1.74}$$

where $\bar{\boldsymbol{q}} \equiv \boldsymbol{q}\xi$. Thus,

$$c(t) \sim \begin{cases} \text{const.} & \text{if } d > 4 \\ -\ln t & \text{if } d = 4 \\ t^{\frac{d}{2}-2} & \text{if } d < 4\,. \end{cases} \tag{1.75}$$

For $d > 4$, mean field theory is qualitatively accurate, with finite corrections. In dimensions $d \leq 4$, the mean field result is overwhelmed by fluctuation contributions as $t \to 0^+$ (*i.e.* as $T \to T_\mathrm{c}^+$). We see that the Ginzburg-Landau mean field theory is sensible provided the fluctuation contributions are small, *i.e.* provided

$$R_*^{-4}\, \mathsf{a}^d\, \xi^{4-d} \ll 1 \,, \tag{1.76}$$

which entails $t \gg t_\mathrm{G}$, where

$$t_\mathrm{G} = \left(\frac{\mathsf{a}}{R_*}\right)^{\frac{2d}{4-d}} \tag{1.77}$$

is the *Ginzburg reduced temperature*. The criterion for the sufficiency of mean field theory, namely $t \gg t_\mathrm{G}$, is known as the *Ginzburg criterion*. The region $|t| < t_\mathrm{G}$ is known as the *critical region*.

In a lattice ferromagnet, as we have seen, $R_* \sim \mathsf{a}$ is on the scale of the lattice spacing itself, hence $t_\mathrm{G} \sim 1$ and the critical regime is very large. Mean field theory then fails quickly as $T \to T_\mathrm{c}$. In a (conventional) three-dimensional superconductor, R_* is on the order of the Cooper pair size, and $R_*/\mathsf{a} \sim 10^2 - 10^3$, hence $t_\mathrm{G} = (a/R_*)^6 \sim 10^{-18} - 10^{-12}$ is negligibly narrow. The mean field theory of the superconducting transition – BCS theory – is then valid essentially all the way to $T = T_\mathrm{c}$.

Another way to think about it is as follows. In dimensions $d > 2$, for $|\boldsymbol{r}|$ fixed and $\xi \to \infty$, one has[6]

$$\big\langle \Psi^*(\boldsymbol{r})\Psi(0)\big\rangle \simeq \frac{C_d}{k_{\rm B}T\,R_*^2}\,\frac{e^{-r/\xi}}{r^{d-2}} \quad , \tag{1.78}$$

where C_d is a dimensionless constant. If we compute the ratio of fluctuations to the mean value over a patch of linear dimension ξ, we have

$$\begin{aligned}\frac{\text{fluctuations}}{\text{mean}} &= \frac{\int^{\xi} d^d\!r\,\langle \Psi^*(\boldsymbol{r})\,\Psi(0)\rangle}{\int^{\xi} d^d\!r\,\langle |\Psi(\boldsymbol{r})|^2\rangle} \\ &\propto \frac{1}{R_*^2\,\xi^d\,|\Psi|^2}\int^{\xi} d^d\!r\,\frac{e^{-r/\xi}}{r^{d-2}} \propto \frac{1}{R_*^2\,\xi^{d-2}\,|\Psi|^2} \quad .\end{aligned} \tag{1.79}$$

Close to the critical point we have $\xi \propto R_*\,|t|^{-\nu}$ and $|\Psi| \propto |t|^{\beta}$, with $\nu = \frac{1}{2}$ and $\beta = \frac{1}{2}$ within mean field theory. Setting the ratio of fluctuations to mean to be small, we recover the Ginzburg criterion.

1.4.6 Domain wall solution

Consider first the simple case of the neutral superfluid. The additional parameter K provides us with a new length scale, $\xi = \sqrt{K/|a|}$, which is called the coherence length. Varying the free energy with respect to $\Psi^*(\boldsymbol{x})$, one obtains

$$\frac{\delta F}{\delta\Psi^*(\boldsymbol{x})} = a\,\Psi(\boldsymbol{x}) + b\,\big|\Psi(\boldsymbol{x})\big|^2\,\Psi(\boldsymbol{x}) - K\nabla^2\Psi(\boldsymbol{x}) \quad . \tag{1.80}$$

Rescaling, we write $\Psi \equiv \big(|a|/b\big)^{1/2}\psi$, and setting the above functional variation to zero, we obtain

$$-\xi^2\nabla^2\psi + \,{\rm sgn}\,(T-T_{\rm c})\,\psi + |\psi|^2\psi = 0 \quad . \tag{1.81}$$

Consider the case of a domain wall when $T < T_{\rm c}$. We assume all spatial variation occurs in the x-direction, and we set $\psi(x=0)=0$ and $\psi(x=\infty)=1$. Furthermore, we take $\psi(x) = f(x)\,e^{i\alpha}$ where α is a constant[7]. We then have $-\xi^2 f''(x) - f + f^3 = 0$, which may be recast as

$$\xi^2\,\frac{d^2\!f}{dx^2} = \frac{\partial}{\partial f}\Big[\tfrac{1}{4}\big(1-f^2\big)^2\Big] \quad . \tag{1.82}$$

This looks just like $F = ma$ if we regard f as the coordinate, x as time, and $-V(f) = \frac{1}{4}\big(1-f^2\big)^2$. Thus, the potential describes an *inverted* double well with symmetric minima at $f = \pm 1$. The solution to the equations of motion is then that the 'particle' rolls starts at 'time' $x = -\infty$ at 'position' $f = +1$ and 'rolls' down, eventually passing the position $f = 0$ exactly at time $x = 0$. Multiplying the above equation by $f'(x)$ and integrating once, we have

$$\xi^2\bigg(\frac{df}{dx}\bigg)^2 = \tfrac{1}{2}\big(1-f^2\big)^2 + C \quad , \tag{1.83}$$

where C is a constant, which is fixed by setting $f(x\to\infty) = +1$, which says $f'(\infty) = 0$, hence $C = 0$. Integrating once more,

$$f(x) = \tanh\bigg(\frac{x-x_0}{\sqrt{2}\,\xi}\bigg) \quad , \tag{1.84}$$

[6]Exactly at $T = T_{\rm c}$, the correlations behave as $\big\langle \Psi^*(\boldsymbol{r})\,\Psi(0)\big\rangle \propto r^{-(d-2+\eta)}$, where η is a critical exponent.

[7]Remember that for a superconductor, phase fluctuations of the order parameter are nonphysical since they are eliiminable by a gauge transformation.

where x_0 is the second constant of integration. This, too, may be set to zero upon invoking the boundary condition $f(0) = 0$. Thus, the width of the domain wall is $\xi(T)$. This solution is valid provided that the local magnetic field averaged over scales small compared to ξ, *i.e.* $\boldsymbol{b} = \langle \boldsymbol{\nabla} \times \boldsymbol{A} \rangle$, is negligible.

The energy per unit area of the domain wall is given by $\tilde{\sigma}$, where

$$\begin{aligned} \tilde{\sigma} &= \int_0^\infty \! dx \, \bigg\{ K \left| \frac{d\Psi}{dx} \right|^2 + a \, |\Psi|^2 + \tfrac{1}{2} \, b \, |\Psi|^4 \bigg\} \\ &= \frac{a^2}{b} \int_0^\infty \! dx \, \bigg\{ \xi^2 \left(\frac{df}{dx} \right)^2 - f^2 + \tfrac{1}{2} \, f^4 \bigg\} \quad . \end{aligned} \tag{1.85}$$

Now we ask: is domain wall formation energetically favorable in the superconductor? To answer, we compute the difference in surface energy between the domain wall state and the uniform superconducting state. We call the resulting difference σ, the true domainwall energy relative to the superconducting state:

$$\begin{aligned} \sigma &= \tilde{\sigma} - \int_0^\infty \! dx \, \bigg(- \frac{H_c^2}{8\pi} \bigg) \\ &= \frac{a^2}{b} \int_0^\infty \! dx \, \bigg\{ \xi^2 \left(\frac{df}{dx} \right)^2 + \tfrac{1}{2} \, \big(1 - f^2\big)^2 \bigg\} \equiv \frac{H_c^2}{8\pi} \, \delta \quad , \end{aligned} \tag{1.86}$$

where we have used $H_c^2 = 4\pi a^2/b$. Invoking the previous result $f' = (1 - f^2)/\sqrt{2}\,\xi$, the parameter δ is given by

$$\delta = 2 \int_0^\infty \! dx \, \big(1 - f^2\big)^2 = 2 \int_0^1 \! df \, \frac{\big(1 - f^2\big)^2}{f'} = \frac{4\sqrt{2}}{3} \, \xi(T) \quad . \tag{1.87}$$

Had we permitted a field to penetrate over a distance $\lambda_L(T)$ in the domain wall state, we'd have obtained

$$\delta(T) = \frac{4\sqrt{2}}{3} \, \xi(T) - \lambda_L(T) \quad . \tag{1.88}$$

Detailed calculations show

$$\delta = \begin{cases} \frac{4\sqrt{2}}{3} \, \xi \approx 1.89 \, \xi & \text{if } \xi \gg \lambda_L \\ 0 & \text{if } \xi = \sqrt{2} \, \lambda_L \\ -\frac{8(\sqrt{2}-1)}{3} \, \lambda_L \approx -1.10 \, \lambda_L & \text{if } \lambda_L \gg \xi \quad . \end{cases} \tag{1.89}$$

Accordingly, we define the Ginzburg-Landau parameter $\kappa \equiv \lambda_L/\xi$, which is temperature-dependent near $T = T_c$, as we'll soon show.

So the story is as follows. In type-I materials, the positive $(\delta > 0)$ N-S surface energy keeps the sample spatially homogeneous for all $H < H_c$. In type-II materials, the negative surface energy causes the system to break into domains, which are vortex structures, as soon as H exceeds the lower critical field H_{c1}. This is known as the *mixed state*.

1.4.7 Scaled Ginzburg-Landau equations

For $T < T_c$, we write

$$\Psi = \sqrt{\frac{|a|}{b}} \, \psi \quad , \qquad \boldsymbol{x} = \lambda_L \, \boldsymbol{r} \quad , \qquad \boldsymbol{A} = \sqrt{2} \, \lambda_L \, H_c \, \boldsymbol{a} \tag{1.90}$$

as well as the GL parameter,

$$\kappa = \frac{\lambda_{\rm L}}{\xi} = \frac{\sqrt{2}\, e^*}{\hbar c}\, H_{\rm c}\, \lambda_{\rm L}^2 \quad . \tag{1.91}$$

The Gibbs free energy is then

$$G = \frac{H_{\rm c}^2 \lambda_{\rm L}^3}{4\pi} \int d^3r \left\{ -|\psi|^2 + \tfrac{1}{2}\,|\psi|^2 + \big|(\kappa^{-1}\boldsymbol{\nabla} + i\boldsymbol{a})\,\psi\big|^2 + (\boldsymbol{\nabla}\times\boldsymbol{a})^2 - 2\boldsymbol{h}\cdot\boldsymbol{\nabla}\times\boldsymbol{a}\right\} \quad . \tag{1.92}$$

Setting $\delta G = 0$, we obtain

$$\begin{gathered}(\kappa^{-1}\boldsymbol{\nabla} + i\boldsymbol{a})^2\,\psi + \psi - |\psi|^2\psi = 0 \\ \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{a} - \boldsymbol{h}) + |\psi|^2\boldsymbol{a} - \frac{i}{2\kappa}\big(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\big) = 0 \quad .\end{gathered} \tag{1.93}$$

The condition that no current flow through the boundary is

$$\hat{\boldsymbol{n}}\cdot\big(\boldsymbol{\nabla} + i\kappa\boldsymbol{a}\big)\psi\Big|_{\partial\Omega} = 0 \quad . \tag{1.94}$$

1.5 Applications of Ginzburg-Landau Theory

The applications of GL theory are numerous. Here we run through some examples.

1.5.1 Domain wall energy

Consider a domain wall interpolating between a normal metal at $x \to -\infty$ and a superconductor at $x \to +\infty$. The difference between the Gibbs free energies is

$$\begin{aligned}\Delta G = G_{\rm s} - G_{\rm n} &= \int d^3x \left\{ a\,|\Psi|^2 + \tfrac{1}{2} b\,|\Psi|^4 + K\big|(\boldsymbol{\nabla} + \tfrac{ie^*}{\hbar c}\,\boldsymbol{A})\Psi\big|^2 + \frac{(B-H)^2}{8\pi}\right\} \\ &= \frac{H_{\rm c}^2\,\lambda_{\rm L}^3}{4\pi}\int d^3r \left[-|\psi|^2 + \tfrac{1}{2}|\psi|^4 + \big|(\kappa^{-1}\boldsymbol{\nabla} + i\boldsymbol{a})\,\psi\big|^2 + (b-h)^2\right] \quad ,\end{aligned} \tag{1.95}$$

with $b = B/\sqrt{2}\,H_{\rm c}$ and $h = H/\sqrt{2}\,H_{\rm c}$. We define

$$\Delta G(T, H_{\rm c}) \equiv \frac{H_{\rm c}^2}{8\pi}\cdot A\,\lambda_{\rm L}\cdot\delta \quad , \tag{1.96}$$

as we did above in Eqn. 1.86, except here δ is rendered dimensionless by scaling it by $\lambda_{\rm L}$. Here A is the cross-sectional area, so δ is a dimensionless domain wall energy per unit area. Integrating by parts and appealing to the Euler-Lagrange equations, we have

$$\int d^3r \left[-|\psi|^2 + |\psi|^4 + \big|(\kappa^{-1}\boldsymbol{\nabla} + i\boldsymbol{a})\,\psi\big|^2\right] = \int d^3r\; \psi^*\Big[-\psi + |\psi|^2\psi - (\kappa^{-1}\boldsymbol{\nabla} + i\boldsymbol{a})^2\,\psi\Big] = 0 \quad , \tag{1.97}$$

and therefore

$$\delta = \int\limits_{-\infty}^{\infty} dx\,\Big[-|\psi|^4 + 2\,(b-h)^2\Big] \quad . \tag{1.98}$$

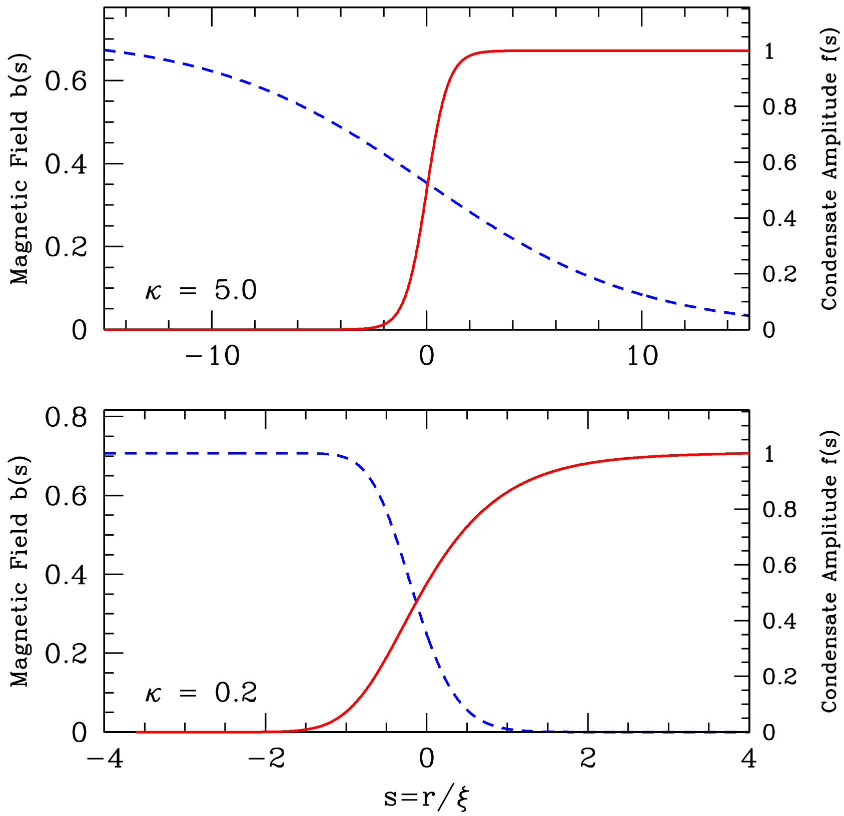

Figure 1.6: Numerical solution to a Ginzburg-Landau domain wall interpolating between normal metal ($x \to -\infty$) and superconducting ($x \to +\infty$) phases, for $H = H_{c2}$. Upper panel corresponds to $\kappa = 5$, and lower panel to $\kappa = 0.2$. Condensate amplitude $f(s)$ is shown in red, and dimensionless magnetic field $b(s) = B(s)/\sqrt{2}\,H_c$ in dashed blue.

Deep in the metal, as $x \to -\infty$, we expect $\psi \to 0$ and $b \to h$. Deep in the superconductor, as $x \to +\infty$, we expect $|\psi| \to 1$ and $b \to 0$. The bulk energy contribution then vanishes for $h = h_c = \frac{1}{\sqrt{2}}$, which means δ is finite, corresponding to the domain wall free energy per unit area.

We take $\psi = f \in \mathbb{R}$, $\boldsymbol{a} = a(x)\,\hat{\boldsymbol{y}}$, so $\boldsymbol{b} = b(x)\,\hat{\boldsymbol{z}}$ with $b(x) = a'(x)$. Thus, $\boldsymbol{\nabla} \times \boldsymbol{b} = -a''(x)\,\hat{\boldsymbol{y}}$, and the Euler-Lagrange equations are

$$\begin{aligned} \frac{1}{\kappa^2}\,\frac{d^2 f}{dx^2} &= \big(a^2 - 1\big) f + f^3 \\ \frac{d^2 a}{dx^2} &= a f^2 \quad . \end{aligned} \tag{1.99}$$

These equations must be solved simultaneously to obtain the full solution. They are equivalent to a nonlinear dynamical system of dimension $N = 4$, where the phase space coordinates are (f, f', a, a'), *i.e.*

$$\frac{d}{dx}\begin{pmatrix} f \\ f' \\ a \\ a' \end{pmatrix} = \begin{pmatrix} f' \\ \kappa^2(a^2-1)f + \kappa^2 f^3 \\ a' \\ a f^2 \end{pmatrix} \quad . \tag{1.100}$$

Four boundary conditions must be provided, which we can take to be

$$f(-\infty) = 0 \quad , \quad a'(-\infty) = \frac{1}{\sqrt{2}} \quad , \quad f(+\infty) = 1 \quad , \quad a'(+\infty) = 0 \quad . \tag{1.101}$$

Usually with dynamical systems, we specify N boundary conditions at some initial value $x = x_0$ and then integrate to the final value, using a Runge-Kutta method. Here we specify $\frac{1}{2}N$ boundary conditions at each of the two ends, which requires we use something such as the *shooting method* to solve the coupled ODEs, which effectively converts the boundary value problem to an initial value problem. In Fig. 1.6, we present such a numerical solution to the above system, for $\kappa = 0.2$ (type-I) and for $\kappa = 5$ (type-II).

Vortex solution

To describe a vortex line of strength $n \in \mathbb{Z}$, we choose cylindrical coordinates (ρ, φ, z), and assume no variation in the vertical (z) direction. We write $\psi(\boldsymbol{r}) = f(\rho)\, e^{in\varphi}$ and $\boldsymbol{a}(\boldsymbol{r}) = a(\rho)\,\hat{\boldsymbol{\varphi}}$. which says $\boldsymbol{b}(\boldsymbol{r}) = b(\rho)\,\hat{\boldsymbol{z}}$ with $b(\rho) = \frac{\partial a}{\partial \rho} + \frac{a}{\rho}$. We then obtain

$$\begin{aligned} \frac{1}{\kappa^2}\bigg(\frac{d^2 f}{d\rho^2} + \frac{1}{\rho}\,\frac{df}{d\rho}\bigg) &= \bigg(\frac{n}{\kappa\rho} + a\bigg)^2 f - f + f^3 \\ \frac{d^2 a}{d\rho^2} + \frac{1}{\rho}\,\frac{da}{d\rho} &= \frac{a}{\rho^2} + \bigg(\frac{n}{\kappa\rho} + a\bigg) f^2 \quad . \end{aligned} \tag{1.102}$$

As in the case of the domain wall, this also corresponds to an $N = 4$ dynamical system boundary value problem, which may be solved numerically using the shooting method.

1.5.2 Thin type-I films : critical field strength

Consider a thin extreme type-I (*i.e.* $\kappa \ll 1$) film. Let the finite dimension of the film be along $\hat{\boldsymbol{x}}$, and write $f = f(x)$, $\boldsymbol{a} = a(x)\,\hat{\boldsymbol{y}}$, so $\boldsymbol{\nabla}\times\boldsymbol{a} = b(x)\,\hat{\boldsymbol{z}} = \frac{\partial a}{\partial x}\,\hat{\boldsymbol{z}}$. We assue $f(x) \in \mathbb{R}$. Now $\boldsymbol{\nabla}\times\boldsymbol{b} = -\frac{\partial^2 a}{\partial x^2}\,\hat{\boldsymbol{y}}$, so we have from the second of Eqs. 1.93 that

$$\frac{d^2 f}{dx^2} = a f^2 \quad , \tag{1.103}$$

while the first of Eqs. 1.93 yields

$$\frac{1}{\kappa^2}\,\frac{d^2 f}{dx^2} + (1 - a^2) f - f^3 = 0 \quad . \tag{1.104}$$

We require $f'(x) = 0$ on the boundaries, which we take to lie at $x = \pm\frac{1}{2}d$. For $\kappa \ll 1$, we have, to a first approximation, $f''(x) = 0$ with $f'(\pm\frac{1}{2}d) = 0$. This yields $f = f_0$, a constant, in which case $a''(x) = f_0^2 a(x)$, yielding

$$a(x) = \frac{h_0\,\sinh(f_0 x)}{f_0\,\cosh(\frac{1}{2} f_0 d)} \qquad , \qquad b(x) = \frac{h_0\,\cosh(f_0 x)}{\cosh(\frac{1}{2} f_0 d)} \quad , \tag{1.105}$$

with $h_0 = H_0/\sqrt{2}\,H_{\mathrm{c}}$ the scaled field outside the superconductor. Note $b(\pm\frac{1}{2}d) = h_0$. To determine the constant f_0, we set $f = f_0 + f_1$ and solve for f_1:

$$-\frac{d^2 f_1}{dx^2} = \kappa^2\Big[\big(1 - a^2(x)\big)\, f_0 - f_0^3\Big] \quad . \tag{1.106}$$

In order for a solution to exist, the RHS must be orthogonal to the zeroth order solution[8], *i.e.* we demand

$$\int\limits_{-d/2}^{d/2} dx\, \Big[1 - a^2(x) - f_0^2\Big] \equiv 0 \quad , \tag{1.107}$$

which requires

$$h_0^2 = \frac{2f_0^2\,(1-f_0^2)\cosh^2(\frac{1}{2}f_0 d)}{\big[\sinh(f_0 d)/f_0 d\,\big] - 1} \quad , \tag{1.108}$$

which should be considered an implicit relation for $f_0(h_0)$. The magnetization is

$$m = \frac{1}{4\pi d}\int\limits_{-d/2}^{d/2} dx\, b(x) - \frac{h_0}{4\pi} = \frac{h_0}{4\pi}\left[\frac{\tanh(\frac{1}{2}f_0 d)}{\frac{1}{2}f_0 d} - 1\right] \quad . \tag{1.109}$$

Note that for $f_0 d \gg 1$, we recover the complete Meissner effect, $h_0 = -4\pi m$. In the opposite limit $f_0 d \ll 1$, we find

$$m \simeq -\frac{f_0^2 d^2 h_0}{48\pi} \quad , \quad h_0^2 \simeq \frac{12(1-f_0^2)}{d^2} \quad \Rightarrow \quad m \simeq -\frac{h_0 d^2}{8\pi}\bigg(1 - \frac{h_0^2 d^2}{12}\bigg) \quad . \tag{1.110}$$

Next, consider the free energy difference,

$$\begin{aligned} G_s - G_n &= \frac{H_c^2 \lambda_L^3}{4\pi}\int\limits_{-d/2}^{d/2} dx\, \Big[-f^2 + \tfrac{1}{2}f^4 + (b-h_0)^2 + \big|(\kappa^{-1}\boldsymbol{\nabla} + i\boldsymbol{a})\,f\big|^2 \Big] \\ &= \frac{H_c^2\lambda_L^3 d}{4\pi}\left[\bigg(1 - \frac{\tanh(\frac{1}{2}f_0 d)}{\frac{1}{2}f_0 d}\bigg)h_0^2 - f_0^2 + \tfrac{1}{2}f_0^4\right] \quad . \end{aligned} \tag{1.111}$$

The critical field $h_0 = h_c$ occurs when $G_s = G_n$, hence

$$h_c^2 = \frac{f_0^2\,(1-\frac{1}{2}f_0^2)}{\left[1 - \frac{\tanh(\frac{1}{2}f_0 d)}{\frac{1}{2}f_0 d}\right]} = \frac{2\,f_0^2\,(1-f_0^2)\cosh^2(\frac{1}{2}f_0 d)}{\big[\sinh(f_0 d)/f_0 d\,\big] - 1} \quad . \tag{1.112}$$

We must eliminate f_0 to determine $h_c(d)$.

When the film is thick we can write $f_0 = 1 - \varepsilon$ with $\varepsilon \ll 1$. Then $df_0 = d(1-\varepsilon) \gg 1$ and we have $h_c^2 \simeq 2d\varepsilon$ and $\varepsilon = h_c^2/2d \ll 1$. We also have

$$h_c^2 \approx \frac{\frac{1}{2}}{1 - \frac{2}{d}} \approx \tfrac{1}{2}\Big(1 + \frac{2}{d}\Big) \quad , \tag{1.113}$$

which says

$$h_c(d) = \tfrac{1}{\sqrt{2}}\big(1 + d^{-1}\big) \quad \Rightarrow \quad H_c(d) = H_c(\infty)\Big(1 + \frac{\lambda_L}{d}\Big) \quad , \tag{1.114}$$

where in the very last equation we restore dimensionful units for d.

For a thin film, we have $f_0 \approx 0$, in which case

$$h_c = \frac{2\sqrt{3}}{d}\sqrt{1 - f_0^2} \quad , \tag{1.115}$$

[8] If $\hat{L} f_1 = R$, then $\langle\, f_0 \,|\, R \,\rangle = \langle\, f_0 \,|\, \hat{L} \,|\, f_1 \,\rangle = \langle\, \hat{L}^\dagger f_0 \,|\, f_1 \,\rangle$. Assuming $\hat{L}$ is self-adjoint, and that $\hat{L} f_0 = 0$, we obtain $\langle\, f_0 \,|\, R \,\rangle = 0$. In our case, the operator $\hat{L}$ is given by $\hat{L} = -d^2/dx^2$.

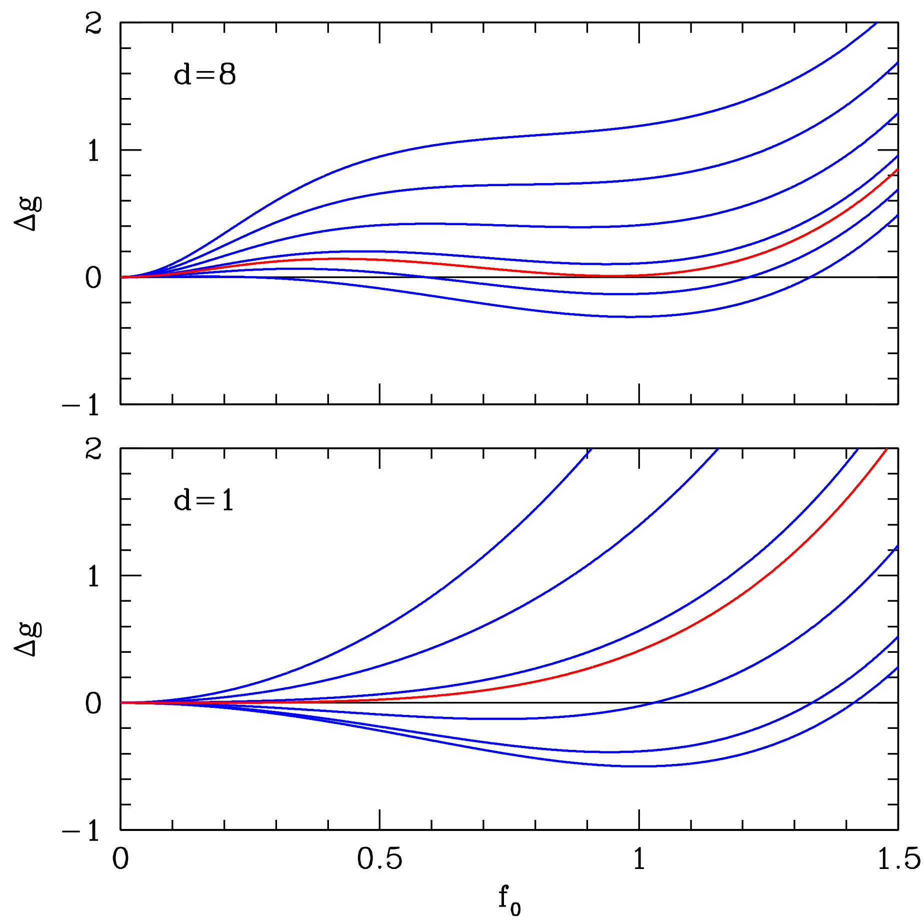

Figure 1.7: Difference in dimensionless free energy density Δg between superconducting and normal state for a thin extreme type-I film of thickness $d\lambda_{\rm L}$. Free energy curves are shown as a function of the amplitude f_0 for several values of the applied field $h_0 = H/\sqrt{2}\,H_{\rm c}(\infty)$ (upper curves correspond to larger h_0 values). Top panel: $d = 8$ curves, with the critical field (in red) at $h_{\rm c} \approx 0.827$ and a first order transition. Lower panel: $d = 1$ curves, with $h_{\rm c} = \sqrt{12} \approx 3.46$ (in red) and a second order transition. The critical thickness is $d_{\rm c} = \sqrt{5}$.

and expanding the hyperbolic tangent, we find

$$h_{\rm c}^2 = \frac{12}{d^2}\big(1 - \tfrac{1}{2}f_0^2\big) \quad . \tag{1.116}$$

This gives

$$f_0 \approx 0 \quad , \quad h_{\rm c} \approx \frac{2\sqrt{3}}{d} \quad \Rightarrow \quad H_{\rm c}(d) = 2\sqrt{6}\,H_{\rm c}(\infty)\,\frac{\lambda_{\rm L}}{d} \quad . \tag{1.117}$$

Note for d large we have $f_0 \approx 1$ at the transition (first order), while for d small we have $f_0 \approx 0$ at the transition (second order). We can see this crossover from first to second order by plotting

$$g = \frac{4\pi}{d\lambda_{\rm L}^3 H_{\rm c}^3}(G_{\rm s} - G_{\rm n}) = \left(1 - \frac{\tanh(\frac{1}{2}f_0 d)}{\frac{1}{2}f_0 d}\right)h_0^2 - f_0^2 + \tfrac{1}{2}f_0^4 \tag{1.118}$$

as a function of f_0 for various values of h_0 and d. Setting $dg/df_0 = 0$ and $d^2g/df_0^2 = 0$ and $f_0 = 0$, we obtain $d_{\rm c} = \sqrt{5}$. See Fig. 1.7. For consistency, we must have $d \ll \kappa^{-1}$.

1.5.3 Critical current of a wire

Consider a wire of radius R and let the total current carried be I. The magnetizing field $\boldsymbol{H}$ is azimuthal, and integrating around the surface of the wire, we obtain

$$2\pi R H_0 = \oint_{r=R} d\boldsymbol{l} \cdot \boldsymbol{H} = \int d\boldsymbol{S} \cdot \boldsymbol{\nabla} \times \boldsymbol{H} = \frac{4\pi}{c} \int d\boldsymbol{S} \cdot \boldsymbol{j} = \frac{4\pi I}{c} \quad . \tag{1.119}$$

Thus,

$$H_0 = H(R) = \frac{2I}{cR} \quad . \tag{1.120}$$

We work in cylindrical coordinates (ρ, φ, z), taking $\boldsymbol{a} = a(\rho)\,\hat{\boldsymbol{z}}$ and $f = f(\rho)$. The scaled GL equations give

$$\big(\kappa^{-1}\boldsymbol{\nabla} + i\boldsymbol{a}\big)^2 f + f - f^3 = 0 \tag{1.121}$$

with[9]

$$\boldsymbol{\nabla} = \hat{\boldsymbol{\rho}}\,\frac{\partial}{\partial\rho} + \frac{\hat{\boldsymbol{\varphi}}}{\rho}\,\frac{\partial}{\partial\varphi} + \hat{\boldsymbol{z}}\,\frac{\partial}{\partial z} \quad . \tag{1.122}$$

Thus,

$$\frac{1}{\kappa^2}\,\frac{\partial^2 f}{\partial\rho^2} + \big(1 - a^2\big) f - f^3 = 0 \quad , \tag{1.123}$$

with $f'(R) = 0$. From $\boldsymbol{\nabla} \times \boldsymbol{b} = -\big(\kappa^{-1}\boldsymbol{\nabla}\theta + \boldsymbol{a}\big)\,|\psi|^2$, where $\arg(\psi) = \theta$, we have $\psi = f \in \mathbb{R}$ hence $\theta = 0$, and therefore

$$\frac{\partial^2 a}{\partial\rho^2} + \frac{1}{\rho}\,\frac{\partial a}{\partial\rho} = a f^2 \quad . \tag{1.124}$$

The magnetic field is

$$\boldsymbol{b} = \boldsymbol{\nabla} \times a(\rho)\,\hat{\boldsymbol{z}} = -\frac{\partial a}{\partial\rho}\,\hat{\boldsymbol{\varphi}} \quad , \tag{1.125}$$

hence $b(\rho) = -\frac{\partial a}{\partial\rho}$, with

$$b(R) = \frac{H(R)}{\sqrt{2}\,H_c} = \frac{\sqrt{2}\,I}{cRH_c} \quad . \tag{1.126}$$

Again, we assume $\kappa \ll 1$, hence $f = f_0$ is the leading order solution to Eqn. 1.123. The vector potential and magnetic field, accounting for boundary conditions, are then given by

$$a(\rho) = -\frac{b(R)\,I_0(f_0\,\rho)}{f_0\,I_1(f_0 R)} \quad , \qquad b(\rho) = \frac{b(R)\,I_1(f_0\,\rho)}{I_1(f_0 R)} \quad , \tag{1.127}$$

where $I_n(z)$ is a modified Bessel function. As in §1.5.2, we determine f_0 by writing $f = f_0 + f_1$ and demanding that f_1 be orthogonal to the uniform solution. This yields the condition

$$\int_0^R d\rho\,\rho\,\Big(1 - f_0^2 - a^2(\rho)\Big) = 0 \quad , \tag{1.128}$$

which gives

$$b^2(R) = \frac{f_0^2\,(1 - f_0^2)\,I_1^2(f_0 R)}{I_0^2(f_0 R) - I_1^2(f_0 R)} \quad . \tag{1.129}$$

[9]Though we don't need to invoke these results, it is good to recall $\frac{\partial\hat{\boldsymbol{\rho}}}{\partial\varphi} = \hat{\boldsymbol{\varphi}}$ and $\frac{\partial\hat{\boldsymbol{\varphi}}}{\partial\varphi} = -\hat{\boldsymbol{\rho}}$.

Thin wire : $R \ll 1$

When $R \ll 1$, we expand the Bessel functions, using

$$I_n(z) = \left(\tfrac{1}{2}z\right)^n \sum_{k=0}^{\infty} \frac{(\frac{1}{4}z^2)^k}{k!\,(k+n)!} \quad . \tag{1.130}$$

Thus

$$\begin{aligned} I_0(z) &= 1 + \tfrac{1}{4}z^2 + \ldots \\ I_1(z) &= \tfrac{1}{2}z + \tfrac{1}{16}z^3 + \ldots \quad , \end{aligned} \tag{1.131}$$

and therefore

$$b^2(R) = \tfrac{1}{4} f_0^4 \big(1 - f_0^2\big) R^2 + \mathcal{O}(R^4) \quad . \tag{1.132}$$

To determine the critical current, we demand that the maximum value of $b(\rho)$ take place at $\rho = R$, yielding

$$\frac{\partial (b^2)}{\partial f_0} = \big(f_0^3 - \tfrac{3}{2} f_0^5\big) R^2 \equiv 0 \quad \Rightarrow \quad f_{0,\mathrm{max}} = \sqrt{\tfrac{2}{3}} \quad . \tag{1.133}$$

From $f_{0,\mathrm{max}}^2 = \frac{2}{3}$, we then obtain

$$b(R) = \frac{R}{3\sqrt{3}} = \frac{\sqrt{2}\, I_\mathrm{c}}{cRH_\mathrm{c}} \quad \Rightarrow \quad I_\mathrm{c} = \frac{cR^2 H_\mathrm{c}}{3\sqrt{6}} \quad . \tag{1.134}$$

The critical current density is then

$$j_\mathrm{c} = \frac{I_\mathrm{c}}{\pi R^2} = \frac{c\,H_\mathrm{c}}{3\sqrt{6}\,\pi\,\lambda_\mathrm{L}} \quad , \tag{1.135}$$

where we have restored physical units.

Thick wire : $1 \ll R \ll \kappa^{-1}$

For a thick wire, we use the asymptotic behavior of $I_n(z)$ for large argument:

$$I_\nu(z) \sim \frac{e^z}{\sqrt{2\pi z}} \sum_{k=0}^{\infty} (-1)^k \, \frac{a_k(\nu)}{z^k} \quad , \tag{1.136}$$

which is known as Hankel's expansion. The expansion coefficients are given by[10]

$$a_k(\nu) = \frac{\big(4\nu^2 - 1^2\big)\big(4\nu^2 - 3^2\big)\cdots\big(4\nu^2 - (2k-1)^2\big)}{8^k\,k!} \quad , \tag{1.137}$$

and we then obtain

$$b^2(R) = f_0^3 (1 - f_0^2) R + \mathcal{O}(R^0) \quad . \tag{1.138}$$

Extremizing with respect to f_0, we obtain $f_{0,\mathrm{max}} = \sqrt{\frac{3}{5}}$ and

$$b_\mathrm{c}(R) = \left(\frac{4 \cdot 3^3}{5^5}\right)^{1/4} R^{1/2} \quad . \tag{1.139}$$

[10] See *e.g.* the *NIST Handbook of Mathematical Functions*, §10.40.1 and §10.17.1.

Restoring units, the critical current of a thick wire is

$$I_c = \frac{3^{3/4}}{5^{5/4}}\, c\, H_c\, R^{3/2}\, \lambda_L^{-1/2} \quad . \tag{1.140}$$

To be consistent, we must have $R \ll \kappa^{-1}$, which explains why our result here does not coincide with the bulk critical current density obtained in Eqn. 1.60.

1.5.4 Magnetic properties of type-II superconductors

Consider an incipient type-II superconductor, when the order parameter is just beginning to form. In this case we can neglect the nonlinear terms in ψ in the Ginzburg-Landau equations 1.93. The first of these equations then yields

$$-\big(\kappa^{-1}\boldsymbol{\nabla} + i\boldsymbol{a}\big)^2\psi = \psi + \overbrace{\mathcal{O}\big(|\psi|^2\psi\big)}^{\approx\, 0} \quad . \tag{1.141}$$

We neglect the second term on the RHS. This is an eigenvalue equation, with the eigenvalue fixed at 1. In fact, this is to be regarded as an equation for $\boldsymbol{a}$, or, more precisely, for the gauge-invariant content of $\boldsymbol{a}$, which is $\boldsymbol{b} = \boldsymbol{\nabla}\times\boldsymbol{a}$. The second of the GL equations says $\boldsymbol{\nabla}\times(\boldsymbol{b}-\boldsymbol{h}) = \mathcal{O}\big(|\psi|^2\big)$, from which we conclude $\boldsymbol{b} = \boldsymbol{h} + \boldsymbol{\nabla}\zeta$, but inspection of the free energy itself tells us $\boldsymbol{\nabla}\zeta = 0$.

We assume $\boldsymbol{b} = h\hat{\boldsymbol{z}}$ and choose a gauge for $\boldsymbol{a}$:

$$\boldsymbol{a} = -\tfrac{1}{2} b\, y\, \hat{\boldsymbol{x}} + \tfrac{1}{2} b\, x\, \hat{\boldsymbol{y}} \quad , \tag{1.142}$$

with $b = h$. We define the operators

$$\pi_x = \frac{1}{i\kappa}\frac{\partial}{\partial x} - \tfrac{1}{2} b\, y \qquad , \qquad \pi_y = \frac{1}{i\kappa}\frac{\partial}{\partial y} + \tfrac{1}{2} b\, x \quad . \tag{1.143}$$

Note that $\big[\pi_x, \pi_y\big] = b/i\kappa$, and that

$$-\big(\kappa^{-1}\boldsymbol{\nabla} + i\boldsymbol{a}\big)^2 = -\frac{1}{\kappa^2}\frac{\partial^2}{\partial z^2} + \pi_x^2 + \pi_y^2 \quad . \tag{1.144}$$

We now define the ladder operators

$$\begin{aligned} \gamma &= \sqrt{\frac{\kappa}{2b}}\,\big(\pi_x - i\pi_y\big) \\ \gamma^\dagger &= \sqrt{\frac{\kappa}{2b}}\,\big(\pi_x + i\pi_y\big) \quad , \end{aligned} \tag{1.145}$$

which satisfy $\big[\gamma, \gamma^\dagger\big] = 1$. Then

$$\hat{L} \equiv -\big(\kappa^{-1}\boldsymbol{\nabla} + i\boldsymbol{a}\big)^2 = -\frac{1}{\kappa^2}\frac{\partial^2}{\partial z^2} + \frac{2b}{\kappa}\big(\gamma^\dagger\gamma + \tfrac{1}{2}\big) \quad . \tag{1.146}$$

The eigenvalues of the operator $\hat{L}$ are therefore

$$\varepsilon_n(k_z) = \frac{k_z^2}{\kappa^2} + \big(n + \tfrac{1}{2}\big)\cdot\frac{2b}{\kappa} \quad . \tag{1.147}$$

The lowest eigenvalue is therefore b/κ. This crosses the threshold value of 1 when $b = \kappa$, *i.e.* when

$$H = \sqrt{2}\,\kappa\, H_c \equiv H_{c2} \quad . \tag{1.148}$$

So, what have we shown? When $b = h < \frac{1}{\sqrt{2}}$, so $H_{c2} < H_c$ (we call H_c the *thermodynamic critical field*), a complete Meissner effect occurs when H is decreased below H_c. The order parameter ψ jumps discontinuously, and the transition across H_c is first order. If $\kappa > \frac{1}{\sqrt{2}}$, then $H_{c2} > H_c$, and for H just below H_{c2} the system wants $\psi \neq 0$. However, a complete Meissner effect cannot occur for $H > H_c$, so for $H_c < H < H_{c2}$ the system is in the so-called *mixed phase*. Recall that $H_c = \phi_L/\sqrt{8}\,\pi\,\xi\lambda_L$, hence

$$H_{c2} = \sqrt{2}\,\kappa\,H_c = \frac{\phi_L}{2\pi\xi^2} \quad . \tag{1.149}$$

Thus, H_{c2} is the field at which neighboring vortex lines, each of which carry flux ϕ_L, are separated by a distance on the order of ξ.

1.5.5 Lower critical field

We now compute the energy of a perfectly straight vortex line, and ask at what field H_{c1} vortex lines first penetrate. Let's consider the regime $\rho > \xi$, where $\psi \simeq e^{i\varphi}$, *i.e.* $|\psi| \simeq 1$. Then the second of the Ginzburg-Landau equations gives

$$\boldsymbol{\nabla} \times \boldsymbol{b} = -\big(\kappa^{-1}\boldsymbol{\nabla}\varphi + \boldsymbol{a}\big) \quad . \tag{1.150}$$

Therefore the Gibbs free energy is

$$G_V = \frac{H_c^2\,\lambda_L^3}{4\pi}\int\! d^3r\,\Big\{ -\tfrac{1}{2} + \boldsymbol{b}^2 + (\boldsymbol{\nabla}\times\boldsymbol{b})^2 - 2\boldsymbol{h}\cdot\boldsymbol{b}\Big\} \quad . \tag{1.151}$$

The first term in the brackets is the condensation energy density $-H_c^2/8\pi$. The second term is the electromagnetic field energy density $\boldsymbol{B}^2/8\pi$. The third term is $\lambda_L^2\,(\boldsymbol{\nabla}\times\boldsymbol{B})^2/8\pi$, and accounts for the kinetic energy density in the superflow.

The energy penalty for a vortex is proportional to its length. We have

$$\begin{aligned}\frac{G_V - G_0}{L} &= \frac{H_c^2\,\lambda_L^2}{4\pi}\int\! d^2\rho\,\Big\{\boldsymbol{b}^2 + (\boldsymbol{\nabla}\times\boldsymbol{b})^2 - 2\,\boldsymbol{h}\cdot\boldsymbol{b}\Big\}\\ &= \frac{H_c^2\,\lambda_L^2}{4\pi}\int\! d^2\rho\,\Big\{\boldsymbol{b}\cdot\big[\boldsymbol{b} + \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{b})\big] - 2\boldsymbol{h}\cdot\boldsymbol{b}\Big\} \quad .\end{aligned} \tag{1.152}$$

The total flux is

$$\int\! d^2\rho\,\boldsymbol{b}(\boldsymbol{\rho}) = -2\pi n\kappa^{-1}\,\hat{\boldsymbol{z}} \quad , \tag{1.153}$$

in units of $\sqrt{2}\,H_c\,\lambda_L^2$. We also have $b(\boldsymbol{\rho}) = -n\kappa^{-1}\,K_0(\rho)$ and, taking the curl of Eqn. 1.150, we have $\boldsymbol{b}+\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{b}) = -2\pi n\kappa^{-1}\,\delta(\boldsymbol{\rho})\,\hat{\boldsymbol{z}}$. As mentioned earlier above, the logarithmic divergence of $b(\rho\to 0)$ is an artifact of the London limit, where the vortices have no core structure. The core can crudely be accounted for by simply replacing $B(0)$ by $B(\xi)$, *i.e.* replacing $b(0)$ by $b(\xi/\lambda_L) = b(\kappa^{-1})$. Then, for $\kappa \gg 1$, after invoking Eqn. 1.67,

$$\frac{G_V - G_0}{L} = \frac{H_c^2\,\lambda_L^2}{4\pi}\Big\{2\pi n^2\kappa^{-2}\ln\big(2\,e^{-C}\kappa\big) + 4\pi n h\kappa^{-1}\Big\} \quad . \tag{1.154}$$

For vortices with vorticity $n = -1$, this first turns negative at a field

$$h_{c1} = \tfrac{1}{2}\kappa^{-1}\ln\big(2\,e^{-C}\kappa\big) \quad . \tag{1.155}$$

With $2\,e^{-C} \simeq 1.23$, we have, restoring units,

$$H_{c1} = \frac{H_c}{\sqrt{2}\,\kappa}\,\ln\big(2\,e^{-C}\kappa\big) = \frac{\phi_L}{4\pi\lambda_L^2}\,\ln(1.23\,\kappa) \quad . \tag{1.156}$$

So we have

$$
\begin{aligned}
H_{\mathrm{c1}} &= \frac{\ln(1.23\,\kappa)}{\sqrt{2}\,\kappa}\,H_{\mathrm{c}} \quad (\kappa \gg 1) \\
H_{\mathrm{c2}} &= \sqrt{2}\,\kappa\,H_{\mathrm{c}} \quad ,
\end{aligned}
\tag{1.157}
$$

where H_{c} is the thermodynamic critical field. Note in general that if E_{v} is the energy of a single vortex, then the lower critical field is given by the relation $H_{\mathrm{c1}}\phi_{\mathrm{L}} = 4\pi E_{\mathrm{v}}$, *i.e.*

$$
H_{\mathrm{c1}} = \frac{4\pi E_{\mathrm{v}}}{\phi_{\mathrm{L}}} \quad . \tag{1.158}
$$

1.5.6 Abrikosov vortex lattice

Consider again the linearized GL equation $-\big(\kappa^{-1}\boldsymbol{\nabla} + i\boldsymbol{a}\big)^2\psi = \psi$ with $\boldsymbol{b} = \boldsymbol{\nabla}\times\boldsymbol{a} = b\,\hat{\boldsymbol{z}}$, with $b = \kappa$, *i.e.* $B = H_{\mathrm{c2}}$. We chose the gauge $\boldsymbol{a} = \frac{1}{2}b\,(-y, x, 0)$. We showed that $\psi(\boldsymbol{\rho})$ with no z-dependence is an eigenfunction with unit eigenvalue. Recall also that $\gamma\,\psi(\boldsymbol{\rho}) = 0$, where

$$
\begin{aligned}
\gamma &= \frac{1}{\sqrt{2}}\left(\frac{1}{i\kappa}\frac{\partial}{\partial x} - \frac{\kappa}{2}\,y - \frac{1}{\kappa}\frac{\partial}{\partial y} - \frac{i\kappa}{2}\,x\right) \\
&= \frac{\sqrt{2}}{i\kappa}\left(\frac{\partial}{\partial w} + \tfrac{1}{4}\kappa^2\bar{w}\right) \quad ,
\end{aligned}
\tag{1.159}
$$

where $w = x + iy$ and $\bar{w} = x - iy$ are complex. To find general solutions of $\gamma\,\psi = 0$, note that

$$
\gamma = \frac{\sqrt{2}}{i\kappa}\,e^{-\kappa^2\bar{w}w/4}\,\frac{\partial}{\partial w}\,e^{+\kappa^2\bar{w}w/4} \quad . \tag{1.160}
$$

Thus, $\gamma\,\psi(x,y)$ is satisfied by any function of the form

$$
\psi(x,y) = f(\bar{w})\,e^{-\kappa^2\bar{w}w/4} \quad . \tag{1.161}
$$

where $f(\bar{w})$ is analytic in the complex coordinate $\bar{w}$. This set of functions is known as the *lowest Landau level*.

The most general such function[11] is of the form

$$
f(\bar{w}) = C\prod_i(\bar{w} - \bar{w}_i) \quad , \tag{1.162}
$$

where each $\bar{w}_i$ is a zero of $f(\bar{w})$. Any analytic function on the plane is, up to a constant, uniquely specified by the positions of its zeros. Note that

$$
\big|\psi(x,y)\big|^2 = |C|^2\,e^{-\kappa^2\bar{w}w/2}\prod_i\big|w - w_i\big|^2 \equiv |C|^2\,e^{-\Phi(\boldsymbol{\rho})} \quad , \tag{1.163}
$$

where

$$
\Phi(\boldsymbol{\rho}) = \tfrac{1}{2}\kappa^2\boldsymbol{\rho}^2 - 2\sum_i \ln\big|\boldsymbol{\rho} - \boldsymbol{\rho}_i\big| \quad . \tag{1.164}
$$

[11]We assume that ψ is square-integrable, which excludes poles in $f(\bar{w})$.

$\Phi(\boldsymbol{\rho})$ may be interpreted as the electrostatic potential of a set of point charges located at $\boldsymbol{\rho}_i$, in the presence of a uniform neutralizing background. To see this, recall that $\nabla^2 \ln \rho = 2\pi\, \delta(\boldsymbol{\rho})$, so

$$\nabla^2\Phi(\boldsymbol{\rho}) = 2\kappa^2 - 4\pi \sum_i \delta\big(\boldsymbol{\rho} - \boldsymbol{\rho}_i\big) \quad . \tag{1.165}$$

Therefore if we are to describe a state where the local density $|\psi|^2$ is uniform on average, we must impose $\langle \nabla^2\Phi \rangle = 0$, which says

$$\Big\langle \sum_i \delta(\boldsymbol{\rho} - \boldsymbol{\rho}_i) \Big\rangle = \frac{\kappa^2}{2\pi} \quad . \tag{1.166}$$

The zeroes $\boldsymbol{\rho}_i$ are of course the positions of (anti)vortices, hence the uniform state has vortex density $n_{\rm v} = \kappa^2/2\pi$. Recall that in these units each vortex carries $2\pi/\kappa$ London flux quanta, which upon restoring units is

$$\frac{2\pi}{\kappa} \cdot \sqrt{2}\, H_{\rm c}\, \lambda_{\rm L}^2 = 2\pi \cdot \sqrt{2}\, H_{\rm c}\, \lambda_{\rm L}\, \xi = \frac{hc}{e^*} = \phi_{\rm L} \quad . \tag{1.167}$$

Multiplying the vortex density $n_{\rm v}$ by the vorticity $2\pi/\kappa$, we obtain the magnetic field strength,

$$b = h = \frac{\kappa^2}{2\pi} \times \frac{2\pi}{\kappa} = \kappa \quad . \tag{1.168}$$

In other words, $H = H_{\rm c2}$.

Just below the upper critical field

Next, we consider the case where H is just below the upper critical field $H_{\rm c2}$. We write $\psi = \psi_0 + \delta\psi$, and $b = \kappa + \delta b$, with $\delta b < 0$. We apply the method of successive approximation, and solve for b using the second GL equation. This yields

$$b = h - \frac{|\psi_0|^2}{2\kappa} \qquad , \qquad \delta b = h - \kappa - \frac{|\psi_0|^2}{2\kappa} \tag{1.169}$$

where $\psi_0(\boldsymbol{\rho})$ is our initial solution for $\delta b = 0$. To see this, note that the second GL equation may be written

$$\boldsymbol{\nabla} \times (\boldsymbol{h} - \boldsymbol{b}) = \tfrac{1}{2}\Big(\psi^*\, \boldsymbol{\pi}\, \psi + \psi\, \boldsymbol{\pi}^*\, \psi^*\Big) = \mathsf{Re}\,\Big(\psi^*\, \boldsymbol{\pi}\, \psi\Big) \quad , \tag{1.170}$$

where $\boldsymbol{\pi} = -i\kappa^{-1}\boldsymbol{\nabla} + \boldsymbol{a}$. On the RHS we now replace ψ by ψ_0 and b by κ, corresponding to our lowest order solution. This means we write $\boldsymbol{\pi} = \boldsymbol{\pi}_0 + \delta\boldsymbol{a}$, with $\boldsymbol{\pi}_0 = -i\kappa^{-1}\boldsymbol{\nabla} + \boldsymbol{a}_0$, $\boldsymbol{a}_0 = \frac{1}{2}\kappa\, \hat{\boldsymbol{z}} \times \boldsymbol{\rho}$, and $\boldsymbol{\nabla} \times \delta\boldsymbol{a} = \delta b\, \hat{\boldsymbol{z}}$. Assuming $h - b = |\psi_0|^2/2\kappa$, we have

$$\begin{aligned} \boldsymbol{\nabla} \times \left(\frac{|\psi_0|^2}{2\kappa}\hat{\boldsymbol{z}}\right) &= \frac{1}{2\kappa}\left[\frac{\partial}{\partial y}\,(\psi_0^*\,\psi_0)\,\hat{\boldsymbol{x}} - \frac{\partial}{\partial x}\,(\psi_0^*\,\psi_0)\,\hat{\boldsymbol{y}}\right] \\ &= \frac{1}{\kappa}\,\mathsf{Re}\,\Big[\psi_0^*\,\partial_y\,\psi_0\,\hat{\boldsymbol{x}} - \psi_0^*\,\partial_x\,\psi_0\,\hat{\boldsymbol{y}}\Big] \\ &= \mathsf{Re}\,\Big[\psi_0^*\, i\pi_{0y}\,\psi_0\,\hat{\boldsymbol{x}} - \psi_0^*\, i\pi_{0x}\,\psi_0\,\hat{\boldsymbol{y}}\Big] = \mathsf{Re}\,\Big[\psi_0^*\,\boldsymbol{\pi}_0\,\psi_0\Big] \quad , \end{aligned} \tag{1.171}$$

since $i\pi_{0y} = \kappa^{-1}\partial_y + ia_{0y}$ and $\mathsf{Re}\,\big[i\psi_0^*\,\psi_0\,a_{0y}\big] = 0$. Note also that since $\gamma\,\psi_0 = 0$ and $\gamma = \frac{1}{\sqrt{2}}\big(\pi_{0x} - i\pi_{0y}\big) = \frac{1}{\sqrt{2}}\pi_0^\dagger$, we have $\pi_{0y}\psi_0 = -i\pi_{0x}\psi_0$ and, equivalently, $\pi_{0x}\psi_0 = i\pi_{0y}\psi_0$.

Inserting this result into the first GL equation yields an inhomogeneous equation for $\delta\psi$. The original equation is

$$\Big(\boldsymbol{\pi}^2 - 1\Big)\psi = -|\psi|^2\psi \quad . \tag{1.172}$$

With $\boldsymbol{\pi} = \boldsymbol{\pi}_0 + \delta\boldsymbol{a}$, we then have

$$\Big(\boldsymbol{\pi}_0^2 - 1\Big)\delta\psi = -\delta\boldsymbol{a}\cdot\boldsymbol{\pi}_0\,\psi_0 - \boldsymbol{\pi}_0\cdot\delta\boldsymbol{a}\,\psi_0 - |\psi_0|^2\psi_0 \quad . \tag{1.173}$$

The RHS of the above equation must be orthogonal to ψ_0, since $\big(\boldsymbol{\pi}_0^2 - 1\big)\psi_0 = 0$. That is to say,

$$\int\! d^2r\;\psi_0^*\,\Big[\delta\boldsymbol{a}\cdot\boldsymbol{\pi}_0 + \boldsymbol{\pi}_0\cdot\delta\boldsymbol{a} + |\psi_0|^2\Big]\psi_0 = 0 \quad . \tag{1.174}$$

Note that

$$\delta\boldsymbol{a}\cdot\boldsymbol{\pi}_0 + \boldsymbol{\pi}_0\cdot\delta\boldsymbol{a} = \tfrac{1}{2}\,\delta a\,\pi_0^\dagger + \tfrac{1}{2}\,\pi_0^\dagger\,\delta a + \tfrac{1}{2}\,\delta\bar{a}\,\pi_0 + \tfrac{1}{2}\,\pi_0\,\delta\bar{a} \quad , \tag{1.175}$$

where

$$\pi_0 = \pi_{0x} + i\pi_{0y} \quad , \quad \pi_0^\dagger = \pi_{0x} - i\pi_{0y} \quad , \quad \delta a = \delta a_x + i\delta a_y \quad , \quad \delta\bar{a} = \delta a_x - i\delta a_y \quad . \tag{1.176}$$

We also have, from Eqn. 1.143,

$$\pi_0 = -2i\kappa^{-1}\big(\partial_{\bar{w}} - \tfrac{1}{4}\kappa^2 w\big) \qquad , \qquad \pi_0^\dagger = -2i\kappa^{-1}\big(\partial_w + \tfrac{1}{4}\kappa^2\bar{w}\big) \quad . \tag{1.177}$$

Note that

$$\begin{aligned} \pi_0^\dagger\,\delta a &= \big[\pi_0^\dagger\,,\,\delta a\big] + \delta a\,\pi_0^\dagger = -2i\kappa^{-1}\,\partial_w\,\delta a + \delta a\,\pi_0^\dagger \\ \delta\bar{a}\,\pi_0 &= \big[\delta\bar{a}\,,\,\pi_0\big] + \pi_0\,\delta\bar{a} = +2i\kappa^{-1}\,\partial_{\bar{w}}\,\delta\bar{a} + \pi_0\,\delta\bar{a} \end{aligned} \tag{1.178}$$

Therefore,

$$\int\! d^2r\;\psi_0^*\,\Big[\delta a\,\pi_0^\dagger + \pi_0\,\delta\bar{a} - i\kappa^{-1}\,\partial_w\,\delta a + i\kappa^{-1}\,\partial_{\bar{w}}\,\delta\bar{a} + |\psi_0|^2\Big]\psi_0 = 0 \quad . \tag{1.179}$$

We now use the fact that $\pi_0^\dagger\,\psi_0 = 0$ and $\psi_0^*\,\pi_0 = 0$ (integrating by parts) to kill off the first two terms inside the square brackets. The third and fourth term combine to give

$$-i\,\partial_w\,\delta a + i\,\partial_{\bar{w}}\,\delta\bar{a} = \partial_x\,\delta a_y - \partial_y\,\delta a_x = \delta b \quad . \tag{1.180}$$

Plugging in our expression for δb, we finally have our prize:

$$\int\! d^2r\,\left[\left(\frac{h}{\kappa} - 1\right)|\psi_0|^2 + \left(1 - \frac{1}{2\kappa^2}\right)|\psi_0|^4\right] = 0 \quad . \tag{1.181}$$

We may write this as

$$\left(1 - \frac{h}{\kappa}\right)\big\langle|\psi_0|^2\big\rangle = \left(1 - \frac{1}{2\kappa^2}\right)\big\langle|\psi_0|^4\big\rangle \quad , \tag{1.182}$$

where

$$\big\langle F(\boldsymbol{\rho})\big\rangle = \frac{1}{A}\int\! d^2\rho\;F(\boldsymbol{\rho}) \tag{1.183}$$

denotes the global spatial average of $F(\boldsymbol{\rho})$. It is customary to define the ratio

$$\beta_{\rm A} \equiv \frac{\big\langle|\psi_0|^4\big\rangle}{\big\langle|\psi_0|^2\big\rangle^2} \quad , \tag{1.184}$$

which depends on the distribution of the zeros $\{\boldsymbol{\rho}_i\}$. Note that

$$\big\langle|\psi_0|^2\big\rangle = \frac{1}{\beta_{\rm A}}\cdot\frac{\big\langle|\psi_0|^4\big\rangle}{\big\langle|\psi_0|^2\big\rangle} = \frac{2\kappa(\kappa - h)}{(2\kappa^2 - 1)\beta_{\rm A}} \quad . \tag{1.185}$$

Now let's compute the Gibbs free energy density. We have

$$\begin{aligned} g_{\rm s} - g_{\rm n} &= -\big\langle|\psi_0|^4\big\rangle + 2\,\big\langle(b-h)^2\big\rangle \\ &= -\bigg(1-\frac{1}{2\kappa^2}\bigg)\big\langle|\psi_0|^4\big\rangle = -\bigg(1-\frac{h}{\kappa}\bigg)\big\langle|\psi_0|^2\big\rangle = -\frac{2\,(\kappa-h)^2}{(2\kappa^2-1)\beta_{\rm A}} \quad . \end{aligned} \tag{1.186}$$

Since $g_{\rm n} = -2\,h^2$, we have, restoring physical units

$$g_{\rm s} = -\frac{1}{8\pi}\bigg[H^2 + \frac{(H_{\rm c2}-H)^2}{(2\kappa^2-1)\beta_{\rm A}}\bigg] \quad . \tag{1.187}$$

The average magnetic field is then

$$\bar{B} = -4\pi\,\frac{\partial g_{\rm s}}{\partial H} = H - \frac{H_{\rm c2}-H}{(2\kappa^2-1)\beta_{\rm A}} \quad , \tag{1.188}$$

hence

$$M = \frac{B-H}{4\pi} = \frac{H-H_{\rm c2}}{4\pi\,(2\kappa^2-1)\,\beta_{\rm A}} \qquad \Rightarrow \qquad \chi = \frac{\partial M}{\partial H} = \frac{1}{4\pi\,(2\kappa^2-1)\,\beta_{\rm A}} \quad . \tag{1.189}$$

Clearly $g_{\rm s}$ is minimized by making $\beta_{\rm A}$ as small as possible, which is achieved by a regular lattice structure. Since $\beta_{\rm A}^{\rm square} = 1.18$ and $\beta_{\rm A}^{\rm triangular} = 1.16$, the triangular lattice just barely wins.

Just above the lower critical field

When H is just slightly above $H_{\rm c1}$, vortex lines penetrate the superconductor, but their density is very low. To see this, we once again invoke the result of Eqn. 1.152, extending that result to the case of many vortices:

$$\frac{G_{\rm VL}-G_0}{L} = \frac{H_{\rm c}^2\,\lambda_{\rm L}^2}{4\pi}\int\! d^2\!\rho\,\Big\{\boldsymbol{b}\cdot\big[\boldsymbol{b}+\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{b})\big] - 2\boldsymbol{h}\cdot\boldsymbol{b}\Big\} \quad . \tag{1.190}$$

Here we have

$$\begin{aligned} \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{b}) + \boldsymbol{b} &= -\frac{2\pi}{\kappa}\sum_i n_i\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}_i) \\ \boldsymbol{b} &= -\frac{1}{\kappa}\sum_i n_i\,K_0\big(|\boldsymbol{\rho}-\boldsymbol{\rho}_i|\big) \quad . \end{aligned} \tag{1.191}$$

Thus, again replacing $K_0(0)$ by $K_0(\kappa^{-1})$ and invoking Eqn. 1.67 for $\kappa \gg 1$,

$$\frac{G_{\rm VL}-G_0}{L} = \frac{H_{\rm c}^2\,\lambda_{\rm L}^2}{\kappa^2}\left\{\tfrac{1}{2}\ln(1.23\,\kappa)\sum_i n_i^2 + \sum_{i<j} n_i\,n_j\,K_0\big(|\boldsymbol{\rho}_i-\boldsymbol{\rho}_j|\big) + \kappa h\sum_i n_i\right\} \quad . \tag{1.192}$$

The first term on the RHS is the self-interaction, cut off at a length scale κ^{-1} (ξ in physical units). The second term is the interaction between different vortex lines. We've assumed a perfectly straight set of vortex lines – no wiggling! The third term arises from $\boldsymbol{B}\cdot\boldsymbol{H}$ in the Gibbs free energy. If we assume a finite density of vortex lines, we may calculate the magnetization. For $H - H_{\rm c1} \ll H_{\rm c1}$, the spacing between the vortices is huge, and since $K_0(r) \simeq (\pi/2r)^{1/2}\exp(-r)$ for large $|r|$, we may safely neglect all but nearest neighbor interaction terms. We assume $n_i = -1$ for all i. Let the vortex lines form a regular lattice of coordination number z and nearest neighbor separation d. Then

$$\frac{G_{\rm VL}-G_0}{L} = \frac{N H_{\rm c}^2\,\lambda_{\rm L}^2}{\kappa^2}\,\Big\{\tfrac{1}{2}\ln(1.23\,\kappa) + \tfrac{1}{2}zK_0(d) - \kappa h\Big\} \quad , \tag{1.193}$$

where N is the total number of vortex lines, given by $N = A/\Omega$ for a lattice with unit cell area Ω. Assuming a triangular lattice, $\Omega = \frac{\sqrt{3}}{2}\, d^2$ and $z = 6$. Then

$$\frac{G_{\rm VL} - G_0}{L} = \frac{H_{\rm c}^2\, \lambda_{\rm L}^2}{\sqrt{3}\, \kappa^2} \Big\{ \big[\ln(1.23\, \kappa) - 2\kappa h \big] d^{-2} + 6 d^{-2} K_0(d) \Big\} \quad . \tag{1.194}$$

Provided $h > h_{\rm c1} = \ln(1.23\, \kappa)/2\kappa$, this is minimized at a finite value of d.

Chapter 2

Response, Resonance, and the Electron Gas

2.1 Response and Resonance

Consider a damped harmonic oscillator subjected to a time-dependent forcing:

$$\ddot{x} + 2\gamma\dot{x} + \omega_0^2 x = f(t) \ , \tag{2.1}$$

where γ is the damping rate ($\gamma > 0$) and ω_0 is the natural frequency in the absence of damping[1]. We adopt the following convention for the Fourier transform of a function $H(t)$:

$$H(t) = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \hat{H}(\omega)\, e^{-i\omega t} \tag{2.2}$$

$$\hat{H}(\omega) = \int\limits_{-\infty}^{\infty} dt\, H(t)\, e^{+i\omega t} \ . \tag{2.3}$$

Note that if $H(t)$ is a real function, then $\hat{H}(-\omega) = \hat{H}^*(\omega)$. In Fourier space, then, eqn. (2.1) becomes

$$(\omega_0^2 - 2i\gamma\omega - \omega^2)\, \hat{\boldsymbol{x}}(\omega) = \hat{f}(\omega) \ , \tag{2.4}$$

with the solution

$$\hat{\boldsymbol{x}}(\omega) = \frac{\hat{f}(\omega)}{\omega_0^2 - 2i\gamma\omega - \omega^2} \equiv \hat{\chi}(\omega)\, \hat{f}(\omega) \tag{2.5}$$

where $\hat{\chi}(\omega)$ is the *susceptibility function*:

$$\hat{\chi}(\omega) = \frac{1}{\omega_0^2 - 2i\gamma\omega - \omega^2} = \frac{-1}{(\omega - \omega_+)(\omega - \omega_-)} \ , \tag{2.6}$$

with

$$\omega_\pm = -i\gamma \pm \sqrt{\omega_0^2 - \gamma^2} \ . \tag{2.7}$$

[1] Note that $f(t)$ has dimensions of acceleration.

The complete solution to (2.1) is then

$$x(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, \frac{\hat{f}(\omega)\, e^{-i\omega t}}{\omega_0^2 - 2i\gamma\omega - \omega^2} + x_{\rm h}(t) \tag{2.8}$$

where $x_{\rm h}(t)$ is the homogeneous solution,

$$x_{\rm h}(t) = A_+ e^{-i\omega_+ t} + A_- e^{-i\omega_- t} \,. \tag{2.9}$$

Since $\mathrm{Im}(\omega_\pm) < 0$, $x_{\rm h}(t)$ is a *transient* which decays in time. The coefficients $A_\pm$ may be chosen to satisfy initial conditions on $x(0)$ and $\dot{x}(0)$, but the system 'loses its memory' of these initial conditions after a finite time, and in steady state all that is left is the inhomogeneous piece, which is completely determined by the forcing.

In the time domain, we can write

$$x(t) = \int_{-\infty}^{\infty} dt' \; \chi(t-t')\, f(t') \tag{2.10}$$

$$\chi(s) \equiv \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \; \hat{\chi}(\omega)\, e^{-i\omega s} \,, \tag{2.11}$$

which brings us to a very important and sensible result:

<u>*Claim*</u>: The response is *causal*, *i.e.* $\chi(t-t') = 0$ when $t < t'$, provided that $\hat{\chi}(\omega)$ is analytic in the upper half plane of the variable ω.

<u>*Proof*</u>: Consider eqn. (2.11). Of $\hat{\chi}(\omega)$ is analytic in the upper half plane, then closing in the UHP we obtain $\chi(s<0) = 0$.

For our example (2.6), we close in the LHP for $s > 0$ and obtain

$$\begin{aligned} \chi(s>0) &= (-2\pi i) \sum_{\omega \in \mathrm{LHP}} \mathrm{Res} \left\{ \frac{1}{2\pi}\, \hat{\chi}(\omega)\, e^{-i\omega s} \right\} \\ &= \frac{i e^{-i\omega_+ s}}{\omega_+ - \omega_-} + \frac{i e^{-i\omega_- s}}{\omega_- - \omega_+} \,, \end{aligned} \tag{2.12}$$

i.e.

$$\chi(s) = \begin{cases} \frac{e^{-\gamma s}}{\sqrt{\omega_0^2 - \gamma^2}} \, \sin\left(\sqrt{\omega_0^2 - \gamma^2}\right) \Theta(s) & \text{if } \omega_0^2 > \gamma^2 \\ \\ \frac{e^{-\gamma s}}{\sqrt{\gamma^2 - \omega_0^2}} \, \sinh\left(\sqrt{\gamma^2 - \omega_0^2}\right) \Theta(s) & \text{if } \omega_0^2 < \gamma^2 \,, \end{cases} \tag{2.13}$$

where $\Theta(s)$ is the step function: $\Theta(s \geq 0) = 1$, $\Theta(s<0) = 0$. Causality simply means that events occuring after the time t cannot influence the state of the system at t. Note that, in general, $\chi(t)$ describes the time-dependent response to a δ-function impulse at $t = 0$.

2.1.1 Energy Dissipation

How much work is done by the force $f(t)$? Since the power applied is $P(t) = f(t)\,\dot{x}(t)$, we have

$$P(t) = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,(-i\omega)\,\hat{\chi}(\omega)\,\hat{f}(\omega)\,e^{-i\omega t} \int\limits_{-\infty}^{\infty} \frac{d\nu}{2\pi}\,\hat{f}^*(\nu)\,e^{+i\nu t} \tag{2.14}$$

$$\Delta E = \int\limits_{-\infty}^{\infty} dt\,P(t) = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,(-i\omega)\,\hat{\chi}(\omega)\,\big|\hat{f}(\omega)\big|^2 \ . \tag{2.15}$$

Separating $\hat{\chi}(\omega)$ into real and imaginary parts,

$$\hat{\chi}(\omega) = \hat{\chi}'(\omega) + i\hat{\chi}''(\omega)\ , \tag{2.16}$$

we find for our example

$$\hat{\chi}'(\omega) = \frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + 4\gamma^2\omega^2} = +\hat{\chi}'(-\omega) \tag{2.17}$$

$$\hat{\chi}''(\omega) = \frac{2\gamma\omega}{(\omega_0^2 - \omega^2)^2 + 4\gamma^2\omega^2} = -\hat{\chi}''(-\omega). \tag{2.18}$$

The energy dissipated may now be written

$$\Delta E = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,\omega\,\hat{\chi}''(\omega)\,\big|\hat{f}(\omega)\big|^2 \ . \tag{2.19}$$

The even function $\hat{\chi}'(\omega)$ is called the *reactive* part of the susceptibility; the odd function $\hat{\chi}''(\omega)$ is the *dissipative* part. When experimentalists measure a *lineshape*, they usually are referring to features in $\omega\,\hat{\chi}''(\omega)$, which describes the absorption rate as a function of driving frequency.

2.2 Kramers-Kronig Relations

Let $\chi(z)$ be a complex function of the complex variable z which is analytic in the upper half plane. Then the following integral must vanish,

$$\oint\limits_{\mathcal{C}} \frac{dz}{2\pi i}\,\frac{\chi(z)}{z-\zeta} = 0\ , \tag{2.20}$$

whenever $\mathrm{Im}(\zeta) \le 0$, where $\mathcal{C}$ is the contour depicted in fig. 2.1.

Now let $\omega \in \mathbb{R}$ be real, and define the complex function $\chi(\omega)$ of the real variable ω by

$$\chi(\omega) \equiv \lim_{\epsilon \to 0^+} \chi(\omega + i\epsilon)\ . \tag{2.21}$$

Assuming $\chi(z)$ vanishes sufficiently rapidly that Jordan's lemma may be invoked (*i.e.* that the integral of $\chi(z)$ along the arc of $\mathcal{C}$ vanishes), we have

$$\begin{aligned} 0 &= \int\limits_{-\infty}^{\infty} \frac{d\nu}{2\pi i}\,\frac{\chi(\nu)}{\nu - \omega + i\epsilon} \\ &= \int\limits_{-\infty}^{\infty} \frac{d\nu}{2\pi i}\,\big[\chi'(\nu) + i\chi''(\nu)\big]\left[\frac{\mathcal{P}}{\nu-\omega} - i\pi\delta(\nu-\omega)\right] \end{aligned} \tag{2.22}$$

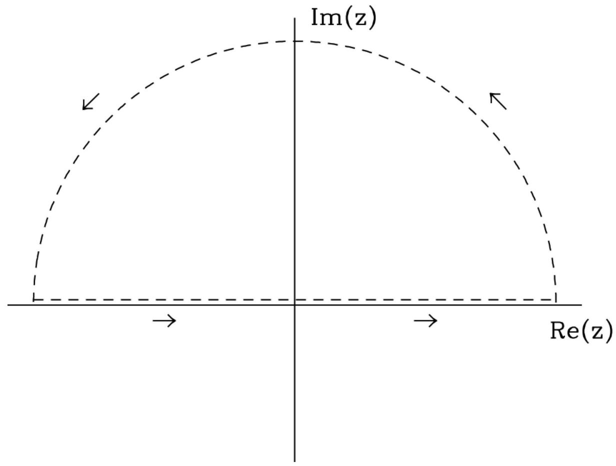

Figure 2.1: The complex integration contour $\mathcal{C}$.

where $\mathcal{P}$ stands for 'principal part'. Taking the real and imaginary parts of this equation reveals the *Kramers-Kronig relations*:

$$\chi'(\omega) = \mathcal{P}\int\limits_{-\infty}^{\infty} \frac{d\nu}{\pi}\,\frac{\chi''(\nu)}{\nu-\omega} \tag{2.23}$$

$$\chi''(\omega) = -\mathcal{P}\int\limits_{-\infty}^{\infty} \frac{d\nu}{\pi}\,\frac{\chi'(\nu)}{\nu-\omega}\ . \tag{2.24}$$

The Kramers-Kronig relations are valid for any function $\chi(z)$ which is analytic in the upper half plane.

If $\chi(z)$ is analytic everywhere off the $\text{Im}(z)=0$ axis, we may write

$$\chi(z) = \int\limits_{-\infty}^{\infty} \frac{d\nu}{\pi}\,\frac{\chi''(\nu)}{\nu-z}\ . \tag{2.25}$$

This immediately yields the result

$$\lim_{\epsilon\to 0^+} \big[\chi(\omega+i\epsilon)-\chi(\omega-i\epsilon)\big] = 2i\,\chi''(\omega)\ . \tag{2.26}$$

As an example, consider the function

$$\chi''(\omega) = \frac{\omega}{\omega^2+\gamma^2}\ . \tag{2.27}$$

Then, choosing $\gamma>0$,

$$\chi(z) = \int\limits_{-\infty}^{\infty} \frac{d\omega}{\pi}\,\frac{1}{\omega-z}\cdot\frac{\omega}{\omega^2+\gamma^2} = \begin{cases} i/(z+i\gamma) & \text{if } \text{Im}(z)>0 \\ \\ -i/(z-i\gamma) & \text{if } \text{Im}(z)<0\ . \end{cases} \tag{2.28}$$

Note that $\chi(z)$ is separately analytic in the UHP and the LHP, but that there is a branch cut along the $\text{Re}(z)$ axis, where $\chi(\omega\pm i\epsilon) = \pm i/(\omega\pm i\gamma)$.

EXERCISE: Show that eqn. (2.26) is satisfied for $\chi(\omega)=\omega/(\omega^2+\gamma^2)$.

If we *analytically continue* $\chi(z)$ from the UHP into the LHP, we find a pole and no branch cut:

$$\tilde{\chi}(z) = \frac{i}{z + i\gamma} \ . \tag{2.29}$$

The pole lies in the LHP at $z = -i\gamma$.

2.3 Quantum Mechanical Response Functions

Now consider a general quantum mechanical system with a Hamiltonian $\mathcal{H}_0$ subjected to a time-dependent perturbation, $\mathcal{H}_1(t)$, where

$$\mathcal{H}_1(t) = -\sum_i Q_i \, \phi_i(t) \ . \tag{2.30}$$

Here, the $\{Q_i\}$ are a set of Hermitian operators, and the $\{\phi_i(t)\}$ are fields or potentials. Some examples:

$$\mathcal{H}_1(t) = \begin{cases} -\boldsymbol{M} \cdot \boldsymbol{B}(t) & \text{magnetic moment – magnetic field} \\ \\ \int d^3\!r \, \varrho(\boldsymbol{r}) \, \phi(\boldsymbol{r}, t) & \text{density – scalar potential} \\ \\ -\frac{1}{c} \int d^3\!r \, \boldsymbol{j}(\boldsymbol{r}) \cdot \boldsymbol{A}(\boldsymbol{r}, t) & \text{electromagnetic current – vector potential} \end{cases}$$

We now ask, what is $\langle Q_i(t) \rangle$? We assume that the lowest order response is linear, *i.e.*

$$\langle Q_i(t) \rangle = \int\limits_{-\infty}^{\infty} \! dt' \ \chi_{ij}(t - t') \, \phi_j(t') + \mathcal{O}(\phi_k \, \phi_l) \ . \tag{2.31}$$

Note that we assume that the $\mathcal{O}(\phi^0)$ term vanishes, which can be assured with a judicious choice of the $\{Q_i\}$[2]. We also assume that the responses are all causal, *i.e.* $\chi_{ij}(t - t') = 0$ for $t < t'$. To compute $\chi_{ij}(t - t')$, we will use first order perturbation theory to obtain $\langle Q_i(t) \rangle$ and then functionally differentiate with respect to $\phi_j(t')$:

$$\chi_{ij}(t - t') = \frac{\delta \big\langle Q_i(t) \big\rangle}{\delta \phi_j(t')} \ . \tag{2.32}$$

The first step is to establish the result,

$$\big|\, \Psi(t) \,\big\rangle = \mathcal{T} \, \exp\Bigg\{ -\frac{i}{\hbar} \int\limits_{t_0}^{t} \! dt' \ \big[\mathcal{H}_0 + \mathcal{H}_1(t') \big] \Bigg\} \big|\, \Psi(t_0) \,\big\rangle \ , \tag{2.33}$$

where $\mathcal{T}$ is the *time ordering operator*, which places earlier times to the right. This is easily derived starting with the Schrödinger equation,

$$i\hbar \frac{d}{dt} \big|\, \Psi(t) \,\big\rangle = \mathcal{H}(t) \big|\, \Psi(t) \,\big\rangle \ , \tag{2.34}$$

where $\mathcal{H}(t) = \mathcal{H}_0 + \mathcal{H}_1(t)$. Integrating this equation from t to $t + dt$ gives

$$\big|\, \Psi(t + dt) \,\big\rangle = \bigg(1 - \frac{i}{\hbar} \mathcal{H}(t) \, dt \bigg) \, \big|\, \Psi(t) \,\big\rangle \tag{2.35}$$

$$\big|\, \Psi(t_0 + N \, dt) \,\big\rangle = \bigg(1 - \frac{i}{\hbar} \mathcal{H}(t_0 + (N-1) dt) \bigg) \cdots \bigg(1 - \frac{i}{\hbar} \mathcal{H}(t_0) \bigg) \, \big|\, \Psi(t_0) \,\big\rangle \ , \tag{2.36}$$

[2] If not, define $\delta Q_i \equiv Q_i - \langle Q_i \rangle_0$ and consider $\langle \delta Q_i(t) \rangle$.

hence

$$\big|\,\Psi(t_2)\,\big\rangle = U(t_2,t_1)\,\big|\,\Psi(t_1)\,\big\rangle \tag{2.37}$$

$$U(t_2,t_1) = \mathcal{T}\exp\bigg\{-\frac{i}{\hbar}\int\limits_{t_1}^{t_2}\!dt\,\mathcal{H}(t)\bigg\}\,. \tag{2.38}$$

$U(t_2,t_1)$ is a unitary operator (*i.e.* $U^\dagger = U^{-1}$), known as the *time evolution operator* between times t_1 and t_2.

EXERCISE: Show that, for $t_1 < t_2 < t_3$ that $U(t_3,t_1) = U(t_3,t_2)\,U(t_2,t_1)$.

If $t_1 < t < t_2$, then differentiating $U(t_2,t_1)$ with respect to $\phi_i(t)$ yields

$$\frac{\delta U(t_2,t_1)}{\delta\phi_j(t)} = \frac{i}{\hbar}\,U(t_2,t)\,Q_j\,U(t,t_1)\;, \tag{2.39}$$

since $\partial\mathcal{H}(t)/\partial\phi_j(t) = -Q_j$. We may therefore write (assuming $t_0 < t,t'$)

$$\begin{aligned}\frac{\delta\big|\,\Psi(t)\,\big\rangle}{\delta\phi_j(t')}\bigg|_{\{\phi_i=0\}} &= \frac{i}{\hbar}\,e^{-i\mathcal{H}_0(t-t')/\hbar}\,Q_j\,e^{-i\mathcal{H}_0(t'-t_0)/\hbar}\,\big|\,\Psi(t_0)\,\big\rangle\Theta(t-t')\\ &= \frac{i}{\hbar}\,e^{-i\mathcal{H}_0 t/\hbar}\,Q_j(t')\,e^{+i\mathcal{H}_0\,t_0/\hbar}\,\big|\,\Psi(t_0)\,\big\rangle\Theta(t-t')\;,\end{aligned} \tag{2.40}$$

where

$$Q_j(t) \equiv e^{i\mathcal{H}_0 t/\hbar}\,Q_j\,e^{-i\mathcal{H}_0 t/\hbar} \tag{2.41}$$

is the operator Q_j in the time-dependent *interaction representation*. Finally, we have

$$\begin{aligned}\chi_{ij}(t-t') &= \frac{\delta}{\delta\phi_j(t')}\,\big\langle\,\Psi(t)\,\big|\,Q_i\,\big|\,\Psi(t)\,\big\rangle\\ &= \frac{\delta\big\langle\,\Psi(t)\,\big|}{\delta\phi_j(t')}\,Q_i\big|\,\Psi(t)\,\big\rangle + \big\langle\,\Psi(t)\,\big|Q_i\,\frac{\delta\big|\,\Psi(t)\,\big\rangle}{\delta\phi_j(t')}\\ &= \bigg\{-\frac{i}{\hbar}\big\langle\,\Psi(t_0)\,\big|\,e^{-i\mathcal{H}_0\,t_0/\hbar}\,Q_j(t')\,e^{+i\mathcal{H}_0 t/\hbar}\,Q_i\,\big|\,\Psi(t)\,\big\rangle\\ &\qquad+\frac{i}{\hbar}\big\langle\,\Psi(t)\,\big|\,Q_i\,e^{-i\mathcal{H}_0 t/\hbar}\,Q_j(t')\,e^{+i\mathcal{H}_0 t_0/\hbar}\,\big|\,\Psi(t_0)\,\big\rangle\bigg\}\,\Theta(t-t')\\ &= \frac{i}{\hbar}\big\langle\big[Q_i(t),Q_j(t')\big]\big\rangle\,\Theta(t-t')\;,\end{aligned} \tag{2.42}$$

were averages are with respect to the wavefunction $\big|\,\Psi\,\big\rangle \equiv \exp(-i\mathcal{H}_0\,t_0/\hbar)\big|\,\Psi(t_0)\,\big\rangle$, with $t_0 \to -\infty$, or, at finite temperature, with respect to a Boltzmann-weighted distribution of such states. To reiterate,

$$\boxed{\chi_{ij}(t-t') = \frac{i}{\hbar}\big\langle\big[Q_i(t),Q_j(t')\big]\big\rangle\,\Theta(t-t')} \tag{2.43}$$

This is sometimes known as the *retarded* response function.

2.3.1 Spectral Representation

We now derive an expression for the response functions in terms of the spectral properties of the Hamiltonian $\mathcal{H}_0$. We stress that $\mathcal{H}_0$ may describe a fully interacting system. Write $\mathcal{H}_0 | n \rangle = \hbar\omega_n | n \rangle$, in which case

$$\begin{aligned}\hat{\chi}_{ij}(\omega) &= \frac{i}{\hbar}\int\limits_0^\infty dt\; e^{i\omega t}\,\big\langle \big[Q_i(t), Q_j(0)\big]\big\rangle \\ &= \frac{i}{\hbar}\int\limits_0^\infty dt\; e^{i\omega t}\,\frac{1}{Z}\sum_{m,n} e^{-\beta\hbar\omega_m}\Big\{\langle\, m \,|\, Q_i \,|\, n \,\rangle\langle\, n \,|\, Q_j \,|\, m \,\rangle\, e^{+i(\omega_m-\omega_n)t} \\ &\qquad\qquad - \langle\, m \,|\, Q_j \,|\, n \,\rangle\langle\, n \,|\, Q_i \,|\, m \,\rangle\, e^{+i(\omega_n-\omega_m)t}\Big\}\ ,\end{aligned} \tag{2.44}$$

where $\beta = 1/k_{\rm B}T$ and Z is the partition function. Regularizing the integrals at $t\to\infty$ with $\exp(-\epsilon t)$ with $\epsilon = 0^+$, we use

$$\int\limits_0^\infty dt\; e^{i(\omega-\Omega+i\epsilon)t} = \frac{i}{\omega-\Omega+i\epsilon} \tag{2.45}$$

to obtain the *spectral representation* of the (retarded) response function[3],

$$\boxed{\hat{\chi}_{ij}(\omega+i\epsilon) = \frac{1}{\hbar Z}\sum_{m,n} e^{-\beta\hbar\omega_m}\left\{\frac{\langle\, m \,|\, Q_j \,|\, n \,\rangle\langle\, n \,|\, Q_i \,|\, m \,\rangle}{\omega-\omega_m+\omega_n+i\epsilon} - \frac{\langle\, m \,|\, Q_i \,|\, n \,\rangle\langle\, n \,|\, Q_j \,|\, m \,\rangle}{\omega+\omega_m-\omega_n+i\epsilon}\right\}} \tag{2.46}$$

We will refer to this as $\hat{\chi}_{ij}(\omega)$; formally $\hat{\chi}_{ij}(\omega)$ has poles or a branch cut (for continuous spectra) along the ${\rm Re}(\omega)$ axis. Diagrammatic perturbation theory does not give us $\hat{\chi}_{ij}(\omega)$, but rather the *time-ordered* response function,

$$\begin{aligned}\chi^{\rm T}_{ij}(t-t') &\equiv \frac{i}{\hbar}\,\big\langle \mathcal{T}\, Q_i(t)\, Q_j(t')\big\rangle \\ &= \frac{i}{\hbar}\,\big\langle Q_i(t)\, Q_j(t')\big\rangle\,\Theta(t-t') + \frac{i}{\hbar}\,\big\langle Q_j(t')\, Q_i(t)\big\rangle\,\Theta(t'-t)\ .\end{aligned} \tag{2.47}$$

The spectral representation of $\hat{\chi}^{\rm T}_{ij}(\omega)$ is

$$\boxed{\hat{\chi}^{\rm T}_{ij}(\omega+i\epsilon) = \frac{1}{\hbar Z}\sum_{m,n} e^{-\beta\hbar\omega_m}\left\{\frac{\langle\, m \,|\, Q_j \,|\, n \,\rangle\langle\, n \,|\, Q_i \,|\, m \,\rangle}{\omega-\omega_m+\omega_n-i\epsilon} - \frac{\langle\, m \,|\, Q_i \,|\, n \,\rangle\langle\, n \,|\, Q_j \,|\, m \,\rangle}{\omega+\omega_m-\omega_n+i\epsilon}\right\}} \tag{2.48}$$

The difference between $\hat{\chi}_{ij}(\omega)$ and $\hat{\chi}^{\rm T}_{ij}(\omega)$ is thus only in the sign of the infinitesimal $\pm i\epsilon$ term in one of the denominators.

Let us now define the real and imaginary parts of the product of expectations values encountered above:

$$\langle\, m \,|\, Q_i \,|\, n \,\rangle\langle\, n \,|\, Q_j \,|\, m \,\rangle \equiv A_{mn}(ij) + iB_{mn}(ij)\ . \tag{2.49}$$

That is[4],

$$A_{mn}(ij) = \frac{1}{2}\langle\, m \,|\, Q_i \,|\, n \,\rangle\langle\, n \,|\, Q_j \,|\, m \,\rangle + \frac{1}{2}\langle\, m \,|\, Q_j \,|\, n \,\rangle\langle\, n \,|\, Q_i \,|\, m \,\rangle \tag{2.50}$$

$$B_{mn}(ij) = \frac{1}{2i}\langle\, m \,|\, Q_i \,|\, n \,\rangle\langle\, n \,|\, Q_j \,|\, m \,\rangle - \frac{1}{2i}\langle\, m \,|\, Q_j \,|\, n \,\rangle\langle\, n \,|\, Q_i \,|\, m \,\rangle. \tag{2.51}$$

[3]The spectral representation is sometimes known as the *Lehmann representation*.

[4]We assume all the Q_i are Hermitian, *i.e.* $Q_i = Q_i^\dagger$.

Note that $A_{mn}(ij)$ is separately symmetric under interchange of either m and n, or of i and j, whereas $B_{mn}(ij)$ is separately antisymmetric under these operations:

$$A_{mn}(ij) = +A_{nm}(ij) = A_{nm}(ji) = +A_{mn}(ji) \tag{2.52}$$

$$B_{mn}(ij) = -B_{nm}(ij) = B_{nm}(ji) = -B_{mn}(ji) \ . \tag{2.53}$$

We define the *spectral densities*

$$\begin{Bmatrix} \varrho^A_{ij}(\omega) \\ \varrho^B_{ij}(\omega) \end{Bmatrix} \equiv \frac{1}{\hbar Z} \sum_{m,n} e^{-\beta\hbar\omega_m} \begin{Bmatrix} A_{mn}(ij) \\ B_{mn}(ij) \end{Bmatrix} \delta(\omega - \omega_n + \omega_m) \ , \tag{2.54}$$

which satisfy

$$\varrho^A_{ij}(\omega) = +\varrho^A_{ji}(\omega) \quad , \quad \varrho^A_{ij}(-\omega) = +e^{-\beta\hbar\omega}\, \varrho^A_{ij}(\omega) \tag{2.55}$$

$$\varrho^B_{ij}(\omega) = -\varrho^B_{ji}(\omega) \quad , \quad \varrho^B_{ij}(-\omega) = -e^{-\beta\hbar\omega}\, \varrho^B_{ij}(\omega) \ . \tag{2.56}$$

In terms of these spectral densities,

$$\hat\chi'_{ij}(\omega) = \mathcal{P}\!\int\limits_{-\infty}^{\infty}\! d\nu\, \frac{2\nu}{\nu^2 - \omega^2}\, \varrho^A_{ij}(\nu) - \pi(1 - e^{-\beta\hbar\omega})\, \varrho^B_{ij}(\omega) = +\hat\chi'_{ij}(-\omega) \tag{2.57}$$

$$\hat\chi''_{ij}(\omega) = \mathcal{P}\!\int\limits_{-\infty}^{\infty}\! d\nu\, \frac{2\omega}{\nu^2 - \omega^2}\, \varrho^B_{ij}(\nu) + \pi(1 - e^{-\beta\hbar\omega})\, \varrho^A_{ij}(\omega) = -\hat\chi''_{ij}(-\omega). \tag{2.58}$$

For the time ordered response functions, we find

$$\hat\chi'^{\,\mathrm{T}}_{ij}(\omega) = \mathcal{P}\!\int\limits_{-\infty}^{\infty}\! d\nu\, \frac{2\nu}{\nu^2 - \omega^2}\, \varrho^A_{ij}(\nu) - \pi(1 + e^{-\beta\hbar\omega})\, \varrho^B_{ij}(\omega) \tag{2.59}$$

$$\hat\chi''^{\,\mathrm{T}}_{ij}(\omega) = \mathcal{P}\!\int\limits_{-\infty}^{\infty}\! d\nu\, \frac{2\omega}{\nu^2 - \omega^2}\, \varrho^B_{ij}(\nu) + \pi(1 + e^{-\beta\hbar\omega})\, \varrho^A_{ij}(\omega) \ . \tag{2.60}$$

Hence, knowledge of either the retarded or the time-ordered response functions is sufficient to determine the full behavior of the other:

$$\big[\hat\chi'_{ij}(\omega) + \hat\chi'_{ji}(\omega)\big] = \big[\hat\chi'^{\,\mathrm{T}}_{ij}(\omega) + \hat\chi'^{\,\mathrm{T}}_{ji}(\omega)\big] \tag{2.61}$$

$$\big[\hat\chi'_{ij}(\omega) - \hat\chi'_{ji}(\omega)\big] = \big[\hat\chi'^{\,\mathrm{T}}_{ij}(\omega) - \hat\chi'^{\,\mathrm{T}}_{ji}(\omega)\big] \times \tanh(\tfrac{1}{2}\beta\hbar\omega) \tag{2.62}$$

$$\big[\hat\chi''_{ij}(\omega) + \hat\chi''_{ji}(\omega)\big] = \big[\hat\chi''^{\,\mathrm{T}}_{ij}(\omega) + \hat\chi''^{\,\mathrm{T}}_{ji}(\omega)\big] \times \tanh(\tfrac{1}{2}\beta\hbar\omega) \tag{2.63}$$

$$\big[\hat\chi''_{ij}(\omega) - \hat\chi''_{ji}(\omega)\big] = \big[\hat\chi''^{\,\mathrm{T}}_{ij}(\omega) - \hat\chi''^{\,\mathrm{T}}_{ji}(\omega)\big] \ . \tag{2.64}$$

2.3.2 Energy Dissipation

The work done on the system must be positive! he rate at which work is done by the external fields is the power dissipated,

$$\begin{aligned} P &= \frac{d}{dt}\, \big\langle\, \Psi(t) \,\big|\, \mathcal{H}(t) \,\big|\, \Psi(t) \,\big\rangle \\ &= \Big\langle \Psi(t) \Big| \frac{\partial \mathcal{H}_1(t)}{\partial t} \Big| \Psi(t) \Big\rangle = -\sum_i \big\langle Q_i(t) \big\rangle\, \dot\phi_i(t) \ , \end{aligned} \tag{2.65}$$

where we have invoked the Feynman-Hellman theorem. The total energy dissipated is thus a functional of the external fields $\{\phi_i(t)\}$:

$$W = \int\limits_{-\infty}^{\infty} dt\, P(t) = -\int\limits_{-\infty}^{\infty} dt \int\limits_{-\infty}^{\infty} dt'\, \chi_{ij}(t-t')\, \dot{\phi}_i(t)\, \phi_j(t')$$

$$= \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, (-i\omega)\, \hat{\phi}_i^*(\omega)\, \hat{\chi}_{ij}(\omega)\, \hat{\phi}_j(\omega)\ . \tag{2.66}$$

Since the $\{Q_i\}$ are Hermitian observables, the $\{\phi_i(t)\}$ must be real fields, in which case $\hat{\phi}_i^*(\omega) = \hat{\phi}_i(-\omega)$, whence

$$W = \int\limits_{-\infty}^{\infty} \frac{d\omega}{4\pi}\, (-i\omega)\big[\hat{\chi}_{ij}(\omega) - \hat{\chi}_{ji}(-\omega)\big]\, \hat{\phi}_i^*(\omega)\, \hat{\phi}_j(\omega)$$

$$= \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \mathcal{M}_{ij}(\omega)\, \hat{\phi}_i^*(\omega)\, \hat{\phi}_j(\omega) \tag{2.67}$$

where

$$\mathcal{M}_{ij}(\omega) \equiv \tfrac{1}{2}(-i\omega)\big[\hat{\chi}_{ij}(\omega) - \hat{\chi}_{ji}(-\omega)\big]$$

$$= \pi\omega\left(1 - e^{-\beta\hbar\omega}\right)\Big(\varrho_{ij}^A(\omega) + i\varrho_{ij}^B(\omega)\Big)\ . \tag{2.68}$$

Note that as a matrix $M(\omega) = M^\dagger(\omega)$, so that $M(\omega)$ has real eigenvalues.

2.3.3 Correlation Functions

We define the *correlation function*

$$S_{ij}(t) \equiv \big\langle Q_i(t)\, Q_j(t') \big\rangle\ , \tag{2.69}$$

which has the spectral representation

$$\hat{S}_{ij}(\omega) = 2\pi\hbar\Big[\varrho_{ij}^A(\omega) + i\varrho_{ij}^B(\omega)\Big]$$

$$= \frac{2\pi}{Z} \sum_{m,n} e^{-\beta\hbar\omega_m}\, \langle\, m \,|\, Q_i \,|\, n \,\rangle \langle\, n \,|\, Q_j \,|\, n \,\rangle\, \delta(\omega - \omega_n + \omega_m)\ . \tag{2.70}$$

Note that

$$\hat{S}_{ij}(-\omega) = e^{-\beta\hbar\omega}\, \hat{S}_{ij}^*(\omega) \qquad , \qquad \hat{S}_{ji}(\omega) = \hat{S}_{ij}^*(\omega)\ . \tag{2.71}$$

and that

$$\boxed{\hat{\chi}_{ij}(\omega) - \hat{\chi}_{ji}(-\omega) = \frac{i}{\hbar}\left(1 - e^{-\beta\hbar\omega}\right)\hat{S}_{ij}(\omega)} \tag{2.72}$$

This result is known as the *fluctuation-dissipation theorem*, as it relates the equilibrium fluctuations $S_{ij}(\omega)$ to the dissipative quantity $\hat{\chi}_{ij}(\omega) - \hat{\chi}_{ji}(-\omega)$.

Time Reversal Symmetry

If the operators Q_i have a definite symmetry under time reversal, say

$$\mathcal{T}\, Q_i \mathcal{T}^{-1} = \eta_i \, Q_i \ , \tag{2.73}$$

then the correlation function satisfies

$$\hat{S}_{ij}(\omega) = \eta_i \, \eta_j \, \hat{S}_{ji}(\omega) \ . \tag{2.74}$$

2.3.4 Continuous Systems

The indices i and j could contain spatial information as well. Typically we will separate out spatial degrees of freedom, and write

$$S_{ij}(\boldsymbol{r}-\boldsymbol{r}', t-t') = \big\langle Q_i(\boldsymbol{r},t)\, Q_j(\boldsymbol{r}',t') \big\rangle \ , \tag{2.75}$$

where we have assumed space and time translation invariance. The Fourier transform is defined as

$$\hat{S}(\boldsymbol{k},\omega) = \int\! d^3\!r \int\limits_{-\infty}^{\infty}\! dt \ e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\, S(\boldsymbol{r},t) \tag{2.76}$$

$$= \frac{1}{V} \int\limits_{-\infty}^{\infty}\! dt \ e^{+i\omega t} \, \big\langle \hat{Q}(\boldsymbol{k},t)\, \hat{Q}(-\boldsymbol{k},0)\big\rangle \ . \tag{2.77}$$

2.4 Density-Density Correlations

In many systems, external probes couple to the number density $n(\boldsymbol{r}) = \sum_{i=1}^N \delta(\boldsymbol{r}-\boldsymbol{r}_i)$, and we may write the perturbing Hamiltonian as

$$\hat{H}_1(t) = -\int\! d^3\!r \, n(\boldsymbol{r})\, U(\boldsymbol{r},t) \ . \tag{2.78}$$

The response $\delta n \equiv n - \langle n \rangle_0$ is given by

$$\begin{aligned} \langle \delta n(\boldsymbol{r},t)\rangle &= \int\! d^3\!r' \!\int\! dt' \, \chi(\boldsymbol{r}-\boldsymbol{r}', t-t')\, U(\boldsymbol{r}',t') \\ \langle \delta \hat{n}(\boldsymbol{q},\omega)\rangle &= \chi(\boldsymbol{q},\omega)\, \hat{U}(\boldsymbol{q},\omega) \ , \end{aligned} \tag{2.79}$$

where

$$\begin{aligned} \chi(\boldsymbol{q},\omega) &= \frac{1}{\hbar V Z} \sum_{m,n} e^{-\beta\hbar\omega_m} \left\{ \frac{\big|\langle\, m \,|\, \hat{n}_{\boldsymbol{q}} \,|\, n \,\rangle\big|^2}{\omega - \omega_m + \omega_n + i\epsilon} - \frac{\big|\langle\, m \,|\, \hat{n}_{\boldsymbol{q}} \,|\, n \,\rangle\big|^2}{\omega + \omega_m - \omega_n + i\epsilon} \right\} \\ &= \frac{1}{\hbar} \int\limits_{-\infty}^{\infty}\! d\nu \, S(\boldsymbol{q},\nu) \left\{ \frac{1}{\omega+\nu+i\epsilon} - \frac{1}{\omega-\nu+i\epsilon} \right\} \end{aligned} \tag{2.80}$$

and

$$S(\boldsymbol{q},\omega) = \frac{2\pi}{VZ} \sum_{m,n} e^{-\beta\hbar\omega_m} \, \big|\langle\, m \,|\, \hat{n}_{\boldsymbol{q}} \,|\, n \,\rangle\big|^2 \, \delta(\omega - \omega_n + \omega_m) \ . \tag{2.81}$$

Note that

$$\hat{n}_{\boldsymbol{q}} = \sum_{i=1}^{N} e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_i} \ , \tag{2.82}$$

and that $\hat{n}^\dagger_{\boldsymbol{q}} = \hat{n}_{-\boldsymbol{q}}$. $S(\boldsymbol{q},\omega)$ is known as the *dynamic structure factor*. In a scattering experiment, where an incident probe (*e.g.* a neutron) interacts with the system via a potential $U(\boldsymbol{r}-\boldsymbol{R})$, where $\boldsymbol{R}$ is the probe particle position, Fermi's Golden Rule says that the rate at which the incident particle deposits momentum $\hbar\boldsymbol{q}$ and energy $\hbar\omega$ into the system is

$$\begin{aligned}\mathcal{I}(\boldsymbol{q},\omega) &= \frac{2\pi}{\hbar Z}\sum_{m,n} e^{-\beta\hbar\omega_m} \left|\langle\, m;\boldsymbol{p}\,|\,\hat{H}_1\,|\,n;\boldsymbol{p}-\hbar\boldsymbol{q}\,\rangle\right|^2 \delta(\omega-\omega_n+\omega_m) \\ &= \frac{1}{\hbar}\left|\hat{U}(\boldsymbol{q})\right|^2 S(\boldsymbol{q},\omega)\ .\end{aligned} \tag{2.83}$$

The quantity $\left|\hat{U}(\boldsymbol{q})\right|^2$ is called the *form factor*. In neutron scattering, the "on-shell" condition requires that the incident energy ε and momentum $\boldsymbol{p}$ are related via the ballistic dispersion $\varepsilon = \boldsymbol{p}^2/2m_{\rm n}$. Similarly, the final energy and momentum are related, hence

$$\varepsilon - \hbar\omega = \frac{\boldsymbol{p}^2}{2m_{\rm n}} - \hbar\omega = \frac{(\boldsymbol{p}-\hbar\boldsymbol{q})^2}{2m_{\rm n}} \qquad \Longrightarrow \qquad \hbar\omega = \frac{\hbar\boldsymbol{q}\cdot\boldsymbol{p}}{m_{\rm n}} - \frac{\hbar^2\boldsymbol{q}^2}{2m_{\rm n}}\ . \tag{2.84}$$

Hence for fixed momentum transfer $\hbar\boldsymbol{q}$, the frequency ω can be adjusted by varying the incident momentum $\boldsymbol{p}$.

Another case of interest is the response of a system to a foreign object moving with trajectory $\boldsymbol{R}(t) = \boldsymbol{V}t$. In this case, $U(\boldsymbol{r},t) = U\big(\boldsymbol{r}-\boldsymbol{R}(t)\big)$, and

$$\begin{aligned}\hat{U}(\boldsymbol{q},\omega) &= \int\! d^3\!r\!\int\! dt\, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\, e^{i\omega t}\, U(\boldsymbol{r}-\boldsymbol{V}t) \\ &= 2\pi\,\delta(\omega-\boldsymbol{q}\cdot\boldsymbol{V})\,\hat{U}(\boldsymbol{q})\end{aligned} \tag{2.85}$$

so that

$$\big\langle \delta n(\boldsymbol{q},\omega)\big\rangle = 2\pi\,\delta(\omega-\boldsymbol{q}\cdot\boldsymbol{V})\,\chi(\boldsymbol{q},\omega)\ . \tag{2.86}$$

2.4.1 Sum Rules

From eqn. (2.81) we find

$$\begin{aligned}\int\limits_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\omega\, S(\boldsymbol{q},\omega) &= \frac{1}{VZ}\sum_{m,n} e^{-\beta\hbar\omega_m}\left|\langle\, m\,|\,\hat{n}_{\boldsymbol{q}}\,|\,n\,\rangle\right|^2 (\omega_n-\omega_m) \\ &= \frac{1}{\hbar VZ}\sum_{m,n} e^{-\beta\hbar\omega_m}\,\langle\, m\,|\,\hat{n}_{\boldsymbol{q}}\,|\,n\,\rangle\,\langle\, n\,|\,[\hat{H},\hat{n}^\dagger_{\boldsymbol{q}}]\,|\,m\,\rangle \\ &= \frac{1}{\hbar V}\big\langle \hat{n}_{\boldsymbol{q}}\,[\hat{H},\hat{n}^\dagger_{\boldsymbol{q}}]\big\rangle = \frac{1}{2\hbar V}\big\langle\big[\hat{n}_{\boldsymbol{q}},[\hat{H},\hat{n}^\dagger_{\boldsymbol{q}}]\big]\big\rangle\ ,\end{aligned} \tag{2.87}$$

where the last equality is guaranteed by $\boldsymbol{q}\to-\boldsymbol{q}$ symmetry. Now if the potential is velocity independent, *i.e.* if

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\boldsymbol{\nabla}_i^{\,2} + V(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N)\ , \tag{2.88}$$

then with $\hat{n}^\dagger_{\boldsymbol{q}} = \sum_{i=1}^N e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}$ we obtain

$$\begin{aligned}
[\hat{H}, \hat{n}^\dagger_{\boldsymbol{q}}] &= -\frac{\hbar^2}{2m} \sum_{i=1}^N \big[\boldsymbol{\nabla}_i^{\,2}, e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}\big] \qquad (2.89)\\
&= \frac{\hbar^2}{2im}\, \boldsymbol{q} \cdot \sum_{i=1}^N \Big(\boldsymbol{\nabla}_i\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i} + e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}\, \boldsymbol{\nabla}_i\Big)\\
\big[\hat{n}_{\boldsymbol{q}}, [\hat{H}, \hat{n}^\dagger_{\boldsymbol{q}}]\big] &= \frac{\hbar^2}{2im}\, \boldsymbol{q} \cdot \sum_{i=1}^N \sum_{j=1}^N \Big[e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_j}, \boldsymbol{\nabla}_i\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i} + e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}\, \boldsymbol{\nabla}_i\Big]\\
&= N\hbar^2 \boldsymbol{q}^2/m \ . \qquad (2.90)
\end{aligned}$$

We have derived the *f-sum rule*:

$$\int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \omega\, S(\boldsymbol{q},\omega) = \frac{N\hbar\boldsymbol{q}^2}{2mV} \ . \qquad (2.91)$$

Note that this integral, which is the first moment of the structure factor, is *independent of the potential*!

$$\int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \omega^n\, S(\boldsymbol{q},\omega) = \frac{1}{\hbar V} \Big\langle \hat{n}_{\boldsymbol{q}} \Big[\overbrace{\hat{H}, \big[\hat{H}, \cdots [\hat{H}}^{n \text{ times}}, \hat{n}^\dagger_{\boldsymbol{q}}] \cdots \big]\Big]\Big\rangle \ . \qquad (2.92)$$

Moments with $n > 1$ in general do depend on the potential. The $n = 0$ moment gives

$$\begin{aligned}
S(\boldsymbol{q}) \equiv \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \omega^n\, S(\boldsymbol{q},\omega) &= \frac{1}{\hbar V} \langle \hat{n}_{\boldsymbol{q}}\, \hat{n}^\dagger_{\boldsymbol{q}} \rangle\\
&= \frac{1}{\hbar} \int d^3\!r\, \langle n(\boldsymbol{r})\, n(0)\rangle\, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} \ , \qquad (2.93)
\end{aligned}$$

which is the Fourier transform of the density-density correlation function.

Compressibility Sum Rule

The isothermal compressibility is given by

$$\kappa_T = -\frac{1}{V} \frac{\partial V}{\partial n}\Big|_T = \frac{1}{n^2} \frac{\partial n}{\partial \mu}\Big|_T \ . \qquad (2.94)$$

Since a constant potential $U(\boldsymbol{r},t)$ is equivalent to a chemical potential shift, we have

$$\langle \delta n\rangle = \chi(0,0)\, \delta\mu \quad \Longrightarrow \quad \kappa_T = \frac{1}{\hbar n^2} \lim_{\boldsymbol{q}\to 0} \int\limits_{-\infty}^{\infty} \frac{d\omega}{\pi}\, \frac{S(\boldsymbol{q},\omega)}{\omega} \ . \qquad (2.95)$$

This is known as the *compressibility sum rule*.

2.5 Structure Factor for the Electron Gas

The dynamic structure factor $S(\boldsymbol{q},\omega)$ tells us about the spectrum of density fluctuations. The density operator $\hat{n}^\dagger_{\boldsymbol{q}} = \sum_i e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}$ increases the wavevector by $\boldsymbol{q}$. At $T = 0$, in order for $\langle\, n \,|\, \hat{n}^\dagger_{\boldsymbol{q}} \,|\, \mathrm{G} \,\rangle$ to be nonzero (where $|\,\mathrm{G}\,\rangle$ is the ground state, *i.e.* the filled Fermi sphere), the state n must correspond to a *particle-hole excitation*. For a given $\boldsymbol{q}$, the maximum excitation frequency is obtained by taking an electron just inside the Fermi sphere, with wavevector $\boldsymbol{k} = k_{\mathrm{F}}\,\hat{\boldsymbol{q}}$ and transferring it to a state outside the Fermi sphere with wavevector $\boldsymbol{k}+\boldsymbol{q}$. For $|\boldsymbol{q}| < 2k_{\mathrm{F}}$, the minimum excitation frequency is zero – one can always form particle-hole excitations with states adjacent to the Fermi sphere. For $|\boldsymbol{q}| > 2k_{\mathrm{F}}$, the minimum excitation frequency is obtained by taking an electron just inside the Fermi sphere with wavevector $\boldsymbol{k} = -k_{\mathrm{F}}\,\hat{\boldsymbol{q}}$ to an unfilled state outside the Fermi sphere with wavevector $\boldsymbol{k}+\boldsymbol{q}$. These cases are depicted graphically in Fig. 2.2.

We therefore have

$$\omega_{\mathrm{max}}(q) = \frac{\hbar q^2}{2m} + \frac{\hbar k_{\mathrm{F}} q}{m} \tag{2.96}$$

$$\omega_{\mathrm{min}}(q) = \begin{cases} 0 & \text{if } q \le 2k_{\mathrm{F}} \\ \frac{\hbar q^2}{2m} - \frac{\hbar k_{\mathrm{F}} q}{m} & \text{if } q > 2k_{\mathrm{F}}\ . \end{cases} \tag{2.97}$$

This is depicted in the left panel of Fig. 2.3. Outside of the region bounded by $\omega_{\mathrm{min}}(q)$ and $\omega_{\mathrm{max}}(q)$, there are no single pair excitations. It is of course easy to create *multiple pair* excitations with arbitrary energy and momentum, as depicted in the right panel of the figure. However, these multipair states do not couple to the ground state $|\,\mathrm{G}\,\rangle$ through a single application of the density operator $\hat{n}^\dagger_{\boldsymbol{q}}$, hence they have zero oscillator strength: $\langle\, n \,|\, \hat{n}^\dagger_{\boldsymbol{q}} \,|\, \mathrm{G} \,\rangle = 0$ for any multipair state $|\, n\,\rangle$.

2.5.1 Explicit $T = 0$ Calculation

We start with

$$S(\boldsymbol{r},t) = \langle n(\boldsymbol{r},t)\, n(0,0)\rangle \tag{2.98}$$

$$= \int\!\frac{d^3k}{(2\pi)^3}\!\int\!\frac{d^3k'}{(2\pi)^3}\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \sum_{i,j} \big\langle e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i(t)}\, e^{i\boldsymbol{k}'\cdot\boldsymbol{r}_j}\big\rangle\ . \tag{2.99}$$

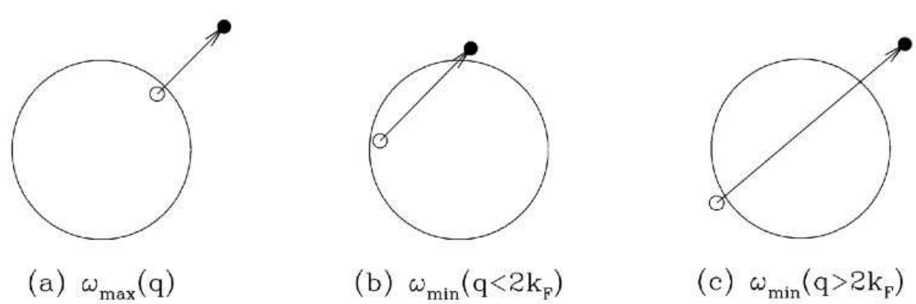

Figure 2.2: Minimum and maximum frequency particle-hole excitations in the free electron gas at $T = 0$. (a) To construct a maximum frequency excitation for a given $\boldsymbol{q}$, create a hole just inside the Fermi sphere at $\boldsymbol{k} = k_{\mathrm{F}}\,\hat{\boldsymbol{q}}$ and an electron at $\boldsymbol{k}' = \boldsymbol{k}+\boldsymbol{q}$. (b) For $|\boldsymbol{q}| < 2k_{\mathrm{F}}$ the minumum excitation frequency is zero. (c) For $|\boldsymbol{q}| > 2k_{\mathrm{F}}$, the minimum excitation frequency is obtained by placing a hole at $\boldsymbol{k} = -k_{\mathrm{F}}\,\hat{\boldsymbol{q}}$ and an electron at $\boldsymbol{k}' = \boldsymbol{k}+\boldsymbol{q}$.

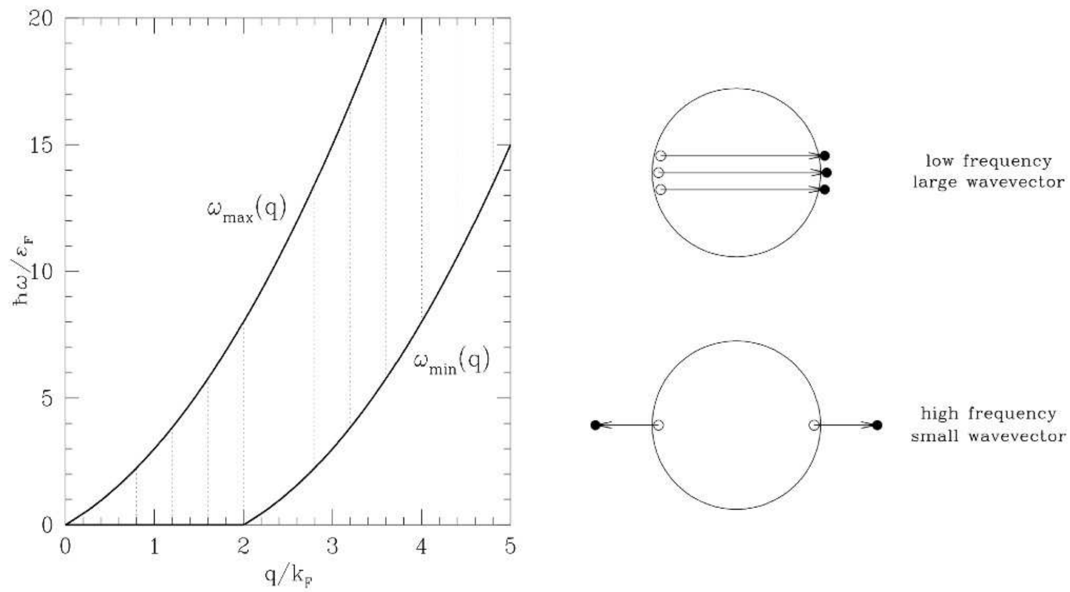

Figure 2.3: Left: Minimum and maximum excitation frequency ω in units of $\varepsilon_{\rm F}/\hbar$ *versus* wavevector q in units of $k_{\rm F}$. Outside the hatched areas, there are no *single pair* excitations. Right: With multiple pair excitations, every part of $(\boldsymbol{q},\omega)$ space is accessible. However, these states to not couple to the ground state $\big|{\rm G}\big\rangle$ through a *single* application of the density operator $\hat{n}^\dagger_{\boldsymbol{q}}$.

The time evolution of the operator $\boldsymbol{r}_i(t)$ is given by $\boldsymbol{r}_i(t) = \boldsymbol{r}_i + \boldsymbol{p}_i t/m$, where $\boldsymbol{p}_i = -i\hbar\boldsymbol{\nabla}_i$. Using the result

$$e^{A+B} = e^A\, e^B\, e^{-\frac{1}{2}[A,B]} \ , \tag{2.100}$$

which is valid when $[A,[A,B]] = [B,[A,B]] = 0$, we have

$$e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i(t)} = e^{i\hbar\boldsymbol{k}^2 t/2m}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m} \ , \tag{2.101}$$

hence

$$S(\boldsymbol{r},t) = \int\!\frac{d^3\!k}{(2\pi)^3}\!\int\!\frac{d^3\!k'}{(2\pi)^3}\, e^{i\hbar\boldsymbol{k}^2 t/2m}\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \sum_{i,j} \big\langle e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i}\, e^{i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m}\, e^{i\boldsymbol{k}'\cdot\boldsymbol{r}_j}\big\rangle \ . \tag{2.102}$$

We now break the sum up into diagonal ($i=j$) and off-diagonal ($i\neq j$) terms.

For the diagonal terms, with $i=j$, we have

$$\begin{aligned}\big\langle e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i}\, e^{i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m}\, e^{i\boldsymbol{k}'\cdot\boldsymbol{r}_i}\big\rangle &= e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{k}' t/m}\, \big\langle e^{i(\boldsymbol{k}-\boldsymbol{k})\cdot\boldsymbol{r}_i}\, e^{i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m}\big\rangle \\ &= e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{k}' t/m}\, \frac{(2\pi)^3}{NV}\, \delta(\boldsymbol{k}-\boldsymbol{k}') \sum_{\boldsymbol{q}} \Theta(k_{\rm F}-q)\, e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m} \ ,\end{aligned} \tag{2.103}$$

since the ground state $|\,{\rm G}\,\rangle$ is a Slater determinant formed of single particle wavefunctions $\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \exp(i\boldsymbol{q}\cdot\boldsymbol{r})/\sqrt{V}$ with $q < k_{\rm F}$.

For $i \neq j$, we must include exchange effects. We then have

$$\begin{aligned}\big\langle e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i}\, e^{i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m}\, e^{i\boldsymbol{k}'\cdot\boldsymbol{r}_j}\big\rangle &= \frac{1}{N(N-1)}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{q}'}\Theta(k_{\rm F}-q)\,\Theta(k_{\rm F}-q') \\ &\qquad\times\int\!\frac{d^3r_i}{V}\!\int\!\frac{d^3r_j}{V}\, e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\Big\{e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i}\, e^{i\boldsymbol{k}'\boldsymbol{r}_j} \\ &\qquad\qquad - e^{i(\boldsymbol{q}-\boldsymbol{q}'-\boldsymbol{k})\cdot\boldsymbol{r}_i}\, e^{i(\boldsymbol{q}'-\boldsymbol{q}+\boldsymbol{k}')\cdot\boldsymbol{r}_j}\Big\} \\ &= \frac{(2\pi)^6}{N(N-1)V^2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{q}'}\Theta(k_{\rm F}-q)\,\Theta(k_{\rm F}-q') \\ &\qquad\times e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\Big\{\delta(\boldsymbol{k})\,\delta(\boldsymbol{k}') - \delta(\boldsymbol{k}-\boldsymbol{k}')\,\delta(\boldsymbol{k}+\boldsymbol{q}'-\boldsymbol{q})\Big\}\ . \end{aligned} \tag{2.104}$$

Summing over the $i=j$ terms gives

$$S_{\rm diag}(\boldsymbol{r},t) = \int\!\frac{d^3k}{(2\pi)^3}\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\, e^{-i\hbar\boldsymbol{k}^2t/2m}\int\!\frac{d^3q}{(2\pi)^3}\,\Theta(k_{\rm F}-q)\, e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\ , \tag{2.105}$$

while the off-diagonal terms yield

$$\begin{aligned} S_{\rm off-diag} &= \int\!\frac{d^3k}{(2\pi)^3}\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\int\!\frac{d^3q}{(2\pi)^3}\!\int\!\frac{d^3q'}{(2\pi)^3}\,\Theta(k_{\rm F}-q)\,\Theta(k_{\rm F}-q') \\ &\qquad\times(2\pi)^3\Big\{\delta(\boldsymbol{k}) - e^{+i\hbar\boldsymbol{k}^2t/2m}\, e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\,\delta(\boldsymbol{q}-\boldsymbol{q}'-\boldsymbol{k})\Big\} \\ &= n^2 - \int\!\frac{d^3k}{(2\pi)^3}\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\, e^{+i\hbar\boldsymbol{k}^2t/2m}\int\!\frac{d^3q}{(2\pi)^3}\Theta(k_{\rm F}-q)\,\Theta(k_{\rm F}-|\boldsymbol{k}-\boldsymbol{q}|)\, e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\ , \end{aligned} \tag{2.106}$$

and hence

$$\begin{aligned} S(\boldsymbol{k},\omega) &= n^2\,(2\pi)^4\,\delta(\boldsymbol{k})\,\delta(\omega) + \int\!\frac{d^3q}{(2\pi)^3}\,\Theta(k_{\rm F}-q)\Big\{2\pi\,\delta\Big(\omega-\frac{\hbar\boldsymbol{k}^2}{2m}-\frac{\hbar\boldsymbol{k}\cdot\boldsymbol{q}}{m}\Big) \\ &\qquad - \Theta(k_{\rm F}-|\boldsymbol{k}-\boldsymbol{q}|)\,2\pi\delta\Big(\omega+\frac{\hbar\boldsymbol{k}^2}{2m}-\frac{\hbar\boldsymbol{k}\cdot\boldsymbol{q}}{m}\Big)\Big\} \\ &= (2\pi)^4 n^2\,\delta(\boldsymbol{k})\,\delta(\omega) + \int\!\frac{d^3q}{(2\pi)^3}\,\Theta(k_{\rm F}-q)\,\Theta(|\boldsymbol{k}+\boldsymbol{q}|-k_{\rm F})\cdot 2\pi\delta\Big(\omega-\frac{\hbar\boldsymbol{k}^2}{2m}-\frac{\hbar\boldsymbol{k}\cdot\boldsymbol{q}}{m}\Big)\ . \end{aligned} \tag{2.107}$$

For nonzero $\boldsymbol{k}$ and ω,

$$\begin{aligned} S(\boldsymbol{k},\omega) &= \frac{1}{2\pi}\int\limits_0^{k_{\rm F}}\!dq\,q^2\int\limits_{-1}^{1}\!dx\,\Theta\big(\sqrt{k^2+q^2+2kqx}-k_{\rm F}\big)\,\delta\Big(\omega-\frac{\hbar k^2}{2m}-\frac{\hbar kq}{m}\,x\Big) \\ &= \frac{m}{2\pi\hbar k}\int\limits_0^{k_{\rm F}}\!dq\,q\,\Theta\Big(\sqrt{q^2+\frac{2m\omega}{\hbar}}-k_{\rm F}\Big)\int\limits_{-1}^{1}\!dx\,\delta\Big(x+\frac{k}{2q}-\frac{m\omega}{\hbar kq}\Big) \\ &= \frac{m}{4\pi\hbar k}\int\limits_0^{k_{\rm F}^2}\!du\,\Theta\Big(u+\frac{2m\omega}{\hbar}-k_{\rm F}^2\Big)\,\Theta\Big(u-\Big|\frac{k}{2}-\frac{m\omega}{\hbar k}\Big|^2\Big)\ . \end{aligned} \tag{2.108}$$

The constraints on u are

$$k_{\rm F}^2 \ge u \ge \max\bigg(k_{\rm F}^2 - \frac{2m\omega}{\hbar} \, , \, \bigg| \frac{k}{2} - \frac{m\omega}{\hbar k} \bigg|^2 \bigg) \ . \tag{2.109}$$

Clearly $\omega > 0$ is required. There are two cases to consider.

The first case is

$$k_{\rm F}^2 - \frac{2m\omega}{\hbar} \ge \bigg| \frac{k}{2} - \frac{m\omega}{\hbar k} \bigg|^2 \quad \Longrightarrow \quad 0 \le \omega \le \frac{\hbar k_{\rm F} k}{m} - \frac{\hbar k^2}{2m} \ , \tag{2.110}$$

which in turn requires $k \le 2k_{\rm F}$. In this case, we have

$$\begin{aligned} S(\boldsymbol{k},\omega) &= \frac{m}{4\pi\hbar k} \bigg\{ k_{\rm F}^2 - \Big(k_{\rm F}^2 - \frac{2m\omega}{\hbar} \Big) \bigg\} \\ &= \frac{m^2 \omega}{2\pi\hbar^2 k} \ . \end{aligned} \tag{2.111}$$

The second case

$$k_{\rm F}^2 - \frac{2m\omega}{\hbar} \le \bigg| \frac{k}{2} - \frac{m\omega}{\hbar k} \bigg|^2 \quad \Longrightarrow \quad \omega \ge \frac{\hbar k_{\rm F} k}{m} - \frac{\hbar k^2}{2m} \ . \tag{2.112}$$

However, we also have that

$$\bigg| \frac{k}{2} - \frac{m\omega}{\hbar k} \bigg|^2 \le k_{\rm F}^2 \ , \tag{2.113}$$

hence ω is restricted to the range

$$\frac{\hbar k}{2m} \, |k - 2k_{\rm F}| \le \omega \le \frac{\hbar k}{2m} \, |k + 2k_{\rm F}| \ . \tag{2.114}$$

The integral in (2.108) then gives

$$S(\boldsymbol{k},\omega) = \frac{m}{4\pi\hbar k} \bigg\{ k_{\rm F}^2 - \bigg| \frac{k}{2} - \frac{m\omega}{\hbar k} \bigg|^2 \bigg\} \ . \tag{2.115}$$

Putting it all together,

$$S(\boldsymbol{k},\omega) = \begin{cases} \frac{mk_{\rm F}}{\pi^2\hbar^2} \cdot \frac{\pi\omega}{2v_{\rm F} k} & \text{if } 0 < \omega \le v_{\rm F} k - \frac{\hbar k^2}{2m} \\ \\ \frac{mk_{\rm F}}{\pi^2\hbar^2} \cdot \frac{\pi k_{\rm F}}{4k} \bigg[1 - \Big(\frac{\omega}{v_{\rm F} k} - \frac{k}{2k_{\rm F}} \Big)^2 \bigg] & \text{if } \Big| v_{\rm F} k - \frac{\hbar k^2}{2m} \Big| \le \omega \le v_{\rm F} k + \frac{\hbar k^2}{2m} \\ \\ 0 & \text{if } \omega \ge v_{\rm F} k + \frac{\hbar k^2}{2m} \ . \end{cases} \tag{2.116}$$

See the various plots in Fig. 2.4

Integrating over all frequency gives the static structure factor,

$$S(\boldsymbol{k}) = \frac{1}{V} \big\langle n_{\boldsymbol{k}}^\dagger \, n_{\boldsymbol{k}} \big\rangle = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, S(\boldsymbol{k},\omega) \ . \tag{2.117}$$

The result is

$$S(\boldsymbol{k}) = \begin{cases} \Big(\frac{3k}{4k_{\rm F}} - \frac{k^3}{16k_{\rm F}^3} \Big) n & \text{if } 0 < k \le 2k_{\rm F} \\ \\ n & \text{if } k \ge 2k_{\rm F} \\ \\ V n^2 & \text{if } k = 0 \ , \end{cases} \tag{2.118}$$

where $n = k_{\rm F}^3 / 6\pi^2$ is the density (per spin polarization).

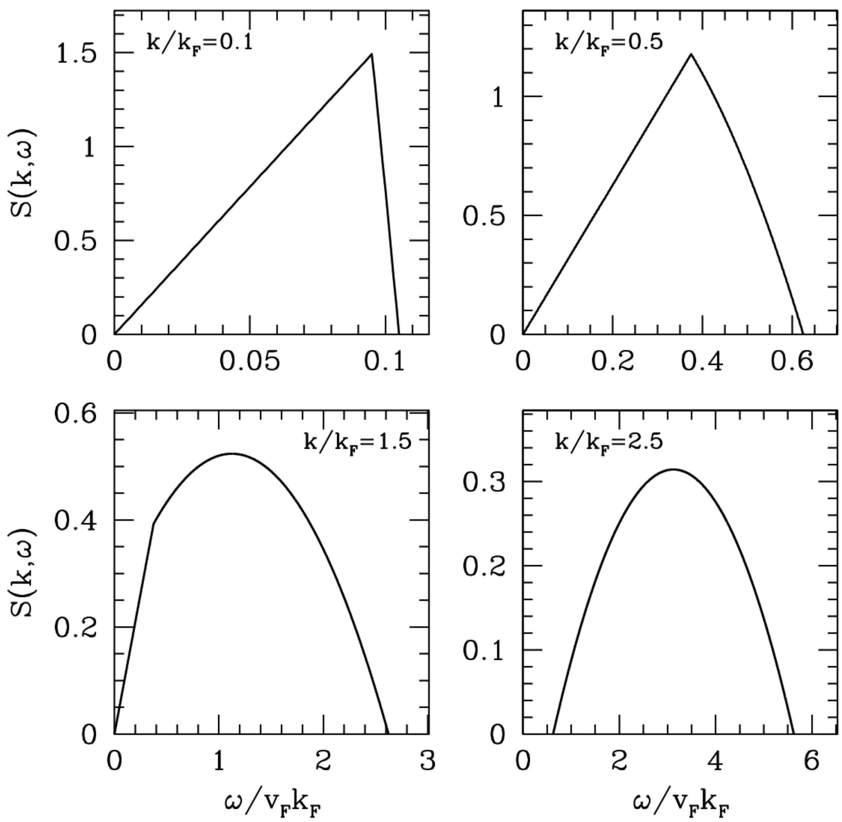

Figure 2.4: The dynamic structure factor $S(k,\omega)$ for the electron gas at various values of $k/k_{\rm F}$.

2.6 Screening and Dielectric Response

2.6.1 Definition of the Charge Response Functions

Consider a many-electron system in the presence of a time-varying external charge density $\rho_{\rm ext}(\boldsymbol{r},t)$. The perturbing Hamiltonian is then

$$\begin{aligned}\hat{H}_1 &= -e\int\! d^3\!r \int\! d^3\!r'\; \frac{n(\boldsymbol{r})\,\rho_{\rm ext}(\boldsymbol{r},t)}{|\boldsymbol{r}-\boldsymbol{r}'|} \\ &= -e\int\!\frac{d^3\!k}{(2\pi)^3}\,\frac{4\pi}{\boldsymbol{k}^2}\,\hat{n}(\boldsymbol{k})\,\hat{\rho}_{\rm ext}(-\boldsymbol{k},t)\ .\end{aligned} \tag{2.119}$$

The induced charge is $-e\,\delta n$, where δn is the induced number density:

$$\delta\hat{n}(\boldsymbol{q},\omega) = \frac{4\pi e}{\boldsymbol{q}^2}\,\chi(\boldsymbol{q},\omega)\,\hat{\rho}_{\rm ext}(\boldsymbol{q},\omega)\ . \tag{2.120}$$

We can use this to determine the dielectric function $\epsilon(\boldsymbol{q},\omega)$:

$$\begin{aligned}\boldsymbol{\nabla}\cdot\boldsymbol{D} &= 4\pi\rho_{\rm ext} \\ \boldsymbol{\nabla}\cdot\boldsymbol{E} &= 4\pi\big(\rho_{\rm ext} - e\,\langle\delta n\rangle\big)\ .\end{aligned} \tag{2.121}$$

In Fourier space,

$$\begin{aligned} i\boldsymbol{q}\cdot\boldsymbol{D}(\boldsymbol{q},\omega) &= 4\pi\hat{\rho}_{\rm ext}(\boldsymbol{q},\omega) \\ i\boldsymbol{q}\cdot\boldsymbol{E}(\boldsymbol{q},\omega) &= 4\pi\hat{\rho}_{\rm ext}(\boldsymbol{q},\omega) - 4\pi e\big\langle\delta\hat{n}(\boldsymbol{q},\omega)\big\rangle\ , \end{aligned} \tag{2.122}$$

so that from $\boldsymbol{D}(\boldsymbol{q},\omega)=\epsilon(\boldsymbol{q},\omega)\,\boldsymbol{E}(\boldsymbol{q},\omega)$ follows

$$\begin{aligned} \frac{1}{\epsilon(\boldsymbol{q},\omega)} = \frac{i\boldsymbol{q}\cdot\boldsymbol{E}(\boldsymbol{q},\omega)}{i\boldsymbol{q}\cdot\boldsymbol{D}(\boldsymbol{q},\omega)} &= 1 - \frac{\delta\hat{n}(\boldsymbol{q},\omega)}{Z\hat{n}_{\rm ext}(\boldsymbol{q},\omega)} \\ &= 1 - \frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi(\boldsymbol{q},\omega)\ . \end{aligned} \tag{2.123}$$

A system is said to exhibit *perfect screening* if

$$\epsilon(\boldsymbol{q}\to 0,\omega=0)=\infty \qquad \Longrightarrow \qquad \lim_{\boldsymbol{q}\to 0}\frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi(\boldsymbol{q},0)=1\ . \tag{2.124}$$

Here, $\chi(\boldsymbol{q},\omega)$ is the usual density-density response function,

$$\chi(\boldsymbol{q},\omega)=\frac{1}{\hbar V}\sum_n \frac{2\omega_{n0}}{\omega_{n0}^2-(\omega+i\epsilon)^2}\,\big|\langle\, n\,|\,\hat{n}_{\boldsymbol{q}}\,|\,0\,\rangle\big|^2\ , \tag{2.125}$$

where we content ourselves to work at $T=0$, and where $\omega_{n0}\equiv\omega_n-\omega_0$ is the excitation frequency for the state $|\,n\,\rangle$.

From $\boldsymbol{j}_{\rm charge}=\sigma\boldsymbol{E}$ and the continuity equation

$$i\boldsymbol{q}\cdot\langle\hat{\boldsymbol{j}}_{\rm charge}(\boldsymbol{q},\omega)\rangle = -ie\omega\langle\hat{n}(\boldsymbol{q},\omega)\rangle = i\sigma(\boldsymbol{q},\omega)\,\boldsymbol{q}\cdot\boldsymbol{E}(\boldsymbol{q},\omega)\ , \tag{2.126}$$

we find

$$\Big(4\pi\hat{\rho}_{\rm ext}(\boldsymbol{q},\omega)-4\pi e\big\langle\delta\hat{n}(\boldsymbol{q},\omega)\big\rangle\Big)\sigma(\boldsymbol{q},\omega) = -i\omega e\big\langle\delta\hat{n}(\boldsymbol{q},\omega)\big\rangle\ , \tag{2.127}$$

or

$$\frac{4\pi i}{\omega}\,\sigma(\boldsymbol{q},\omega)=\frac{\big\langle\delta\hat{n}(\boldsymbol{q},\omega)\big\rangle}{e^{-1}\hat{\rho}_{\rm ext}(\boldsymbol{q},\omega)-\big\langle\delta\hat{n}(\boldsymbol{q},\omega)\big\rangle}=\frac{1-\epsilon^{-1}(\boldsymbol{q},\omega)}{\epsilon^{-1}(\boldsymbol{q}\omega)}=\epsilon(\boldsymbol{q},\omega)-1\ . \tag{2.128}$$

Thus, we arrive at

$$\boxed{\frac{1}{\epsilon(\boldsymbol{q},\omega)}=1-\frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi(\boldsymbol{q},\omega) \qquad , \qquad \epsilon(\boldsymbol{q},\omega)=1+\frac{4\pi i}{\omega}\,\sigma(\boldsymbol{q},\omega)} \tag{2.129}$$

Taken together, these two equations allow us to relate the conductivity and the charge response function,

$$\sigma(\boldsymbol{q},\omega)=-\frac{i\omega}{\boldsymbol{q}^2}\,\frac{e^2\chi(\boldsymbol{q},\omega)}{1-\frac{4\pi e^2}{\boldsymbol{q}^2}\chi(\boldsymbol{q},\omega)}\ . \tag{2.130}$$

2.6.2 Static Screening: Thomas-Fermi Approximation

Imagine a time-independent, slowly varying electrical potential $\phi(\boldsymbol{r})$. We may define the 'local chemical potential' $\widetilde{\mu}(\boldsymbol{r})$ as

$$\mu\equiv\widetilde{\mu}(\boldsymbol{r})-e\phi(\boldsymbol{r})\ , \tag{2.131}$$

where μ is the bulk chemical potential. The local chemical potential is related to the local density by local thermodynamics. At $T = 0$,

$$\begin{aligned}\widetilde{\mu}(\boldsymbol{r}) &\equiv \frac{\hbar^2}{2m}\, k_{\rm F}^2(\boldsymbol{r}) = \frac{\hbar^2}{2m}\Big(3\pi^2 n + 3\pi^2 \delta n(\boldsymbol{r})\Big)^{2/3} \\ &= \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}\left\{1 + \frac{2}{3}\,\frac{\delta n(\boldsymbol{r})}{n} + \ldots\right\} ,\end{aligned} \tag{2.132}$$

hence, to lowest order,

$$\delta n(\boldsymbol{r}) = \frac{3en}{2\mu}\,\phi(\boldsymbol{r}) \; . \tag{2.133}$$

This makes sense – a positive potential induces an increase in the local electron number density. In Fourier space,

$$\langle \delta\hat{n}(\boldsymbol{q},\omega=0)\rangle = \frac{3en}{2\mu}\,\hat{\phi}(\boldsymbol{q},\omega=0) \; . \tag{2.134}$$

Poisson's equation is $-\nabla^2\phi = 4\pi\rho_{\rm tot}$, *i.e.*

$$\begin{aligned} i\boldsymbol{q}\cdot\boldsymbol{E}(\boldsymbol{q},0) &= \boldsymbol{q}^2\,\hat{\phi}(\boldsymbol{q},0) \\ &= 4\pi\hat{\rho}_{\rm ext}(\boldsymbol{q},0) - 4\pi e\,\langle\delta\hat{n}(\boldsymbol{q},0)\rangle \\ &= 4\pi\hat{\rho}_{\rm ext}(\boldsymbol{q},0) - \frac{6\pi n e^2}{\mu}\,\hat{\phi}(\boldsymbol{q},0) \; , \end{aligned} \tag{2.135}$$

and defining the Thomas-Fermi wavevector $q_{\rm TF}$ by

$$q_{\rm TF}^2 \equiv \frac{6\pi n e^2}{\mu} \; , \tag{2.136}$$

we have

$$\hat{\phi}(\boldsymbol{q},0) = \frac{4\pi\hat{\rho}_{\rm ext}(\boldsymbol{q},0)}{\boldsymbol{q}^2 + q_{\rm TF}^2} \; , \tag{2.137}$$

hence

$$e\,\langle\delta\hat{n}(\boldsymbol{q},0)\rangle = \frac{q_{\rm TF}^2}{\boldsymbol{q}^2 + q_{\rm TF}^2}\cdot\hat{\rho}_{\rm ext}(\boldsymbol{q},0) \quad\Longrightarrow\quad \boxed{\epsilon(\boldsymbol{q},0) = 1 + \frac{q_{\rm TF}^2}{\boldsymbol{q}^2}} \tag{2.138}$$

Note that $\epsilon(\boldsymbol{q}\to 0,\omega=0)=\infty$, so there is perfect screening.

For a general electronic density of states $g(\varepsilon)$, we have $\delta n(\boldsymbol{r}) = e\phi(\boldsymbol{r})\,g(\varepsilon_{\rm F})$, where $g(\varepsilon_{\rm F})$ is the DOS at the Fermi energy. Invoking Poisson's equation then yields $q_{\rm TF} = \sqrt{4\pi e^2\,g(\varepsilon_{\rm F})}$.

The Thomas-Fermi wavelength is $\lambda_{\rm TF} = q_{\rm TF}^{-1}$, and for free electrons may be written as

$$\lambda_{\rm TF} = \left(\frac{\pi}{12}\right)^{1/6}\sqrt{r_s}\,a_{\rm B} \simeq 0.800\,\sqrt{r_s}\,a_{\rm B} \; , \tag{2.139}$$

where r_s is the dimensionless free electron sphere radius, in units of the Bohr radius $a_{\rm B} = \hbar^2/me^2 = 0.529$Å, defined by $\frac{4}{3}\,\pi(r_s a_{\rm B})^3\,n = 1$, hence $r_s \propto n^{-1/3}$. Small r_s corresponds to high density. Since Thomas-Fermi theory is a statistical theory, it can only be valid if there are many particles within a sphere of radius $\lambda_{\rm TF}$, *i.e.* $\frac{4}{3}\,\pi\lambda_{\rm TF}^3\,n > 1$, or $r_s \lesssim (\pi/12)^{1/3} \simeq 0.640$. TF theory is applicable only in the high density limit.

In the presence of a δ-function external charge density $\rho_{\rm ext}(\boldsymbol{r}) = Ze\,\delta(\boldsymbol{r})$, we have $\hat{\rho}_{\rm ext}(\boldsymbol{q},0) = Ze$ and

$$\langle\delta\hat{n}(\boldsymbol{q},0)\rangle = \frac{Zq_{\rm TF}^2}{\boldsymbol{q}^2 + q_{\rm TF}^2} \quad\Longrightarrow\quad \boxed{\langle\delta n(\boldsymbol{r})\rangle = \frac{Ze^{-r/\lambda_{\rm TF}}}{4\pi r}} \tag{2.140}$$

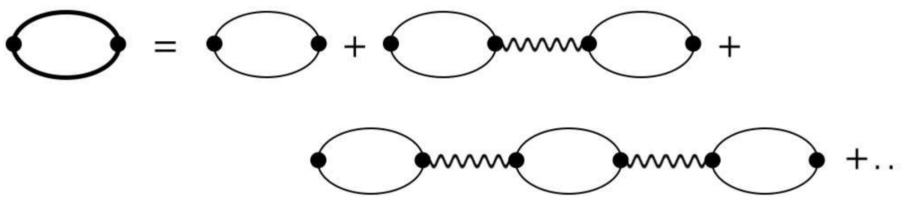

Figure 2.5: Perturbation expansion for RPA susceptibility bubble. Each bare bubble contributes a factor $\chi^0(\boldsymbol{q},\omega)$ and each wavy interaction line $\hat{v}(\boldsymbol{q})$. The infinite series can be summed, yielding eqn. 2.151.

Note the decay on the scale of $\lambda_{\rm TF}$. Note also the perfect screening:

$$e\,\langle \delta\hat{n}(\boldsymbol{q}\to 0,\omega=0)\rangle = \hat{\rho}_{\rm ext}(\boldsymbol{q}\to 0,\omega=0) = Ze\ . \tag{2.141}$$

2.6.3 High Frequency Behavior of $\epsilon(\boldsymbol{q},\omega)$

We have

$$\epsilon^{-1}(\boldsymbol{q},\omega) = 1 - \frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi(\boldsymbol{q},\omega) \tag{2.142}$$

and, at $T=0$,

$$\chi(\boldsymbol{q},\omega) = \frac{1}{\hbar V}\sum_j \big|\langle\, j\,|\,\hat{n}^\dagger_{\boldsymbol{q}}\,|\,0\,\rangle\big|^2 \left\{ \frac{1}{\omega+\omega_{j0}+i\epsilon} - \frac{1}{\omega-\omega_{j0}+i\epsilon}\right\}\ , \tag{2.143}$$

where the number density operator is

$$\hat{n}^\dagger_{\boldsymbol{q}} = \begin{cases} \sum_i e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i} & (1^{\rm st}\text{ quantized}) \\ \\ \sum_{\boldsymbol{k}} \psi^\dagger_{\boldsymbol{k}+\boldsymbol{q}}\,\psi_{\boldsymbol{k}} & (2^{\rm nd}\text{ quantized: } \{\psi_{\boldsymbol{k}},\psi^\dagger_{\boldsymbol{k}'}\} = \delta_{\boldsymbol{k}\boldsymbol{k}'})\ . \end{cases} \tag{2.144}$$

Taking the limit $\omega\to\infty$, we find

$$\chi(\boldsymbol{q},\omega\to\infty) = -\frac{2}{\hbar V\omega^2}\sum_j \big|\langle\, j\,|\,\hat{n}^\dagger_{\boldsymbol{q}}\,|\,0\,\rangle\big|^2\,\omega_{j0} = -\frac{2}{\hbar\omega^2}\int\limits_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,\omega'\,S(\boldsymbol{q},\omega')\ . \tag{2.145}$$

Invoking the f-sum rule, the above integral is $n\hbar\boldsymbol{q}^2/2m$, hence

$$\chi(\boldsymbol{q},\omega\to\infty) = -\frac{n\boldsymbol{q}^2}{m\omega^2}\ , \tag{2.146}$$

and

$$\epsilon^{-1}(\boldsymbol{q},\omega\to\infty) = 1 + \frac{\omega_{\rm p}^2}{\omega^2}\ , \tag{2.147}$$

where

$$\omega_{\rm p} \equiv \sqrt{\frac{4\pi n e^2}{m}} \tag{2.148}$$

is the *plasma frequency*.

2.6.4 Random Phase Approximation (RPA)

The electron charge appears nowhere in the free electron gas response function $\chi^0(\boldsymbol{q},\omega)$. An interacting electron gas certainly does know about electron charge, since the Coulomb repulsion between electrons is part of the Hamiltonian. The idea behind the RPA is to obtain an approximation to the interacting $\chi(\boldsymbol{q},\omega)$ from the noninteracting $\chi^0(\boldsymbol{q},\omega)$ by self-consistently adjusting the charge so that the perturbing charge density is not $\rho_{\rm ext}(\boldsymbol{r})$, but rather $\rho_{\rm ext}(\boldsymbol{r},t) - e\,\langle \delta n(\boldsymbol{r},t)\rangle$. Thus, we write

$$
\begin{aligned}
e\,\langle \delta\hat{n}(\boldsymbol{q},\omega)\rangle &= \frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi^{\rm RPA}(\boldsymbol{q},\omega)\,\hat{\rho}_{\rm ext}(\boldsymbol{q},\omega)\\
&= \frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi^0(\boldsymbol{q},\omega)\,\Big\{\hat{\rho}_{\rm ext}(\boldsymbol{q},\omega) - e\,\langle \delta\hat{n}(\boldsymbol{q},\omega)\rangle\Big\}\ ,
\end{aligned}
\tag{2.149}
$$

which gives

$$
\boxed{\chi^{\rm RPA}(\boldsymbol{q},\omega) = \frac{\chi^0(\boldsymbol{q},\omega)}{1 + \frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi^0(\boldsymbol{q},\omega)}}
\tag{2.150}
$$

Several comments are in order.

1. If the electron-electron interaction were instead given by a general $\hat{v}(\boldsymbol{q})$ rather than the specific Coulomb form $\hat{v}(\boldsymbol{q}) = 4\pi e^2/\boldsymbol{q}^2$, we would obtain

$$
\chi^{\rm RPA}(\boldsymbol{q},\omega) = \frac{\chi^0(\boldsymbol{q},\omega)}{1 + \hat{v}(\boldsymbol{q})\,\chi^0(\boldsymbol{q},\omega)}\ .
\tag{2.151}
$$

2. Within the RPA, there is perfect screening:

$$
\lim_{\boldsymbol{q}\to 0} \frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi^{\rm RPA}(\boldsymbol{q},\omega) = 1\ .
\tag{2.152}
$$

3. The RPA expression may be expanded in an infinite series,

$$
\chi^{\rm RPA} = \chi^0 - \chi^0\,\hat{v}\,\chi^0 + \chi^0\,\hat{v}\,\chi^0\,\hat{v}\,\chi^0 - \ldots\ ,
\tag{2.153}
$$

which has a diagrammatic interpretation, depicted in Fig. 2.5. The perturbative expansion in the interaction $\hat{v}$ may be resummed to yield the RPA result.

4. The RPA dielectric function takes the simple form

$$
\epsilon^{\rm RPA}(\boldsymbol{q},\omega) = 1 + \frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi^0(\boldsymbol{q},\omega)\ .
\tag{2.154}
$$

5. Explicitly,

$$
\begin{aligned}
{\rm Re}\,\epsilon^{\rm RPA}(\boldsymbol{q},\omega) = 1 + \frac{q_{\rm TF}^2}{q^2}\Bigg\{\frac{1}{2} + \frac{k_{\rm F}}{4q}\Bigg[\bigg(1 - \frac{(\omega - \hbar q^2/2m)^2}{(v_{\rm F} q)^2}\bigg)\ln\bigg|\frac{\omega - v_{\rm F} q - \hbar q^2/2m}{\omega + v_{\rm F} q - \hbar q^2/2m}\bigg|\\
+ \bigg(1 - \frac{(\omega - \hbar q^2/2m)^2}{(v_{\rm F} q)^2}\bigg)\ln\bigg|\frac{\omega - v_{\rm F} q + \hbar q^2/2m}{\omega + v_{\rm F} q + \hbar q^2/2m}\bigg|\Bigg]\Bigg\}
\end{aligned}
\tag{2.155}
$$

and

$$\operatorname{Im}\epsilon^{\mathrm{RPA}}(\boldsymbol{q},\omega)=\begin{cases}\frac{\pi\omega}{2v_{\mathrm{F}}q}\cdot\frac{q_{\mathrm{TF}}^2}{q^2} & \text{if } 0\le\omega\le v_{\mathrm{F}}q-\hbar q^2/2m\\[2ex] \frac{\pi k_{\mathrm{F}}}{4q}\left(1-\frac{(\omega-\hbar q^2/2m)^2}{(v_{\mathrm{F}}q)^2}\right)\frac{q_{\mathrm{TF}}^2}{q^2} & \text{if } v_{\mathrm{F}}q-\hbar q^2/2m\le\omega\le v_{\mathrm{F}}q+\hbar q^2/2m\\[2ex] 0 & \text{if } \omega>v_{\mathrm{F}}q+\hbar q^2/2m\end{cases} \tag{2.156}$$

6. Note that

$$\epsilon^{\mathrm{RPA}}(\boldsymbol{q},\omega\to\infty)=1-\frac{\omega_{\mathrm{p}}^2}{\omega^2}\ , \tag{2.157}$$

in agreement with the f-sum rule, and

$$\epsilon^{\mathrm{RPA}}(\boldsymbol{q}\to 0,\omega=0)=1+\frac{q_{\mathrm{TF}}^2}{q^2}\ , \tag{2.158}$$

in agreement with Thomas-Fermi theory.

7. At $\omega=0$ we have

$$\epsilon^{\mathrm{RPA}}(\boldsymbol{q},0)=1+\frac{q_{\mathrm{TF}}^2}{q^2}\left\{\frac{1}{2}+\frac{k_{\mathrm{F}}}{2q}\left(1-\frac{q^2}{4k_{\mathrm{F}}^2}\right)\ln\left|\frac{q+2k_{\mathrm{F}}}{2-2k_{\mathrm{F}}}\right|\right\}\ , \tag{2.159}$$

which is real and which has a singularity at $q=2k_{\mathrm{F}}$. This means that the long-distance behavior of $\langle\delta n(\boldsymbol{r})\rangle$ must oscillate. For a local charge perturbation, $\rho_{\mathrm{ext}}(\boldsymbol{r})=Ze\,\delta(\boldsymbol{r})$, we have

$$\langle\delta n(\boldsymbol{r})\rangle=\frac{Z}{2\pi^2 r}\int_0^\infty\!dq\,q\sin(qr)\left\{1-\frac{1}{\epsilon(\boldsymbol{q},0)}\right\}\ , \tag{2.160}$$

and within the RPA one finds for long distances

$$\langle\delta n(\boldsymbol{r})\rangle\sim\frac{Z\cos(2k_{\mathrm{F}}r)}{r^3}\ , \tag{2.161}$$

rather than the Yukawa form familiar from Thomas-Fermi theory.

2.6.5 Plasmons

The RPA response function diverges when $\hat{v}(\boldsymbol{q})\,\chi^0(\boldsymbol{q},\omega)=-1$. For a given value of $\boldsymbol{q}$, this occurs for a specific value (or for a discrete set of values) of ω, *i.e.* it defines a dispersion relation $\omega=\Omega(\boldsymbol{q})$. The poles of χ^{RPA} and are identified with elementary excitations of the electron gas known as *plasmons*.

To find the plasmon dispersion, we first derive a result for $\chi^0(\boldsymbol{q},\omega)$, starting with

$$\begin{aligned}\chi^0(\boldsymbol{q},t)&=\frac{i}{\hbar V}\langle\big[\hat{n}(\boldsymbol{q},t),\hat{n}(-\boldsymbol{q},0)\big]\rangle\\&=\frac{i}{\hbar V}\langle\Big[\sum_{\boldsymbol{k}\sigma}\psi^\dagger_{\boldsymbol{k},\sigma}\,\psi_{\boldsymbol{k}+\boldsymbol{q},\sigma},\sum_{\boldsymbol{k}',\sigma'}\psi^\dagger_{\boldsymbol{k}',\sigma'}\,\psi_{\boldsymbol{k}'-\boldsymbol{q},\sigma'}\Big]\rangle\,e^{i(\varepsilon(\boldsymbol{k})-\varepsilon(\boldsymbol{k}+\boldsymbol{q}))t/\hbar}\,\Theta(t)\ ,\end{aligned} \tag{2.162}$$

where $\varepsilon(\boldsymbol{k})$ is the noninteracting electron dispersion. For a free electron gas, $\varepsilon(\boldsymbol{k})=\hbar^2\boldsymbol{k}^2/2m$. Next, using

$$\big[AB,CD\big]=A\big\{B,C\big\}D-\big\{A,C\big\}BD+CA\big\{B,D\big\}-C\big\{A,D\big\}B \tag{2.163}$$

we obtain

$$\chi^0(\boldsymbol{q},t) = \frac{i}{\hbar V}\sum_{\boldsymbol{k}\sigma}(f_{\boldsymbol{k}} - f_{\boldsymbol{k}+\boldsymbol{q}})\, e^{i(\varepsilon(\boldsymbol{k})-\varepsilon(\boldsymbol{k}+\boldsymbol{q}))t/\hbar}\,\Theta(t) \;, \tag{2.164}$$

and therefore

$$\boxed{\chi^0(\boldsymbol{q},\omega) = 2\int\!\frac{d^3\!k}{(2\pi)^3}\;\frac{f_{\boldsymbol{k}+\boldsymbol{q}} - f_{\boldsymbol{k}}}{\hbar\omega - \varepsilon(\boldsymbol{k}+\boldsymbol{q}) + \varepsilon(\boldsymbol{k}) + i\epsilon}}\;. \tag{2.165}$$

Here,

$$f_{\boldsymbol{k}} = \frac{1}{e^{(\varepsilon(\boldsymbol{k})-\mu)/k_{\rm B}T} + 1} \tag{2.166}$$

is the Fermi distribution. At $T = 0$, $f_{\boldsymbol{k}} = \Theta(k_{\rm F} - k)$, and for $\omega \gg v_{\rm F} q$ we can expand $\chi^0(\boldsymbol{q},\omega)$ in powers of ω^{-2}, yielding

$$\chi^0(\boldsymbol{q},\omega) = -\frac{k_{\rm F}^3}{3\pi^2}\cdot\frac{q^2}{m\omega^2}\bigg\{1 + \frac{3}{5}\bigg(\frac{\hbar k_{\rm F} q}{m\omega}\bigg)^{\!2} + \ldots\bigg\} \;, \tag{2.167}$$

so the resonance condition becomes

$$\begin{aligned} 0 &= 1 + \frac{4\pi e^2}{q^2}\,\chi^0(\boldsymbol{q},\omega) \\ &= 1 - \frac{\omega_{\rm p}^2}{\omega^2}\cdot\bigg\{1 + \frac{3}{5}\bigg(\frac{v_{\rm F} q}{\omega}\bigg)^{\!2} + \ldots\bigg\} \;. \end{aligned} \tag{2.168}$$

This gives the dispersion

$$\omega = \omega_{\rm p}\,\bigg\{1 + \frac{3}{10}\bigg(\frac{v_{\rm F} q}{\omega_{\rm p}}\bigg)^{\!2} + \ldots\bigg\} \;. \tag{2.169}$$

For the noninteracting electron gas, the energy of the particle-hole continuum is bounded by $\omega_{\rm min}(q)$ and $\omega_{\rm max}(q)$, which are given below in Eqs. 2.97 and 2.96. Eventually the plasmon penetrates the particle-hole continuum, at which point it becomes heavily damped, since it can decay into particle-hole excitations.

2.6.6 Jellium

Finally, consider an electron gas in the presence of a neutralizing ionic background. We assume one species of ion with mass $M_{\rm i}$ and charge $+Z_{\rm i}e$, and we smear the ionic charge into a continuum as an approximation. This nonexistent material is known in the business of many-body physics as *jellium*. Let the ion number density be $n_{\rm i}$, and the electron number density be $n_{\rm e}$. Then Laplace's equation says

$$\nabla^2\phi = -4\pi\rho_{\rm charge} = -4\pi e\big(n_{\rm i} - n_{\rm e} + n_{\rm ext}\big) \quad , \tag{2.170}$$

where $n_{\rm ext} = \rho_{\rm ext}/e$, where $\rho_{\rm ext}$ is the test charge density, regarded as a perturbation to the jellium. The ions move according to

$$M_{\rm i}\,\frac{d\boldsymbol{v}}{dt} = Z_{\rm i} e\boldsymbol{E} = -Z_{\rm i} e\,\boldsymbol{\nabla}\phi \quad . \tag{2.171}$$

They also satisfy continuity, which to lowest order in small quantities is governed by the equation

$$n_{\rm i}^0\,\boldsymbol{\nabla}\!\cdot\!\boldsymbol{v} + \frac{\partial n_{\rm i}}{\partial t} = 0 \quad , \tag{2.172}$$

where n_i^0 is the average ionic number density. Taking the time derivative of the above equation, and invoking Newton's law for the ion's as well as Laplace, we find

$$-\frac{\partial^2 n_{\rm i}(\boldsymbol{x},t)}{\partial t^2} = \frac{4\pi n_{\rm i}^0 Z_{\rm i} e^2}{M_{\rm i}} \Big(n_{\rm i}(\boldsymbol{x},t) + n_{\rm ext}(\boldsymbol{x},t) - n_{\rm e}(\boldsymbol{x},t)\Big) \quad . \tag{2.173}$$

In Fourier space,

$$\omega^2\, \hat{n}_{\rm i}(\boldsymbol{q},\omega) = \Omega_{\rm p,i}^2 \Big(\hat{n}_{\rm i}(\boldsymbol{q},\omega) + \hat{n}_{\rm ext}(\boldsymbol{q},\omega) - \hat{n}_{\rm e}(\boldsymbol{q},\omega)\Big) \quad , \tag{2.174}$$

where

$$\Omega_{\rm p,i} = \sqrt{\frac{4\pi n_{\rm i}^0 Z_{\rm i} e^2}{M_{\rm i}}} \tag{2.175}$$

is the ionic plasma frequency. Typically $\Omega_{\rm p,i} \approx 10^{13}\,{\rm s}^{-1}$.

Since the ionic mass $M_{\rm i}$ is much greater than the electron mass, the ionic plasma frequency is much greater than the electron plasma frequency. We assume that the ions may be regarded as 'slow' and that the electrons respond according to Eqn. 2.120, *viz.*

$$\hat{n}_{\rm e}(\boldsymbol{q},\omega) = \frac{4\pi e}{\boldsymbol{q}^2}\, \chi_{\rm e}(\boldsymbol{q},\omega) \Big(\hat{n}_{\rm i}(\boldsymbol{q},\omega) + \hat{n}_{\rm ext}(\boldsymbol{q},\omega)\Big) \quad . \tag{2.176}$$

We then have

$$\frac{\omega^2}{\Omega_{\rm p,i}^2}\, \hat{n}_{\rm i}(\boldsymbol{q},\omega) = \frac{\hat{n}_{\rm i}(\boldsymbol{q},\omega) + \hat{n}_{\rm ext}(\boldsymbol{q},\omega)}{\epsilon_{\rm e}(\boldsymbol{q},\omega)} \quad . \tag{2.177}$$

From this equation, we obtain $\hat{n}_{\rm i}(\boldsymbol{q},\omega)$ and then $n_{\rm tot} \equiv n_{\rm i} - n_{\rm e} + n_{\rm ext}$. We thereby obtain

$$\hat{n}_{\rm tot}(\boldsymbol{q},\omega) = \frac{\hat{n}_{\rm ext}(\boldsymbol{q},\omega)}{\epsilon_{\rm e}(\boldsymbol{q},\omega) - \frac{\Omega_{\rm p,i}^2}{\omega^2}} \quad . \tag{2.178}$$

Finally, the dielectric function of the jellium system is given by

$$\begin{aligned}\epsilon(\boldsymbol{q},\omega) &= \frac{\hat{n}_{\rm ext}(\boldsymbol{q},\omega)}{\hat{n}_{\rm tot}(\boldsymbol{q},\omega)} \\ &= \epsilon_{\rm e}(\boldsymbol{q},\omega) - \frac{\omega^2}{\Omega_{\rm p,i}^2} \quad .\end{aligned} \tag{2.179}$$

At frequencies low compared to the electron plasma frequency, we approximate $\epsilon_{\rm e}(\boldsymbol{q},\omega)$ by the Thomas-Fermi form, $\epsilon_{\rm e}(\boldsymbol{q},\omega) \approx \big(q^2 + q_{\rm TF}^2\big)/q^2$. Then

$$\epsilon(\boldsymbol{q},\omega) \approx 1 + \frac{q_{\rm TF}^2}{q^2} - \frac{\Omega_{\rm p,i}^2}{\omega^2} \quad . \tag{2.180}$$

The zeros of this function, given by $\epsilon(\boldsymbol{q},\omega_{\boldsymbol{q}}) = 0$, occur for

$$\omega_{\boldsymbol{q}} = \frac{\Omega_{\rm p,i}\, q}{\sqrt{q^2 + q_{\rm TF}^2}} \quad . \tag{2.181}$$

This allows us to write

$$\frac{4\pi e^2}{\boldsymbol{q}^2}\, \frac{1}{\epsilon(\boldsymbol{q},\omega)} = \frac{4\pi e^2}{\boldsymbol{q}^2 + q_{\rm TF}^2} \cdot \frac{\omega^2}{\omega^2 - \omega_{\boldsymbol{q}}^2} \quad . \tag{2.182}$$

This is interpreted as the effective interaction between charges in the jellium model, arising from both electronic and ionic screening. Note that the interaction is negative, *i.e.* attractive, for $\omega^2 < \omega_{\boldsymbol{q}}^2$. At frequencies high compared to $\omega_{\boldsymbol{q}}$, but low compared to the electronic plasma frequency, the effective potential is of the Yukawa form. Only the electrons then participate in screening, because the phonons are too slow.

2.7 Electromagnetic Response

Consider an interacting system consisting of electrons of charge $-e$ in the presence of a time-varying electromagnetic field. The electromagnetic field is given in terms of the 4-potential $A^\mu = (A^0, \boldsymbol{A})$:

$$\begin{aligned} \boldsymbol{E} &= -\boldsymbol{\nabla} A^0 - \frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t} \\ \boldsymbol{B} &= \boldsymbol{\nabla} \times \boldsymbol{A} \,. \end{aligned} \tag{2.183}$$

The Hamiltonian for an N-particle system is

$$\begin{aligned} \hat{H}(A^\mu) &= \sum_{i=1}^{N} \bigg\{ \frac{1}{2m}\Big(\boldsymbol{p}_i + \frac{e}{c}\boldsymbol{A}(\boldsymbol{x}_i, t)\Big)^2 - eA^0(\boldsymbol{x}_i, t) + U(\boldsymbol{x}_i)\bigg\} + \sum_{i<j} v(\boldsymbol{x}_i - \boldsymbol{x}_j) \\ &= \hat{H}(0) - \frac{1}{c}\int\! d^3\!x \; j^{\mathrm{p}}_\mu(\boldsymbol{x})\, A^\mu(\boldsymbol{x}, t) + \frac{e^2}{2mc^2}\int\! d^3\!x \; n(\boldsymbol{x})\, \boldsymbol{A}^2(\boldsymbol{x}, t) \,, \end{aligned} \tag{2.184}$$

where we have defined

$$n(\boldsymbol{x}) \equiv \sum_{i=1}^{N} \delta(\boldsymbol{x} - \boldsymbol{x}_i) \tag{2.185}$$

$$\boldsymbol{j}^{\mathrm{p}}(\boldsymbol{x}) \equiv -\frac{e}{2m}\sum_{i=1}^{N} \Big\{ \boldsymbol{p}_i \,\delta(\boldsymbol{x} - \boldsymbol{x}_i) + \delta(\boldsymbol{x} - \boldsymbol{x}_i)\, \boldsymbol{p}_i \Big\} \tag{2.186}$$

$$j^{\mathrm{p}}_0(\boldsymbol{x}) \equiv n(\boldsymbol{x}) ec \,. \tag{2.187}$$

Throughout this discussion we invoke covariant/contravariant notation, using the metric

$$g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} , \tag{2.188}$$

so that if $j^\mu = (j^0, j^1, j^2, j^3) \equiv (j^0, \boldsymbol{j})$, then

$$\begin{aligned} j_\mu &= g_{\mu\nu}\, j^\nu = (-j^0, j^1, j^2, j^3) \\ j_\mu A^\mu &= j^\mu g_{\mu\nu}\, A^\nu = -j^0 A^0 + \boldsymbol{j} \cdot \boldsymbol{A} \equiv j \cdot A \quad . \end{aligned} \tag{2.189}$$

The quantity $j^{\mathrm{p}}_\mu(\boldsymbol{x})$ is known as the *paramagnetic current density*. The physical current density $j_\mu(\boldsymbol{x})$ also contains a *diamagnetic* contribution:

$$\begin{aligned} j_\mu(\boldsymbol{x}) &= -c\,\frac{\delta \hat{H}}{\delta A^\mu(\boldsymbol{x})} = j^{\mathrm{p}}_\mu(\boldsymbol{x}) + j^{\mathrm{d}}_\mu(\boldsymbol{x}) \\ \boldsymbol{j}^{\mathrm{d}}(\boldsymbol{x}) &= -\frac{e^2}{mc}\, n(\boldsymbol{x}) \boldsymbol{A}(\boldsymbol{x}) = -\frac{e}{mc^2}\, j^{\mathrm{p}}_0(\boldsymbol{x})\, \boldsymbol{A}(\boldsymbol{x}) \quad . \end{aligned} \tag{2.190}$$

The temporal component of the diamagnetic current is zero: $j^{\mathrm{d}}_0(\boldsymbol{x}) = 0$. The electromagnetic response tensor $K_{\mu\nu}$ is defined via

$$\big\langle j_\mu(\boldsymbol{x}, t)\big\rangle = -\frac{c}{4\pi}\int\! d^3\!x' \!\int\! dt \; K_{\mu\nu}(\boldsymbol{x}t; \boldsymbol{x}'t')\, A^\nu(\boldsymbol{x}', t') \,, \tag{2.191}$$

valid to first order in the external 4-potential A^μ. From

$$\begin{aligned} \big\langle j^{\rm p}_\mu(\boldsymbol{x},t)\big\rangle &= \frac{i}{\hbar c}\int\! d^3x' \!\int\! dt'\,\big\langle \big[j^{\rm p}_\mu(\boldsymbol{x},t), j^{\rm p}_\nu(\boldsymbol{x}',t')\big]\big\rangle\,\Theta(t-t')\,A^\nu(\boldsymbol{x}',t') \\ \big\langle j^{\rm d}_\mu(\boldsymbol{x},t)\big\rangle &= -\frac{e}{mc^2}\,\big\langle j^{\rm p}_0(\boldsymbol{x},t)\big\rangle\,A^\mu(\boldsymbol{x},t)\,(1-\delta_{\mu 0})\ , \end{aligned} \tag{2.192}$$

we conclude

$$\begin{aligned} K_{\mu\nu}(\boldsymbol{x}t;\boldsymbol{x}'t') = \frac{4\pi}{i\hbar c^2}\,&\Big\langle \big[j^{\rm p}_\mu(\boldsymbol{x},t), j^{\rm p}_\nu(\boldsymbol{x}',t')\big]\Big\rangle\,\Theta(t-t') \\ &+\frac{4\pi e}{mc^3}\,\big\langle j^{\rm p}_0(\boldsymbol{x},t)\big\rangle\,\delta(\boldsymbol{x}-\boldsymbol{x}')\,\delta(t-t')\,\delta_{\mu\nu}\,(1-\delta_{\mu 0})\ . \end{aligned} \tag{2.193}$$

The first term is sometimes known as the *paramagnetic response kernel*, $K^{\rm p}_{\mu\nu}(x;x') = (4\pi i/i\hbar c^2)\big\langle\big[j^{\rm p}_\mu(x), j^{\rm p}_\nu(x')\big]\big\rangle\,\Theta(t-t')$ is not directly calculable by perturbation theory. Rather, one obtains the time-ordered response function $K^{\rm p;T}_{\mu\nu}(x;x') = (4\pi/i\hbar c^2)\big\langle \mathcal{T} j^{\rm p}_\mu(x)\, j^{\rm p}_\nu(x')\big\rangle$, where $x^\mu \equiv (ct,\boldsymbol{x})$.

Second Quantized Notation

In the presence of an electromagnetic field described by the 4-potential $A^\mu = (c\phi, \boldsymbol{A})$, the Hamiltonian of an interacting electron system takes the form

$$\begin{aligned} \hat H = \sum_\sigma \int\! d^3x\,\psi^\dagger_\sigma(\boldsymbol{x})\bigg\{\frac{1}{2m}\Big(\frac{\hbar}{i}\boldsymbol{\nabla}+\frac{e}{c}\boldsymbol{A}\Big)^2 - eA^0(\boldsymbol{x}) + U(\boldsymbol{x})\bigg\}\,\psi_\sigma(\boldsymbol{x}) \\ +\frac{1}{2}\sum_{\sigma,\sigma'}\int\! d^3x\!\int\! d^3x'\,\psi^\dagger_\sigma(\boldsymbol{x})\,\psi^\dagger_{\sigma'}(\boldsymbol{x}')\,v(\boldsymbol{x}-\boldsymbol{x}')\,\psi_{\sigma'}(\boldsymbol{x}')\,\psi_\sigma(\boldsymbol{x})\ , \end{aligned} \tag{2.194}$$

where $v(\boldsymbol{x}-\boldsymbol{x}')$ is a two-body interaction, *e.g.* $e^2/|\boldsymbol{x}-\boldsymbol{x}'|$, and $U(\boldsymbol{x})$ is the external scalar potential. Expanding in powers of A^μ,

$$\hat H(A^\mu) = \hat H(0) - \frac{1}{c}\int\! d^3x\, j^{\rm p}_\mu(\boldsymbol{x})\,A^\mu(\boldsymbol{x}) + \frac{e^2}{2mc^2}\sum_\sigma\int\! d^3x\,\psi^\dagger_\sigma(\boldsymbol{x})\,\psi_\sigma(\boldsymbol{x})\,\boldsymbol{A}^2(\boldsymbol{x})\ , \tag{2.195}$$

where the paramagnetic current density $j^{\rm p}_\mu(\boldsymbol{x})$ is defined by

$$\begin{aligned} j^{\rm p}_0(\boldsymbol{x}) &= c\,e\sum_\sigma \psi^\dagger_\sigma(\boldsymbol{x})\,\psi_\sigma(\boldsymbol{x}) \\ \boldsymbol{j}^{\rm p}(\boldsymbol{x}) &= \frac{ie\hbar}{2m}\sum_\sigma\Big\{\psi^\dagger_\sigma(\boldsymbol{x})\,\boldsymbol{\nabla}\,\psi_\sigma(\boldsymbol{x}) - \Big(\boldsymbol{\nabla}\psi^\dagger_\sigma(\boldsymbol{x})\Big)\,\psi_\sigma(\boldsymbol{x})\Big\}\ . \end{aligned} \tag{2.196}$$

2.7.1 Gauge Invariance and Charge Conservation

In Fourier space, with $q^\mu = (\omega/c, \boldsymbol{q})$, we have, for homogeneous systems,

$$\big\langle j_\mu(q)\big\rangle = -\frac{c}{4\pi}\,K_{\mu\nu}(q)\,A^\nu(q)\ . \tag{2.197}$$

Note our convention on Fourier transforms:

$$\begin{aligned} H(x) &= \int\!\frac{d^4k}{(2\pi)^4}\,\hat H(k)\,e^{+ik\cdot x} \\ \hat H(k) &= \int\! d^4x\,H(x)\,e^{-ik\cdot x}\ , \end{aligned} \tag{2.198}$$

where $k \cdot x \equiv k_\mu x^\mu = \boldsymbol{k} \cdot \boldsymbol{x} - \omega t$. Under a gauge transformation, $A^\mu \to A^\mu + \partial^\mu \Lambda$, *i.e.*

$$A^\mu(q) \to A^\mu(q) + i\Lambda(q)\, q^\mu \; , \tag{2.199}$$

where Λ is an arbitrary scalar function. Since the physical current must be unchanged by a gauge transformation, we conclude that $K_{\mu\nu}(q)\, q^\nu = 0$. We also have the continuity equation, $\partial^\mu j_\mu = 0$, the Fourier space version of which says $q^\mu\, j_\mu(q) = 0$, which in turn requires $q^\mu\, K_{\mu\nu}(q) = 0$. Therefore,

$$\boxed{\sum_\mu q^\mu\, K_{\mu\nu}(q) = \sum_\nu K_{\mu\nu}(q)\, q^\nu = 0} \tag{2.200}$$

In fact, the above conditions are identical owing to the reciprocity relations,

$$\begin{aligned} \mathrm{Re}\, K_{\mu\nu}(q) &= +\mathrm{Re}\, K_{\nu\mu}(-q) \\ \mathrm{Im}\, K_{\mu\nu}(q) &= -\mathrm{Im}\, K_{\nu\mu}(-q) \; , \end{aligned} \tag{2.201}$$

which follow from the spectral representation of $K_{\mu\nu}(q)$. Thus,

$$\boxed{\text{gauge invariance} \Longleftrightarrow \text{charge conservation}} \tag{2.202}$$

2.7.2 A Sum Rule

If we work in a gauge where $A^0 = 0$, then $\boldsymbol{E} = -c^{-1}\dot{\boldsymbol{A}}$, hence $\boldsymbol{E}(q) = iq^0 \boldsymbol{A}(q)$, and

$$\begin{aligned} \big\langle j_i(q) \big\rangle &= -\frac{c}{4\pi}\, K_{ij}(q)\, A^j(q) \\ &= -\frac{c}{4\pi}\, K_{ij}(q)\, \frac{c}{i\omega}\, E^j(q) \\ &\equiv \sigma_{ij}(q)\, E^j(q) \; . \end{aligned} \tag{2.203}$$

Thus, the conductivity tensor is given by

$$\sigma_{ij}(\boldsymbol{q},\omega) = \frac{ic^2}{4\pi\omega}\, K_{ij}(\boldsymbol{q},\omega) \; . \tag{2.204}$$

If, in the $\omega \to 0$ limit, the conductivity is to remain finite, then we must have

$$\int\! d^3\!x \int_0^\infty \! dt \, \Big\langle \big[j^{\mathrm{p}}_i(\boldsymbol{x},t), j^{\mathrm{p}}_j(0,0) \big] \Big\rangle \, e^{+i\omega t} = \frac{ie^2 n}{m}\, \delta_{ij} \; , \tag{2.205}$$

where n is the electron number density. This relation is spontaneously violated in a superconductor, where $\sigma(\omega) \propto \omega^{-1}$ as $\omega \to 0$.

2.7.3 Longitudinal and Transverse Response

In an isotropic system, the spatial components of $K_{\mu\nu}$ may be resolved into longitudinal and transverse components, since the only preferred spatial vector is $\boldsymbol{q}$ itself. Thus, we may write

$$K_{ij}(\boldsymbol{q},\omega) = K_\parallel(\boldsymbol{q},\omega)\, \hat{q}_i\, \hat{q}_j + K_\perp(\boldsymbol{q},\omega)\, \big(\delta_{ij} - \hat{q}_i\, \hat{q}_j\big) \; , \tag{2.206}$$

where $\hat{q}_i \equiv q_i/|\boldsymbol{q}|$. We now invoke current conservation, which says $q^\mu\, K_{\mu\nu}(q) = 0$. When $\nu = j$ is a spatial index,

$$q^0\, K_{0j} + q^i\, K_{ij} = \frac{\omega}{c}\, K_{0j} + K_{\parallel}\, q_j \ , \tag{2.207}$$

which yields

$$\boxed{K_{0j}(\boldsymbol{q},\omega) = -\frac{c}{\omega}\, q^j\, K_{\parallel}(\boldsymbol{q},\omega) = K_{j0}(\boldsymbol{q},\omega)} \tag{2.208}$$

In other words, the three components of $K_{0j}(q)$ are in fact completely determined by $K_{\parallel}(q)$ and q itself. When $\nu = 0$,

$$0 = q^0\, K_{00} + q^i\, K_{i0} = \frac{\omega}{c}\, K_{00} - \frac{c}{\omega}\, \boldsymbol{q}^2\, K_{\parallel} \ , \tag{2.209}$$

which says

$$\boxed{K_{00}(\boldsymbol{q},\omega) = \frac{c^2}{\omega^2}\, \boldsymbol{q}^2\, K_{\parallel}(\boldsymbol{q},\omega)} \tag{2.210}$$

Thus, of the 10 freedoms of the symmetric 4×4 tensor $K_{\mu\nu}(q)$, there are only two independent ones – the functions $K_{\parallel}(q)$ and $K_{\perp}(q)$.

2.7.4 Neutral Systems

In neutral systems, we define the number density and number current density as

$$\begin{aligned} n(\boldsymbol{x}) &= \sum_{i=1}^N \delta(\boldsymbol{x} - \boldsymbol{x}_i) \\ \boldsymbol{j}(\boldsymbol{x}) &= \frac{1}{2m} \sum_{i=1}^N \Big\{ \boldsymbol{p}_i\, \delta(\boldsymbol{x} - \boldsymbol{x}_i) + \delta(\boldsymbol{x} - \boldsymbol{x}_i)\, \boldsymbol{p}_i \Big\} \ . \end{aligned} \tag{2.211}$$

The charge and current susceptibilities are then given by

$$\begin{aligned} \chi(\boldsymbol{x},t) &= \frac{i}{\hbar}\, \big\langle \big[n(\boldsymbol{x},t), n(0,0) \big] \big\rangle\, \Theta(t) \\ \chi_{ij}(\boldsymbol{x},t) &= \frac{i}{\hbar}\, \big\langle \big[j_i(\boldsymbol{x},t), j_j(0,0) \big] \big\rangle\, \Theta(t) \ . \end{aligned} \tag{2.212}$$

We define the longitudinal and transverse susceptibilities for homogeneous systems according to

$$\chi_{ij}(\boldsymbol{q},\omega) = \chi_{\parallel}(\boldsymbol{q},\omega)\, \hat{q}_i\, \hat{q}_j + \chi_{\perp}(\boldsymbol{q},\omega)\, (\delta_{ij} - \hat{q}_i\, \hat{q}_j) \ . \tag{2.213}$$

From the continuity equation,

$$\boldsymbol{\nabla} \cdot \boldsymbol{j} + \frac{\partial n}{\partial t} = 0 \tag{2.214}$$

follows the relation

$$\chi_{\parallel}(\boldsymbol{q},\omega) = \frac{n}{m} + \frac{\omega^2}{\boldsymbol{q}^2}\, \chi(\boldsymbol{q},\omega) \ . \tag{2.215}$$

EXERCISE: Derive eqn. (2.215).

The relation between $K_{\mu\nu}(q)$ and the neutral susceptibilities defined above is then

$$\begin{aligned} K_{00}(\boldsymbol{x},t) &= -4\pi e^2\,\chi(\boldsymbol{x},t) \\ K_{ij}(\boldsymbol{x},t) &= \frac{4\pi e^2}{c^2}\bigg\{\frac{n}{m}\,\delta(\boldsymbol{x})\,\delta(t) - \chi_{ij}(\boldsymbol{x},t)\bigg\}\ , \end{aligned} \tag{2.216}$$

and therefore

$$\begin{aligned} K_{\parallel}(\boldsymbol{q},\omega) &= \frac{4\pi e^2}{c^2}\bigg\{\frac{n}{m} - \chi_{\parallel}(\boldsymbol{q},\omega)\bigg\} \\ K_{\perp}(\boldsymbol{q},\omega) &= \frac{4\pi e^2}{c^2}\bigg\{\frac{n}{m} - \chi_{\perp}(\boldsymbol{q},\omega)\bigg\}\ . \end{aligned} \tag{2.217}$$

2.7.5 The Meissner Effect and Superfluid Density

Suppose we apply an electromagnetic field $\boldsymbol{E}$. We adopt a gauge in which $A^0 = 0$, in which case $\boldsymbol{E} = -c^{-1}\dot{\boldsymbol{A}}$. As always, $\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}$. To satisfy Maxwell's equations, we have $\boldsymbol{q}\cdot\boldsymbol{A}(\boldsymbol{q},\omega) = 0$, *i.e.* $\boldsymbol{A}(\boldsymbol{q},\omega)$ is purely transverse. But then

$$\big\langle \boldsymbol{j}(\boldsymbol{q},\omega)\big\rangle = -\frac{c}{4\pi}\,K_{\perp}(\boldsymbol{q},\omega)\,\boldsymbol{A}(\boldsymbol{q},\omega)\ . \tag{2.218}$$

This leads directly to the Meissner effect whenever $\lim_{\boldsymbol{q}\to 0} K_{\perp}(\boldsymbol{q},0)$ is finite. To see this, we write

$$\begin{aligned} \boldsymbol{\nabla}\times\boldsymbol{B} = \boldsymbol{\nabla}\,(\boldsymbol{\nabla}\cdot\boldsymbol{A}) - \boldsymbol{\nabla}^{\,2}\boldsymbol{A} &= \frac{4\pi}{c}\,\boldsymbol{j} + \frac{1}{c}\frac{\partial\boldsymbol{E}}{\partial t} \\ &= \frac{4\pi}{c}\Big(-\frac{c}{4\pi}\Big)\,K_{\perp}(-i\boldsymbol{\nabla}, i\,\partial_t)\,\boldsymbol{A} - \frac{1}{c^2}\frac{\partial^2\boldsymbol{A}}{\partial t^2}\quad , \end{aligned} \tag{2.219}$$

which yields

$$\Big(\boldsymbol{\nabla}^{\,2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\Big)\boldsymbol{A} = K_{\perp}(-i\boldsymbol{\nabla}, i\,\partial_t)\boldsymbol{A}\ . \tag{2.220}$$

In the static limit, $\boldsymbol{\nabla}^{\,2}\boldsymbol{A} = K_{\perp}(i\boldsymbol{\nabla},0)\boldsymbol{A}$, and we define

$$\frac{1}{\lambda_{\rm L}^2} \equiv \lim_{\boldsymbol{q}\to 0} K_{\perp}(\boldsymbol{q},0)\ . \tag{2.221}$$

$\lambda_{\rm L}$ is the *London penetration depth*, which is related to the *superfluid density* $n_{\rm s}$ by

$$\begin{aligned} n_{\rm s} &\equiv \frac{mc^2}{4\pi e^2\lambda_{\rm L}^2} \\ &= n - m\lim_{\boldsymbol{q}\to 0}\chi_{\perp}(\boldsymbol{q},0)\ . \end{aligned} \tag{2.222}$$

Ideal Bose Gas

We start from the susceptibility,

$$\chi_{ij}(\boldsymbol{q},t) = \frac{i}{\hbar V}\,\big\langle\big[j_i(\boldsymbol{q},t), j_j(-\boldsymbol{q},0)\big]\big\rangle\,\Theta(t)\quad , \tag{2.223}$$

where the current operator is given by

$$j_i(\boldsymbol{q}) = \frac{\hbar}{2m} \sum_{\boldsymbol{k}} (2k_i + q_i)\, \psi^\dagger_{\boldsymbol{k}}\, \psi_{\boldsymbol{k}+\boldsymbol{q}} \ . \tag{2.224}$$

For the free Bose gas, with dispersion $\omega_{\boldsymbol{k}} = \hbar \boldsymbol{k}^2/2m$,

$$j_i(\boldsymbol{q},t) = (2k_i + q_i)\, e^{i(\omega_{\boldsymbol{k}} - \omega_{\boldsymbol{k}+\boldsymbol{q}})t}\, \psi^\dagger_{\boldsymbol{k}}\, \psi_{\boldsymbol{k}+\boldsymbol{q}} \quad , \tag{2.225}$$

hence

$$\begin{aligned}\big[j_i(\boldsymbol{q},t), j_j(-\boldsymbol{q},0)\big] &= \frac{\hbar^2}{4m^2} \sum_{\boldsymbol{k},\boldsymbol{k}'} (2k_i + q_i)(2k'_j - q_j)\, e^{i(\omega_{\boldsymbol{k}} - \omega_{\boldsymbol{k}+\boldsymbol{q}})t} \\ &\qquad\qquad \times \big[\psi^\dagger_{\boldsymbol{k}}\, \psi_{\boldsymbol{k}+\boldsymbol{q}} \,,\, \psi^\dagger_{\boldsymbol{k}'}\, \psi_{\boldsymbol{k}'-\boldsymbol{q}}\big]\end{aligned} \tag{2.226}$$

Using

$$[AB, CD] = A\,[B,C]\,D + AC\,[B,D] + C\,[A,D]\,B + [A,C]\,DB \ , \tag{2.227}$$

we obtain

$$\big[j_i(\boldsymbol{q},t), j_j(-\boldsymbol{q},0)\big] = \frac{\hbar^2}{4m^2} \sum_{\boldsymbol{k}} (2k_i + q_i)(2k_j + q_j)\, e^{i(\omega_{\boldsymbol{k}} - \omega_{\boldsymbol{k}+\boldsymbol{q}})t} \, \big\{ n^0(\omega_{\boldsymbol{k}}) - n^0(\omega_{\boldsymbol{k}+\boldsymbol{q}}) \big\} \ , \tag{2.228}$$

where $n^0(\omega)$ is the equilibrium Bose distribution,[5]

$$n^0(\omega) = \frac{1}{e^{\beta\hbar\omega}\, e^{-\beta\mu} - 1} \ . \tag{2.229}$$

Thus,

$$\begin{aligned}\chi_{ij}(\boldsymbol{q},\omega) &= \frac{\hbar}{4m^2 V} \sum_{\boldsymbol{k}} (2k_i + q_i)(2k_j + q_j)\, \frac{n^0(\omega_{\boldsymbol{k}+\boldsymbol{q}}) - n^0(\omega_{\boldsymbol{k}})}{\omega + \omega_{\boldsymbol{k}} - \omega_{\boldsymbol{k}+\boldsymbol{q}} + i\epsilon} \\ &= \frac{\hbar n_0}{4m^2} \left\{ \frac{1}{\omega + \omega_{\boldsymbol{q}} + i\epsilon} - \frac{1}{\omega - \omega_{\boldsymbol{q}} + i\epsilon} \right\} q_i\, q_j \\ &\qquad + \frac{\hbar}{m^2} \int \!\frac{d^3\!k}{(2\pi)^3}\, \frac{n^0(\omega_{\boldsymbol{k}+\boldsymbol{q}/2}) - n^0(\omega_{\boldsymbol{k}-\boldsymbol{q}/2})}{\omega + \omega_{\boldsymbol{k}-\boldsymbol{q}/2} - \omega_{\boldsymbol{k}+\boldsymbol{q}/2} + i\epsilon}\, k_i\, k_j \ ,\end{aligned} \tag{2.230}$$

where $n_0 = N_0/V$ is the condensate number density. Taking the $\omega = 0$ and $\boldsymbol{q} \to 0$ limit yields

$$\chi_{ij}(\boldsymbol{q} \to 0, 0) = \frac{n_0}{m}\, \hat{q}_i\, \hat{q}_j + \frac{n'}{m}\, \delta_{ij} \ , \tag{2.231}$$

where n' is the density of uncondensed bosons. From this we read off

$$\chi_{\parallel}(\boldsymbol{q} \to 0, 0) = \frac{n}{m} \qquad , \qquad \chi_{\perp}(\boldsymbol{q} \to 0, 0) = \frac{n'}{m} \ , \tag{2.232}$$

where $n = n_0 + n'$ is the total boson number density. The superfluid density, according to (2.222), is $n_{\rm s} = n_0(T)$. In fact, the ideal Bose gas is *not* a superfluid. Its excitation spectrum is too 'soft' - any superflow is unstable toward decay into single particle excitations.

[5]Recall that $\mu = 0$ in the condensed phase.

2.8 Electron-phonon Hamiltonian

Let $\boldsymbol{R}_i = \boldsymbol{R}_i^0 + \delta\boldsymbol{R}_i$ denote the position of the i^{th} ion, and let $U(\boldsymbol{r}) = -Ze^2\exp(-r/\lambda_{\text{TF}})/r$ be the electron-ion interaction. Expanding in terms of the ionic displacements $\delta\boldsymbol{R}_i$,

$$\hat{H}_{\text{el-ion}} = \sum_i U(\boldsymbol{r}-\boldsymbol{R}_i^0) - \sum_i \delta\boldsymbol{R}_i \cdot \boldsymbol{\nabla} U(\boldsymbol{r}-\boldsymbol{R}_i^0) \ , \tag{2.233}$$

where i runs from 1 to N_{ion}, the number of ions[6]. The deviation $\delta\boldsymbol{R}_i$ may be expanded in terms of the vibrational normal modes of the lattice, *i.e.* the phonons, as

$$\delta R_i^\alpha = \frac{1}{\sqrt{N_{\text{ion}}}} \sum_{\boldsymbol{q}\lambda} \left(\frac{\hbar}{2\,\omega_\lambda(\boldsymbol{q})}\right)^{1/2} \hat{\mathrm{e}}_\lambda^\alpha(\boldsymbol{q})\, e^{i\boldsymbol{q}\cdot\boldsymbol{R}_i^0}\, (a_{\boldsymbol{q}\lambda} + a^\dagger_{-\boldsymbol{q}\lambda}) \ . \tag{2.234}$$

The phonon polarization vectors satisfy $\hat{\boldsymbol{e}}_\lambda(\boldsymbol{q}) = \hat{\boldsymbol{e}}^*_\lambda(-\boldsymbol{q})$ as well as the generalized orthonormality relations

$$\begin{aligned} \sum_\alpha \hat{\mathrm{e}}_\lambda^\alpha(\boldsymbol{q})\, \hat{\mathrm{e}}_{\lambda'}^\alpha(-\boldsymbol{q}) &= M^{-1}\,\delta_{\lambda\lambda'} \\ \sum_\lambda \hat{e}_\lambda^\alpha(\boldsymbol{q})\, \hat{e}_\lambda^\beta(-\boldsymbol{q}) &= M^{-1}\delta_{\alpha\beta} \ , \end{aligned} \tag{2.235}$$

where M is the ionic mass. The number of unit cells in the crystal is $N_{\text{ion}} = V/\Omega$, where Ω is the Wigner-Seitz cell volume. Again, we approximate Bloch states by plane waves $\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \exp(i\boldsymbol{k}\cdot\boldsymbol{r})/\sqrt{V}$, in which case

$$\langle\, \boldsymbol{k}' \,|\, \boldsymbol{\nabla} U(\boldsymbol{r}-\boldsymbol{R}_i^0)\,|\, \boldsymbol{k}\,\rangle = -\frac{i}{V}\, e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}_i^0}\, \frac{4\pi Ze^2\,(\boldsymbol{k}-\boldsymbol{k}')}{(\boldsymbol{k}-\boldsymbol{k}')^2 + \lambda_{\text{TF}}^{-2}} \ . \tag{2.236}$$

The sum over lattice sites gives

$$\sum_{i=1}^{N_{\text{ion}}} e^{i(\boldsymbol{k}-\boldsymbol{k}'+\boldsymbol{q})\cdot\boldsymbol{R}_i^0} = N_{\text{ion}}\,\delta_{\boldsymbol{k}',\boldsymbol{k}+\boldsymbol{q}\ \text{mod}\ \boldsymbol{G}} \ , \tag{2.237}$$

so that

$$\hat{H}_{\text{el-ph}} = \frac{1}{\sqrt{V}} \sum_{\substack{\boldsymbol{k}\boldsymbol{k}'\sigma \\ \boldsymbol{q}\lambda\boldsymbol{G}}} g_\lambda(\boldsymbol{k},\boldsymbol{k}')\,(a^\dagger_{\boldsymbol{q}\lambda} + a_{-\boldsymbol{q}\lambda})\,\psi^\dagger_{\boldsymbol{k}\sigma}\,\psi_{\boldsymbol{k}'\sigma}\,\delta_{\boldsymbol{k}',\boldsymbol{k}+\boldsymbol{q}+\boldsymbol{G}} \quad , \tag{2.238}$$

with

$$g_\lambda(\boldsymbol{k},\boldsymbol{k}+\boldsymbol{q}+\boldsymbol{G}) = -i\left(\frac{\hbar}{2\,\Omega\,\omega_\lambda(\boldsymbol{q})}\right)^{1/2} \frac{4\pi Ze^2}{(\boldsymbol{q}+\boldsymbol{G})^2 + \lambda_{\text{TF}}^{-2}}\,(\boldsymbol{q}+\boldsymbol{G})\cdot\hat{\boldsymbol{e}}^*_\lambda(\boldsymbol{q}) \ . \tag{2.239}$$

In an isotropic solid[7] ('jellium'), the phonon polarization at wavevector $\boldsymbol{q}$ either is parallel to $\boldsymbol{q}$ (longitudinal waves), or perpendicular to $\boldsymbol{q}$ (transverse waves). We see that only longitudinal waves couple to the electrons. This is because transverse waves do not result in any local accumulation of charge density, and it is to the charge density that electrons couple, via the Coulomb interaction.

Restricting our attention to the longitudinal phonon, we have $\hat{\boldsymbol{e}}_{\text{L}}(\boldsymbol{q}) = \hat{\boldsymbol{q}}/\sqrt{M}$ and hence, for small $\boldsymbol{q} = \boldsymbol{k}'-\boldsymbol{k}$,

$$g_{\text{L}}(\boldsymbol{k},\boldsymbol{k}+\boldsymbol{q}) = -i\left(\frac{\hbar}{2M\Omega}\right)^{1/2} \frac{4\pi Ze^2}{q^2+\lambda_{\text{TF}}^{-2}}\, c_{\text{L}}^{-1/2}\, q^{1/2} \ , \tag{2.240}$$

[6]We assume a Bravais lattice, for simplicity.
[7]The jellium model ignores $\boldsymbol{G} \neq 0$ *Umklapp* processes.

Metal	Θ_s	Θ_D	λ_{el-ph}	Metal	Θ_s	Θ_D	λ_{el-ph}
Na	220	150	0.47	Au	310	170	0.08
K	150	100	0.25	Be	1940	1000	0.59
Cu	490	315	0.16	Al	910	394	0.90
Ag	340	215	0.12	In	300	129	1.05

Table 2.1: Electron-phonon interaction parameters for some metals. Temperatures are in Kelvins.

where c_L is the longitudinal phonon velocity. Thus, for small $\boldsymbol{q}$ we that the electron-longitudinal phonon coupling $g_L(\boldsymbol{k}, \boldsymbol{k}+\boldsymbol{q}) \equiv g_{\boldsymbol{q}}$ satisfies

$$|g_{\boldsymbol{q}}|^2 = \lambda_{el-ph} \cdot \frac{\hbar c_L q}{g(\varepsilon_F)} \ , \tag{2.241}$$

where $g(\varepsilon_F)$ is the electronic density of states, and where the dimensionless *electron-phonon coupling constant* is

$$\lambda_{el-ph} = \frac{Z^2}{2Mc_L^2\,\Omega g(\varepsilon_F)} = \frac{2Z}{3}\,\frac{m^*}{M}\left(\frac{\varepsilon_F}{k_B\Theta_s}\right)^2 \ , \tag{2.242}$$

with $\Theta_s \equiv \hbar c_L k_F / k_B$. Table 2.1 lists Θ_s, the Debye temperature Θ_D, and the electron-phonon coupling λ_{el-ph} for various metals.

Chapter 3

BCS Theory of Superconductivity

3.1 Binding and Dimensionality

Consider a spherically symmetric potential $U(\boldsymbol{r}) = -U_0\,\Theta(a-r)$. Are there bound states, *i.e.* states in the eigenspectrum of negative energy? What role does dimension play? It is easy to see that if $U_0 > 0$ is large enough, there are always bound states. A trial state completely localized within the well has kinetic energy $T_0 \simeq \hbar^2/ma^2$, while the potential energy is $-U_0$, so if $U_0 > \hbar^2/ma^2$, we have a variational state with energy $E = T_0 - U_0 < 0$, which is of course an upper bound on the true ground state energy.

What happens, though, if $U_0 < T_0$? We again appeal to a variational argument. Consider a Gaussian or exponentially localized wavefunction with characteristic size $\xi \equiv \lambda a$, with $\lambda > 1$. The variational energy is then

$$E \simeq \frac{\hbar^2}{m\xi^2} - U_0\left(\frac{a}{\xi}\right)^d = T_0\,\lambda^{-2} - U_0\,\lambda^{-d} \quad . \tag{3.1}$$

Extremizing with respect to λ, we obtain $-2T_0\,\lambda^{-3} + d\,U_0\,\lambda^{-(d+1)}$ and $\lambda = \big(d\,U_0/2T_0\big)^{1/(d-2)}$. Inserting this into our expression for the energy, we find

$$E = \left(\frac{2}{d}\right)^{2/(d-2)}\left(1 - \frac{2}{d}\right) T_0^{d/(d-2)}\,U_0^{-2/(d-2)} \quad . \tag{3.2}$$

We see that for $d=1$ we have $\lambda = 2T_0/U_0$ and $E = -U_0^2/4T_0 < 0$. In $d=2$ dimensions, we have $E = (T_0 - U_0)/\lambda^2$, which says $E \geq 0$ unless $U_0 > T_0$. For weak attractive $U(\boldsymbol{r})$, the minimum energy solution is $E \to 0^+$, with $\lambda \to \infty$. It turns out that $d = 2$ is a marginal dimension, and we shall show that we always get localized states with a ballistic dispersion and an attractive potential well. For $d > 2$ we have $E > 0$ which suggests that we cannot have bound states unless $U_0 > T_0$, in which case $\lambda \leq 1$ and we must appeal to the analysis in the previous paragraph.

We can firm up this analysis a bit by considering the Schrödinger equation,

$$-\frac{\hbar^2}{2m}\,\nabla^2\psi(\boldsymbol{x}) + V(\boldsymbol{x})\,\psi(\boldsymbol{x}) = E\,\psi(\boldsymbol{x}) \quad . \tag{3.3}$$

Fourier transforming, we have

$$\varepsilon(\boldsymbol{k})\,\hat{\psi}(\boldsymbol{k}) + \int\!\frac{d^dk'}{(2\pi)^d}\,\hat{V}(\boldsymbol{k}-\boldsymbol{k}')\,\hat{\psi}(\boldsymbol{k}') = E\,\hat{\psi}(\boldsymbol{k}) \quad , \tag{3.4}$$

where $\varepsilon(\boldsymbol{k}) = \hbar^2\boldsymbol{k}^2/2m$. We may now write $\hat{V}(\boldsymbol{k}-\boldsymbol{k}') = \sum_n \lambda_n\, \alpha_n(\boldsymbol{k})\, \alpha_n^*(\boldsymbol{k}')$, which is a decomposition of the Hermitian matrix $\hat{V}_{\boldsymbol{k},\boldsymbol{k}'} \equiv \hat{V}(\boldsymbol{k}-\boldsymbol{k}')$ into its (real) eigenvalues λ_n and eigenvectors $\alpha_n(\boldsymbol{k})$. Let's approximate $V_{\boldsymbol{k},\boldsymbol{k}'}$ by its leading eigenvalue, which we call λ, and the corresponding eigenvector $\alpha(\boldsymbol{k})$. That is, we write $\hat{V}_{\boldsymbol{k},\boldsymbol{k}'} \simeq \lambda\, \alpha(\boldsymbol{k})\, \alpha^*(\boldsymbol{k}')$. We then have

$$\hat{\psi}(\boldsymbol{k}) = \frac{\lambda\, \alpha(\boldsymbol{k})}{E-\varepsilon(\boldsymbol{k})} \int \frac{d^dk'}{(2\pi)^d}\, \alpha^*(\boldsymbol{k}')\, \hat{\psi}(\boldsymbol{k}') \quad . \tag{3.5}$$

Multiply the above equation by $\alpha^*(\boldsymbol{k})$ and integrate over $\boldsymbol{k}$, resulting in

$$\frac{1}{\lambda} = \int \frac{d^dk}{(2\pi)^d}\, \frac{\big|\alpha(\boldsymbol{k})\big|^2}{E-\varepsilon(\boldsymbol{k})} = \frac{1}{\lambda} = \int_0^\infty \!d\varepsilon\, \frac{g(\varepsilon)}{E-\varepsilon}\, \big|\alpha(\varepsilon)\big|^2 \quad , \tag{3.6}$$

where $g(\varepsilon)$ is the density of states $g(\varepsilon) = \mathsf{Tr}\, \delta\big(\varepsilon - \varepsilon(\boldsymbol{k})\big)$. Here, we assume that $\alpha(\boldsymbol{k}) = \alpha(k)$ is isotropic. It is generally the case that if $V_{\boldsymbol{k},\boldsymbol{k}'}$ is isotropic, *i.e.* if it is invariant under a simultaneous $\mathsf{O}(3)$ rotation $\boldsymbol{k} \to R\boldsymbol{k}$ and $\boldsymbol{k}' \to R\boldsymbol{k}'$, then so will be its lowest eigenvector. Furthermore, since $\varepsilon = \hbar^2k^2/2m$ is a function of the scalar $k = |\boldsymbol{k}|$, this means $\alpha(k)$ can be considered a function of ε. We then have

$$\frac{1}{|\lambda|} = \int_0^\infty \!d\varepsilon\, \frac{g(\varepsilon)}{|E|+\varepsilon}\, \big|\alpha(\varepsilon)\big|^2 \quad , \tag{3.7}$$

where we have we assumed an attractive potential ($\lambda < 0$), and, as we are looking for a bound state, $E < 0$.

If $\alpha(0)$ and $g(0)$ are finite, then in the limit $|E| \to 0$ we have

$$\frac{1}{|\lambda|} = g(0)\, |\alpha(0)|^2\, \ln\big(1/|E|\big) + \text{finite} \,. \tag{3.8}$$

This equation may be solved for arbitrarily small $|\lambda|$ because the RHS of Eqn. 3.7 diverges as $|E| \to 0$. If, on the other hand, $g(\varepsilon) \sim \varepsilon^p$ where $p > 0$, then the RHS is finite even when $E = 0$. In this case, bound states can only exist for $|\lambda| > \lambda_c$, where

$$\lambda_c = 1 \Bigg/ \int_0^\infty \!d\varepsilon\, \frac{g(\varepsilon)}{\varepsilon}\, \big|\alpha(\varepsilon)\big|^2 \quad . \tag{3.9}$$

Typically the integral has a finite upper limit, given by the bandwidth B. For the ballistic dispersion, one has $g(\varepsilon) \propto \varepsilon^{(d-2)/2}$, so $d = 2$ is the marginal dimension. In dimensions $d \leq 2$, bound states for for arbitrarily weak attractive potentials.

3.2 Cooper's Problem

In 1956, Leon Cooper considered the problem of two electrons interacting in the presence of a quiescent Fermi sea. The background electrons comprising the Fermi sea enter the problem only through their *Pauli blocking*. Since spin and total momentum are conserved, Cooper first considered a zero momentum singlet,

$$|\,\Psi\,\rangle = \sum_{\boldsymbol{k}} A_{\boldsymbol{k}}\, \big(c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} - c^\dagger_{\boldsymbol{k}\downarrow} c^\dagger_{-\boldsymbol{k}\uparrow}\big) |\,\mathrm{F}\,\rangle \quad , \tag{3.10}$$

where $|\,\mathrm{F}\,\rangle$ is the filled Fermi sea, $|\,\mathrm{F}\,\rangle = \prod_{|\boldsymbol{p}|<k_\mathrm{F}} c^\dagger_{\boldsymbol{p}\uparrow} c^\dagger_{\boldsymbol{p}\downarrow}\,|\,0\,\rangle$. Only states with $k > k_\mathrm{F}$ contribute to the RHS of Eqn. 3.10, due to Pauli blocking. The real space wavefunction is

$$\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2) = \sum_{\boldsymbol{k}} A_{\boldsymbol{k}}\, e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)} \big(|\!\uparrow_1\downarrow_2\rangle - |\!\downarrow_1\uparrow_2\rangle\big) \quad , \tag{3.11}$$

with $A_{\boldsymbol{k}} = A_{-\boldsymbol{k}}$ to enforce symmetry of the orbital part. It should be emphasized that this is a two-particle wavefunction, and not an $(N+2)$-particle wavefunction, with N the number of electrons in the Fermi sea. Again, the Fermi sea in this analysis has no dynamics of its own. Its presence is reflected only in the restriction $k > k_\mathrm{F}$ for the states which participate in the Cooper pair.

The many-body Hamiltonian is written

$$\hat{H} = \sum_{\boldsymbol{k}\sigma} \varepsilon_{\boldsymbol{k}}\, c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \tfrac{1}{2} \sum_{\boldsymbol{k}_1\sigma_1} \sum_{\boldsymbol{k}_2\sigma_2} \sum_{\boldsymbol{k}_3\sigma_3} \sum_{\boldsymbol{k}_4\sigma_4} \langle\, \boldsymbol{k}_1\sigma_1, \boldsymbol{k}_2\sigma_2 \,|\, v \,|\, \boldsymbol{k}_3\sigma_3, \boldsymbol{k}_4\sigma_4 \,\rangle\, c^\dagger_{\boldsymbol{k}_1\sigma_1} c^\dagger_{\boldsymbol{k}_2\sigma_2} c_{\boldsymbol{k}_4\sigma_4} c_{\boldsymbol{k}_3\sigma_3} \,. \tag{3.12}$$

We treat $|\,\Psi\,\rangle$ as a variational state, which means we set

$$\frac{\delta}{\delta A^*_{\boldsymbol{k}}} \frac{\langle\,\Psi\,|\,\hat{H}\,|\,\Psi\,\rangle}{\langle\,\Psi\,|\,\Psi\,\rangle} = 0 \quad , \tag{3.13}$$

resulting in

$$(E - E_0)\, A_{\boldsymbol{k}} = 2\varepsilon_{\boldsymbol{k}}\, A_{\boldsymbol{k}} + \sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\, A_{\boldsymbol{k}'} \quad , \tag{3.14}$$

where

$$V_{\boldsymbol{k},\boldsymbol{k}'} = \langle\, \boldsymbol{k}\!\uparrow, -\boldsymbol{k}\!\downarrow \,|\, v \,|\, \boldsymbol{k}'\!\uparrow, -\boldsymbol{k}'\!\downarrow \,\rangle = \frac{1}{V}\int\! d^3\!r\; v(\boldsymbol{r})\, e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} \quad . \tag{3.15}$$

Here $E_0 = \langle\,\mathrm{F}\,|\,\hat{H}\,|\,\mathrm{F}\,\rangle$ is the energy of the Fermi sea.

We write $\varepsilon_{\boldsymbol{k}} = \varepsilon_\mathrm{F} + \xi_{\boldsymbol{k}}$, and we define $E \equiv E_0 + 2\varepsilon_\mathrm{F} + W$. Then

$$W\, A_{\boldsymbol{k}} = 2\xi_{\boldsymbol{k}}\, A_{\boldsymbol{k}} + \sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\, A_{\boldsymbol{k}'} \quad . \tag{3.16}$$

If $V_{\boldsymbol{k},\boldsymbol{k}'}$ is rotationally invariant, meaning it is left unchanged by $\boldsymbol{k} \to R\boldsymbol{k}$ and $\boldsymbol{k}' \to R\boldsymbol{k}'$ where $R \in \mathsf{O}(3)$, then we may write

$$V_{\boldsymbol{k},\boldsymbol{k}'} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} V_\ell(k,k')\, Y^\ell_m(\hat{\boldsymbol{k}})\, Y^\ell_{-m}(\hat{\boldsymbol{k}}') \quad . \tag{3.17}$$

We assume that $V_l(k,k')$ is *separable*, meaning we can write

$$V_\ell(k,k') = \frac{1}{V}\, \lambda_\ell\, \alpha_\ell(k)\, \alpha^*_\ell(k') \quad . \tag{3.18}$$

This simplifies matters and affords us an exact solution, for now we take $A_{\boldsymbol{k}} = A_k\, Y^\ell_m(\hat{\boldsymbol{k}})$ to obtain a solution in the ℓ angular momentum channel:

$$W_\ell\, A_k = 2\xi_k\, A_k + \lambda_\ell\, \alpha_\ell(k) \cdot \frac{1}{V} \sum_{k'} \alpha^*_\ell(k')\, A_{k'} \quad , \tag{3.19}$$

which may be recast as

$$A_k = \frac{\lambda_\ell\, \alpha_\ell(k)}{W_\ell - 2\xi_k} \cdot \frac{1}{V} \sum_{k'} \alpha^*_\ell(k')\, A_{k'} \quad . \tag{3.20}$$

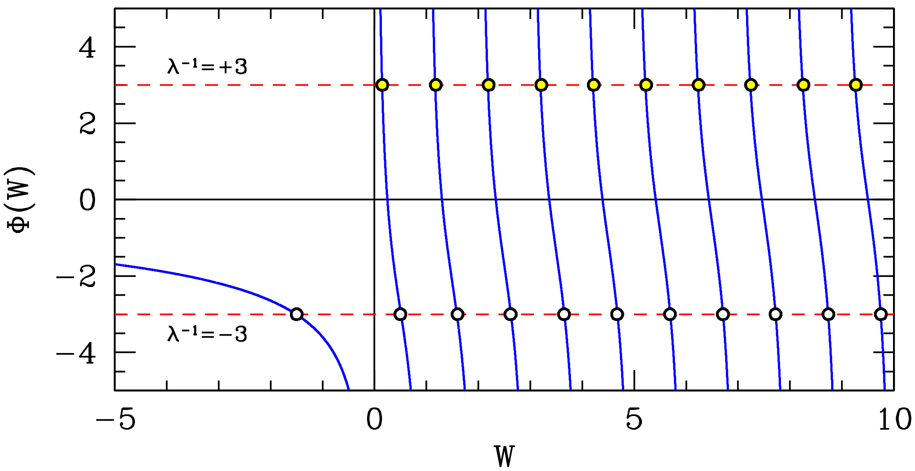

Figure 3.1: Graphical solution to the Cooper problem. A bound state exists for arbitrarily weak $\lambda < 0$.

Now multiply by α_k^* and sum over k to obtain

$$\frac{1}{\lambda_\ell} = \frac{1}{V} \sum_k \frac{\left|\alpha_\ell(k)\right|^2}{W_\ell - 2\xi_k} \equiv \Phi(W_\ell) \quad . \tag{3.21}$$

We solve this for W_ℓ.

We may find a graphical solution. Recall that the sum is restricted to $k > k_{\rm F}$, and that $\xi_k \geq 0$. The denominator on the RHS of Eqn. 3.21 changes sign as a function of W_ℓ every time $\frac{1}{2}W_\ell$ passes through one of the ξ_k values[1]. A sketch of the graphical solution is provided in Fig. 3.1. One sees that if $\lambda_\ell < 0$, *i.e.* if the potential is attractive, then a bound state exists. This is true for arbitrarily weak $|\lambda_\ell|$, a situation not usually encountered in three-dimensional problems, where there is usually a critical strength of the attractive potential in order to form a bound state[2]. This is a density of states effect – by restricting our attention to electrons near the Fermi level, where the DOS is roughly constant at $g(\varepsilon_{\rm F}) = m^* k_{\rm F}/\pi^2\hbar^2$, rather than near $\boldsymbol{k} = 0$, where $g(\varepsilon)$ vanishes as $\sqrt{\varepsilon}$, the pairing problem is effectively rendered two-dimensional. We can make further progress by assuming a particular form for $\alpha_\ell(k)$:

$$\alpha_\ell(k) = \begin{cases} 1 & \text{if } 0 < \xi_k < B_\ell \\ 0 & \text{otherwise} \end{cases} \quad , \tag{3.22}$$

where B_ℓ is an effective bandwidth for the ℓ channel. Then

$$1 = \tfrac{1}{2}\,|\lambda_\ell| \int\limits_0^{B_\ell} \! d\xi \, \frac{g(\varepsilon_{\rm F} + \xi)}{\left|W_\ell\right| + 2\xi} \quad . \tag{3.23}$$

The factor of $\frac{1}{2}$ is because it is the DOS per spin here, and not the total DOS. We assume $g(\varepsilon)$ does not vary significantly in the vicinity of $\varepsilon = \varepsilon_{\rm F}$, and pull $g(\varepsilon_{\rm F})$ out from the integrand. Integrating and solving for $\left|W_\ell\right|$,

$$\left|W_\ell\right| = \frac{2B_\ell}{\exp\!\left(\frac{4}{|\lambda_\ell|\, g(\varepsilon_{\rm F})}\right) - 1} \quad . \tag{3.24}$$

[1] We imagine quantizing in a finite volume, so the allowed k values are discrete.
[2] For example, the ^{2}He molecule is unbound, despite the attractive $-1/r^6$ van der Waals attractive tail in the interatomic potential.

In the *weak coupling* limit, where $|\lambda_\ell|\, g(\varepsilon_{\rm F}) \ll 1$, we have

$$\big|W_\ell\big| \simeq 2B_\ell\,\exp\!\left(-\frac{4}{|\lambda_\ell|\,g(\varepsilon_{\rm F})}\right) \quad . \tag{3.25}$$

As we shall see when we study BCS theory, the factor in the exponent is twice too large. The coefficient $2B_\ell$ will be shown to be the Debye energy of the phonons; we will see that it is only over a narrow range of energies about the Fermi surface that the effective electron-electron interaction is attractive. For strong coupling,

$$|W_\ell| = \tfrac{1}{2}\,|\lambda_\ell|\,g(\varepsilon_{\rm F}) \quad . \tag{3.26}$$

Finite momentum Cooper pair

We can construct a finite momentum Cooper pair as follows:

$$|\,\Psi_{\boldsymbol q}\,\rangle = \sum_{\boldsymbol k} A_{\boldsymbol k}\,\big(c^\dagger_{\boldsymbol k+\frac{1}{2}\boldsymbol q\uparrow}c^\dagger_{-\boldsymbol k+\frac{1}{2}\boldsymbol q\downarrow} - c^\dagger_{\boldsymbol k+\frac{1}{2}\boldsymbol q\downarrow}c^\dagger_{-\boldsymbol k+\frac{1}{2}\boldsymbol q\uparrow}\big)\,|\,{\rm F}\,\rangle \quad . \tag{3.27}$$

This wavefunction is a momentum eigenstate, with total momentum $\boldsymbol P = \hbar\boldsymbol q$. The eigenvalue equation is then

$$W A_{\boldsymbol k} = \big(\xi_{\boldsymbol k+\frac{1}{2}\boldsymbol q} + \xi_{-\boldsymbol k+\frac{1}{2}\boldsymbol q}\big)A_{\boldsymbol k} + \sum_{\boldsymbol k'} V_{\boldsymbol k,\boldsymbol k'}\,A_{\boldsymbol k'} \quad . \tag{3.28}$$

Assuming $\xi_{\boldsymbol k} = \xi_{-\boldsymbol k}$,

$$\xi_{\boldsymbol k+\frac{1}{2}\boldsymbol q} + \xi_{-\boldsymbol k+\frac{1}{2}\boldsymbol q} = 2\,\xi_{\boldsymbol k} + \tfrac{1}{4}\,q^\alpha q^\beta\,\frac{\partial^2\xi_{\boldsymbol k}}{\partial k^\alpha\,\partial k^\beta} + \ldots \quad . \tag{3.29}$$

The binding energy is thus reduced by an amount proportional to q^2; the $\boldsymbol q = 0$ Cooper pair has the greatest binding energy[3].

Mean square radius of the Cooper pair

We have

$$\begin{aligned}\big\langle \boldsymbol r^2\big\rangle &= \frac{\int\! d^3\!r\,\big|\Psi(\boldsymbol r)\big|^2\,\boldsymbol r^2}{\int\! d^3\!r\,\big|\Psi(\boldsymbol r)\big|^2} = \frac{\int\! d^3\!k\,\big|\boldsymbol\nabla_{\boldsymbol k} A_{\boldsymbol k}\big|^2}{\int\! d^3\!k\,\big|A_{\boldsymbol k}\big|^2} \\ &\simeq \frac{g(\varepsilon_{\rm F})\,\xi'(k_{\rm F})^2 \int_0^\infty\! d\xi\,\big|\frac{\partial A}{\partial \xi}\big|^2}{g(\varepsilon_{\rm F})\int_0^\infty\! d\xi\,|A|^2}\end{aligned} \tag{3.30}$$

with $A(\xi) = -C/\big(|W| + 2\xi\big)$ and thus $A'(\xi) = 2C/\big(|W| + 2\xi\big)^2$, where C is a constant independent of ξ. Ignoring the upper cutoff on ξ at B_ℓ, we have

$$\big\langle \boldsymbol r^2\big\rangle = 4\,\xi'(k_{\rm F})^2\cdot\frac{\int_{|W|}^\infty du\,u^{-4}}{\int_{|W|}^\infty du\,u^{-2}} = \tfrac{4}{3}\,(\hbar v_{\rm F})^2\,|W|^{-2} \quad , \tag{3.31}$$

[3]We assume the matrix $\partial_\alpha\partial_\beta\,\xi_{\boldsymbol k}$ is positive definite.

where we have used $\xi'(k_{\rm F}) = \hbar v_{\rm F}$. Thus, $R_{\rm RMS} = 2\hbar v_{\rm F}/\sqrt{3}\,|W|$. In the weak coupling limit, where $|W|$ is exponentially small in $1/|\lambda|$, the Cooper pair radius is huge. Indeed it is so large that many other Cooper pairs have their centers of mass within the radius of any given pair. This feature is what makes the BCS mean field theory of superconductivity so successful. Recall in our discussion of the Ginzburg criterion in §1.4.5, we found that mean field theory was qualitatively correct down to the Ginzburg reduced temperature $t_{\rm G} = ({\sf a}/R_*)^{2d/(4-d)}$, *i.e.* $t_{\rm G} = ({\sf a}/R_*)^6$ for $d = 3$. In this expression, R_* should be the mean Cooper pair size, and ${\sf a}$ a microscopic length (*i.e.* lattice constant). Typically $R_*/{\sf a} \sim 10^2 - 10^3$, so $t_{\rm G}$ is very tiny indeed.

3.3 Effective attraction due to phonons

The solution to Cooper's problem provided the first glimpses into the pairing nature of the superconducting state. But why should $V_{\boldsymbol{k},\boldsymbol{k}'}$ be attractive? One possible mechanism is an *induced* attraction due to phonons.

3.3.1 Electron-phonon Hamiltonian

In §2.8 we derived the electron-phonon Hamiltonian,

$$\hat{H}_{\rm el-ph} = \frac{1}{\sqrt{V}} \sum_{\substack{\boldsymbol{k},\boldsymbol{k}'\sigma \\ \boldsymbol{q},\lambda,\boldsymbol{G}}} g_\lambda(\boldsymbol{k},\boldsymbol{k}')\,(a^\dagger_{\boldsymbol{q}\lambda} + a_{-\boldsymbol{q}\lambda})\, c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}'\sigma}\, \delta_{\boldsymbol{k}',\boldsymbol{k}+\boldsymbol{q}+\boldsymbol{G}} \quad , \tag{3.32}$$

where $c^\dagger_{\boldsymbol{k}\sigma}$ creates an electron in state $|\,\boldsymbol{k}\,\sigma\,\rangle$ and $a^\dagger_{\boldsymbol{q}\lambda}$ creates a phonon in state $|\,\boldsymbol{q}\,\lambda\,\rangle$, where λ is the phonon polarization state. $\boldsymbol{G}$ is a reciprocal lattice vector, and

$$g_\lambda(\boldsymbol{k},\boldsymbol{k}') = -i \left(\frac{\hbar}{2\Omega\,\omega_\lambda(\boldsymbol{q})}\right)^{1/2} \frac{4\pi Z e^2}{(\boldsymbol{q}+\boldsymbol{G})^2 + \lambda_{\rm TF}^{-2}}\,(\boldsymbol{q}+\boldsymbol{G})\cdot\hat{\boldsymbol{e}}^*_\lambda(\boldsymbol{q}) \ . \tag{3.33}$$

is the electron-phonon coupling constant, with $\hat{\boldsymbol{e}}_\lambda(\boldsymbol{q})$ the phonon polarization vector, Ω the Wigner-Seitz unit cell volume, and $\omega_\lambda(\boldsymbol{q})$ the phonon frequency dispersion of the λ branch.

Recall that in an isotropic 'jellium' solid, the phonon polarization at wavevector $\boldsymbol{q}$ either is parallel to $\boldsymbol{q}$ (longitudinal waves), or perpendicular to $\boldsymbol{q}$ (transverse waves). We then have that only longitudinal waves couple to the electrons. This is because transverse waves do not result in any local accumulation of charge density, and the Coulomb interaction couples electrons to density fluctuations. Restricting our attention to the longitudinal phonon, we found for small $\boldsymbol{q}$ the electron-longitudinal phonon coupling $g_{\rm L}(\boldsymbol{k},\boldsymbol{k}+\boldsymbol{q}) \equiv g_{\boldsymbol{q}}$ satisfies

$$|g_{\boldsymbol{q}}|^2 = \lambda_{\rm el-ph}\cdot\frac{\hbar c_{\rm L} q}{g(\varepsilon_{\rm F})} \ , \tag{3.34}$$

where $g(\varepsilon_{\rm F})$ is the electronic density of states, $c_{\rm L}$ is the longitudinal phonon speed, and where the dimensionless *electron-phonon coupling constant* is

$$\lambda_{\rm el-ph} = \frac{Z^2}{2Mc_{\rm L}^2\,\Omega\, g(\varepsilon_{\rm F})} = \frac{2Z}{3}\,\frac{m^*}{M}\left(\frac{\varepsilon_{\rm F}}{k_{\rm B}\Theta_{\rm s}}\right)^2 \ , \tag{3.35}$$

with $\Theta_{\rm s} \equiv \hbar c_{\rm L} k_{\rm F}/k_{\rm B}$.

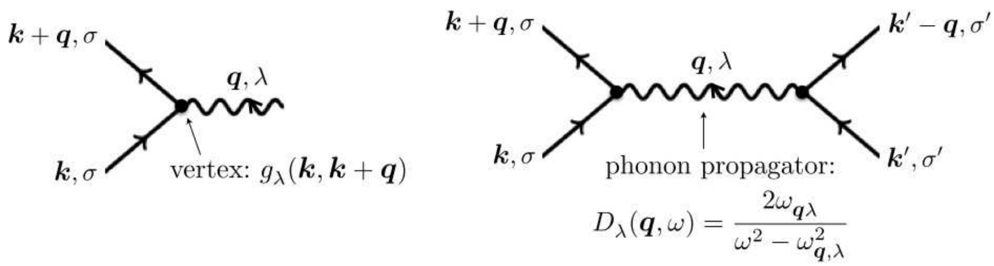

Figure 3.2: Feynman diagrams for electron-phonon processes.

3.3.2 Effective interaction between electrons

Consider now the problem of two particle scattering $|\,\boldsymbol{k}\,\sigma\,,\,-\boldsymbol{k}\,\,-\sigma\,\rangle\to|\,\boldsymbol{k}'\,\sigma\,,\,-\boldsymbol{k}'\,\,-\sigma\,\rangle$. We assume no phonons are present in the initial state, *i.e.* we work at $T=0$. The initial state energy is $E_{\rm i}=2\xi_{\boldsymbol{k}}$ and the final state energy is $E_{\rm f}=2\xi_{\boldsymbol{k}'}$. There are two intermediate states:[4]

$$\begin{aligned}|\,{\rm I}_1\,\rangle&=|\,\boldsymbol{k}'\,\sigma\,,\,-\boldsymbol{k}\,\,-\sigma\,\rangle\otimes|\,-\,\boldsymbol{q}\,\lambda\,\rangle\\ |\,{\rm I}_2\,\rangle&=|\,\boldsymbol{k}\,\sigma\,,\,-\boldsymbol{k}'\,\,-\sigma\,\rangle\otimes|\,+\,\boldsymbol{q}\,\lambda\,\rangle\quad,\end{aligned}\tag{3.36}$$

with $\boldsymbol{k}'=\boldsymbol{k}+\boldsymbol{q}$ in each case. The energies of these intermediate states are

$$E_1=\xi_{-\boldsymbol{k}}+\xi_{\boldsymbol{k}'}+\hbar\omega_{-\boldsymbol{q}\,\lambda}\qquad,\qquad E_2=\xi_{\boldsymbol{k}}+\xi_{-\boldsymbol{k}'}+\hbar\omega_{\boldsymbol{q}\,\lambda}\quad.\tag{3.37}$$

The second order matrix element is then

$$\begin{aligned}\langle\,\boldsymbol{k}'\,\sigma\,,\,-\boldsymbol{k}'\,\,-\sigma\,|\,\hat H_{\rm indirect}\,|\,\boldsymbol{k}\,\sigma\,,\,-\boldsymbol{k}\,\,-\sigma\,\rangle&=\sum_n\langle\,\boldsymbol{k}\,\sigma\,,\,-\boldsymbol{k}\,\,-\sigma\,|\,\hat H_{\rm el-ph}\,|\,n\,\rangle\langle\,n\,|\,\hat H_{\rm el-ph}\,|\,\boldsymbol{k}'\,\sigma\,,\,-\boldsymbol{k}'\,\,-\sigma\,\rangle\\ &\qquad\times\left(\frac{1}{E_{\rm f}-E_n}+\frac{1}{E_{\rm i}-E_n}\right)\\ &=\big|g_{\boldsymbol{k}'-\boldsymbol{k}}\big|^2\left(\frac{1}{\xi_{\boldsymbol{k}'}-\xi_{\boldsymbol{k}}-\omega_{\boldsymbol{q}}}+\frac{1}{\xi_{\boldsymbol{k}}-\xi_{\boldsymbol{k}'}-\omega_{\boldsymbol{q}}}\right)\quad.\end{aligned}\tag{3.38}$$

Here we have assumed $\xi_{\boldsymbol{k}}=\xi_{-\boldsymbol{k}}$ and $\omega_{\boldsymbol{q}}=\omega_{-\boldsymbol{q}'}$ and we have chosen λ to correspond to the longitudinal acoustic phonon branch. We add this to the Coulomb interaction $\hat v\big(|\boldsymbol{k}-\boldsymbol{k}'|\big)$ to get the net effective interaction between electrons,

$$\langle\,\boldsymbol{k}\,\sigma\,,\,-\boldsymbol{k}\,\,-\sigma\,|\,\hat H_{\rm eff}\,|\,\boldsymbol{k}'\,\sigma\,,\,-\boldsymbol{k}'\,\,-\sigma\,\rangle=\hat v\big(|\boldsymbol{k}-\boldsymbol{k}'|\big)+\big|g_{\boldsymbol{q}}\big|^2\times\frac{2\omega_{\boldsymbol{q}}}{(\xi_{\boldsymbol{k}}-\xi_{\boldsymbol{k}'})^2-(\hbar\omega_{\boldsymbol{q}})^2}\quad,\tag{3.39}$$

where $\boldsymbol{k}'=\boldsymbol{k}+\boldsymbol{q}$. We see that the effective interaction can be attractive, but only of $|\xi_{\boldsymbol{k}}-\xi_{\boldsymbol{k}'}|<\hbar\omega_{\boldsymbol{q}}$.

Another way to evoke this effective attraction is via the jellium model studied in §2.6.6. There we found the effective interaction between unit charges was given by

$$\hat V_{\rm eff}(\boldsymbol{q},\omega)=\frac{4\pi e^2}{\boldsymbol{q}^2\,\epsilon(\boldsymbol{q},\omega)}\tag{3.40}$$

where

$$\frac{1}{\epsilon(\boldsymbol{q},\omega)}\simeq\frac{q^2}{q^2+q^2_{\rm TF}}\left\{1+\frac{\omega^2_{\boldsymbol{q}}}{\omega^2-\omega^2_{\boldsymbol{q}}}\right\}\quad,\tag{3.41}$$

[4]The annihilation operator in the Hamiltonian $\hat H_{\rm el-ph}$ can act on either of the two electrons.

where the first term in the curly brackets is due to Thomas-Fermi screening (§2.6.2) and the second from ionic screening (§2.6.6). Recall that the Thomas-Fermi wavevector is given by $q_{\text{TF}} = \sqrt{4\pi e^2 g(\varepsilon_{\text{F}})}$, where $g(\varepsilon_{\text{F}})$ is the electronic density of states at the Fermi level, and that $\omega_{\boldsymbol{q}} = \Omega_{\text{p,i}}\, q/\sqrt{q^2+q^2_{\text{TF}}}$, where $\Omega_{\text{p,i}} = \sqrt{4\pi n^0_{\text{i}} Z_{\text{i}} e^2/M_{\text{i}}}$ is the ionic plasma frequency.

3.4 Reduced BCS Hamiltonian

The operator which creates a Cooper pair with total momentum $\boldsymbol{q}$ is $b^\dagger_{\boldsymbol{k},\boldsymbol{q}} + b^\dagger_{-\boldsymbol{k},\boldsymbol{q}}$, where

$$b^\dagger_{\boldsymbol{k},\boldsymbol{q}} = c^\dagger_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\uparrow}\, c^\dagger_{-\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\downarrow} \tag{3.42}$$

is a composite operator which creates the state $|\, \boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\uparrow\,,\, -\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\downarrow\rangle$. We learned from the solution to the Cooper problem that the $\boldsymbol{q}=0$ pairs have the greatest binding energy. This motivates consideration of the so-called *reduced BCS Hamiltonian*,

$$\hat{H}_{\text{red}} = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}}\, c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\, b^\dagger_{\boldsymbol{k},0}\, b_{\boldsymbol{k}',0} \quad . \tag{3.43}$$

The most general form for a momentum-conserving interaction is[5]

$$\hat{V} = \frac{1}{2V}\sum_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}\sum_{\sigma,\sigma'} \hat{u}_{\sigma\sigma'}(\boldsymbol{k},\boldsymbol{p},\boldsymbol{q})\, c^\dagger_{\boldsymbol{k}+\boldsymbol{q}\,\sigma}\, c^\dagger_{\boldsymbol{p}-\boldsymbol{q}\,\sigma'}\, c_{\boldsymbol{p}\,\sigma'}\, c_{\boldsymbol{k}\,\sigma} \quad . \tag{3.44}$$

Taking $\boldsymbol{p}=-\boldsymbol{k}$, $\sigma'=-\sigma$, and defining $\boldsymbol{k}'\equiv\boldsymbol{k}+\boldsymbol{q}$, we have

$$\hat{V} \to \frac{1}{2V}\sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} \hat{v}(\boldsymbol{k},\boldsymbol{k}')\, c^\dagger_{\boldsymbol{k}'\sigma}\, c^\dagger_{-\boldsymbol{k}'\,-\sigma}\, c_{-\boldsymbol{k}\,-\sigma}\, c_{\boldsymbol{k}\sigma} \quad , \tag{3.45}$$

where $\hat{v}(\boldsymbol{k},\boldsymbol{k}') = \hat{u}_{\uparrow\downarrow}(\boldsymbol{k},-\boldsymbol{k},\boldsymbol{k}'-\boldsymbol{k})$, which is equivalent to $\hat{H}_{\text{red}}$.

If $V_{\boldsymbol{k},\boldsymbol{k}'}$ is attractive, then the ground state will have no pair $(\boldsymbol{k}\uparrow,\, -\boldsymbol{k}\downarrow)$ occupied by a single electron; the pair states are either empty or doubly occupied. In that case, the reduced BCS Hamiltonian may be written as[6]

$$H^0_{\text{red}} = \sum_{\boldsymbol{k}} 2\varepsilon_{\boldsymbol{k}}\, b^\dagger_{\boldsymbol{k},0}\, b_{\boldsymbol{k},0} + \sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\, b^\dagger_{\boldsymbol{k},0}\, b_{\boldsymbol{k}',0} \quad . \tag{3.46}$$

This has the innocent appearance of a noninteracting bosonic Hamiltonian – an exchange of Cooper pairs restores the many-body wavefunction without a sign change because the Cooper pair is a composite object consisting of an even number of fermions[7]. However, this is not quite correct, because the operators $b_{\boldsymbol{k},0}$ and $b_{\boldsymbol{k}',0}$ do not satisfy canonical bosonic commutation relations. Rather,

$$\begin{aligned} \big[b_{\boldsymbol{k},0}\,,\, b_{\boldsymbol{k}',0}\big] = \big[b^\dagger_{\boldsymbol{k},0}\,,\, b^\dagger_{\boldsymbol{k}',0}\big] &= 0 \\ \big[b_{\boldsymbol{k},0}\,,\, b^\dagger_{\boldsymbol{k}',0}\big] &= \big(1 - c^\dagger_{\boldsymbol{k}\uparrow} c_{\boldsymbol{k}\uparrow} - c^\dagger_{-\boldsymbol{k}\downarrow} c_{-\boldsymbol{k}\downarrow}\big)\, \delta_{\boldsymbol{k}\boldsymbol{k}'} \quad . \end{aligned} \tag{3.47}$$

Because of this, $\hat{H}^0_{\text{red}}$ cannot naïvely be diagonalized. The extra terms inside the round brackets on the RHS arise due to the Pauli blocking effects. Indeed, one has $(b^\dagger_{\boldsymbol{k},0})^2 = 0$, so $b^\dagger_{\boldsymbol{k},0}$ is no ordinary boson operator.

[5] See the discussion in Appendix I, §3.13.

[6] Spin rotation invariance and a singlet Cooper pair requires that $V_{\boldsymbol{k},\boldsymbol{k}'} = V_{\boldsymbol{k},-\boldsymbol{k}'} = V_{-\boldsymbol{k},\boldsymbol{k}'}$.

[7] Recall that the atom ^{4}He, which consists of six fermions (two protons, two neutrons, and two electrons), is a boson, while ^{3}He, which has only one neutron and thus five fermions, is itself a fermion.

Figure 3.3: John Bardeen, Leon Cooper, and J. Robert Schrieffer.

Suppose, though, we try a mean field Hartree-Fock approach. We write

$$b_{\boldsymbol{k},0} = \langle b_{\boldsymbol{k},0}\rangle + \overbrace{\big(b_{\boldsymbol{k},0} - \langle b_{\boldsymbol{k},0}\rangle\big)}^{\delta b_{\boldsymbol{k},0}} \quad , \tag{3.48}$$

and we neglect terms in $\hat{H}_{\rm red}$ proportional to $\delta b^\dagger_{\boldsymbol{k},0}\,\delta b_{\boldsymbol{k}',0}$. We have

$$\hat{H}_{\rm red} = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}}\, c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'} \Big(\overbrace{-\langle b^\dagger_{\boldsymbol{k},0}\rangle\,\langle b_{\boldsymbol{k}',0}\rangle}^{\text{energy shift}} + \overbrace{\langle b_{\boldsymbol{k}',0}\rangle\, b^\dagger_{\boldsymbol{k},0} + \langle b^\dagger_{\boldsymbol{k},0}\rangle\, b_{\boldsymbol{k}',0}}^{\text{keep this}} + \overbrace{\delta b^\dagger_{\boldsymbol{k},0}\,\delta b_{\boldsymbol{k}',0}}^{\text{drop this!}} \Big) \quad . \tag{3.49}$$

Dropping the last term, which is quadratic in fluctuations, we obtain

$$\hat{H}^{\rm MF}_{\rm red} = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}}\, c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k}} \big(\Delta_{\boldsymbol{k}}\, c^\dagger_{\boldsymbol{k}\uparrow}\, c^\dagger_{-\boldsymbol{k}\downarrow} + \Delta^*_{\boldsymbol{k}}\, c_{-\boldsymbol{k}\downarrow}\, c_{\boldsymbol{k}\uparrow}\big) - \sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\,\langle b^\dagger_{\boldsymbol{k},0}\rangle\,\langle b_{\boldsymbol{k}',0}\rangle \quad , \tag{3.50}$$

where

$$\Delta_{\boldsymbol{k}} = \sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\,\big\langle c_{-\boldsymbol{k}'\downarrow}\, c_{\boldsymbol{k}'\uparrow}\big\rangle \qquad , \qquad \Delta^*_{\boldsymbol{k}} = \sum_{\boldsymbol{k}'} V^*_{\boldsymbol{k},\boldsymbol{k}'}\,\big\langle c^\dagger_{\boldsymbol{k}'\uparrow}\, c^\dagger_{-\boldsymbol{k}'\downarrow}\big\rangle \quad . \tag{3.51}$$

The first thing to notice about $\hat{H}^{\rm MF}_{\rm red}$ is that it does not preserve particle number, *i.e.* it does not commute with $\hat{N} = \sum_{\boldsymbol{k},\sigma} c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$. Accordingly, we are practically forced to work in the grand canonical ensemble, and we define the grand canonical Hamiltonian $\hat{K} \equiv \hat{H} - \mu\hat{N}$.

3.5 Solution of the mean field Hamiltonian

We now subtract $\mu\hat{N}$ from Eqn. 3.50, and define $\hat{K}_{\rm BCS} \equiv \hat{H}^{\rm MF}_{\rm red} - \mu\hat{N}$. Thus,

$$\hat{K}_{\rm BCS} = \sum_{\boldsymbol{k}} \begin{pmatrix} c^\dagger_{\boldsymbol{k}\uparrow} & c_{-\boldsymbol{k}\downarrow} \end{pmatrix} \overbrace{\begin{pmatrix} \xi_{\boldsymbol{k}} & \Delta_{\boldsymbol{k}} \\ \Delta^*_{\boldsymbol{k}} & -\xi_{\boldsymbol{k}} \end{pmatrix}}^{K_{\boldsymbol{k}}} \begin{pmatrix} c_{\boldsymbol{k}\uparrow} \\ c^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix} + K_0 \quad , \tag{3.52}$$

with $\xi_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}} - \mu$, and where

$$K_0 = \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} - \sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'} \, \langle c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} \rangle \, \langle c_{-\boldsymbol{k}'\downarrow} \, c_{\boldsymbol{k}'\uparrow} \rangle \tag{3.53}$$

is a constant. This problem may be brought to diagonal form via a unitary transformation,

$$\begin{pmatrix} c_{\boldsymbol{k}\uparrow} \\ c^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix} = \overbrace{\begin{pmatrix} \cos\vartheta_{\boldsymbol{k}} & -\sin\vartheta_{\boldsymbol{k}}\, e^{i\phi_{\boldsymbol{k}}} \\ \sin\vartheta_{\boldsymbol{k}}\, e^{-i\phi_{\boldsymbol{k}}} & \cos\vartheta_{\boldsymbol{k}} \end{pmatrix}}^{U_{\boldsymbol{k}}} \begin{pmatrix} \gamma_{\boldsymbol{k}\uparrow} \\ \gamma^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix} \quad . \tag{3.54}$$

In order for the $\gamma_{\boldsymbol{k}\sigma}$ operators to satisfy fermionic anticommutation relations, the matrix $U_{\boldsymbol{k}}$ must be unitary[8]. We then have

$$\begin{aligned} c_{\boldsymbol{k}\sigma} &= \cos\vartheta_{\boldsymbol{k}}\, \gamma_{\boldsymbol{k}\sigma} - \sigma \sin\vartheta_{\boldsymbol{k}}\, e^{i\phi_{\boldsymbol{k}}}\, \gamma^\dagger_{-\boldsymbol{k}\,-\sigma} \\ \gamma_{\boldsymbol{k}\sigma} &= \cos\vartheta_{\boldsymbol{k}}\, c_{\boldsymbol{k}\sigma} + \sigma \sin\vartheta_{\boldsymbol{k}}\, e^{i\phi_{\boldsymbol{k}}}\, c^\dagger_{-\boldsymbol{k}\,-\sigma} \quad . \end{aligned} \tag{3.55}$$

EXERCISE: Verify that $\{\gamma_{\boldsymbol{k}\sigma}\, ,\, \gamma^\dagger_{\boldsymbol{k}'\sigma'}\} = \delta_{\boldsymbol{k}\boldsymbol{k}'}\, \delta_{\sigma\sigma'}$.

We now must compute the transformed Hamiltonian. Dropping the $\boldsymbol{k}$ subscript for notational convenience, we have

$$\begin{aligned} \widetilde{K} = U^\dagger\, K\, U &= \begin{pmatrix} \cos\vartheta & \sin\vartheta\, e^{i\phi} \\ -\sin\vartheta\, e^{-i\phi} & \cos\vartheta \end{pmatrix} \begin{pmatrix} \xi & \Delta \\ \Delta^* & -\xi \end{pmatrix} \begin{pmatrix} \cos\vartheta & -\sin\vartheta\, e^{i\phi} \\ \sin\vartheta\, e^{-i\phi} & \cos\vartheta \end{pmatrix} \\ &= \begin{pmatrix} (\cos^2\!\vartheta - \sin^2\!\vartheta)\, \xi + \sin\vartheta\cos\vartheta\, (\Delta\, e^{-i\phi} + \Delta^* e^{i\phi}) & \Delta\cos^2\!\vartheta - \Delta^* e^{2i\phi} \sin^2\!\vartheta - 2\xi \sin\vartheta\cos\vartheta\, e^{i\phi} \\ \Delta^* \cos^2\!\vartheta - \Delta e^{-2i\phi} \sin^2\!\vartheta - 2\xi\sin\vartheta\cos\vartheta\, e^{-i\phi} & (\sin^2\!\vartheta - \cos^2\!\vartheta)\, \xi - \sin\vartheta\cos\vartheta\, (\Delta\, e^{-i\phi} + \Delta^* e^{i\phi}) \end{pmatrix} . \end{aligned} \tag{3.56}$$

We now use our freedom to choose ϑ and ϕ to render $\widetilde{K}$ diagonal. That is, we demand $\phi = \arg(\Delta)$ and

$$2\xi \sin\vartheta\cos\vartheta = \Delta\, (\cos^2\!\vartheta - \sin^2\!\vartheta) \quad . \tag{3.57}$$

This says $\tan(2\vartheta) = \Delta/\xi$, which means

$$\cos(2\vartheta) = \frac{\xi}{E} \quad , \quad \sin(2\vartheta) = \frac{\Delta}{E} \quad , \quad E = \sqrt{\xi^2 + \Delta^2} \quad . \tag{3.58}$$

The upper left element of $\widetilde{K}$ then becomes

$$(\cos^2\!\vartheta - \sin^2\!\vartheta)\, \xi + \sin\vartheta\cos\vartheta\, (\Delta\, e^{-i\phi} + \Delta^* e^{i\phi}) = \frac{\xi^2}{E} + \frac{\Delta^2}{E} = E \quad , \tag{3.59}$$

and thus $\widetilde{K} = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$. This unitary transformation, which mixes particle and hole states, is called a *Bogoliubov transformation*, because it was first discovered by Valatin.

Restoring the $\boldsymbol{k}$ subscript, we have $\phi_{\boldsymbol{k}} = \arg(\Delta_{\boldsymbol{k}})$, and $\tan(2\vartheta_{\boldsymbol{k}}) = |\Delta_{\boldsymbol{k}}|/\xi_{\boldsymbol{k}}$, which means

$$\cos(2\vartheta_{\boldsymbol{k}}) = \frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}} \quad , \quad \sin(2\vartheta_{\boldsymbol{k}}) = \frac{|\Delta_{\boldsymbol{k}}|}{E_{\boldsymbol{k}}} \quad , \quad E_{\boldsymbol{k}} = \sqrt{\xi^2_{\boldsymbol{k}} + |\Delta_{\boldsymbol{k}}|^2} \quad . \tag{3.60}$$

[8] The most general 2×2 unitary matrix is of the above form, but with each row multiplied by an independent phase. These phases may be absorbed into the definitions of the fermion operators themselves. After absorbing these harmless phases, we have written the most general unitary transformation.

Assuming that $\Delta_{\boldsymbol{k}}$ is not strongly momentum-dependent, we see that the dispersion $E_{\boldsymbol{k}}$ of the excitations has a nonzero minimum at $\xi_{\boldsymbol{k}} = 0$, *i.e.* at $k = k_{\rm F}$. This minimum value of $E_{\boldsymbol{k}}$ is called the *superconducting energy gap*.

We may further write

$$\cos\vartheta_{\boldsymbol{k}} = \sqrt{\frac{E_{\boldsymbol{k}} + \xi_{\boldsymbol{k}}}{2E_{\boldsymbol{k}}}} \qquad , \qquad \sin\vartheta_{\boldsymbol{k}} = \sqrt{\frac{E_{\boldsymbol{k}} - \xi_{\boldsymbol{k}}}{2E_{\boldsymbol{k}}}} \quad . \tag{3.61}$$

The grand canonical BCS Hamiltonian then becomes

$$\hat{K}_{\rm BCS} = \sum_{\boldsymbol{k},\sigma} E_{\boldsymbol{k}}\, \gamma^\dagger_{\boldsymbol{k}\sigma}\, \gamma_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k}} (\xi_{\boldsymbol{k}} - E_{\boldsymbol{k}}) - \sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\, \langle c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} \rangle\, \langle c_{-\boldsymbol{k}'\downarrow}\, c_{\boldsymbol{k}'\uparrow} \rangle \quad . \tag{3.62}$$

Finally, what of the ground state wavefunction itself? We must have $\gamma_{\boldsymbol{k}\sigma} |\, \mathrm{G}\, \rangle = 0$. This leads to

$$|\, \mathrm{G}\, \rangle = \prod_{\boldsymbol{k}} \big(\cos\vartheta_{\boldsymbol{k}} - \sin\vartheta_{\boldsymbol{k}}\, e^{i\phi_{\boldsymbol{k}}}\, c^\dagger_{\boldsymbol{k}\uparrow}\, c^\dagger_{-\boldsymbol{k}\downarrow} \big)\, |\, 0\, \rangle \quad . \tag{3.63}$$

Note that $\langle\, \mathrm{G} \,|\, \mathrm{G}\, \rangle = 1$. J. R. Schrieffer conceived of this wavefunction during a subway ride in New York City sometime during the winter of 1957. At the time he was a graduate student at the University of Illinois.

Sanity check

It is good to make contact with something familiar, such as the case $\Delta_{\boldsymbol{k}} = 0$. Note that $\xi_{\boldsymbol{k}} < 0$ for $k < k_{\rm F}$ and $\xi_{\boldsymbol{k}} > 0$ for $k > k_{\rm F}$. We now have

$$\cos\vartheta_{\boldsymbol{k}} = \Theta(k - k_{\rm F}) \qquad , \qquad \sin\vartheta_{\boldsymbol{k}} = \Theta(k_{\rm F} - k) \quad . \tag{3.64}$$

Note that the wavefunction $|\, \mathrm{G}\, \rangle$ in Eqn. 3.63 correctly describes a filled Fermi sphere out to $k = k_{\rm F}$. Furthermore, the constant on the RHS of Eqn. 3.62 is $2\sum_{k<k_{\rm F}} \xi_{\boldsymbol{k}}$, which is the Landau free energy of the filled Fermi sphere. What of the excitations? We are free to take $\phi_{\boldsymbol{k}} = 0$. Then

$$\begin{aligned} k < k_{\rm F} \ &: \ \gamma^\dagger_{\boldsymbol{k}\sigma} = \sigma\, c_{-\boldsymbol{k}\, -\sigma} \\ k > k_{\rm F} \ &: \ \gamma^\dagger_{\boldsymbol{k}\sigma} = c^\dagger_{\boldsymbol{k}\sigma} \quad . \end{aligned} \tag{3.65}$$

Thus, the elementary excitations are holes below $k_{\rm F}$ and electrons above $k_{\rm F}$. All we have done, then, is to effect a (unitary) particle-hole transformation on those states lying within the Fermi sea.

3.6 Self-consistency

We now demand that the following two conditions hold:

$$\begin{aligned} N &= \sum_{\boldsymbol{k}\sigma} \langle c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}\sigma} \rangle \\ \Delta_{\boldsymbol{k}} &= \sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\, \langle c_{-\boldsymbol{k}'\downarrow}\, c_{\boldsymbol{k}'\uparrow} \rangle \quad , \end{aligned} \tag{3.66}$$

the second of which is from Eqn. 3.51. Thus, we need

$$\begin{aligned} \langle c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}\sigma} \rangle &= \big\langle (\cos\vartheta_{\boldsymbol{k}}\, \gamma^\dagger_{\boldsymbol{k}\sigma} - \sigma \sin\vartheta_{\boldsymbol{k}}\, e^{-i\phi_{\boldsymbol{k}}}\, \gamma_{-\boldsymbol{k}\, -\sigma})(\cos\vartheta_{\boldsymbol{k}}\, \gamma_{\boldsymbol{k}\sigma} - \sigma \sin\vartheta_{\boldsymbol{k}}\, e^{i\phi_{\boldsymbol{k}}}\, \gamma^\dagger_{-\boldsymbol{k}\, -\sigma}) \big\rangle \\ &= \cos^2\!\vartheta_{\boldsymbol{k}}\, f_{\boldsymbol{k}} + \sin^2\!\vartheta_{\boldsymbol{k}}\, (1 - f_{\boldsymbol{k}}) = \frac{1}{2} - \frac{\xi_{\boldsymbol{k}}}{2E_{\boldsymbol{k}}} \tanh\!\big(\tfrac{1}{2}\beta E_{\boldsymbol{k}}\big) \quad , \end{aligned} \tag{3.67}$$

where

$$f_{\boldsymbol{k}} = \langle \gamma^\dagger_{\boldsymbol{k}\sigma}\, \gamma_{\boldsymbol{k}\sigma} \rangle = \frac{1}{e^{\beta E_{\boldsymbol{k}}} + 1} = \tfrac{1}{2} - \tfrac{1}{2} \tanh\big(\tfrac{1}{2}\beta E_{\boldsymbol{k}}\big) \tag{3.68}$$

is the Fermi function, with $\beta = 1/k_{\rm B}T$. We also have

$$\begin{aligned}\langle c_{-\boldsymbol{k}\,-\sigma}\, c_{\boldsymbol{k}\sigma} \rangle &= \big\langle (\cos\vartheta_{\boldsymbol{k}}\, \gamma_{-\boldsymbol{k}\,-\sigma} + \sigma \sin\vartheta_{\boldsymbol{k}}\, e^{i\phi_{\boldsymbol{k}}}\, \gamma^\dagger_{\boldsymbol{k}\sigma})(\cos\vartheta_{\boldsymbol{k}}\, \gamma_{\boldsymbol{k}\sigma} - \sigma \sin\vartheta_{\boldsymbol{k}}\, e^{i\phi_{\boldsymbol{k}}}\, \gamma^\dagger_{-\boldsymbol{k}\,-\sigma}) \big\rangle \\ &= \sigma \sin\vartheta_{\boldsymbol{k}} \cos\vartheta_{\boldsymbol{k}}\, e^{i\phi_{\boldsymbol{k}}}\, \big(2f_{\boldsymbol{k}} - 1\big) = -\frac{\sigma\Delta_{\boldsymbol{k}}}{2E_{\boldsymbol{k}}}\, \tanh\big(\tfrac{1}{2}\beta E_{\boldsymbol{k}}\big) \quad . \end{aligned} \tag{3.69}$$

Let's evaluate at $T = 0$:

$$\begin{aligned} N &= \sum_{\boldsymbol{k}} \bigg(1 - \frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\bigg) \\ \Delta_{\boldsymbol{k}} &= -\sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\, \frac{\Delta_{\boldsymbol{k}'}}{2E_{\boldsymbol{k}'}} \quad . \end{aligned} \tag{3.70}$$

The second of these is known as the BCS gap equation. Note that $\Delta_{\boldsymbol{k}} = 0$ is always a solution of the gap equation.

To proceed further, we need a model for $V_{\boldsymbol{k},\boldsymbol{k}'}$. We shall assume

$$V_{\boldsymbol{k},\boldsymbol{k}'} = \begin{cases} -v/V & \text{if } |\xi_{\boldsymbol{k}}| < \hbar\omega_{\rm D} \text{ and } |\xi_{\boldsymbol{k}'}| < \hbar\omega_{\rm D} \\ 0 & \text{otherwise} \quad . \end{cases} \tag{3.71}$$

Here $v > 0$, so the interaction is attractive, but only when $\xi_{\boldsymbol{k}}$ and $\xi_{\boldsymbol{k}'}$ are within an energy $\hbar\omega_{\rm D}$ of zero. For phonon-mediated superconductivity, $\omega_{\rm D}$ is the Debye frequency, which is the phonon bandwidth.

3.6.1 Solution at zero temperature

We first solve the second of Eqns. 3.70, by assuming

$$\Delta_{\boldsymbol{k}} = \begin{cases} \Delta\, e^{i\phi} & \text{if } |\xi_{\boldsymbol{k}}| < \hbar\omega_{\rm D} \\ 0 & \text{otherwise} \quad , \end{cases} \tag{3.72}$$

with Δ real. We then have[9]

$$\begin{aligned} \Delta &= +v \int \frac{d^3\!k}{(2\pi)^3}\, \frac{\Delta}{2E_{\boldsymbol{k}}}\, \Theta\big(\hbar\omega_{\rm D} - |\xi_{\boldsymbol{k}}|\big) \\ &= \tfrac{1}{2} v\, g(\varepsilon_{\rm F}) \int\limits_0^{\hbar\omega_{\rm D}} \!d\xi\, \frac{\Delta}{\sqrt{\xi^2 + \Delta^2}} \quad . \end{aligned} \tag{3.73}$$

Cancelling out the common factors of Δ on each side, we obtain

$$1 = \tfrac{1}{2} v\, g(\varepsilon_{\rm F}) \int\limits_0^{\hbar\omega_{\rm D}/\Delta} \!ds\, (1 + s^2)^{-1/2} = \tfrac{1}{2} v\, g(\varepsilon_{\rm F})\, \sinh^{-1}\big(\hbar\omega_{\rm D}/\Delta\big) \quad . \tag{3.74}$$

[9]We assume the density of states $g(\varepsilon)$ is slowly varying in the vicinity of the chemical potential and approximate it at $g(\varepsilon_{\rm F})$. In fact, we should more properly call it $g(\mu)$, but as a practical matter $\mu \simeq \varepsilon_{\rm F}$ at temperatures low enough to be in the superconducting phase. Note that $g(\varepsilon_{\rm F})$ is the total DOS for both spin species. In the literature, one often encounters the expression $N(0)$, which is the DOS per spin at the Fermi level, *i.e.* $N(0) = \frac{1}{2}\, g(\varepsilon_{\rm F})$.

Thus, writing $\Delta_0 \equiv \Delta(0)$ for the zero temperature gap,

$$\Delta_0 = \frac{\hbar\omega_{\rm D}}{\sinh\big(2/g(\varepsilon_{\rm F})\, v\big)} \simeq 2\hbar\omega_{\rm D} \exp\bigg(-\frac{2}{g(\varepsilon_{\rm F})\, v}\bigg) \quad , \tag{3.75}$$

where $g(\varepsilon_{\rm F})$ is the total electronic DOS (for both spin species) at the Fermi level. Notice that, as promised, the argument of the exponent is one half as large as what we found in our solution of the Cooper problem, in Eqn. 3.25.

3.6.2 Condensation energy

We now evaluate the zero temperature expectation of $\hat{K}_{\rm BCS}$ from Eqn. 3.62. To get the correct answer, it is essential that we retain the term corresponding to the constant energy shift in the mean field Hamiltonian, *i.e.* the last term on the RHS of Eqn. 3.62. Invoking the gap equation $\Delta_{\boldsymbol{k}} = \sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'} \, \langle c_{-\boldsymbol{k}'\downarrow} \, c_{\boldsymbol{k}'\uparrow} \rangle$, we have

$$\langle \, {\rm G} \, | \, \hat{K}_{\rm BCS} \, | \, {\rm G} \, \rangle = \sum_{\boldsymbol{k}} \Bigg(\xi_{\boldsymbol{k}} - E_{\boldsymbol{k}} + \frac{|\Delta_{\boldsymbol{k}}|^2}{2E_{\boldsymbol{k}}} \Bigg) \quad . \tag{3.76}$$

From this we subtract the ground state energy of the metallic phase, *i.e.* when $\Delta_{\boldsymbol{k}} = 0$, which is $2\sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} \, \Theta(k_{\rm F} - k)$. The difference is the condensation energy. Adopting the model interaction potential in Eqn. 3.71, we have

$$\begin{aligned} E_{\rm s} - E_{\rm n} &= \sum_{\boldsymbol{k}} \bigg(\xi_{\boldsymbol{k}} - E_{\boldsymbol{k}} + \frac{|\Delta_{\boldsymbol{k}}|^2}{2E_{\boldsymbol{k}}} - 2\xi_{\boldsymbol{k}} \, \Theta(k_{\rm F} - k) \bigg) \\ &= 2 \sum_{\boldsymbol{k}} \, (\xi_{\boldsymbol{k}} - E_{\boldsymbol{k}}) \, \Theta(\xi_{\boldsymbol{k}}) \, \Theta(\hbar\omega_{\rm D} - \xi_{\boldsymbol{k}}) + \sum_{\boldsymbol{k}} \frac{\Delta_0^2}{2E_{\boldsymbol{k}}} \, \Theta\big(\hbar\omega_{\rm D} - |\xi_{\boldsymbol{k}}|\big) \quad , \end{aligned} \tag{3.77}$$

where we have linearized about $k = k_{\rm F}$. We then have

$$\begin{aligned} E_{\rm s} - E_{\rm n} &= V g(\varepsilon_{\rm F}) \, \Delta_0^2 \int\limits_0^{\hbar\omega_{\rm D}/\Delta_0} \! ds \, \bigg(s - \sqrt{s^2 + 1} + \frac{1}{2\sqrt{s^2+1}} \bigg) \\ &= \tfrac{1}{2} \, V g(\varepsilon_{\rm F}) \, \Delta_0^2 \Big(x^2 - x\sqrt{1 + x^2} \Big) \approx -\tfrac{1}{4} \, V g(\varepsilon_{\rm F}) \, \Delta_0^2 \quad , \end{aligned} \tag{3.78}$$

where $x \equiv \hbar\omega_{\rm D}/\Delta_0$. The condensation energy density is therefore $-\frac{1}{4} \, g(\varepsilon_{\rm F}) \, \Delta_0^2$, which may be equated with $-H_{\rm c}^2/8\pi$, where $H_{\rm c}$ is the thermodynamic critical field. Thus, we find

$$H_{\rm c}(0) = \sqrt{2\pi g(\varepsilon_{\rm F})} \, \Delta_0 \quad , \tag{3.79}$$

which relates the thermodynamic critical field to the superconducting gap, at $T = 0$.

3.7 Coherence factors and quasiparticle energies

When $\Delta_{\boldsymbol{k}} = 0$, we have $E_{\boldsymbol{k}} = |\xi_{\boldsymbol{k}}|$. When $\hbar\omega_{\rm D} \ll \varepsilon_{\rm F}$, there is a very narrow window surrounding $k = k_{\rm F}$ where $E_{\boldsymbol{k}}$ departs from $|\xi_{\boldsymbol{k}}|$, as shown in the bottom panel of Fig. 3.4. Note the *energy gap* in the quasiparticle dispersion, where the minimum excitation energy is given by[10]

$$\min_{\boldsymbol{k}} E_{\boldsymbol{k}} = E_{k_{\rm F}} = \Delta_0 \quad . \tag{3.80}$$

[10]Here we assume, without loss of generality, that Δ is real.

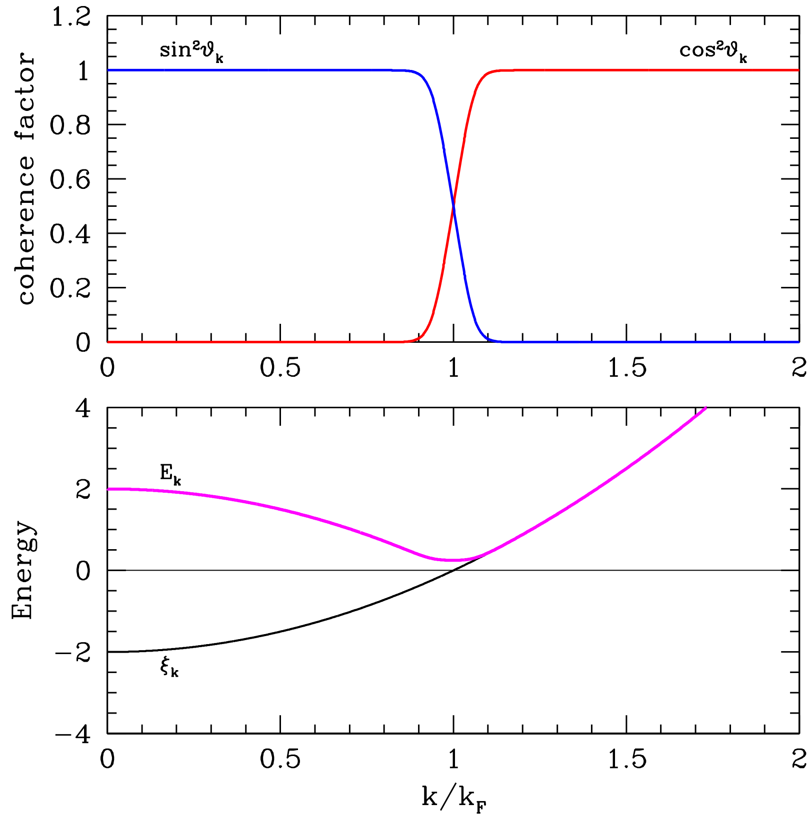

Figure 3.4: Top panel: BCS coherence factors $\sin^2\vartheta_{\boldsymbol{k}}$ (blue) and $\cos^2\vartheta_{\boldsymbol{k}}$ (red). Bottom panel: the functions $\xi_{\boldsymbol{k}}$ (black) and $E_{\boldsymbol{k}}$ (magenta). The minimum value of the magenta curve is the superconducting gap Δ_0.

In the top panel of Fig. 3.4 we plot the coherence factors $\sin^2\vartheta_{\boldsymbol{k}}$ and $\cos^2\vartheta_{\boldsymbol{k}}$. Note that $\sin^2\vartheta_{\boldsymbol{k}}$ approaches unity for $k < k_{\rm F}$ and $\cos^2\vartheta_{\boldsymbol{k}}$ approaches unity for $k > k_{\rm F}$, aside for the narrow window of width $\delta k \simeq \Delta_0/\hbar v_{\rm F}$. Recall that

$$\gamma^\dagger_{\boldsymbol{k}\sigma} = \cos\vartheta_{\boldsymbol{k}}\, c^\dagger_{\boldsymbol{k}\sigma} + \sigma\sin\vartheta_{\boldsymbol{k}}\, e^{-i\phi_{\boldsymbol{k}}}\, c_{-\boldsymbol{k}\,-\sigma} \quad . \tag{3.81}$$

Thus we see that the quasiparticle creation operator $\gamma^\dagger_{\boldsymbol{k}\sigma}$ creates an electron in the state $|\,\boldsymbol{k}\,\sigma\,\rangle$ when $\cos^2\vartheta_{\boldsymbol{k}} \simeq 1$, and a hole in the state $|\,-\boldsymbol{k}\;-\sigma\,\rangle$ when $\sin^2\vartheta_{\boldsymbol{k}} \simeq 1$. In the aforementioned narrow window $|k - k_{\rm F}| \lesssim \Delta_0/\hbar v_{\rm F}$, the quasiparticle creates a linear combination of electron and hole states. Typically $\Delta_0 \sim 10^{-4}\,\varepsilon_{\rm F}$, since metallic Fermi energies are on the order of tens of thousands of Kelvins, while Δ_0 is on the order of Kelvins or tens of Kelvins. Thus, $\delta k \lesssim 10^{-3} k_{\rm F}$. The difference between the superconducting state and the metallic state all takes place within an onion skin at the Fermi surface!

Note that for the model interaction $V_{\boldsymbol{k},\boldsymbol{k}'}$ of Eqn. 3.71, the solution $\Delta_{\boldsymbol{k}}$ in Eqn. 3.72 is actually *discontinuous* when $\xi_{\boldsymbol{k}} = \pm\hbar\omega_{\rm D}$, *i.e.* when $k = k^*_\pm \equiv k_{\rm F} \pm \omega_{\rm D}/v_{\rm F}$. Therefore, the energy dispersion $E_{\boldsymbol{k}}$ is also discontinuous along these surfaces. However, the magnitude of the discontinuity is

$$\delta E = \sqrt{(\hbar\omega_{\rm D})^2 + \Delta_0^2} - \hbar\omega_{\rm D} \approx \frac{\Delta_0^2}{2\hbar\omega_{\rm D}} \quad . \tag{3.82}$$

Therefore $\delta E/E_{k^*_\pm} \approx \Delta_0^2/2(\hbar\omega_{\rm D})^2 \propto \exp\big(-4/g(\varepsilon_{\rm F})\,v\big)$, which is very tiny in weak coupling, where $g(\varepsilon_{\rm F})\,v \ll 1$. Note that the ground state is largely unaffected for electronic states in the vicinity of this (unphysical) energy discontinuity. The coherence factors are distinguished from those of a Fermi liquid only in regions where $\langle c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow}\rangle$ is appreciable, which requires $\xi_{\boldsymbol{k}}$ to be on the order of $\Delta_{\boldsymbol{k}}$. This only happens when $|k - k_{\rm F}| \lesssim \Delta_0/\hbar v_{\rm F}$, as discussed in the previous paragraph. In a more physical model, the interaction $V_{\boldsymbol{k},\boldsymbol{k}'}$ and the solution $\Delta_{\boldsymbol{k}}$ would not be discontinuous functions of $\boldsymbol{k}$.

3.8 Number and Phase

The BCS ground state wavefunction $|\,{\rm G}\,\rangle$ was given in Eqn. 3.63. Consider the state

$$|\,{\rm G}(\alpha)\,\rangle = \prod_{\boldsymbol{k}} \Big(\cos\vartheta_{\boldsymbol{k}} - e^{i\alpha}\, e^{i\phi_{\boldsymbol{k}}} \sin\vartheta_{\boldsymbol{k}}\, c^\dagger_{\boldsymbol{k}\uparrow}\, c^\dagger_{-\boldsymbol{k}\downarrow}\Big)\,|\,0\,\rangle \quad . \tag{3.83}$$

This is the ground state when the gap function $\Delta_{\boldsymbol{k}}$ is multiplied by the uniform phase factor $e^{i\alpha}$. We shall here abbreviate $|\,\alpha\,\rangle \equiv |\,{\rm G}(\alpha)\,\rangle$.

Now consider the action of the number operator on $|\,\alpha\,\rangle$:

$$\begin{aligned}\hat{N}\,|\,\alpha\,\rangle &= \sum_{\boldsymbol{k}} \big(c^\dagger_{\boldsymbol{k}\uparrow} c_{\boldsymbol{k}\uparrow} + c^\dagger_{-\boldsymbol{k}\downarrow} c_{-\boldsymbol{k}\downarrow}\big)\,|\,\alpha\,\rangle \\ &= -2\sum_{\boldsymbol{k}} e^{i\alpha}\, e^{i\phi_{\boldsymbol{k}}}\, \sin\vartheta_{\boldsymbol{k}}\, c^\dagger_{\boldsymbol{k}\uparrow}\, c^\dagger_{-\boldsymbol{k}\downarrow} \prod_{\boldsymbol{k}'\neq\boldsymbol{k}} \Big(\cos\vartheta_{\boldsymbol{k}'} - e^{i\alpha}\, e^{i\phi_{\boldsymbol{k}'}} \sin\vartheta_{\boldsymbol{k}'}\, c^\dagger_{\boldsymbol{k}'\uparrow}\, c^\dagger_{-\boldsymbol{k}'\downarrow}\Big)\,|\,0\,\rangle \\ &= \frac{2}{i}\,\frac{\partial}{\partial\alpha}\,|\,\alpha\,\rangle \quad .\end{aligned} \tag{3.84}$$

If we define the number of Cooper pairs as $\hat{M} \equiv \frac{1}{2}\hat{N}$, then we may identify $\hat{M} = \frac{1}{i}\frac{\partial}{\partial\alpha}$. Furthermore, we may project $|\,{\rm G}\,\rangle$ onto a state of definite particle number by defining

$$|\,M\,\rangle = \int\limits_{-\pi}^{\pi} \frac{d\alpha}{2\pi}\, e^{-iM\alpha}\,|\,\alpha\,\rangle \quad . \tag{3.85}$$

The state $|\,M\,\rangle$ has $N = 2M$ particles, *i.e.* M Cooper pairs. One can easily compute the number fluctuations in the state $|\,{\rm G}(\alpha)\,\rangle$:

$$\frac{\langle\,\alpha\,|\,\hat{N}^2\,|\,\alpha\,\rangle - \langle\,\alpha\,|\,\hat{N}\,|\,\alpha\,\rangle^2}{\langle\,\alpha\,|\,\hat{N}\,|\,\alpha\,\rangle} = \frac{2\int\! d^3\!k\, \sin^2\!\vartheta_{\boldsymbol{k}}\, \cos^2\!\vartheta_{\boldsymbol{k}}}{\int\! d^3\!k\, \sin^2\!\vartheta_{\boldsymbol{k}}} \quad . \tag{3.86}$$

Thus, $(\Delta N)_{\rm RMS} \propto \sqrt{\langle N\rangle}$. Note that $(\Delta N)_{\rm RMS}$ vanishes in the Fermi liquid state, where $\sin\vartheta_{\boldsymbol{k}}\cos\vartheta_{\boldsymbol{k}} = 0$.

3.9 Finite temperature

The gap equation at finite temperature takes the form

$$\Delta_{\boldsymbol{k}} = -\sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\, \frac{\Delta_{\boldsymbol{k}'}}{2E_{\boldsymbol{k}'}}\, \tanh\!\bigg(\frac{E_{\boldsymbol{k}'}}{2k_{\rm B}T}\bigg) \quad . \tag{3.87}$$

It is easy to see that we have no solutions other than the trivial one $\Delta_{\boldsymbol{k}} = 0$ in the $T \to \infty$ limit, for the gap equation then becomes $\sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\, \Delta_{\boldsymbol{k}'} = -4k_{\rm B}T\, \Delta_{\boldsymbol{k}'}$ and if the eigenspectrum of $V_{\boldsymbol{k},\boldsymbol{k}'}$ is bounded, there is no solution for $k_{\rm B}T$ greater than the largest eigenvalue of $-V_{\boldsymbol{k},\boldsymbol{k}'}$.

To find the critical temperature where the gap collapses, again we assume the forms in Eqns. 3.71 and 3.72, in which case we have

$$1 = \tfrac{1}{2}\, g(\varepsilon_{\rm F})\, v \int\limits_0^{\hbar\omega_{\rm D}} \frac{d\xi}{\sqrt{\xi^2+\Delta^2}}\, \tanh\!\bigg(\frac{\sqrt{\xi^2+\Delta^2}}{2k_{\rm B}T}\bigg) \quad . \tag{3.88}$$

It is clear that $\Delta(T)$ is a decreasing function of temperature, which vanishes at $T=T_{\rm c}$, where $T_{\rm c}$ is determined by the equation

$$\int\limits_0^{\Lambda/2} ds\, s^{-1} \tanh(s) = \frac{2}{g(\varepsilon_{\rm F})\, v} \quad , \tag{3.89}$$

where $\Lambda = \hbar\omega_{\rm D}/k_{\rm B}T_{\rm c}$. One finds, for large Λ ,

$$\begin{aligned} I(\Lambda) = \int\limits_0^{\Lambda/2} ds\, s^{-1} \tanh(s) &= \ln\big(\tfrac{1}{2}\Lambda\big) \tanh\big(\tfrac{1}{2}\Lambda\big) - \int\limits_0^{\Lambda/2} ds\, \frac{\ln s}{\cosh^2 s} \\ &= \ln\Lambda + \ln\big(2\,e^{\rm C}/\pi\big) + \mathcal{O}\big(e^{-\Lambda/2}\big) \quad , \end{aligned} \tag{3.90}$$

where ${\rm C} = 0.57721566\ldots$ is the Euler-Mascheroni constant. One has $2\,e^{\rm C}/\pi = 1.134$, so

$$k_{\rm B}T_{\rm c} = 1.134\,\hbar\omega_{\rm D}\, e^{-2/g(\varepsilon_{\rm F})\, v} \quad . \tag{3.91}$$

Comparing with Eqn. 3.75, we obtain the famous result

$$2\Delta(0) = 2\pi e^{-\rm C}\, k_{\rm B}T_{\rm c} \simeq 3.52\, k_{\rm B}T_{\rm c} \quad . \tag{3.92}$$

As we shall derive presently, just below the critical temperature, one has

$$\Delta(T) = 1.734\,\Delta(0)\left(1-\frac{T}{T_{\rm c}}\right)^{1/2} \simeq 3.06\, k_{\rm B}T_{\rm c}\left(1-\frac{T}{T_{\rm c}}\right)^{1/2} \quad . \tag{3.93}$$

3.9.1 Isotope effect

The prefactor in Eqn. 3.91 is proportional to the Debye energy $\hbar\omega_{\rm D}$. Thus,

$$\ln T_{\rm c} = \ln\omega_{\rm D} - \frac{2}{g(\varepsilon_{\rm F})\, v} + {\rm const.} \quad . \tag{3.94}$$

If we imagine varying only the mass of the ions, via isotopic substitution, then $g(\varepsilon_{\rm F})$ and v do not change, and we have

$$\delta\ln T_{\rm c} = \delta\ln\omega_{\rm D} = -\tfrac{1}{2}\,\delta\ln M \quad , \tag{3.95}$$

where M is the ion mass. Thus, isotopically increasing the ion mass leads to a concomitant reduction in $T_{\rm c}$ according to BCS theory. This is fairly well confirmed in experiments on low $T_{\rm c}$ materials.

3.9.2 Landau free energy of a superconductor

Quantum statistical mechanics of noninteracting fermions applied to $\hat{K}_{\rm BCS}$ in Eqn. 3.62 yields the Landau free energy

$$\varOmega_{\rm s} = -2k_{\rm B}T\sum_{\boldsymbol{k}} \ln\big(1+e^{-E_{\boldsymbol{k}}/k_{\rm B}T}\big) + \sum_{\boldsymbol{k}}\left\{\xi_{\boldsymbol{k}} - E_{\boldsymbol{k}} + \frac{|\Delta_{\boldsymbol{k}}|^2}{2E_{\boldsymbol{k}}}\,\tanh\!\bigg(\frac{E_{\boldsymbol{k}}}{2k_{\rm B}T}\bigg)\right\} \quad . \tag{3.96}$$

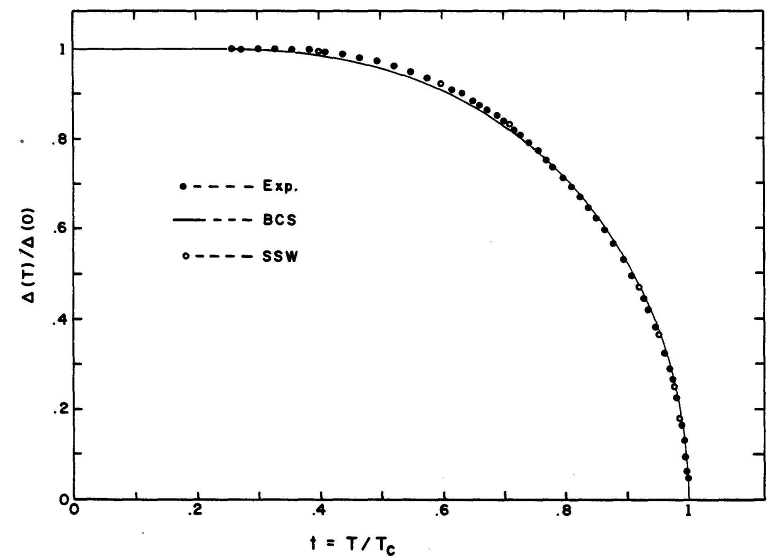

Figure 3.5: Temperature dependence of the energy gap in Pb as determined by tunneling *versus* prediction of BCS theory. From R. F. Gasparovic, B. N. Taylor, and R. E. Eck, *Sol. State Comm.* **4**, 59 (1966). Deviations from the BCS theory are accounted for by numerical calculations at strong coupling by Swihart, Scalapino, and Wada (1965).

The corresponding result for the normal state ($\Delta_{\boldsymbol{k}} = 0$) is

$$\Omega_{\rm n} = -2k_{\rm B}T \sum_{\boldsymbol{k}} \ln\big(1 + e^{-|\xi_{\boldsymbol{k}}|/k_{\rm B}T}\big) + \sum_{\boldsymbol{k}} \Big(\xi_{\boldsymbol{k}} - |\xi_{\boldsymbol{k}}|\Big) \quad . \tag{3.97}$$

Thus, the difference is

$$\Omega_{\rm s} - \Omega_{\rm n} = -2k_{\rm B}T \sum_{\boldsymbol{k}} \ln\left(\frac{1 + e^{-E_{\boldsymbol{k}}/k_{\rm B}T}}{1 + e^{-|\xi_{\boldsymbol{k}}|/k_{\rm B}T}}\right) + \sum_{\boldsymbol{k}} \left\{ |\xi_{\boldsymbol{k}}| - E_{\boldsymbol{k}} + \frac{|\Delta_{\boldsymbol{k}}|^2}{2E_{\boldsymbol{k}}} \tanh\left(\frac{E_{\boldsymbol{k}}}{2k_{\rm B}T}\right)\right\} \quad . \tag{3.98}$$

We now invoke the model interaction in Eqn. 3.71. Recall that the solution to the gap equation is of the form $\Delta_{\boldsymbol{k}}(T) = \Delta(T)\,\Theta\big(\hbar\omega_{\rm D} - |\xi_{\boldsymbol{k}}|\big)$. We then have

$$\begin{aligned} \frac{\Omega_{\rm s} - \Omega_{\rm n}}{V} &= \frac{\Delta^2}{v} - \tfrac{1}{2}\, g(\varepsilon_{\rm F})\, \Delta^2 \left\{ \frac{\hbar\omega_{\rm D}}{\Delta} \sqrt{1 + \left(\frac{\hbar\omega_{\rm D}}{\Delta}\right)^2} - \left(\frac{\hbar\omega_{\rm D}}{\Delta}\right)^2 + \sinh^{-1}\left(\frac{\hbar\omega_{\rm D}}{\Delta}\right)\right\} \\ &\qquad - 2\, g(\varepsilon_{\rm F})\, k_{\rm B}T\, \Delta \int\limits_0^\infty \! ds\, \ln\left(1 + e^{-\sqrt{1+s^2}\,\Delta/k_{\rm B}T}\right) + \tfrac{1}{6}\,\pi^2\, g(\varepsilon_{\rm F})\, (k_{\rm B}T)^2 \quad . \end{aligned} \tag{3.99}$$

We will now expand this result in the vicinity of $T = 0$ and $T = T_{\rm c}$. In the weak coupling limit, throughout this entire region we have $\Delta \ll \hbar\omega_{\rm D}$, so we proceed to expand in the small ratio, writing

$$\begin{aligned} \frac{\Omega_{\rm s} - \Omega_{\rm n}}{V} &= -\tfrac{1}{4}\, g(\varepsilon_{\rm F})\, \Delta^2 \left\{ 1 + 2\ln\left(\frac{\Delta_0}{\Delta}\right) - \left(\frac{\Delta}{2\hbar\omega_{\rm D}}\right)^2 + \mathcal{O}(\Delta^4)\right\} \\ &\qquad - 2\, g(\varepsilon_{\rm F})\, k_{\rm B}T\Delta \int\limits_0^\infty \! ds\, \ln\left(1 + e^{-\sqrt{1+s^2}\,\Delta/k_{\rm B}T}\right) + \tfrac{1}{6}\,\pi^2\, g(\varepsilon_{\rm F})\, (k_{\rm B}T)^2 \quad . \end{aligned} \tag{3.100}$$

where $\Delta_0 = \Delta(0) = \pi e^{-C}\, k_B T_c$. The asymptotic analysis of this expression in the limits $T \to 0^+$ and $T \to T_c^-$ is discussed in the appendix §3.14.

$T \to 0^+$

In the limit $T \to 0$, we find

$$\frac{\Omega_s - \Omega_n}{V} = -\tfrac{1}{4}\, g(\varepsilon_F)\, \Delta^2 \left\{ 1 + 2\ln\!\left(\frac{\Delta_0}{\Delta}\right) + \mathcal{O}(\Delta^2) \right\} - g(\varepsilon_F)\sqrt{2\pi (k_B T)^3 \Delta}\; e^{-\Delta/k_B T} + \tfrac{1}{6}\,\pi^2\, g(\varepsilon_F)\,(k_B T)^2 \quad . \tag{3.101}$$

Differentiating the above expression with respect to Δ, we obtain a self-consistent equation for the gap $\Delta(T)$ at low temperatures:

$$\ln\!\left(\frac{\Delta}{\Delta_0}\right) = -\sqrt{\frac{2\pi k_B T}{\Delta}}\; e^{-\Delta/k_B T}\left(1 - \frac{k_B T}{2\Delta} + \ldots\right) \tag{3.102}$$

Thus,

$$\Delta(T) = \Delta_0 - \sqrt{2\pi \Delta_0 k_B T}\; e^{-\Delta_0/k_B T} + \ldots \quad . \tag{3.103}$$

Substituting this expression into Eqn. 3.101, we find

$$\frac{\Omega_s - \Omega_n}{V} = -\tfrac{1}{4}\, g(\varepsilon_F)\, \Delta_0^2 - g(\varepsilon_F)\sqrt{2\pi \Delta_0\, (k_B T)^3}\; e^{-\Delta_0/k_B T} + \tfrac{1}{6}\,\pi^2\, g(\varepsilon_F)\,(k_B T)^2 \quad . \tag{3.104}$$

Equating this with the condensation energy density, $-H_c^2(T)/8\pi$, and invoking our previous result, $\Delta_0 = \pi e^{-C}\, k_B T_c$, we find

$$H_c(T) = H_c(0)\left\{ 1 - \overbrace{\tfrac{1}{3}\, e^{2C}}^{\approx 1.057} \left(\frac{T}{T_c}\right)^2 + \ldots \right\} \quad , \tag{3.105}$$

where $H_c(0) = \sqrt{2\pi\, g(\varepsilon_F)}\; \Delta_0$.

$T \to T_c^-$

In this limit, one finds

$$\frac{\Omega_s - \Omega_n}{V} = \tfrac{1}{2}\, g(\varepsilon_F)\, \ln\!\left(\frac{T}{T_c}\right)\Delta^2 + \frac{7\,\zeta(3)}{32\pi^2}\,\frac{g(\varepsilon_F)}{(k_B T)^2}\,\Delta^4 + \mathcal{O}(\Delta^6) \quad . \tag{3.106}$$

This is of the standard Landau form,

$$\frac{\Omega_s - \Omega_n}{V} = \tilde{a}(T)\,\Delta^2 + \tfrac{1}{2}\,\tilde{b}(T)\,\Delta^4 \quad , \tag{3.107}$$

with coefficients

$$\tilde{a}(T) = \tfrac{1}{2}\, g(\varepsilon_F)\left(\frac{T}{T_c} - 1\right) \qquad , \qquad \tilde{b} = \frac{7\,\zeta(3)}{16\pi^2}\,\frac{g(\varepsilon_F)}{(k_B T_c)^2} \quad , \tag{3.108}$$

working here to lowest nontrivial order in $T - T_c$. The head capacity jump, according to Eqn. 1.44, is

$$c_s(T_c^-) - c_n(T_c^+) = \frac{T_c\big[\tilde{a}'(T_c)\big]^2}{\tilde{b}(T_c)} = \frac{4\pi^2}{7\,\zeta(3)}\, g(\varepsilon_F)\, k_B^2 T_c \quad . \tag{3.109}$$

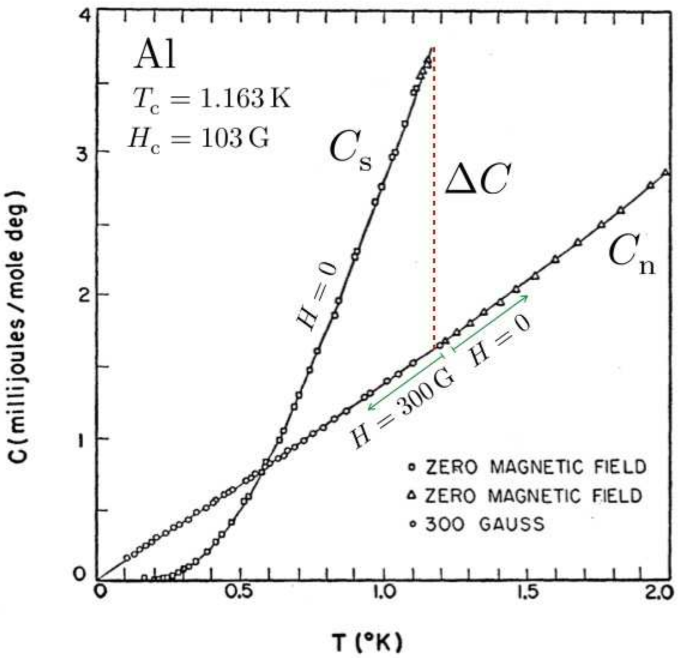

Figure 3.6: Heat capacity in aluminum at low temperatures, from N. K. Phillips, *Phys. Rev. 114*, **3** (1959). The zero field superconducting transition occurs at $T_c = 1.163$ K. Comparison with normal state C below T_c is made possible by imposing a magnetic field $H > H_c$. This destroys the superconducting state, but has little effect on the metal. A jump ΔC is observed at T_c, quantitatively in agreement BCS theory.

The normal state heat capacity at $T = T_c$ is $c_n = \frac{1}{3}\pi^2 g(\varepsilon_F)\, k_B^2 T_c$, hence

$$\frac{c_s(T_c^-) - c_n(T_c^+)}{c_n(T_c^+)} = \frac{12}{7\,\zeta(3)} = 1.43 \quad . \tag{3.110}$$

This universal ratio is closely reproduced in many experiments; see, for example, Fig. 3.6.

The order parameter is given by

$$\Delta^2(T) = -\frac{\tilde{a}(T)}{\tilde{b}(T)} = \frac{8\pi^2 (k_B T_c)^2}{7\,\zeta(3)} \left(1 - \frac{T}{T_c}\right) = \frac{8\, e^{2C}}{7\,\zeta(3)} \left(1 - \frac{T}{T_c}\right) \Delta^2(0) \quad , \tag{3.111}$$

where we have used $\Delta(0) = \pi\, e^{-C}\, k_B T_c$. Thus,

$$\frac{\Delta(T)}{\Delta(0)} = \overbrace{\left(\frac{8\, e^{2C}}{7\,\zeta(3)}\right)^{1/2}}^{\approx 1.734} \left(1 - \frac{T}{T_c}\right)^{1/2} \quad . \tag{3.112}$$

The thermodynamic critical field just below T_c is obtained by equating the energies $-\tilde{a}^2/2\tilde{b}$ and $-H_c^2/8\pi$. Therefore

$$\frac{H_c(T)}{H_c(0)} = \left(\frac{8\, e^{2C}}{7\,\zeta(3)}\right)^{1/2} \left(1 - \frac{T}{T_c}\right) \simeq 1.734 \left(1 - \frac{T}{T_c}\right) \quad . \tag{3.113}$$

3.10 Paramagnetic Susceptibility

Suppose we add a weak magnetic field, the effect of which is described by the perturbation Hamiltonian

$$\hat{H}_1 = -\mu_{\rm B} H \sum_{\boldsymbol{k},\sigma} \sigma\, c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}\sigma} = -\mu_{\rm B} H \sum_{\boldsymbol{k},\sigma} \sigma\, \gamma^\dagger_{\boldsymbol{k}\sigma}\, \gamma_{\boldsymbol{k}\sigma} \quad . \tag{3.114}$$

The shift in the Landau free energy due to the field is then $\Delta\Omega_{\rm s}(T,V,\mu,H) = \Omega_{\rm s}(T,V,\mu,H) - \Omega_{\rm s}(T,V,\mu,0)$. We have

$$\begin{aligned} \Delta\Omega_{\rm s}(T,V,\mu,H) &= -k_{\rm B}T \sum_{\boldsymbol{k},\sigma} \ln\!\left(\frac{1+e^{-\beta(E_{\boldsymbol{k}}+\sigma\mu_{\rm B}H)}}{1+e^{-\beta E_{\boldsymbol{k}}}}\right) \\ &= -\beta\,(\mu_{\rm B}H)^2 \sum_{\boldsymbol{k}} \frac{e^{\beta E_{\boldsymbol{k}}}}{\big(e^{\beta E_{\boldsymbol{k}}}+1\big)^2} + \mathcal{O}(H^4) \quad . \end{aligned} \tag{3.115}$$

The magnetic susceptibility is then

$$\chi_{\rm s} = -\frac{1}{V}\,\frac{\partial^2\Delta\Omega_{\rm s}}{\partial H^2} = g(\varepsilon_{\rm F})\,\mu_{\rm B}^2\,\mathcal{Y}(T) \quad , \tag{3.116}$$

where

$$\mathcal{Y}(T) = 2\int\limits_0^\infty\! d\xi \left(-\frac{\partial f}{\partial E}\right) = \tfrac{1}{2}\beta \int\limits_0^\infty\! d\xi\ {\rm sech}^2\Big(\tfrac{1}{2}\beta\sqrt{\xi^2+\Delta^2}\Big) \tag{3.117}$$

is the *Yoshida function*. Note that $\mathcal{Y}(T_{\rm c}) = \int\limits_0^\infty\! du\ {\rm sech}^2 u = 1$, and $\mathcal{Y}(T\to 0) \simeq (2\pi\beta\Delta)^{1/2}\exp(-\beta\Delta)$, which is exponentially suppressed. Since $\chi_{\rm n} = g(\varepsilon_{\rm F})\,\mu_{\rm B}^2$ is the normal state Pauli susceptibility, we have that the ratio of superconducting to normal state susceptibilities is $\chi_{\rm s}(T)/\chi_{\rm n}(T) = \mathcal{Y}(T)$. This vanishes exponentially as $T\to 0$ because it takes a finite energy Δ to create a Bogoliubov quasiparticle out of the spin singlet BCS ground state.

In metals, the nuclear spins experience a shift in their resonance energy in the presence of an external magnetic field, due to their coupling to conduction electrons via the hyperfine interaction. This is called the *Knight shift*, after Walter Knight, who first discovered this phenomenon at Berkeley in 1949. The magnetic field polarizes the metallic conduction electrons, which in turn impose an extra effective field, through the hyperfine coupling, on the nuclei. In superconductors, the electrons remain unpolarized in a weak magnetic field owing to the superconducting gap. Thus there is no Knight shift.

As we have seen from the Ginzburg-Landau theory, when the field is sufficiently strong, superconductivity is destroyed (type I), or there is a mixed phase at intermediate fields where magnetic flux penetrates the superconductor in the form of vortex lines. Our analysis here is valid only for weak fields.

3.11 Finite Momentum Condensate

The BCS reduced Hamiltonian of Eqn. 3.43 involved interactions between $\boldsymbol{q}=0$ Cooper pairs only. In fact, we could just as well have taken

$$\hat{H}_{\rm red} = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}}\, c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{p}} V_{\boldsymbol{k},\boldsymbol{k}'}\, b^\dagger_{\boldsymbol{k},\boldsymbol{p}}\, b_{\boldsymbol{k}',\boldsymbol{p}} \quad . \tag{3.118}$$

where $b^\dagger_{\boldsymbol{k},\boldsymbol{p}} = c^\dagger_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{p}\uparrow}\, c^\dagger_{-\boldsymbol{k}+\frac{1}{2}\boldsymbol{p}\uparrow}$, provided the mean field was $\langle b_{\boldsymbol{k},\boldsymbol{p}}\rangle = \Delta_{\boldsymbol{k}}\,\delta_{\boldsymbol{p},0}$. What happens, though, if we take

$$\big\langle\, b_{\boldsymbol{k},\boldsymbol{p}}\,\big\rangle = \big\langle c_{-\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\downarrow}\, c_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\uparrow}\big\rangle\,\delta_{\boldsymbol{p},\boldsymbol{q}} \quad , \tag{3.119}$$

corresponding to a finite momentum condensate? We then obtain

$$\hat{K}_{\rm BCS} = \sum_{\boldsymbol{k}} \begin{pmatrix} c^\dagger_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\uparrow} & c_{-\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\downarrow} \end{pmatrix} \begin{pmatrix} \omega_{\boldsymbol{k},\boldsymbol{q}} + \nu_{\boldsymbol{k},\boldsymbol{q}} & \Delta_{\boldsymbol{k},\boldsymbol{q}} \\ \Delta^*_{\boldsymbol{k},\boldsymbol{q}} & -\omega_{\boldsymbol{k},\boldsymbol{q}} + \nu_{\boldsymbol{k},\boldsymbol{q}} \end{pmatrix} \begin{pmatrix} c_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\uparrow} \\ c^\dagger_{-\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\downarrow} \end{pmatrix} + \sum_{\boldsymbol{k}} \Big(\xi_{\boldsymbol{k}} - \Delta_{\boldsymbol{k},\boldsymbol{q}} \, \langle b^\dagger_{\boldsymbol{k},\boldsymbol{q}}\rangle\Big) \quad , \tag{3.120}$$

where

$$\omega_{\boldsymbol{k},\boldsymbol{q}} = \tfrac{1}{2}\Big(\xi_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}} + \xi_{-\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}}\Big) \qquad\qquad \xi_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}} = \omega_{\boldsymbol{k},\boldsymbol{q}} + \nu_{\boldsymbol{k},\boldsymbol{q}} \tag{3.121}$$

$$\nu_{\boldsymbol{k},\boldsymbol{q}} = \tfrac{1}{2}\Big(\xi_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}} - \xi_{-\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}}\Big) \qquad\qquad \xi_{-\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}} = \omega_{\boldsymbol{k},\boldsymbol{q}} - \nu_{\boldsymbol{k},\boldsymbol{q}} \quad . \tag{3.122}$$

Note that $\omega_{\boldsymbol{k},\boldsymbol{q}}$ is even under reversal of either $\boldsymbol{k}$ or $\boldsymbol{q}$, while $\nu_{\boldsymbol{k},\boldsymbol{q}}$ is odd under reversal of either $\boldsymbol{k}$ or $\boldsymbol{q}$. That is,

$$\omega_{\boldsymbol{k},\boldsymbol{q}} = \omega_{-\boldsymbol{k},\boldsymbol{q}} = \omega_{\boldsymbol{k},-\boldsymbol{q}} = \omega_{-\boldsymbol{k},-\boldsymbol{q}} \qquad , \qquad \nu_{\boldsymbol{k},\boldsymbol{q}} = -\nu_{-\boldsymbol{k},\boldsymbol{q}} = -\nu_{\boldsymbol{k},-\boldsymbol{q}} = \nu_{-\boldsymbol{k},-\boldsymbol{q}} \quad . \tag{3.123}$$

We now make a Bogoliubov transformation,

$$\begin{aligned} c_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\uparrow} &= \cos\vartheta_{\boldsymbol{k},\boldsymbol{q}}\, \gamma_{\boldsymbol{k},\boldsymbol{q},\uparrow} - \sin\vartheta_{\boldsymbol{k},\boldsymbol{q}}\, e^{i\phi_{\boldsymbol{k},\boldsymbol{q}}}\, \gamma^\dagger_{-\boldsymbol{k},\boldsymbol{q},\downarrow} \\ c^\dagger_{-\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\downarrow} &= \cos\vartheta_{\boldsymbol{k},\boldsymbol{q}}\, \gamma^\dagger_{-\boldsymbol{k},\boldsymbol{q},\downarrow} + \sin\vartheta_{\boldsymbol{k},\boldsymbol{q}}\, e^{i\phi_{\boldsymbol{k},\boldsymbol{q}}}\, \gamma_{\boldsymbol{k},\boldsymbol{q},\uparrow} \end{aligned} \tag{3.124}$$

with

$$\cos\vartheta_{\boldsymbol{k},\boldsymbol{q}} = \sqrt{\frac{E_{\boldsymbol{k},\boldsymbol{q}} + \omega_{\boldsymbol{k},\boldsymbol{q}}}{2E_{\boldsymbol{k},\boldsymbol{q}}}} \qquad\qquad \phi_{\boldsymbol{k},\boldsymbol{q}} = \textsf{arg}(\Delta_{\boldsymbol{k},\boldsymbol{q}}) \tag{3.125}$$

$$\sin\vartheta_{\boldsymbol{k},\boldsymbol{q}} = \sqrt{\frac{E_{\boldsymbol{k},\boldsymbol{q}} - \omega_{\boldsymbol{k},\boldsymbol{q}}}{2E_{\boldsymbol{k},\boldsymbol{q}}}} \qquad\qquad E_{\boldsymbol{k},\boldsymbol{q}} = \sqrt{\omega^2_{\boldsymbol{k},\boldsymbol{q}} + |\Delta_{\boldsymbol{k},\boldsymbol{q}}|^2} \quad . \tag{3.126}$$

We then obtain

$$\hat{K}_{\rm BCS} = \sum_{\boldsymbol{k},\sigma} (E_{\boldsymbol{k},\boldsymbol{q}} + \nu_{\boldsymbol{k},\boldsymbol{q}})\, \gamma^\dagger_{\boldsymbol{k},\boldsymbol{q},\sigma} \gamma_{\boldsymbol{k},\boldsymbol{q},\sigma} + \sum_{\boldsymbol{k}} \Big(\xi_{\boldsymbol{k}} - E_{\boldsymbol{k},\boldsymbol{q}} + \Delta_{\boldsymbol{k},\boldsymbol{q}}\, \langle b^\dagger_{\boldsymbol{k},\boldsymbol{q}}\rangle\Big) \, . \tag{3.127}$$

Next, we compute the quantum statistical averages

$$\begin{aligned} \big\langle c^\dagger_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\uparrow}\, c_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\uparrow}\big\rangle &= \cos^2\!\vartheta_{\boldsymbol{k},\boldsymbol{q}}\, f(E_{\boldsymbol{k},\boldsymbol{q}} + \nu_{\boldsymbol{k},\boldsymbol{q}}) + \sin^2\!\vartheta_{\boldsymbol{k},\boldsymbol{q}} \Big[1 - f(E_{\boldsymbol{k},\boldsymbol{q}} - \nu_{\boldsymbol{k},\boldsymbol{q}})\Big] \\ &= \frac{1}{2}\bigg(1 + \frac{\omega_{\boldsymbol{k},\boldsymbol{q}}}{E_{\boldsymbol{k},\boldsymbol{q}}}\bigg)\, f(E_{\boldsymbol{k},\boldsymbol{q}} + \nu_{\boldsymbol{k},\boldsymbol{q}}) + \frac{1}{2}\bigg(1 - \frac{\omega_{\boldsymbol{k},\boldsymbol{q}}}{E_{\boldsymbol{k},\boldsymbol{q}}}\bigg) \Big[1 - f(E_{\boldsymbol{k},\boldsymbol{q}} - \nu_{\boldsymbol{k},\boldsymbol{q}})\Big] \end{aligned} \tag{3.128}$$

and

$$\begin{aligned} \big\langle c^\dagger_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\uparrow}\, c^\dagger_{-\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\downarrow}\big\rangle &= -\sin\vartheta_{\boldsymbol{k},\boldsymbol{q}} \cos\vartheta_{\boldsymbol{k},\boldsymbol{q}}\, e^{-i\phi_{\boldsymbol{k},\boldsymbol{q}}} \Big[1 - f(E_{\boldsymbol{k},\boldsymbol{q}} + \nu_{\boldsymbol{k},\boldsymbol{q}}) - f(E_{\boldsymbol{k},\boldsymbol{q}} - \nu_{\boldsymbol{k},\boldsymbol{q}})\Big] \\ &= -\frac{\Delta^*_{\boldsymbol{k},\boldsymbol{q}}}{2E_{\boldsymbol{k},\boldsymbol{q}}} \Big[1 - f(E_{\boldsymbol{k},\boldsymbol{q}} + \nu_{\boldsymbol{k},\boldsymbol{q}}) - f(E_{\boldsymbol{k},\boldsymbol{q}} - \nu_{\boldsymbol{k},\boldsymbol{q}})\Big] \quad . \end{aligned} \tag{3.129}$$

3.11.1 Gap equation for finite momentum condensate

We may now solve the $T=0$ gap equation,

$$1 = -\sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\,\frac{1}{2E_{\boldsymbol{k}',\boldsymbol{q}}} = \tfrac{1}{2}\,g(\varepsilon_{\rm F})\,v\int\limits_0^{\hbar\omega_{\rm D}}\frac{d\xi}{\sqrt{(\xi+b_{\boldsymbol{q}})^2+|\Delta_{0,\boldsymbol{q}}|^2}} \quad . \tag{3.130}$$

Here we have assumed the interaction $V_{\boldsymbol{k},\boldsymbol{k}'}$ of Eqn. 3.71, and we take

$$\Delta_{\boldsymbol{k},\boldsymbol{q}} = \Delta_{0,\boldsymbol{q}}\,\Theta\big(\hbar\omega_{\rm D}-|\xi_{\boldsymbol{k}}|\big) \quad . \tag{3.131}$$

We have also written $\omega_{\boldsymbol{k},\boldsymbol{q}} = \xi_{\boldsymbol{k}} + b_{\boldsymbol{q}}$. This form is valid for quadratic $\xi_{\boldsymbol{k}} = \frac{\hbar^2\boldsymbol{k}^2}{2m^*} - \mu$, in which case $b_{\boldsymbol{q}} = \hbar^2\boldsymbol{q}^2/8m^*$. We take $\Delta_{0,\boldsymbol{q}} \in \mathbb{R}$. We may now compute the critical wavevector $q_{\rm c}$ at which the $T=0$ gap collapses:

$$1 = \tfrac{1}{2}\,g(\varepsilon_{\rm F})\,g\,\ln\!\bigg(\frac{\hbar\omega_{\rm D}+b_{q_{\rm c}}}{b_{q_{\rm c}}}\bigg) \qquad \Rightarrow \qquad b_{q_{\rm c}} \simeq \hbar\omega_{\rm D}\,e^{-2/g(\varepsilon_{\rm F})\,v} = \tfrac{1}{2}\,\Delta_0 \quad , \tag{3.132}$$

whence $q_{\rm c} = 2\sqrt{m^*\Delta_0}\,/\hbar$. Here we have assumed weak coupling, *i.e.* $g(\varepsilon_{\rm F})\,v \ll 1$

Next, we compute the gap $\Delta_{0,\boldsymbol{q}}$. We have

$$\sinh^{-1}\!\bigg(\frac{\hbar\omega_{\rm D}+b_{\boldsymbol{q}}}{\Delta_{0,\boldsymbol{q}}}\bigg) = \frac{2}{g(\varepsilon_{\rm F})\,v} + \sinh^{-1}\!\bigg(\frac{b_{\boldsymbol{q}}}{\Delta_{0,\boldsymbol{q}}}\bigg) \quad . \tag{3.133}$$

Assuming $b_{\boldsymbol{q}} \ll \Delta_{0,\boldsymbol{q}}$, we obtain

$$\Delta_{0,\boldsymbol{q}} = \Delta_0 - b_{\boldsymbol{q}} = \Delta_0 - \frac{\hbar^2\boldsymbol{q}^2}{8m^*} \quad . \tag{3.134}$$

3.11.2 Supercurrent

We assume a quadratic dispersion $\varepsilon_{\boldsymbol{k}} = \hbar^2\boldsymbol{k}^2/2m^*$, so $\boldsymbol{v}_{\boldsymbol{k}} = \hbar\boldsymbol{k}/m^*$. The current density is then given by

$$\begin{aligned}\boldsymbol{j} &= \frac{2e\hbar}{m^*V}\sum_{\boldsymbol{k}}\,(\boldsymbol{k}+\tfrac{1}{2}\boldsymbol{q})\big\langle\, c^\dagger_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\uparrow}\,c_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\uparrow}\big\rangle \\ &= \frac{ne\hbar}{2m^*}\,\boldsymbol{q} + \frac{2e\hbar}{m^*V}\sum_{\boldsymbol{k}}\boldsymbol{k}\,\big\langle\, c^\dagger_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\uparrow}\,c_{\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}\uparrow}\big\rangle \quad ,\end{aligned} \tag{3.135}$$

where $n=N/V$ is the total electron number density. Appealing to Eqn. 3.128, we have

$$\begin{aligned}\boldsymbol{j} = \frac{e\hbar}{m^*V}\sum_{\boldsymbol{k}}\boldsymbol{k}\,\bigg\{&\Big[1+f(E_{\boldsymbol{k},\boldsymbol{q}}+\nu_{\boldsymbol{k},\boldsymbol{q}})-f(E_{\boldsymbol{k},\boldsymbol{q}}-\nu_{\boldsymbol{k},\boldsymbol{q}})\Big] \\ &+\frac{\omega_{\boldsymbol{k},\boldsymbol{q}}}{E_{\boldsymbol{k},\boldsymbol{q}}}\Big[f(E_{\boldsymbol{k},\boldsymbol{q}}+\nu_{\boldsymbol{k},\boldsymbol{q}})+f(E_{\boldsymbol{k},\boldsymbol{q}}-\nu_{\boldsymbol{k},\boldsymbol{q}})-1\Big]\bigg\} + \frac{ne\hbar}{2m^*}\,\boldsymbol{q}\end{aligned} \tag{3.136}$$

We now write $f(E_{\boldsymbol{k},\boldsymbol{q}}\pm\nu_{\boldsymbol{k},\boldsymbol{q}}) = f(E_{\boldsymbol{k},\boldsymbol{q}}) \pm f'(E_{\boldsymbol{k},\boldsymbol{q}})\,\nu_{\boldsymbol{k},\boldsymbol{q}} + \ldots$, obtaining

$$\boldsymbol{j} = \frac{e\hbar}{m^*V}\sum_{\boldsymbol{k}}\boldsymbol{k}\,\Big[1+2\,\nu_{\boldsymbol{k},\boldsymbol{q}}\,f'(E_{\boldsymbol{k},\boldsymbol{q}})\Big] + \frac{ne\hbar}{2m^*}\,\boldsymbol{q} \quad . \tag{3.137}$$

For the ballistic dispersion, $\nu_{\boldsymbol{k},\boldsymbol{q}} = \hbar^2 \boldsymbol{k}\cdot\boldsymbol{q}/2m^*$, so

$$\begin{aligned}\boldsymbol{j} - \frac{ne\hbar}{2m^*}\,\boldsymbol{q} &= \frac{e\hbar}{m^* V}\,\frac{\hbar^2}{m^*}\sum_{\boldsymbol{k}}(\boldsymbol{q}\cdot\boldsymbol{k})\,\boldsymbol{k}\,f'(E_{\boldsymbol{k},\boldsymbol{q}}) \\ &= \frac{e\hbar^3}{3{m^*}^2 V}\boldsymbol{q}\sum_{\boldsymbol{k}}\boldsymbol{k}^2\,f'(E_{\boldsymbol{k},\boldsymbol{q}}) \simeq \frac{ne\hbar}{m^*}\,\boldsymbol{q}\int_0^\infty d\xi\,\frac{\partial f}{\partial E}\quad,\end{aligned} \tag{3.138}$$

where we have set $\boldsymbol{k}^2 = k_F^2$ inside the sum, since it is only appreciable in the vicinity of $k = k_F$, and we have invoked $g(\varepsilon_F) = m^* k_F/\pi^2\hbar^2$ and $n = k_F^3/3\pi^2$. Thus,

$$\boldsymbol{j} = \frac{ne\hbar}{2m^*}\left(1 + 2\int_0^\infty d\xi\,\frac{\partial f}{\partial E}\right)\boldsymbol{q} \equiv \frac{n_s(T)\,e\hbar\boldsymbol{q}}{2m^*}\quad. \tag{3.139}$$

This defines the superfluid density,

$$n_s(T) = n\left(1 + 2\int_0^\infty d\xi\,\frac{\partial f}{\partial E}\right)\quad. \tag{3.140}$$

Note that the second term in round brackets on the RHS is always negative. Thus, at $T = 0$, we have $n_s = n$, but at $T = T_c$, where the gap vanishes, we find $n_s(T_c) = 0$, since $E = |\xi|$ and $f(0) = \frac{1}{2}$. We may write $n_s(T) = n - n_n(T)$, where $n_n(T) = n\,\mathcal{Y}(T)$ is the normal fluid density.

Ginzburg-Landau theory

We may now expand the free energy near $T = T_c$ at finite condensate $\boldsymbol{q}$. We will only quote the result. One finds

$$\frac{\Omega_s - \Omega_n}{V} = \tilde{a}(T)\,|\Delta|^2 + \tfrac{1}{2}\,\tilde{b}(T)\,|\Delta|^4 + \frac{n\,\tilde{b}(T)}{g(\varepsilon_F)}\,\frac{\hbar^2\boldsymbol{q}^2}{2m^*}\,|\Delta|^2\quad, \tag{3.141}$$

where the Landau coefficients $\tilde{a}(T)$ and $\tilde{b}(T)$ are given in Eqn. 3.108. Identifying the last term as $\tilde{K}\,|\boldsymbol{\nabla}\Delta|^2$, where $\tilde{K}$ is the stiffness, we have

$$\tilde{K} = \frac{\hbar^2}{2m^*}\,\frac{n\,\tilde{b}(T)}{g(\varepsilon_F)}\quad. \tag{3.142}$$

3.12 Effect of repulsive interactions

Let's modify our model in Eqns. 3.71 and 3.72 and write

$$V_{\boldsymbol{k},\boldsymbol{k}'} = \begin{cases} (v_C - v_p)/V & \text{if } |\xi_{\boldsymbol{k}}| < \hbar\omega_D \text{ and } |\xi_{\boldsymbol{k}'}| < \hbar\omega_D \\ v_C/V & \text{otherwise} \end{cases} \tag{3.143}$$

and

$$\Delta_{\boldsymbol{k}} = \begin{cases} \Delta_0 & \text{if } |\xi_{\boldsymbol{k}}| < \hbar\omega_D \\ \Delta_1 & \text{otherwise}\quad. \end{cases} \tag{3.144}$$

Here $-v_p < 0$ is the attractive interaction mediated by phonons, while $v_C > 0$ is the Coulomb repulsion. We presume $v_p > v_C$ so that there is a net attraction at low energies, although below we will show this assumption is overly pessimistic. We take $\Delta_{0,1}$ both to be real.

At $T=0$, the gap equation then gives

$$\begin{aligned}\Delta_0 &= \tfrac{1}{2}\, g(\varepsilon_{\rm F})\,(v_{\rm p}-v_{\rm C})\int\limits_0^{\hbar\omega_{\rm D}}\! d\xi\, \frac{\Delta_0}{\sqrt{\xi^2+\Delta_0^2}} - \tfrac{1}{2}\, g(\varepsilon_{\rm F})\, v_{\rm C}\int\limits_{\hbar\omega_{\rm D}}^{B}\! d\xi\, \frac{\Delta_1}{\sqrt{\xi^2+\Delta_1^2}} \\ \Delta_1 &= -\tfrac{1}{2}\, g(\varepsilon_{\rm F})\, v_{\rm C}\int\limits_0^{\hbar\omega_{\rm D}}\! d\xi\, \frac{\Delta_0}{\sqrt{\xi^2+\Delta_0^2}} - \tfrac{1}{2}\, g(\varepsilon_{\rm F})\, v_{\rm C}\int\limits_{\hbar\omega_{\rm D}}^{B}\! d\xi\, \frac{\Delta_1}{\sqrt{\xi^2+\Delta_1^2}} \quad ,\end{aligned} \tag{3.145}$$

where $\hbar\omega_{\rm D}$ is once again the Debye energy, and B is the full electronic bandwidth. Performing the integrals, and assuming $\Delta_{0,1} \ll \hbar\omega_{\rm D} \ll B$, we obtain

$$\begin{aligned}\Delta_0 &= \tfrac{1}{2}\, g(\varepsilon_{\rm F})\,(v_{\rm p}-v_{\rm C})\,\Delta_0\, \ln\!\bigg(\frac{2\hbar\omega_{\rm D}}{\Delta_0}\bigg) - \tfrac{1}{2}\, g(\varepsilon_{\rm F})\, v_{\rm C}\,\Delta_1 \ln\!\bigg(\frac{B}{\hbar\omega_{\rm D}}\bigg) \\ \Delta_1 &= -\tfrac{1}{2}\, g(\varepsilon_{\rm F})\, v_{\rm C}\,\Delta_0\, \ln\!\bigg(\frac{2\hbar\omega_{\rm D}}{\Delta_0}\bigg) - \tfrac{1}{2}\, g(\varepsilon_{\rm F})\, v_{\rm C}\,\Delta_1 \ln\!\bigg(\frac{B}{\hbar\omega_{\rm D}}\bigg) \quad .\end{aligned} \tag{3.146}$$

The second of these equations gives

$$\Delta_1 = -\frac{\frac{1}{2} g(\varepsilon_{\rm F})\, v_{\rm C} \ln(2\hbar\omega_{\rm D}/\Delta_0)}{1+\frac{1}{2} g(\varepsilon_{\rm F})\, v_{\rm C}\, \ln(B/\hbar\omega_{\rm D})}\,\Delta_0 \quad . \tag{3.147}$$

Inserting this into the first equation then results in

$$\frac{2}{g(\varepsilon_{\rm F})\, v_{\rm p}} = \ln\!\bigg(\frac{2\hbar\omega_{\rm D}}{\Delta_0}\bigg)\cdot\bigg\{1-\frac{v_{\rm C}}{v_{\rm p}}\cdot\frac{1}{1+\frac{1}{2}\, g(\varepsilon_{\rm F})\, \ln(B/\hbar\omega_{\rm D})}\bigg\} \quad . \tag{3.148}$$

This has a solution only if the attractive potential $v_{\rm p}$ is greater than the repulsive factor $v_{\rm C}\Big/\big[1+\frac{1}{2}\, g(\varepsilon_{\rm F})\, v_{\rm C} \ln(B/\hbar\omega_{\rm D})\big]$. Note that it is a renormalized and reduced value of the bare repulsion $v_{\rm C}$ which enters here. Thus, it is possible to have

$$v_{\rm C} > v_{\rm p} > \frac{v_{\rm C}}{1+\frac{1}{2}\, g(\varepsilon_{\rm F})\, v_{\rm C} \ln(B/\hbar\omega_{\rm D})} \quad , \tag{3.149}$$

so that $v_{\rm C} > v_{\rm p}$ and the potential is *always* repulsive, yet still the system is superconducting!

Working at finite temperature, we must include factors of $\tanh\!\Big(\frac{1}{2}\beta\sqrt{\xi^2+\Delta_{0,1}^2}\,\Big)$ inside the appropriate integrands in Eqn. 3.145, with $\beta = 1/k_{\rm B}T$. The equation for $T_{\rm c}$ is then obtained by examining the limit $\Delta_{0,1} \to 0$, with the ratio $r \equiv \Delta_1/\Delta_0$ finite. We then have

$$\begin{aligned}\frac{2}{g(\varepsilon_{\rm F})} &= (v_{\rm p}-v_{\rm C})\int\limits_0^{\widetilde\Omega}\! ds\, s^{-1}\, \tanh(s) - r\, v_{\rm C}\int\limits_{\widetilde\Omega}^{\widetilde B}\! ds\, s^{-1}\, \tanh(s) \\ \frac{2}{g(\varepsilon_{\rm F})} &= -r^{-1}\, v_{\rm C}\int\limits_0^{\widetilde\Omega}\! ds\, s^{-1}\, \tanh(s) - v_{\rm C}\int\limits_{\widetilde\Omega}^{\widetilde B}\! ds\, s^{-1}\, \tanh(s) \quad ,\end{aligned} \tag{3.150}$$

where $\widetilde\Omega \equiv \hbar\omega_{\rm D}/2k_{\rm B}T_{\rm c}$ and $\widetilde B \equiv B/2k_{\rm B}T_{\rm c}$. We now use

$$\int\limits_0^{\Lambda}\! ds\, s^{-1}\, \tanh(s) = \ln\Lambda + \ln\big(\overbrace{4e^{\rm C}/\pi}^{\approx 2.268}\big) + \mathcal{O}\big(e^{-\Lambda}\big) \tag{3.151}$$

to obtain

$$\frac{2}{g(\varepsilon_{\rm F})\, v_{\rm p}} = \ln\!\left(\frac{1.134\,\hbar\omega_{\rm D}}{k_{\rm B}T_{\rm c}}\right) \cdot \left\{ 1 - \frac{v_{\rm C}}{v_{\rm p}} \cdot \frac{1}{1 + \frac{1}{2}\, g(\varepsilon_{\rm F})\, \ln(B/\hbar\omega_{\rm D})} \right\} \quad . \tag{3.152}$$

Comparing with Eqn. 3.148, we see that once again we have $2\Delta_0(T=0) = 3.52\, k_{\rm B}T_{\rm c}$. Note, however, that

$$k_{\rm B}T_{\rm c} = 1.134\,\hbar\omega_{\rm D}\, \exp\!\left(-\frac{2}{g(\varepsilon_{\rm F})\, v_{\rm eff}}\right) \quad , \tag{3.153}$$

where

$$v_{\rm eff} = v_{\rm p} - \frac{v_{\rm C}}{1 + \frac{1}{2}\, g(\varepsilon_{\rm F}) \ln(B/\hbar\omega_{\rm D})} \quad . \tag{3.154}$$

It is customary to define

$$\lambda \equiv \tfrac{1}{2}\, g(\varepsilon_{\rm F})\, v_{\rm p} \qquad , \qquad \mu \equiv \tfrac{1}{2}\, g(\varepsilon_{\rm F})\, v_{\rm C} \qquad , \qquad \mu^* \equiv \frac{\mu}{1 + \mu \ln(B/\hbar\omega_{\rm D})} \quad , \tag{3.155}$$

so that

$$k_{\rm B}T_{\rm c} = 1.134\,\hbar\omega_{\rm D}\, e^{-1/(\lambda-\mu^*)} \quad , \quad \Delta_0 = 2\hbar\omega_{\rm D}\, e^{-1/(\lambda-\mu^*)} \quad , \quad \Delta_1 = -\frac{\mu^*\Delta_0}{\lambda - \mu^*} \quad . \tag{3.156}$$

Since μ^* depends on $\omega_{\rm D}$, the isotope effect is modified:

$$\delta \ln T_{\rm c} = \delta \ln \omega_{\rm D} \cdot \left\{ 1 - \frac{\mu^2}{1 + \mu \ln(B/\hbar\omega_{\rm D})} \right\} \quad . \tag{3.157}$$

3.13 Appendix I : General Variational Formulation

We consider a more general grand canonical Hamiltonian of the form

$$\hat{K} = \sum_{\boldsymbol{k}\sigma} (\varepsilon_{\boldsymbol{k}} - \mu)\, c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}\sigma} + \frac{1}{2V} \sum_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}} \sum_{\sigma,\sigma'} \hat{u}_{\sigma\sigma'}(\boldsymbol{k},\boldsymbol{p},\boldsymbol{q})\, c^\dagger_{\boldsymbol{k}+\boldsymbol{q}\,\sigma}\, c^\dagger_{\boldsymbol{p}-\boldsymbol{q}\,\sigma'}\, c_{\boldsymbol{p}\,\sigma'}\, c_{\boldsymbol{k}\,\sigma} \quad . \tag{3.158}$$

In order that the Hamiltonian be Hermitian, we may require, without loss of generality,

$$\hat{u}^*_{\sigma\sigma'}(\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}) = \hat{u}_{\sigma\sigma'}(\boldsymbol{k}+\boldsymbol{q}\,,\, \boldsymbol{p}-\boldsymbol{q}\,,\, -\boldsymbol{q}) \quad . \tag{3.159}$$

In addition, spin rotation invariance says that $\hat{u}_{\uparrow\uparrow}(\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}) = \hat{u}_{\downarrow\downarrow}(\boldsymbol{k},\boldsymbol{p},\boldsymbol{q})$ and $\hat{u}_{\uparrow\downarrow}(\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}) = \hat{u}_{\downarrow\uparrow}(\boldsymbol{k},\boldsymbol{p},\boldsymbol{q})$. We now take the thermal expectation of $\hat{K}$ using a density matrix derived from the BCS Hamiltonian,

$$\hat{K}_{\rm BCS} = \sum_{\boldsymbol{k}} \begin{pmatrix} c^\dagger_{\boldsymbol{k}\uparrow} & c_{-\boldsymbol{k}\downarrow} \end{pmatrix} \begin{pmatrix} \xi_{\boldsymbol{k}} & \Delta_{\boldsymbol{k}} \\ \Delta^*_{\boldsymbol{k}} & -\xi_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} c_{\boldsymbol{k}\uparrow} \\ c^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix} + K_0 \quad . \tag{3.160}$$

The energy shift K_0 will not be important in our subsequent analysis. From the BCS Hamiltonian,

$$\begin{aligned} \langle c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}'\sigma'} \rangle &= n_{\boldsymbol{k}}\, \delta_{\boldsymbol{k},\boldsymbol{k}'}\, \delta_{\sigma\sigma'} \\ \langle c^\dagger_{\boldsymbol{k}\sigma}\, c^\dagger_{\boldsymbol{k}'\sigma'} \rangle &= \Psi^*_{\boldsymbol{k}}\, \delta_{\boldsymbol{k}',-\boldsymbol{k}}\, \varepsilon_{\sigma\sigma'} \quad , \end{aligned} \tag{3.161}$$

where $\varepsilon_{\sigma\sigma'} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. We don't yet need the detailed forms of $n_{\boldsymbol{k}}$ and $\Psi_{\boldsymbol{k}}$ either. Using Wick's theorem, we find

$$\langle \hat{K} \rangle = \sum_{\boldsymbol{k}} 2(\varepsilon_{\boldsymbol{k}} - \mu)\, n_{\boldsymbol{k}} + \sum_{\boldsymbol{k},\boldsymbol{k}'} W_{\boldsymbol{k},\boldsymbol{k}'}\, n_{\boldsymbol{k}}\, n_{\boldsymbol{k}'} - \sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\, \Psi^*_{\boldsymbol{k}}\, \Psi_{\boldsymbol{k}'} \quad , \tag{3.162}$$

where

$$\begin{aligned} W_{\boldsymbol{k},\boldsymbol{k}'} &= \frac{1}{V}\Big\{\hat{u}_{\uparrow\uparrow}(\boldsymbol{k},\boldsymbol{k}',0) + \hat{u}_{\uparrow\downarrow}(\boldsymbol{k},\boldsymbol{k}',0) - \hat{u}_{\uparrow\uparrow}(\boldsymbol{k},\boldsymbol{k}',\boldsymbol{k}'-\boldsymbol{k})\Big\} \\ V_{\boldsymbol{k},\boldsymbol{k}'} &= -\frac{1}{V}\,\hat{u}_{\uparrow\downarrow}(\boldsymbol{k}',-\boldsymbol{k}',\boldsymbol{k}-\boldsymbol{k}') \quad . \end{aligned} \tag{3.163}$$

We may assume $W_{\boldsymbol{k},\boldsymbol{k}'}$ is real and symmetric, and $V_{\boldsymbol{k},\boldsymbol{k}'}$ is Hermitian.

Now let's vary $\langle\hat{K}\rangle$ by changing the distribution. We have

$$\delta\langle\hat{K}\rangle = 2\sum_{\boldsymbol{k}}\bigg(\varepsilon_{\boldsymbol{k}} - \mu + \sum_{\boldsymbol{k}'} W_{\boldsymbol{k},\boldsymbol{k}'}\,n_{\boldsymbol{k}'}\bigg)\delta n_{\boldsymbol{k}} + \sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\Big(\Psi^*_{\boldsymbol{k}}\,\delta\Psi_{\boldsymbol{k}'} + \delta\Psi^*_{\boldsymbol{k}}\,\Psi_{\boldsymbol{k}'}\Big) \quad . \tag{3.164}$$

On the other hand,

$$\delta\langle\hat{K}_{\rm BCS}\rangle = 2\sum_{\boldsymbol{k}}\Big(\xi_{\boldsymbol{k}}\,\delta n_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}}\,\delta\Psi^*_{\boldsymbol{k}} + \Delta^*_{\boldsymbol{k}}\,\delta\Psi_{\boldsymbol{k}}\Big) \quad . \tag{3.165}$$

Setting these variations to be equal, we obtain

$$\begin{aligned} \xi_{\boldsymbol{k}} &= \varepsilon_{\boldsymbol{k}} - \mu + \sum_{\boldsymbol{k}'} W_{\boldsymbol{k},\boldsymbol{k}'}\,n_{\boldsymbol{k}'} \\ &= \varepsilon_{\boldsymbol{k}} - \mu + \sum_{\boldsymbol{k}'} W_{\boldsymbol{k},\boldsymbol{k}'}\left[\frac{1}{2} - \frac{\xi_{\boldsymbol{k}'}}{2E_{\boldsymbol{k}'}}\tanh\!\big(\tfrac{1}{2}\beta E_{\boldsymbol{k}'}\big)\right] \end{aligned} \tag{3.166}$$

and

$$\begin{aligned} \Delta_{\boldsymbol{k}} &= \sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\,\Psi_{\boldsymbol{k}'} \\ &= -\sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'}\,\frac{\Delta_{\boldsymbol{k}'}}{2E_{\boldsymbol{k}'}}\,\tanh\!\big(\tfrac{1}{2}\beta E_{\boldsymbol{k}'}\big) \quad . \end{aligned} \tag{3.167}$$

These are to be regarded as self-consistent equations for $\xi_{\boldsymbol{k}}$ and $\Delta_{\boldsymbol{k}}$.

3.14 Appendix II : Superconducting Free Energy

We start with the Landau free energy difference from Eqn. 3.100,

$$\begin{aligned} \frac{\Omega_{\rm s} - \Omega_{\rm n}}{V} = -\tfrac{1}{4}\,g(\varepsilon_{\rm F})\,\Delta^2\left\{1 + 2\ln\!\left(\frac{\Delta_0}{\Delta}\right) - \left(\frac{\Delta}{2\hbar\omega_{\rm D}}\right)^{\!2} + \mathcal{O}(\Delta^4)\right\} \\ - 2\,g(\varepsilon_{\rm F})\,\Delta^2\,I(\delta) + \tfrac{1}{6}\,\pi^2\,g(\varepsilon_{\rm F})\,(k_{\rm B}T)^2 \quad , \end{aligned} \tag{3.168}$$

where

$$I(\delta) = \frac{1}{\delta}\int\limits_0^\infty\! ds\;\ln\Big(1 + e^{-\delta\sqrt{1+s^2}}\Big) \ . \tag{3.169}$$

We now proceed to examine the integral $I(\delta)$ in the limits $\delta \to \infty$ (*i.e.* $T \to 0^+$) and $\delta \to 0^+$ (*i.e.* $T \to T_{\rm c}^-$, where $\Delta \to 0$).

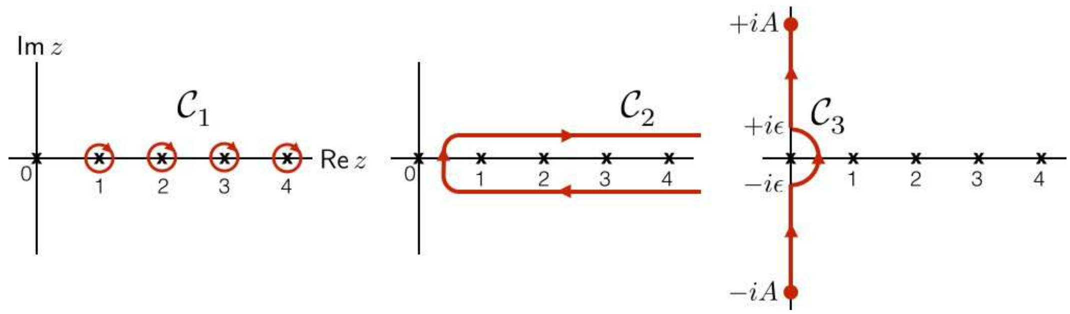

Figure 3.7: Contours for complex integration for calculating $I(\delta)$ as described in the text.

When $\delta \to \infty$, we may safely expand the logarithm in a Taylor series, and

$$I(\delta) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n\delta}\, K_1(n\delta) \quad , \tag{3.170}$$

where $K_1(\delta)$ is the modified Bessel function, also called the MacDonald function. Asymptotically, we have[11]

$$K_1(z) = \left(\frac{\pi}{2z}\right)^{1/2} e^{-z} \cdot \Big\{1 + \mathcal{O}\big(z^{-1}\big)\Big\} \quad . \tag{3.171}$$

We may then retain only the $n=1$ term to leading nontrivial order. This immediately yields the expression in Eqn. 3.101.

The limit $\delta \to 0$ is much more subtle. We begin by integrating once by parts, to obtain

$$I(\delta) = \int_1^{\infty} \! dt\, \frac{\sqrt{t^2-1}}{e^{\delta t}+1} \quad . \tag{3.172}$$

We now appeal to the tender mercies of `Mathematica`. Alas, this avenue is to no avail, for the program gags when asked to expand $I(\delta)$ for small δ. We need something better than `Mathematica`. We need Professor Michael Fogler.

Fogler says[12]: start by writing Eqn. 3.170 in the form

$$I(\delta) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n\delta}\, K_1(n\delta) = +\int_{\mathcal{C}_1} \! \frac{dz}{2\pi i}\, \frac{\pi}{\sin \pi z}\, \frac{K_1(\delta z)}{\delta z} \quad . \tag{3.173}$$

The initial contour $\mathcal{C}_1$ consists of a disjoint set of small loops circling the points $z = \pi n$, where $n \in \mathbb{Z}_+$. Note that the sense of integration is clockwise rather than counterclockwise. This accords with an overall minus sign in the RHS above, because the residues contain a factor of $\cos(\pi n) = (-1)^n$ rather than the desired $(-1)^{n-1}$. Following Fig. 3.7, the contour may now be deformed into $\mathcal{C}_2$, and then into $\mathcal{C}_3$. Contour $\mathcal{C}_3$ lies along the imaginary z axis, aside from a small semicircle of radius $\epsilon \to 0$ avoiding the origin, and terminates at $z = \pm iA$. We will later take $A \to \infty$, but for the moment we consider $1 \ll A \ll \delta^{-1}$. So long as $A \gg 1$, the denominator $\sin \pi z = i \sinh \pi u$, with $z = iu$, will be exponentially large at $u = \pm A$, so we are safe in making this initial truncation. We demand $A \ll \delta^{-1}$, however, which means $|\delta z| \ll 1$ everywhere along $\mathcal{C}_3$. *This allows us to expand $K_1(\delta z)$ for small values of*

[11]See, *e.g.*, the *NIST Handbook of Mathematical Functions*, §10.25.
[12]M. Fogler, private communications.

the argument. One has

$$\frac{K_1(w)}{w} = \frac{1}{w^2} + \tfrac{1}{2}\ln w\,\Big(1 + \tfrac{1}{8}w^2 + \tfrac{1}{192}w^4 + \ldots\Big) + \big(\mathrm{C} - \ln 2 - \tfrac{1}{2}\big) + \tfrac{1}{16}\big(C - \ln 2 - \tfrac{5}{4}\big)w^2 + \tfrac{1}{384}\big(C - \ln 2 - \tfrac{5}{3}\big)w^4 + \ldots \quad , \tag{3.174}$$

where $\mathrm{C} \simeq 0.577216$ is the Euler-Mascheroni constant. The integral is then given by

$$I(\delta) = \int\limits_{\epsilon}^{A}\frac{du}{2\pi i}\,\frac{\pi}{\sinh\pi u}\left[\frac{K_1(i\delta u)}{i\delta u} - \frac{K_1(-i\delta u)}{-i\delta u}\right] + \int\limits_{-\pi/2}^{\pi/2}\frac{d\theta}{2\pi}\,\frac{\pi\epsilon\,e^{i\theta}}{\sin\big(\pi\epsilon\,e^{i\theta}\big)}\,\frac{K_1\big(\delta\epsilon\,e^{i\theta}\big)}{\delta\epsilon\,e^{i\theta}} \quad . \tag{3.175}$$

Using the above expression for $K_1(w)/w$, we have

$$\frac{K_1(i\delta u)}{i\delta u} - \frac{K_1(-i\delta u)}{-i\delta u} = \frac{i\pi}{2}\Big(1 - \tfrac{1}{8}\delta^2 u^2 + \tfrac{1}{192}\delta^4 u^4 + \ldots\Big) \quad . \tag{3.176}$$

At this point, we may take $A \to \infty$. The integral along the two straight parts of the $\mathcal{C}_3$ contour is then

$$\begin{aligned} I_1(\delta) &= \tfrac{1}{4}\pi\int\limits_{\epsilon}^{\infty}\frac{du}{\sinh\pi u}\Big(1 - \tfrac{1}{8}\delta^2 u^2 + \tfrac{1}{192}\delta^4 u^4 + \ldots\Big) \\ &= -\tfrac{1}{4}\ln\tanh\big(\tfrac{1}{2}\pi\epsilon\big) - \frac{7\,\zeta(3)}{64\,\pi^2}\,\delta^2 + \frac{31\,\zeta(5)}{512\,\pi^4}\,\delta^4 + \mathcal{O}\big(\delta^6\big) \quad . \end{aligned} \tag{3.177}$$

The integral around the semicircle is

$$\begin{aligned} I_2(\delta) &= \int\limits_{-\pi/2}^{\pi/2}\frac{d\theta}{2\pi}\,\frac{1}{1 - \frac{1}{6}\pi^2\epsilon^2\,e^{2i\theta}}\left\{\frac{1}{\delta^2\epsilon^2\,e^{2i\theta}} + \tfrac{1}{2}\ln\big(\delta\epsilon\,e^{i\theta}\big) + \tfrac{1}{2}(\mathrm{C} - \ln 2 - \tfrac{1}{2}) + \ldots\right\} \\ &= \int\limits_{-\pi/2}^{\pi/2}\frac{d\theta}{2\pi}\Big(1 + \tfrac{1}{6}\pi^2\epsilon^2\,e^{2i\theta} + \ldots\Big)\left\{\frac{e^{-2i\theta}}{\delta^2\epsilon^2} + \tfrac{1}{2}\ln(\delta\epsilon) + \tfrac{i}{2}\theta + \tfrac{1}{2}(\mathrm{C} - \ln 2 - \tfrac{1}{2}) + \ldots\right\} \\ &= \frac{\pi^2}{12\,\delta^2} + \tfrac{1}{4}\ln\delta + \tfrac{1}{4}\ln\epsilon + \tfrac{1}{4}(\mathrm{C} - \ln 2 - \tfrac{1}{2}) + \mathcal{O}\big(\epsilon^2\big) \quad . \end{aligned} \tag{3.178}$$

We now add the results to obtain $I(\delta) = I_1(\delta) + I_2(\delta)$. Note that there are divergent pieces, each proportional to $\ln\epsilon$, which cancel as a result of this addition. The final result is

$$I(\delta) = \frac{\pi^2}{12\,\delta^2} + \tfrac{1}{4}\ln\!\left(\frac{2\delta}{\pi}\right) + \tfrac{1}{4}(\mathrm{C} - \ln 2 - \tfrac{1}{2}) - \frac{7\,\zeta(3)}{64\,\pi^2}\,\delta^2 + \frac{31\,\zeta(5)}{512\,\pi^4}\,\delta^4 + \mathcal{O}\big(\delta^6\big) \quad . \tag{3.179}$$

Inserting this result in Eqn. 3.168 above, we thereby recover Eqn. 3.106.

Chapter 4

Applications of BCS Theory

4.1 Quantum XY Model for Granular Superconductors

Consider a set of superconducting grains, each of which is large enough to be modeled by BCS theory, but small enough that the self-capacitance (*i.e.* Coulomb interaction) cannot be neglected. The Coulomb energy of the $j^{\rm th}$ grain is written as

$$\hat{U}_j = \frac{2e^2}{C_j}\big(\hat{M}_j - \bar{M}_j\big)^2 \quad , \tag{4.1}$$

where $\hat{M}_j$ is the operator which counts the number of Cooper pairs on grain j, and $\bar{M}_j$ is the mean number of pairs in equilibrium, which is given by half the total ionic charge on the grain. The capacitance C_j is a geometrical quantity which is proportional to the radius of the grain, assuming the grain is roughly spherical. For very large grains, the Coulomb interaction is negligible. It should be stressed that here we are accounting for only the long wavelength part of the Coulomb interaction, which is proportional to $4\pi\big|\delta\hat{\rho}(q_{\rm min})\big|^2/q_{\rm min}^2$, where $q_{\rm min} \sim 1/R_j$ is the inverse grain size. The remaining part of the Coulomb interaction is included in the BCS part of the Hamiltonian for each grain.

We assume that $\hat{K}_{{\rm BCS}\,,\,j}$ describes a simple s-wave superconductor with gap $\Delta_j = |\Delta_j|\, e^{i\phi_j}$. We saw in chapter 3 how ϕ_j is conjugate to the Cooper pair number operator $\hat{M}_j$, with

$$\hat{M}_j = \frac{1}{i}\,\frac{\partial}{\partial\phi_j} \quad . \tag{4.2}$$

The operator which adds one Cooper pair to grain j is therefore $e^{i\phi_j}$, because

$$\hat{M}_j\, e^{i\phi_j} = e^{i\phi_j}\,(\hat{M}_j + 1) \quad . \tag{4.3}$$

Thus, accounting for the hopping of Cooper pairs between neighboring grains, the effective Hamiltonian for a granular superconductor should be given by

$$\hat{H}_{\rm gr} = -\tfrac{1}{2}\sum_{i,j} J_{ij}\big(e^{i\phi_i}\, e^{-i\phi_j} + e^{-i\phi_i}\, e^{i\phi_j}\big) + \sum_i \frac{2e^2}{C_j}\big(\hat{M}_j - \bar{M}_j\big)^2 \quad , \tag{4.4}$$

where J_{ij} is the hopping matrix element for the Cooper pairs, here assumed to be real.

Before we calculate J_{ij}, note that we can eliminate the constants $\bar{M}_i$ from the Hamiltonian via the unitary transformation $\hat{H}_{\rm gr} \to \hat{H}'_{\rm gr} = V^\dagger \hat{H}_{\rm gr} V$, where $V = \prod_j e^{i\,[\bar{M}_j]\,\phi_j}$, where $[\bar{M}_j]$ is defined as the integer nearest to $\bar{M}_j$. The difference, $\delta\bar{M}_j = \bar{M}_j - [\bar{M}_j]$, cannot be removed. This transformation commutes with the hopping part of $\hat{H}_{\rm gr}$, so, after dropping the prime on $\hat{H}'_{\rm gr}$, we are left with

$$\hat{H}_{\rm gr} = \sum_j \frac{2e^2}{C_j}\left(\frac{1}{i}\frac{\partial}{\partial\phi_j} - \delta\bar{M}_j\right)^2 - \sum_{i,j} J_{ij}\cos(\phi_i - \phi_j) \quad . \tag{4.5}$$

In the presence of an external magnetic field,

$$\hat{H}_{\rm gr} = \sum_j \frac{2e^2}{C_j}\left(\frac{1}{i}\frac{\partial}{\partial\phi_j} - \delta\bar{M}_j\right)^2 - \sum_{i,j} J_{ij}\cos(\phi_i - \phi_j - \mathcal{A}_{ij}) \quad , \tag{4.6}$$

where

$$\mathcal{A}_{ij} = \frac{2e}{\hbar c}\int\limits_{\boldsymbol{R}_i}^{\boldsymbol{R}_j} d\boldsymbol{l}\cdot\boldsymbol{A} \tag{4.7}$$

is a lattice vector potential, with $\boldsymbol{R}_i$ the position of grain i.

4.1.1 No disorder

In a perfect lattice of identical grains, with $J_{ij} = J$ for nearest neighbors, $\delta\bar{M}_j = 0$ and $2e^2/C_j = U$ for all j, we have

$$\hat{H}_{\rm gr} = -U\sum_i \frac{\partial^2}{\partial\phi_i^2} - 2J\sum_{\langle ij\rangle}\cos(\phi_i - \phi_j) \quad , \tag{4.8}$$

where $\langle ij\rangle$ indicates a nearest neighbor pair. This model, known as the *quantum rotor model*, features competing interactions. The potential energy, proportional to U, favors each grain being in a state $\psi(\phi_i) = 1$, corresponding to $M = 0$, which minimizes the Coulomb interaction. However, it does a poor job with the hopping, since $\big\langle\cos(\phi_i - \phi_j)\big\rangle = 0$ in this state. The kinetic (hopping) energy, proportional to J, favors that all grains be coherent with $\phi_i = \alpha$ for all i, where α is a constant. This state has significant local charge fluctuations which cost Coulomb energy – an infinite amount, in fact! Some sort of compromise must be reached. One important issue is whether the ground state exhibits a finite order parameter $\langle e^{i\phi_i}\rangle$.

The model has been simulated numerically using a cluster Monte Carlo algorithm[1], and is known to exhibit a quantum phase transition between superfluid and insulating states at a critical value of J/U. The superfluid state is that in which $\langle e^{i\phi_i}\rangle \neq 0$.

4.1.2 Self-consistent harmonic approximation

The self-consistent harmonic approximation (SCHA) is a variational approach in which we approximate the ground state wavefunction as a Gaussian function of the many phase variables $\{\phi_i\}$. Specifically, we write

$$\Psi[\phi] = \mathcal{C}\,\exp\big(-\tfrac{1}{4}\,A_{ij}\,\phi_i\,\phi_j\big) \quad , \tag{4.9}$$

[1] See F. Alet and E. Sørensen, *Phys. Rev. E* **67**, 015701(R) (2003) and references therein.

where $\mathcal{C}$ is a normalization constant. The matrix elements A_{ij} is assumed to be a function of the separation $\boldsymbol{R}_i - \boldsymbol{R}_j$, where $\boldsymbol{R}_i$ is the position of lattice site i. We define the *generating function*

$$Z[\mathcal{J}] = \int\!D\phi\,\big|\Psi[\phi]\big|^2\,e^{-\mathcal{J}_i\,\phi_i} = Z[0]\,\exp\big(\tfrac{1}{2}\,\mathcal{J}_i\,A^{-1}_{ij}\,\mathcal{J}_j\big) \quad . \tag{4.10}$$

Here $\mathcal{J}_i$ is a *source field* with respect to which we differentiate in order to compute correlation functions, as we shall see. Here $D\phi = \prod_i d\phi_i$, and all the phase variables are integrated over the $\phi_i \in (-\infty, +\infty)$. Right away we see something is fishy, since in the original model there is a periodicity under $\phi_i \to \phi_i + 2\pi$ at each site. The individual basis functions are $\psi_n(\phi) = e^{in\phi}$, corresponding to $M = n$ Cooper pairs. Taking linear combinations of these basis states preserves the 2π periodicity, but this is not present in our variational wavefunction. Nevertheless, we can extract some useful physics using the SCHA.

The first order of business is to compute the correlator

$$\langle\,\Psi\,|\,\phi_i\,\phi_j\,|\,\Psi\,\rangle = \frac{1}{Z[0]}\,\frac{\partial^2 Z[\mathcal{J}]}{\partial\mathcal{J}_i\,\partial\mathcal{J}_j}\bigg|_{\mathcal{J}=0} = A^{-1}_{ij} \quad . \tag{4.11}$$

This means that

$$\langle\,\Psi\,|\,e^{i(\phi_i-\phi_j)}\,|\,\Psi\,\rangle = e^{-\langle(\phi_i-\phi_j)^2\rangle/2} = e^{-(A^{-1}_{ii}-A^{-1}_{ij})} \quad . \tag{4.12}$$

Here we have used that $\langle e^Q\rangle = e^{\langle Q^2\rangle/2}$ where Q is a sum of Gaussian-distributed variables. Next, we need

$$\begin{aligned}\langle\,\Psi\,|\,\frac{\partial^2}{\partial\phi_i^2}\,|\,\Psi\,\rangle &= -\langle\,\Psi\,|\,\frac{\partial}{\partial\phi_i}\,\tfrac{1}{2}\,A_{ik}\,\phi_k\,|\,\Psi\,\rangle \\ &= -\tfrac{1}{2}\,A_{ii} + \tfrac{1}{4}\,A_{ik}\,A_{li}\,\langle\,\Psi\,|\,\phi_k\,\phi_l\,|\,\Psi\,\rangle = -\tfrac{1}{4}\,A_{ii} \quad .\end{aligned} \tag{4.13}$$

Thus, the variational energy per site is

$$\begin{aligned}\frac{1}{N}\,\langle\,\Psi\,|\,\hat{H}_{\text{gr}}\,|\,\Psi\,\rangle &= \tfrac{1}{4}\,U A_{ii} - zJ\,e^{-(A^{-1}_{ii}-A^{-1}_{ij})} \\ &= \tfrac{1}{4}U\!\int\!\frac{d^dk}{(2\pi)^d}\,\hat{A}(\boldsymbol{k}) - zJ\,\exp\left\{-\!\int\!\frac{d^dk}{(2\pi)^d}\,\frac{1-\gamma_{\boldsymbol{k}}}{\hat{A}(\boldsymbol{k})}\right\} \quad ,\end{aligned} \tag{4.14}$$

where z is the lattice coordination number ($N_{\text{links}} = \frac{1}{2}zN$),

$$\gamma_{\boldsymbol{k}} = \frac{1}{z}\sum_{\boldsymbol{\delta}} e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}} \tag{4.15}$$

is a sum over the z nearest neighbor vectors $\boldsymbol{\delta}$, and $\hat{A}(\boldsymbol{k})$ is the Fourier transform of A_{ij},

$$A_{ij} = \int\!\frac{d^dk}{(2\pi)^d}\,\hat{A}(\boldsymbol{k})\,e^{i(\boldsymbol{R}_i-\boldsymbol{R}_j)} \quad . \tag{4.16}$$

Note that $\hat{A}^*(\boldsymbol{k}) = \hat{A}(-\boldsymbol{k})$ since $\hat{A}(\boldsymbol{k})$ is the (discrete) Fourier transform of a real quantity.

We are now in a position to vary the energy in Eqn. 4.14 with respect to the variational parameters $\{\hat{A}(\boldsymbol{k})\}$. Taking the functional derivative with respect to $\hat{A}(\boldsymbol{k})$, we find

$$(2\pi)^d\,\frac{\delta(E_{\text{gr}}/N)}{\delta\hat{A}(\boldsymbol{k})} = \tfrac{1}{4}\,U - \frac{1-\gamma_{\boldsymbol{k}}}{\hat{A}^2(\boldsymbol{k})}\cdot zJ\,e^{-W} \quad , \tag{4.17}$$

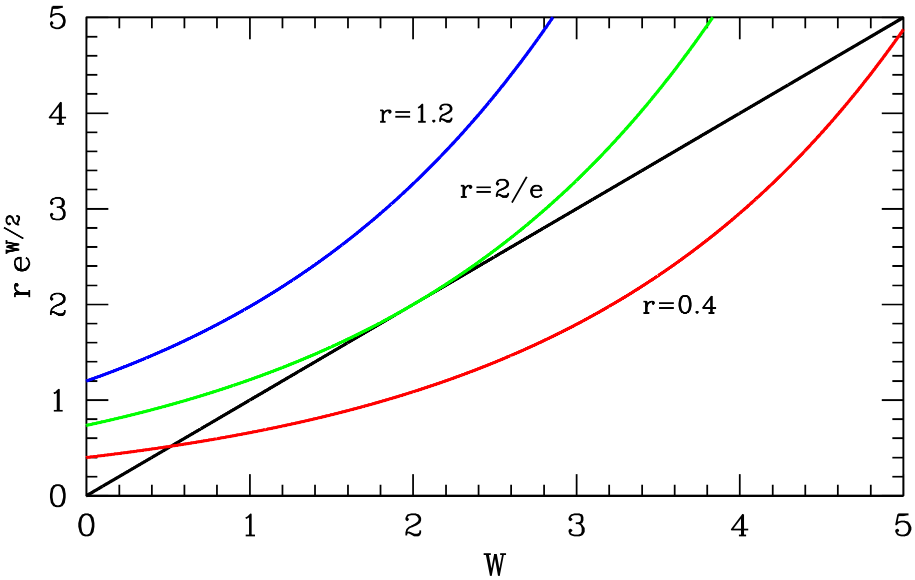

Figure 4.1: Graphical solution to the SCHA equation $W = r\,\exp\left(\frac{1}{2}W\right)$ for three representative values of r. The critical value is $r_c = 2/e = 0.73576$.

where

$$W = \int \frac{d^dk}{(2\pi)^d}\,\frac{1-\gamma_{\boldsymbol{k}}}{\hat{A}(\boldsymbol{k})} \quad . \tag{4.18}$$

We now have

$$\hat{A}(\boldsymbol{k}) = 2\left(\frac{zJ}{U}\right)^{1/2} e^{-W/2}\sqrt{1-\gamma_{\boldsymbol{k}}} \quad . \tag{4.19}$$

Inserting this into our expression for W, we obtain the self-consistent equation

$$W = r\,e^{W/2} \quad ; \quad r = C_d\left(\frac{U}{4zJ}\right)^{1/2} \quad , \quad C_d \equiv \int \frac{d^dk}{(2\pi)^d}\,\sqrt{1-\gamma_{\boldsymbol{k}}} \quad . \tag{4.20}$$

One finds $C_{d=1} = 0.900316$ for the linear chain, $C_{d=2} = 0.958091$ for the square lattice, and $C_{d=3} = 0.974735$ on the cubic lattice.

The graphical solution to $W = r\,\exp\left(\frac{1}{2}W\right)$ is shown in Fig. 4.1. One sees that for $r > r_c = 2/e \simeq 0.73576$, there is no solution. In this case, the variational wavefunction should be taken to be $\Psi = 1$, which is a product of $\psi_{n=0}$ states on each grain, corresponding to fixed charge $M_i = 0$ and maximally fluctuating phase. In this case we must restrict each $\phi_i \in [0, 2\pi]$. When $r < r_c$, though, there are two solutions for W. The larger of the two is spurious, and the smaller one is the physical one. As J/U increases, *i.e.* r decreases, the size of $\hat{A}(\boldsymbol{k})$ increases, which means that A^{-1}_{ij} decreases in magnitude. This means that the correlation in Eqn. 4.12 is growing, and the phase variables are localized. The SCHA predicts a spurious first order phase transition; the real superfluid-insulator transition is continuous (second-order)[2].

[2]That the SCHA gives a spurious first order transition was recognized by E. Pytte, *Phys. Rev. Lett.* **28**, 895 (1971).

4.1.3 Calculation of the Cooper pair hopping amplitude

Finally, let us compute J_{ij}. We do so by working to second order in perturbation theory in the *electron* hopping Hamiltonian

$$\hat{H}_{\text{hop}} = -\frac{1}{(V_i\, V_j)^{1/2}} \sum_{\langle ij\rangle} \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} \Big(t_{ij}(\boldsymbol{k},\boldsymbol{k}')\, c^\dagger_{i,\boldsymbol{k},\sigma}\, c_{j,\boldsymbol{k}',\sigma} + t^*_{ij}(\boldsymbol{k},\boldsymbol{k}')\, c^\dagger_{j,\boldsymbol{k}',\sigma}\, c_{i,\boldsymbol{k},\sigma}\Big) \quad . \tag{4.21}$$

Here $t_{ij}(\boldsymbol{k},\boldsymbol{k}')$ is the amplitude for an electron of wavevector $\boldsymbol{k}'$ in grain j to hop to a state of wavevector $\boldsymbol{k}$ in grain i. To simplify matters we will assume the grains are identical in all respects other than their overall phases. We'll write the fermion destruction operators on grain i as $c_{\boldsymbol{k}\sigma}$ and those on grain j as $\tilde{c}_{\boldsymbol{k}\sigma}$. We furthermore assume $t_{ij}(\boldsymbol{k},\boldsymbol{k}') = t$ is real and independent of $\boldsymbol{k}$ and $\boldsymbol{k}'$. Only spin polarization, and not momentum, is preserved in the hopping process. Then

$$\hat{H}_{\text{hop}} = -\frac{t}{V} \sum_{\boldsymbol{k},\boldsymbol{k}'} \big(c^\dagger_{\boldsymbol{k}\sigma}\, \tilde{c}_{\boldsymbol{k}'\sigma} + \tilde{c}^\dagger_{\boldsymbol{k}'\sigma}\, c_{\boldsymbol{k}\sigma}\big) \quad . \tag{4.22}$$

Each grain is described by a BCS model. The respective Bogoliubov transformations are

$$\begin{aligned} c_{\boldsymbol{k}\sigma} &= \cos\vartheta_{\boldsymbol{k}}\, \gamma_{\boldsymbol{k}\sigma} - \sigma \sin\vartheta_{\boldsymbol{k}}\, e^{i\phi}\, \gamma^\dagger_{-\boldsymbol{k}\,-\sigma} \\ \tilde{c}_{\boldsymbol{k}\sigma} &= \cos\tilde{\vartheta}_{\boldsymbol{k}}\, \tilde{\gamma}_{\boldsymbol{k}\sigma} - \sigma \sin\tilde{\vartheta}_{\boldsymbol{k}}\, e^{i\tilde{\phi}}\, \tilde{\gamma}^\dagger_{-\boldsymbol{k}\,-\sigma} \quad . \end{aligned} \tag{4.23}$$

Second order perturbation says that the ground state energy $\mathcal{E}$ is

$$\mathcal{E} = \mathcal{E}_0 - \sum_n \frac{\big|\langle\, n\,|\, \hat{H}_{\text{hop}}\,|\,\text{G}\,\rangle\big|^2}{\mathcal{E}_n - \mathcal{E}_0} \quad , \tag{4.24}$$

where $|\,\text{G}\,\rangle = |\,\text{G}_i\,\rangle \otimes |\,\text{G}_j\,\rangle$ is a product of BCS ground states on the two grains. Clearly the only intermediate states $|\,n\,\rangle$ which can couple to $|\,\text{G}\,\rangle$ through a single application of $\hat{H}_{\text{hop}}$ are states of the form

$$|\,\boldsymbol{k},\boldsymbol{k}',\sigma\,\rangle = \gamma^\dagger_{\boldsymbol{k}\sigma}\, \tilde{\gamma}^\dagger_{-\boldsymbol{k}'\,-\sigma}\,|\,\text{G}\,\rangle \quad , \tag{4.25}$$

and for this state

$$\langle\, \boldsymbol{k},\boldsymbol{k}',\sigma\,|\, \hat{H}_{\text{hop}}\,|\,\text{G}\,\rangle = -\sigma\Big(\cos\vartheta_{\boldsymbol{k}} \sin\tilde{\vartheta}_{\boldsymbol{k}'}\, e^{i\tilde{\phi}} + \sin\vartheta_{\boldsymbol{k}} \cos\tilde{\vartheta}_{\boldsymbol{k}'}\, e^{i\phi}\Big) \tag{4.26}$$

The energy of this intermediate state is

$$E_{\boldsymbol{k},\boldsymbol{k}',\sigma} = E_{\boldsymbol{k}} + E_{\boldsymbol{k}'} + \frac{e^2}{C} \quad , \tag{4.27}$$

where we have included the contribution from the charging energy of each grain. Then we find[3]

$$\mathcal{E}^{(2)} = \mathcal{E}_0' - J\cos(\phi - \tilde{\phi}\,) \quad , \tag{4.28}$$

where

$$J = \frac{|t|^2}{V^2} \sum_{\boldsymbol{k},\boldsymbol{k}'} \frac{\Delta_{\boldsymbol{k}}}{E_{\boldsymbol{k}}} \cdot \frac{\Delta_{\boldsymbol{k}'}}{E_{\boldsymbol{k}'}} \cdot \frac{1}{E_{\boldsymbol{k}} + E_{\boldsymbol{k}'} + (e^2/C)} \quad . \tag{4.29}$$

For a general set of dissimilar grains,

$$J_{ij} = \frac{|t_{ij}|^2}{V_i V_j} \sum_{\boldsymbol{k},\boldsymbol{k}'} \frac{\Delta_{i,\boldsymbol{k}}}{E_{i,\boldsymbol{k}}} \cdot \frac{\Delta_{j,\boldsymbol{k}'}}{E_{j,\boldsymbol{k}'}} \cdot \frac{1}{E_{i,\boldsymbol{k}} + E_{j,\boldsymbol{k}'} + (e^2/2C_{ij})} \quad , \tag{4.30}$$

where $C_{ij}^{-1} = C_i^{-1} + C_j^{-1}$.

[3] There is no factor of two arising from a spin sum since we are summing over all $\boldsymbol{k}$ and $\boldsymbol{k}'$, and therefore summing over spin would overcount the intermediate states $|n\rangle$ by a factor of two.

4.2 Tunneling

We follow the very clear discussion in §9.3 of G. Mahan's *Many Particle Physics*. Consider two bulk samples, which we label left (L) and right (R). The Hamiltonian is taken to be

$$\hat{H} = \hat{H}_{\rm L} + \hat{H}_{\rm R} + \hat{H}_{\rm T} \quad , \tag{4.31}$$

where $\hat{H}_{\rm L,R}$ are the bulk Hamiltonians, and

$$\hat{H}_{\rm T} = -\sum_{i,j,\sigma} \big(T_{ij}\, c^\dagger_{{\rm L}\,i\,\sigma}\, c_{{\rm R}\,j\,\sigma} + T^*_{ij}\, c^\dagger_{{\rm R}\,j\,\sigma}\, c_{{\rm L}\,i\,\sigma} \big) \quad . \tag{4.32}$$

The indices i and j label single particle electron states (*not* Bogoliubov quasiparticles) in the two banks. As we shall discuss below, we can take them to correspond to Bloch wavevectors in a particular energy band. In a nonequilibrium setting we work in the grand canonical ensemble, with

$$\hat{K} = \hat{H}_{\rm L} - \mu_{\rm L}\, \hat{N}_{\rm L} + \hat{H}_{\rm R} - \mu_{\rm R}\, \hat{N}_{\rm R} + \hat{H}_{\rm T} \quad . \tag{4.33}$$

The difference between the chemical potentials is $\mu_{\rm R} - \mu_{\rm L} = eV$, where V is the voltage bias. The current flowing from left to right is

$$I(t) = e\, \Big\langle \frac{d\hat{N}_{\rm L}}{dt} \Big\rangle \quad . \tag{4.34}$$

Note that if $N_{\rm L}$ is increasing in time, this means an electron number current flows from right to left, and hence an electrical current (of fictitious positive charges) flows from left to right. We use perturbation theory in $\hat{H}_{\rm T}$ to compute $I(t)$. Note that expectations such as $\langle\, \Psi_{\rm L}\,|\, c_{{\rm L}i}\,|\, \Psi_{\rm L}\,\rangle$ vanish, while $\langle\, \Psi_{\rm L}\,|\, c_{{\rm L}i}\, c_{{\rm L}j}\,|\, \Psi_{\rm L}\,\rangle$ may not if $|\, \Psi_{\rm L}\,\rangle$ is a BCS state.

A few words on the labels i and j: We will assume the left and right samples can be described as perfect crystals, so i and j will represent crystal momentum eigenstates. The only exception to this characterization will be that we assume their respective surfaces are sufficiently rough to destroy conservation of momentum in the plane of the surface. Momentum perpendicular to the surface is also not conserved, since the presence of the surface breaks translation invariance in this direction. The matrix element T_{ij} will be dominated by the behavior of the respective single particle electron wavefunctions in the vicinity of their respective surfaces. As there is no reason for the respective wavefunctions to be coherent, they will in general disagree in sign in random fashion. We then expect the overlap to be proportional to $\sqrt{A}$, on the basis of the Central Limit Theorem. Adding in the plane wave normalization factors, we therefore approximate

$$T_{ij} = T_{\boldsymbol{q},\boldsymbol{k}} \approx \bigg(\frac{A}{V_{\rm L} V_{\rm R}} \bigg)^{1/2} t\big(\xi_{{\rm L}\,\boldsymbol{q}}\,,\, \xi_{{\rm R}\,\boldsymbol{k}}\big) \quad , \tag{4.35}$$

where $\boldsymbol{q}$ and $\boldsymbol{k}$ are the wavevectors of the Bloch electrons on the left and right banks, respectively. Note that we presume spin is preserved in the tunneling process, although wavevector is not.

4.2.1 Perturbation theory

We begin by noting

$$\begin{aligned} \frac{d\hat{N}_{\rm L}}{dt} &= \frac{i}{\hbar}\big[\hat{H}, \hat{N}_{\rm L}\big] = \frac{i}{\hbar}\big[\hat{H}_{\rm T}\,,\, \hat{N}_{\rm L}\big] \\ &= -\frac{i}{\hbar} \sum_{i,j,\sigma} \big(T_{ij}\, c^\dagger_{{\rm L}\,i\,\sigma}\, c_{{\rm R}\,j\,\sigma} - T^*_{ij}\, c^\dagger_{{\rm R}\,j\,\sigma}\, c_{{\rm L}\,i\,\sigma} \big) \quad . \end{aligned} \tag{4.36}$$

First order perturbation theory then gives

$$| \Psi(t) \rangle = e^{-i\hat{H}_0(t-t_0)/\hbar} \, | \Psi(t_0) \rangle - \frac{i}{\hbar} \, e^{-i\hat{H}_0 t/\hbar} \int\limits_{t_0}^{t} dt_1 \; \hat{H}_{\rm T}(t_1) \, e^{i\hat{H}_0 t_0/\hbar} \, | \Psi(t_0) \rangle + \mathcal{O}\big(\hat{H}_{\rm T}^2\big) \quad , \tag{4.37}$$

where $\hat{H}_0 = \hat{H}_{\rm L} + \hat{H}_{\rm R}$ and

$$\hat{H}_{\rm T}(t) = e^{i\hat{H}_0 t/\hbar} \, \hat{H}_{\rm T} \, e^{-i\hat{H}_0 t/\hbar} \tag{4.38}$$

is the perturbation (hopping) Hamiltonian in the interaction representation. To lowest order in $\hat{H}_{\rm T}$, then,

$$\langle \, \Psi(t) \, | \, \hat{I} \, | \, \Psi(t) \, \rangle = -\frac{i}{\hbar} \int\limits_{t_0}^{t} dt_1 \; \langle \, \tilde{\Psi}(t_0) \, | \, \big[\hat{I}(t) \, , \, \hat{H}_{\rm T}(t_1) \big] \, | \, \tilde{\Psi}(t_0) \, \rangle \quad , \tag{4.39}$$

where $| \, \tilde{\Psi}(t_0) \, \rangle = e^{i\hat{H}_0 t_0/\hbar} \, | \, \Psi(t_0) \, \rangle$. Setting $t_0 = -\infty$, and averaging over a thermal ensemble of initial states, we have

$$I(t) = -\frac{i}{\hbar} \int\limits_{-\infty}^{t} dt' \, \big\langle \big[\hat{I}(t) \, , \, \hat{H}_{\rm T}(t') \big] \big\rangle \quad , \tag{4.40}$$

where $\hat{I}(t) = e\dot{\hat{N}}_{\rm L}(t) = (+e) \, e^{i\hat{H}_0 t/\hbar} \, \dot{\hat{N}}_{\rm L} \, e^{-i\hat{H}_0 t/\hbar}$ is the current flowing from *right* to *left*. Note that it is the electron charge $-e$ that enters here and not the Cooper pair charge, since $\hat{H}_{\rm T}$ describes electron hopping.

There remains a *caveat* which we have already mentioned. The chemical potentials $\mu_{\rm L}$ and $\mu_{\rm R}$ differ according to

$$\mu_{\rm R} - \mu_{\rm L} = eV \quad , \tag{4.41}$$

where V is the bias voltage. If $V > 0$, then $\mu_{\rm R} > \mu_{\rm L}$, which means an electron current flows from right to left, and an electrical current (*i.e.* the direction of positive charge flow) from left to right. We must work in an ensemble described by $\hat{K}_0$, where

$$\hat{K}_0 = \hat{H}_{\rm L} - \mu_{\rm L} \hat{N}_{\rm L} + \hat{H}_{\rm R} - \mu_{\rm R} \hat{N}_{\rm R} \quad . \tag{4.42}$$

We now separate $\hat{H}_{\rm T}$ into its component processes, writing $\hat{H}_{\rm T} = \hat{H}^+_{\rm T} + \hat{H}^-_{\rm T}$, with

$$\hat{H}^+_{\rm T} = -\sum_{i,j,\sigma} T_{ij} \, c^\dagger_{{\rm L}\, i\, \sigma} \, c_{{\rm R}\, j\, \sigma} \qquad , \qquad \hat{H}^-_{\rm T} = -\sum_{i,j,\sigma} T^*_{ij} \, c^\dagger_{{\rm R}\, j\, \sigma} \, c_{{\rm L}\, i\, \sigma} \quad . \tag{4.43}$$

Thus, $\hat{H}^+_{\rm T}$ describes hops from R to L, while $\hat{H}^-_{\rm T}$ describes hops from L to R. Note that $\hat{H}^-_{\rm T} = (\hat{H}^+_{\rm T})^\dagger$. Therefore $\hat{H}_{\rm T}(t) = \hat{H}^+_{\rm T}(t) + \hat{H}^-_{\rm T}(t)$, where[4]

$$\begin{aligned} \hat{H}^\pm_{\rm T}(t) &= e^{i(\hat{K}_0 + \mu_{\rm L} \hat{N}_{\rm L} + \mu_{\rm R} \hat{N}_{\rm R})t/\hbar} \, \hat{H}^\pm_{\rm T} \, e^{-i(\hat{K}_0 + \mu_{\rm L} \hat{N}_{\rm L} + \mu_{\rm R} \hat{N}_{\rm R})t/\hbar} \\ &= e^{\mp ieVt/\hbar} \, e^{i\hat{K}_0 t/\hbar} \, \hat{H}^\pm_{\rm T} \, e^{-i\hat{K}_0 t/\hbar} \quad . \end{aligned} \tag{4.44}$$

Note that the current operator is

$$\hat{I} = \frac{ie}{\hbar} \, \big[\hat{H}_{\rm T} \, , \, N_{\rm L} \big] = \frac{ie}{\hbar} \Big(\hat{H}^-_{\rm T} - \hat{H}^+_{\rm T} \Big) \quad . \tag{4.45}$$

We then have

$$\begin{aligned} I(t) &= \frac{e}{\hbar^2} \int\limits_{-\infty}^{t} dt' \, \Big\langle \big[e^{ieVt/\hbar} \, \hat{H}^-_{\rm T}(t) - e^{-ieVt/\hbar} \, \hat{H}^+_{\rm T}(t) \, , \, e^{ieVt'/\hbar} \, \hat{H}^-_{\rm T}(t') + e^{-ieVt'/\hbar} \, \hat{H}^+_{\rm T}(t') \big] \Big\rangle \\ &= I_{\rm N}(t) + I_{\rm J}(t) \quad , \end{aligned} \tag{4.46}$$

[4]We make use of the fact that $\hat{N}_{\rm L} + \hat{N}_{\rm R}$ is conserved and commutes with $\hat{H}^\pm_{\rm T}$.

where

$$I_{\rm N}(t) = \frac{e}{\hbar^2} \int\limits_{-\infty}^{\infty} dt'\, \Theta(t-t') \left\{ e^{+i\Omega(t-t')} \left\langle \left[\hat{H}^-_{\rm T}(t)\,,\, \hat{H}^+_{\rm T}(t') \right] \right\rangle - e^{-i\Omega(t-t')} \left\langle \left[\hat{H}^+_{\rm T}(t)\,,\, \hat{H}^-_{\rm T}(t') \right] \right\rangle \right\} \tag{4.47}$$

and

$$I_{\rm J}(t) = \frac{e}{\hbar^2} \int\limits_{-\infty}^{\infty} dt'\, \Theta(t-t') \left\{ e^{+i\Omega(t+t')} \left\langle \left[\hat{H}^-_{\rm T}(t)\,,\, \hat{H}^-_{\rm T}(t') \right] \right\rangle - e^{-i\Omega(t+t')} \left\langle \left[\hat{H}^+_{\rm T}(t)\,,\, \hat{H}^+_{\rm T}(t') \right] \right\rangle \right\}\,, \tag{4.48}$$

with $\Omega \equiv eV/\hbar$. $I_{\rm N}(t)$ is the usual *single particle tunneling current*, which is present both in normal metals as well as in superconductors. $I_{\rm J}(t)$ is the *Josephson pair tunneling current*, which is only present when the ensemble average is over states of indefinite particle number.

4.2.2 The single particle tunneling current $I_{\rm N}$

We now proceed to evaluate the so-called single-particle current $I_{\rm N}$ in Eqn. 4.47. This current is present, under voltage bias, between normal metal and normal metal, between normal metal and superconductor, and between superconductor and superconductor. It is convenient to define the quantities

$$\begin{aligned} \mathcal{X}_{\sf r}(t-t') &\equiv -i\,\Theta(t-t') \left\langle \left[\hat{H}^-_{\rm T}(t)\,,\, \hat{H}^+_{\rm T}(t') \right] \right\rangle \\ \mathcal{X}_{\sf a}(t-t') &\equiv -i\,\Theta(t-t') \left\langle \left[\hat{H}^-_{\rm T}(t')\,,\, \hat{H}^+_{\rm T}(t) \right] \right\rangle \quad , \end{aligned} \tag{4.49}$$

which differ by the order of the time values of the operators inside the commutator. We then have

$$\begin{aligned} I_{\rm N} &= \frac{ie}{\hbar^2} \int\limits_{-\infty}^{\infty} dt\, \left\{ e^{+i\Omega t}\, \mathcal{X}_{\sf r}(t) + e^{-i\Omega t}\, \mathcal{X}_{\sf a}(t) \right\} \\ &= \frac{ie}{\hbar^2} \Big(\widetilde{\mathcal{X}}_{\sf r}(\Omega) + \widetilde{\mathcal{X}}_{\sf a}(-\Omega) \Big) \quad , \end{aligned} \tag{4.50}$$

where $\widetilde{\mathcal{X}}_{\sf a}(\Omega)$ is the Fourier transform of $\mathcal{X}_{\sf a}(t)$ into the frequency domain. As we shall show presently, $\widetilde{\mathcal{X}}_{\sf a}(-\Omega) = -\widetilde{\mathcal{X}}^*_{\sf r}(\Omega)$, so we have

$$I_{\rm N}(V) = -\frac{2e}{\hbar^2}\, {\sf Im}\, \widetilde{\mathcal{X}}_{\sf r}(eV/\hbar) \quad . \tag{4.51}$$

Proof that $\tilde{\mathcal{X}}_{\sf a}(\Omega) = -\widetilde{\mathcal{X}}^*_{\sf r}(-\Omega)$: Consider the general case

$$\begin{aligned} \mathcal{X}_{\sf r}(t) &= -i\,\Theta(t) \left\langle \left[\hat{A}(t)\,,\, \hat{A}^\dagger(0) \right] \right\rangle \\ \mathcal{X}_{\sf a}(t) &= -i\,\Theta(t) \left\langle \left[\hat{A}(0)\,,\, \hat{A}^\dagger(t) \right] \right\rangle \quad . \end{aligned} \tag{4.52}$$

We now spectrally decompose these expressions, inserting complete sets of states in between products of operators. One finds

$$\begin{aligned} \widetilde{\mathcal{X}}_{\sf r}(\omega) &= -i \int\limits_{-\infty}^{\infty} dt\, \Theta(t) \sum_{m,n} P_m \left\{ \left| \langle\, m \,|\, \hat{A} \,|\, n \,\rangle \right|^2 e^{i(\omega_m - \omega_n)t} - \left| \langle\, m \,|\, \hat{A}^\dagger \,|\, n \,\rangle \right|^2 e^{-i(\omega_m - \omega_n)t} \right\} e^{i\omega t} \\ &= \sum_{m,n} P_m \left\{ \frac{\left| \langle\, m \,|\, \hat{A} \,|\, n \,\rangle \right|^2}{\omega + \omega_m - \omega_n + i\epsilon} - \frac{\left| \langle\, m \,|\, \hat{A}^\dagger \,|\, n \,\rangle \right|^2}{\omega - \omega_m + \omega_n + i\epsilon} \right\} \quad , \end{aligned} \tag{4.53}$$

where the eigenvalues of $\hat{K}$ are written $\hbar\omega_m$, and $P_m = e^{-\hbar\omega_m/k_\mathrm{B}T}/\,\Xi$ is the thermal probability for state $|\,m\,\rangle$, where Ξ is the grand partition function. The corresponding expression for $\widetilde{\mathcal{X}}_\mathsf{a}(\omega)$ is

$$\widetilde{\mathcal{X}}_\mathsf{a}(\omega) = \sum_{m,n} P_m \left\{ \frac{\big|\langle\, m\,|\,\hat{A}\,|\,n\,\rangle\big|^2}{\omega - \omega_m + \omega_n + i\epsilon} - \frac{\big|\langle\, m\,|\,\hat{A}^\dagger\,|\,n\,\rangle\big|^2}{\omega + \omega_m - \omega_n + i\epsilon} \right\} \quad , \tag{4.54}$$

whence follows $\widetilde{\mathcal{X}}_\mathsf{a}(-\omega) = -\widetilde{\mathcal{X}}^*_\mathsf{r}(\omega)$. QED. Note that in general

$$\begin{aligned} \mathcal{Z}(t) = -i\,\Theta(t)\,\big\langle \hat{A}(t)\,\hat{B}(0)\big\rangle &= -i\,\Theta(t)\sum_{m,n} P_m\,\langle\, m\,|\,e^{i\hat{K}t/\hbar}\,\hat{A}\,e^{-i\hat{K}t/\hbar}\,|\,n\,\rangle\langle\, n\,|\,\hat{B}\,|\,m\,\rangle \\ &= -i\,\Theta(t)\sum_{m,n} P_m\,\langle\, m\,|\,\hat{A}\,|\,n\,\rangle\langle\, n\,|\,\hat{B}\,|\,m\,\rangle\, e^{i(\omega_m-\omega_n)t} \quad , \end{aligned} \tag{4.55}$$

the Fourier transform of which is

$$\widetilde{\mathcal{Z}}(\omega) = \int\limits_{-\infty}^{\infty}\! dt\; e^{i\omega t}\,\mathcal{Z}(t) = \sum_{m,n} P_m\,\frac{\langle\, m\,|\,\hat{A}\,|\,n\,\rangle\langle\, n\,|\,\hat{B}\,|\,m\,\rangle}{\omega + \omega_m - \omega_n + i\epsilon} \quad . \tag{4.56}$$

If we define the *spectral density* $\rho(\omega)$ as

$$\rho(\omega) = 2\pi \sum_{m,n} P_{m,n}\langle\, m\,|\,\hat{A}\,|\,n\,\rangle\langle\, n\,|\,\hat{B}\,|\,m\,\rangle\,\delta(\omega + \omega_m - \omega_n) \quad , \tag{4.57}$$

then we have

$$\widetilde{\mathcal{Z}}(\omega) = \int\limits_{-\infty}^{\infty}\!\frac{d\nu}{2\pi}\,\frac{\rho(\nu)}{\omega - \nu + i\epsilon} \quad . \tag{4.58}$$

Note that $\rho(\omega)$ is real if $B = A^\dagger$.

Evaluation of $\widetilde{\mathcal{X}}_\mathsf{r}(\omega)$: We must compute

$$\begin{aligned} \mathcal{X}_\mathsf{r}(t) &= -i\,\Theta(t)\sum_{i,j,\sigma}\sum_{k,l,\sigma'} T^*_{kl}\,T_{ij}\,\Big\langle\Big[c^\dagger_{\mathrm{R}\,j\,\sigma}(t)\,c_{\mathrm{L}\,i\,\sigma}(t)\,,\,c^\dagger_{\mathrm{L}\,k\,\sigma'}(0)\,c_{\mathrm{R}\,l\,\sigma'}(0)\Big]\Big\rangle \\ &= -i\,\Theta(t)\sum_{\boldsymbol{q},\boldsymbol{k},\sigma} |T_{\boldsymbol{q},\boldsymbol{k}}|^2 \Big\{ \big\langle c^\dagger_{\mathrm{R}\,\boldsymbol{k}\,\sigma}(t)\,c_{\mathrm{R}\,\boldsymbol{k}\,\sigma}(0)\big\rangle\,\big\langle c_{\mathrm{L}\,\boldsymbol{q}\,\sigma}(t)\,c^\dagger_{\mathrm{L}\,\boldsymbol{q}\,\sigma}(0)\big\rangle \\ &\qquad\qquad - \big\langle c^\dagger_{\mathrm{L}\,\boldsymbol{q}\,\sigma}(0)\,c_{\mathrm{L}\,\boldsymbol{q}\,\sigma}(t)\big\rangle\,\big\langle c_{\mathrm{R}\,\boldsymbol{k}\,\sigma}(0)\,c^\dagger_{\mathrm{R}\,\boldsymbol{k}\,\sigma}(t)\big\rangle\Big\} \end{aligned} \tag{4.59}$$

Note how we have taken $j = l \to \boldsymbol{k}$ and $i = k \to \boldsymbol{q}$, since *in each bank* wavevector is assumed to be a good quantum number. We now invoke the Bogoliubov transformation,

$$c_{\boldsymbol{k}\sigma} = u_{\boldsymbol{k}}\,\gamma_{\boldsymbol{k}\sigma} - \sigma\,v_{\boldsymbol{k}}\,e^{i\phi}\,\gamma^\dagger_{-\boldsymbol{k}\,-\sigma} \quad , \tag{4.60}$$

where we write $u_{\boldsymbol{k}} = \cos\vartheta_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}} = \sin\vartheta_{\boldsymbol{k}}$. We then have

$$\begin{aligned} \big\langle c^\dagger_{\mathrm{R}\,\boldsymbol{k}\,\sigma}(t)\,c_{\mathrm{R}\,\boldsymbol{k}\,\sigma}(0)\big\rangle &= u^2_{\boldsymbol{k}}\,e^{iE_{\boldsymbol{k}}t/\hbar}\,f(E_{\boldsymbol{k}}) + v^2_{\boldsymbol{k}}\,e^{-iE_{\boldsymbol{k}}t/\hbar}\,\big[1 - f(E_{\boldsymbol{k}})\big] \\ \big\langle c_{\mathrm{L}\,\boldsymbol{q}\,\sigma}(t)\,c^\dagger_{\mathrm{L}\,\boldsymbol{q}\,\sigma}(0)\big\rangle &= u^2_{\boldsymbol{q}}\,e^{-iE_{\boldsymbol{q}}t/\hbar}\,\big[1 - f(E_{\boldsymbol{q}})\big] + v^2_{\boldsymbol{q}}\,e^{iE_{\boldsymbol{q}}t/\hbar}\,f(E_{\boldsymbol{q}}) \\ \big\langle c^\dagger_{\mathrm{L}\,\boldsymbol{q}\,\sigma}(0)\,c_{\mathrm{L}\,\boldsymbol{q}\,\sigma}(t)\big\rangle &= u^2_{\boldsymbol{q}}\,e^{-iE_{\boldsymbol{q}}t/\hbar}\,f(E_{\boldsymbol{q}}) + v^2_{\boldsymbol{q}}\,e^{iE_{\boldsymbol{q}}t/\hbar}\,\big[1 - f(E_{\boldsymbol{q}})\big] \\ \big\langle c_{\mathrm{R}\,\boldsymbol{k}\,\sigma}(0)\,c^\dagger_{\mathrm{R}\,\boldsymbol{k}\,\sigma}(t)\big\rangle &= u^2_{\boldsymbol{k}}\,e^{iE_{\boldsymbol{k}}t/\hbar}\,\big[1 - f(E_{\boldsymbol{k}})\big] + v^2_{\boldsymbol{k}}\,e^{-iE_{\boldsymbol{k}}t/\hbar}\,f(E_{\boldsymbol{k}}) \quad . \end{aligned} \tag{4.61}$$

We now appeal to Eqn. 4.35 and convert the $\boldsymbol{q}$ and $\boldsymbol{k}$ sums to integrals over $\xi_{\mathrm{L}\,\boldsymbol{q}}$ and $\xi_{\mathrm{R}\,\boldsymbol{k}}$. Pulling out the DOS factors $g_{\mathrm{L}} \equiv g_{\mathrm{L}}(\mu_{\mathrm{L}})$ and $g_{\mathrm{R}} \equiv g_{\mathrm{R}}(\mu_{\mathrm{R}})$, as well as the hopping integral $t \equiv t\big(\xi_{\mathrm{L}\,\boldsymbol{q}} = 0\,,\,\xi_{\mathrm{R}\,\boldsymbol{k}} = 0\big)$ from the integrand, we have

$$\begin{aligned}\mathcal{X}_{\mathsf{r}}(t) = -i\,\Theta(t) \times \tfrac{1}{2}\, g_{\mathrm{L}}\, g_{\mathrm{R}}\, |t|^2 A \int\limits_{-\infty}^{\infty}\! d\xi \int\limits_{-\infty}^{\infty}\! d\xi' \times \\ \bigg\{ \Big[u^2\, e^{-iEt/\hbar}\,(1-f) + v^2\, e^{iEt/\hbar}\, f\Big] \times \Big[u'^2\, e^{iE't/\hbar}\, f' + v'^2\, e^{-iE't/\hbar}\,(1-f')\Big] \\ - \Big[u^2\, e^{-iEt/\hbar}\, f + v^2\, e^{iEt/\hbar}\,(1-f)\Big] \times \Big[u'^2\, e^{iE't/\hbar}\,(1-f') + v'^2\, e^{-iE't/\hbar}\, f'\Big] \bigg\} \quad ,\end{aligned} \tag{4.62}$$

where unprimed quantities correspond to the left bank (L) and primed quantities to the right bank (R). The ξ and ξ' integrals are simplified by the fact that in $u^2 = (E+\xi)/2E$ and $v^2 = (E-\xi)/2E$, *etc.* The terms proportional to ξ and ξ' and to $\xi\xi'$ drop out because everything else in the integrand is even in ξ and ξ' separately. Thus, we may replace u^2, v^2, u'^2, and v'^2 all by $\frac{1}{2}$. We now compute the Fourier transform, and we can read off the results using

$$-i\int\limits_0^{\infty}\! dt\; e^{i\omega t}\, e^{i\Omega t}\, e^{-\epsilon t} = \frac{1}{\omega + \Omega + i\epsilon} \quad . \tag{4.63}$$

We then obtain

$$\begin{aligned}\widetilde{\mathcal{X}}_{\mathsf{r}}(\omega) = \tfrac{1}{8}\,\hbar\, g_{\mathrm{L}}\, g_{\mathrm{R}}\, |t|^2 A \int\limits_{-\infty}^{\infty}\! d\xi \int\limits_{-\infty}^{\infty}\! d\xi' \, \Bigg\{ \frac{2\,(f'-f)}{\hbar\omega + E' - E + i\epsilon} + \frac{1-f-f'}{\hbar\omega - E - E' + i\epsilon} \\ - \frac{1-f-f'}{\hbar\omega + E + E' + i\epsilon} \Bigg\} \quad .\end{aligned} \tag{4.64}$$

Therefore,

$$\begin{aligned} I_{\mathrm{N}}(V,T) &= -\frac{2e}{\hbar^2}\, \mathsf{Im}\, \widetilde{\mathcal{X}}_{\mathsf{r}}(eV/\hbar) \\ &= \frac{\pi e}{\hbar}\, g_{\mathrm{L}}\, g_{\mathrm{R}}\, |t|^2 A \int\limits_0^{\infty}\! d\xi \int\limits_0^{\infty}\! d\xi' \, \bigg\{ (1-f-f')\Big[\delta(E+E'-eV) - \delta(E+E'+eV)\Big] \\ &\qquad\qquad + 2\,(f'-f)\,\delta(E'-E+eV) \bigg\} \quad . \end{aligned} \tag{4.65}$$

Single particle tunneling current in NIN junctions

We now evaluate I_{N} from Eqn. 4.65 for the case where both banks are normal metals. In this case, $E = \xi$ and $E' = \xi'$. (No absolute value symbol is needed since the ξ and ξ' integrals run over the positive real numbers.) At zero temperature, we have $f = 0$ and thus

$$\begin{aligned} I_{\mathrm{N}}(V, T=0) &= \frac{\pi e}{\hbar}\, g_{\mathrm{L}}\, g_{\mathrm{R}}\, |t|^2 A \int\limits_0^{\infty}\! d\xi \int\limits_0^{\infty}\! d\xi' \, \Big[\delta(\xi+\xi'-eV) - \delta(\xi+\xi'+eV)\Big] \\ &= \frac{\pi e}{\hbar}\, g_{\mathrm{L}}\, g_{\mathrm{R}}\, |t|^2 A \int\limits_0^{eV}\! d\xi = \frac{\pi e^2}{\hbar}\, g_{\mathrm{L}}\, g_{\mathrm{R}}\, |t|^2 A\, V \quad . \end{aligned} \tag{4.66}$$

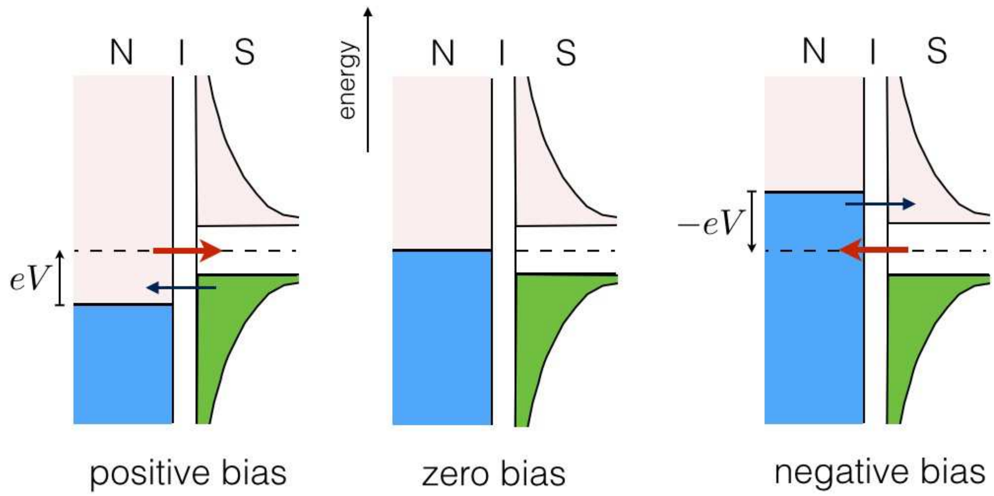

Figure 4.2: NIS tunneling for positive bias (left), zero bias (center), and negative bias (right). The left bank is maintained at an electrical potential V with respect to the right, hence $\mu_{R} = \mu_{L} + eV$. Blue regions indicate occupied fermionic states in the metal. Green regions indicate occupied electronic states in the superconductor. Light red regions indicate unoccupied states. Tunneling from or into the metal can only take place when its Fermi level lies outside the superconductor's gap region, meaning $|eV| > \Delta$, where V is the bias voltage. The arrow indicates the direction of electron number current. Black arrows indicate direction of electron current. Thick red arrows indicate direction of electrical current.

We thus identify the normal state conductance of the junction as

$$G_{N} \equiv \frac{\pi e^2}{\hbar}\, g_{L}\, g_{R}\, |t|^2 A \quad . \tag{4.67}$$

Single particle tunneling current in NIS junctions

Consider the case where one of the banks is a superconductor and the other a normal metal. We will assume $V > 0$ and work at $T = 0$. From Eqn. 4.65, we then have

$$\begin{aligned} I_{N}(V, T=0) &= \frac{G_{N}}{e} \int_0^\infty \! d\xi \int_0^\infty \! d\xi' \; \delta(\xi + E' - eV) = \frac{G_{N}}{e} \int_0^\infty \! d\xi \; \Theta(eV - E) \\ &= \frac{G_{N}}{e} \int_\Delta^{eV} \! dE \; \frac{E}{\sqrt{E^2 - \Delta^2}} = G_n \sqrt{V^2 - (\Delta/e)^2} \quad . \end{aligned} \tag{4.68}$$

The zero temperature conductance of the NIS junction is therefore

$$G_{NIS}(V) = \frac{dI}{dV} = \frac{G_{N} eV}{\sqrt{(eV)^2 - \Delta^2}} \quad . \tag{4.69}$$

Hence the ratio G_{NIS}/G_{NIN} is

$$\frac{G_{NIS}(V)}{G_{NIN}(V)} = \frac{eV}{\sqrt{(eV)^2 - \Delta^2}} \quad . \tag{4.70}$$

It is to be understood that these expressions are to be multiplied by $\mathrm{sgn}(V)\, \Theta\big(e|V| - \Delta\big)$ to obtain the full result valid at all voltages.

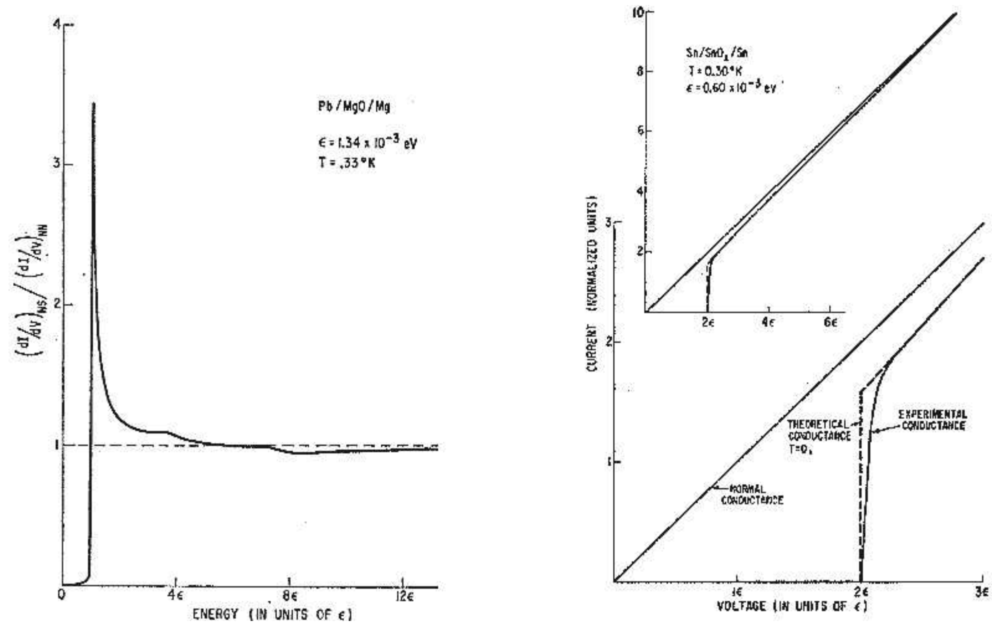

Figure 4.3: Tunneling data by Giaever *et al.* from *Phys. Rev.* **126**, 941 (1962). Left: normalized NIS tunneling conductance in a Pb/MgO/Mg sandwich junction. Pb is a superconductor for $T < T_c^{\rm Pb} = 7.19\,{\rm K}$, and Mg is a metal. A thin MgO layer provides a tunnel barrier. Right: I-V characteristic for a SIS junction Sn/SnO$_x$/Sn. Sn is a superconductor for $T < T_c^{\rm Sn} = 2.32\,{\rm K}$.

Superconducting density of states

We define

$$\begin{aligned} n_{\rm S}(E) &= 2\int \frac{d^3k}{(2\pi)^d}\,\delta(E - E_{\boldsymbol{k}}) \simeq g(\mu)\int\limits_{-\infty}^{\infty} d\xi\,\delta\Big(E - \sqrt{\xi^2+\Delta^2}\Big) \\ &= g(\mu)\,\frac{2E}{\sqrt{E^2-\Delta^2}}\,\Theta(E-\Delta) \quad . \end{aligned} \tag{4.71}$$

This is the density of energy states per unit volume for elementary excitations in the superconducting state. Note that there is an *energy gap* of size Δ, and that the missing states from this region pile up for $E \gtrsim \Delta$, resulting in a (integrable) divergence of $n_{\rm S}(E)$. In the limit $\Delta \to 0$, we have $n_{\rm S}(E) = 2\,g(\mu)\,\Theta(E)$. The factor of two arises because $n_{\rm S}(E)$ is the total density of states, which includes particle excitations above $k_{\rm F}$ as well as hole excitations below $k_{\rm F}$, both of which contribute $g(\mu)$. If $\Delta(\xi)$ is energy-dependent in the vicinity of $\xi = 0$, then we have

$$n(E) = g(\mu)\cdot\frac{E}{\xi}\cdot\frac{1}{1+\frac{\Delta}{\xi}\frac{d\Delta}{d\xi}}\Bigg|_{\xi=\sqrt{E^2-\Delta^2(\xi)}} \quad . \tag{4.72}$$

Here, $\xi = \sqrt{E^2 - \Delta^2(\xi)}$ is an implicit relation for $\xi(E)$.

The function $n_{\rm S}(E)$ vanishes for $E < 0$. We can, however, make a particle-hole transformation on the Bogoliubov operators, so that

$$\gamma_{\boldsymbol{k}\sigma} = \psi_{\boldsymbol{k}\sigma}\,\Theta(\xi_{\boldsymbol{k}}) + \psi^\dagger_{-\boldsymbol{k}\,-\sigma}\,\Theta(-\xi_{\boldsymbol{k}}) \quad . \tag{4.73}$$

We then have, up to constants,

$$\hat{K}_{\text{BCS}} = \sum_{\boldsymbol{k}\sigma} \mathcal{E}_{\boldsymbol{k}\sigma}\, \psi^\dagger_{\boldsymbol{k}\sigma}\, \psi_{\boldsymbol{k}\sigma} \quad , \tag{4.74}$$

where

$$\mathcal{E}_{\boldsymbol{k}\sigma} = \begin{cases} +E_{\boldsymbol{k}\sigma} & \text{if } \xi_{\boldsymbol{k}} > 0 \\ -E_{\boldsymbol{k}\sigma} & \text{if } \xi_{\boldsymbol{k}} < 0 \end{cases} \quad . \tag{4.75}$$

The density of states for the ψ particles is then

$$\widetilde{n}_{\text{S}}(\mathcal{E}) = \frac{g_{\text{S}}\,|\mathcal{E}|}{\sqrt{\mathcal{E}^2 - \Delta^2}}\,\Theta\big(|\mathcal{E}| - \Delta\big) \quad , \tag{4.76}$$

were g_{S} is the metallic DOS at the Fermi level in the superconducting bank, *i.e.* above T_{c}. Note that $\widetilde{n}_{\text{S}}(-\mathcal{E}) = \widetilde{n}_{\text{S}}(\mathcal{E})$ is now an even function of $\mathcal{E}$, and that half of the weight from $n_{\text{S}}(E)$ has now been assigned to negative $\mathcal{E}$ states. The interpretation of Fig. 4.2 follows by writing

$$I_{\text{N}}(V, T=0) = \frac{G_{\text{N}}}{e g_{\text{S}}} \int\limits_0^{eV} \! d\mathcal{E}\; n_{\text{S}}(\mathcal{E}) \quad . \tag{4.77}$$

Note that this is properly odd under $V \to -V$. If $V > 0$, the tunneling current is proportional to the integral of the superconducting density of states from $\mathcal{E} = \Delta$ to $\mathcal{E} = eV$. Since $\widetilde{n}_{\text{S}}(\mathcal{E})$ vanishes for $|\mathcal{E}| < \Delta$, the tunnel current vanishes if $|eV| < \Delta$.

<u>**Single particle tunneling current in SIS junctions**</u>

We now come to the SIS case, where both banks are superconducting. From Eqn. 4.65, we have ($T = 0$)

$$\begin{aligned} I_{\text{N}}(V, T=0) &= \frac{G_{\text{N}}}{e} \int\limits_0^\infty \! d\xi \int\limits_0^\infty \! d\xi'\; \delta(E + E' - eV) \qquad (4.78) \\ &= \frac{G_{\text{N}}}{e} \int\limits_0^\infty \! dE \int\limits_0^\infty \! dE'\; \frac{E}{\sqrt{E^2 - \Delta_{\text{L}}^2}}\, \frac{E'}{\sqrt{E'^{\,2} - \Delta_{\text{R}}^2}} \Big[\delta(E + E' - eV) - \delta(E + E' + eV)\Big] \quad . \end{aligned}$$

While this integral has no general analytic form, we see that $I_{\text{N}}(V) = -I_{\text{N}}(-V)$, and that the threshold voltage V^* below which $I_{\text{N}}(V)$ vanishes is given by $eV^* = \Delta_{\text{L}} + \Delta_{\text{R}}$. For the special case $\Delta_{\text{L}} = \Delta_{\text{R}} \equiv \Delta$, one has

$$I_{\text{N}}(V) = \frac{G_{\text{N}}}{e} \left\{ \frac{(eV)^2}{eV + 2\Delta}\, \mathbb{K}(x) - (eV + 2\Delta)\Big(\mathbb{K}(x) - \mathbb{E}(x)\Big) \right\} \quad , \tag{4.79}$$

where $x = (eV - 2\Delta)/(eV + 2\Delta)$ and $\mathbb{K}(x)$ and $\mathbb{E}(x)$ are complete elliptic integrals of the first and second kinds, respectively. We may also make progress by setting $eV = \Delta_{\text{L}} + \Delta_{\text{R}} + e\,\delta V$. One then has

$$I_{\text{N}}(V^* + \delta V) = \frac{G_{\text{N}}}{e} \int\limits_0^\infty \! d\xi_{\text{L}} \int\limits_0^\infty \! d\xi_{\text{R}}\; \delta\bigg(e\,\delta V - \frac{\xi_{\text{L}}^2}{2\Delta_{\text{L}}} - \frac{\xi_{\text{R}}^2}{2\Delta_{\text{R}}}\bigg) = \frac{\pi G_{\text{N}}}{2e}\sqrt{\Delta_{\text{L}}\,\Delta_{\text{R}}} \quad . \tag{4.80}$$

Thus, the SIS tunnel current jumps discontinuously at $V = V^*$. At finite temperature, there is a smaller local maximum in I_{N} for $V = |\Delta_{\text{L}} - \Delta_{\text{R}}|/e$.

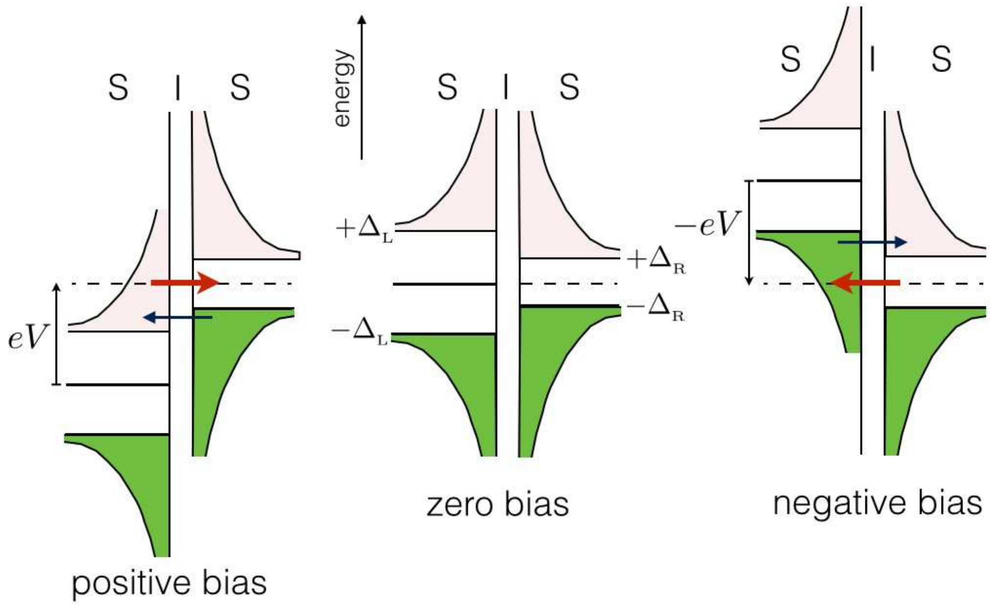

Figure 4.4: SIS tunneling for positive bias (left), zero bias (center), and negative bias (right). Green regions indicate occupied electronic states in each superconductor, where $\tilde{n}_{\rm s}(\mathcal{E}) > 0$.

4.2.3 The Josephson pair tunneling current $I_{\rm J}$

Earlier we obtained the expression

$$I_{\rm J}(t) = \frac{e}{\hbar^2}\int\limits_{-\infty}^{\infty} dt'\;\Theta(t-t')\,\Big\{ e^{+i\Omega(t+t')}\,\Big\langle\big[\hat{H}^-_{\rm T}(t)\,,\,\hat{H}^-_{\rm T}(t')\big]\Big\rangle - e^{-i\Omega(t+t')}\,\Big\langle\big[\hat{H}^+_{\rm T}(t)\,,\,\hat{H}^+_{\rm T}(t')\big]\Big\rangle\Big\} \quad . \tag{4.81}$$

Proceeding in analogy to the case for $I_{\rm N}$, define now the anomalous response functions,

$$\begin{aligned}\mathcal{Y}_{\sf r}(t-t') &= -i\,\Theta(t-t')\,\Big\langle\big[\hat{H}^+_{\rm T}(t)\,,\,\hat{H}^+_{\rm T}(t')\big]\Big\rangle\\ \mathcal{Y}_{\sf a}(t-t') &= -i\,\Theta(t-t')\,\Big\langle\big[\hat{H}^-_{\rm T}(t')\,,\,\hat{H}^-_{\rm T}(t)\big]\Big\rangle \quad .\end{aligned} \tag{4.82}$$

The spectral representations of these response functions are

$$\begin{aligned}\widetilde{\mathcal{Y}}_{\sf r}(\omega) &= \sum_{m,n} P_m\,\bigg\{\frac{\langle\, m\,|\,\hat{H}^+_{\rm T}\,|\,n\,\rangle\langle\, n\,|\,\hat{H}^+_{\rm T}\,|\,m\,\rangle}{\omega+\omega_m-\omega_n+i\epsilon} - \frac{\langle\, m\,|\,\hat{H}^+_{\rm T}\,|\,n\,\rangle\langle\, n\,|\,\hat{H}^+_{\rm T}\,|\,m\,\rangle}{\omega-\omega_m+\omega_n+i\epsilon}\bigg\}\\ \widetilde{\mathcal{Y}}_{\sf a}(\omega) &= \sum_{m,n} P_m\,\bigg\{\frac{\langle\, m\,|\,\hat{H}^-_{\rm T}\,|\,n\,\rangle\langle\, n\,|\,\hat{H}^-_{\rm T}\,|\,m\,\rangle}{\omega-\omega_m+\omega_n+i\epsilon} - \frac{\langle\, m\,|\,\hat{H}^-_{\rm T}\,|\,n\,\rangle\langle\, n\,|\,\hat{H}^-_{\rm T}\,|\,m\,\rangle}{\omega+\omega_m-\omega_n+i\epsilon}\bigg\} \quad ,\end{aligned} \tag{4.83}$$

from which we see $\widetilde{\mathcal{Y}}_{\mathsf{a}}(\omega) = -\widetilde{\mathcal{Y}}^*_{\mathsf{r}}(-\omega)$. The Josephson current is then given by

$$
\begin{aligned}
I_{\mathrm{J}}(t) &= -\frac{ie}{\hbar^2}\int\limits_{-\infty}^{\infty}\!dt'\,\Big\{e^{-2i\Omega t}\,\mathcal{Y}_{\mathsf{r}}(t-t')\,e^{+i\Omega(t-t')} + e^{+2i\Omega t}\,\mathcal{Y}_{\mathsf{a}}(t-t')\,e^{-i\Omega(t-t')}\Big\} \\
&= \frac{2e}{\hbar^2}\,\mathsf{Im}\Big[e^{-2i\Omega t}\,\widetilde{\mathcal{Y}}_{\mathsf{r}}(\Omega)\Big] \quad ,
\end{aligned}
\tag{4.84}
$$

where $\Omega = eV/\hbar$.

Plugging in our expressions for $\hat{H}^{\pm}_{\mathrm{T}}$, we have

$$
\begin{aligned}
\mathcal{Y}_{\mathsf{r}}(t) &= -i\,\Theta(t)\sum_{\boldsymbol{k},\boldsymbol{q},\sigma} T_{\boldsymbol{k},\boldsymbol{q}}\,T_{-\boldsymbol{k},-\boldsymbol{q}}\,\Big\langle\Big[c^\dagger_{\mathrm{L}\,\boldsymbol{q}\,\sigma}(t)\,c_{\mathrm{R}\,\boldsymbol{k}\,\sigma}(t)\,,\,c^\dagger_{\mathrm{L}\,-\boldsymbol{q}\,-\sigma}(0)\,c_{\mathrm{R}\,-\boldsymbol{k}\,-\sigma}(0)\Big]\Big\rangle \\
&= 2i\,\Theta(t)\sum_{\boldsymbol{q},\boldsymbol{k}} T_{\boldsymbol{k},\boldsymbol{q}}\,T_{-\boldsymbol{k},-\boldsymbol{q}}\,\Big\{\big\langle c^\dagger_{\mathrm{L}\,\boldsymbol{q}\uparrow}(t)\,c^\dagger_{\mathrm{L}\,-\boldsymbol{q}\downarrow}(0)\big\rangle\,\big\langle c_{\mathrm{R}\,\boldsymbol{k}\uparrow}(t)\,c_{\mathrm{R}\,-\boldsymbol{k}\downarrow}(0)\big\rangle \\
&\qquad\qquad - \big\langle c^\dagger_{\mathrm{L}\,-\boldsymbol{q}\downarrow}(0)\,c^\dagger_{\mathrm{L}\,\boldsymbol{q}\uparrow}(t)\big\rangle\,\big\langle c_{\mathrm{R}\,-\boldsymbol{k}\downarrow}(0)\,c_{\mathrm{R}\,\boldsymbol{k}\uparrow}(t)\big\rangle\Big\} \quad .
\end{aligned}
\tag{4.85}
$$

Again we invoke Bogoliubov,

$$
c_{\boldsymbol{k}\uparrow} = u_{\boldsymbol{k}}\,\gamma_{\boldsymbol{k}\uparrow} - v_{\boldsymbol{k}}\,e^{i\phi}\,\gamma^\dagger_{-\boldsymbol{k}\downarrow} \qquad\qquad c^\dagger_{\boldsymbol{k}\uparrow} = u_{\boldsymbol{k}}\,\gamma^\dagger_{\boldsymbol{k}\uparrow} - v_{\boldsymbol{k}}\,e^{-i\phi}\,\gamma_{-\boldsymbol{k}\downarrow} \tag{4.86}
$$

$$
c_{-\boldsymbol{k}\downarrow} = u_{\boldsymbol{k}}\,\gamma_{-\boldsymbol{k}\downarrow} + v_{\boldsymbol{k}}\,e^{i\phi}\,\gamma^\dagger_{\boldsymbol{k}\uparrow} \qquad\qquad c^\dagger_{-\boldsymbol{k}\downarrow} = u_{\boldsymbol{k}}\,\gamma^\dagger_{-\boldsymbol{k}\downarrow} + v_{\boldsymbol{k}}\,e^{-i\phi}\,\gamma_{\boldsymbol{k}\uparrow} \tag{4.87}
$$

to obtain

$$
\begin{aligned}
\big\langle c^\dagger_{\mathrm{L}\,\boldsymbol{q}\uparrow}(t)\,c^\dagger_{\mathrm{L}\,-\boldsymbol{q}\downarrow}(0)\big\rangle &= u_{\boldsymbol{q}}\,v_{\boldsymbol{q}}\,e^{-i\phi_{\mathrm{L}}}\,\Big\{e^{iE_{\boldsymbol{q}}t/\hbar}\,f(E_{\boldsymbol{q}}) - e^{-iE_{\boldsymbol{q}}t/\hbar}\,\big[1-f(E_{\boldsymbol{q}})\big]\Big\} \\
\big\langle c_{\mathrm{R}\,\boldsymbol{k}\uparrow}(t)\,c_{\mathrm{R}\,-\boldsymbol{k}\downarrow}(0)\big\rangle &= u_{\boldsymbol{k}}\,v_{\boldsymbol{k}}\,e^{+i\phi_{\mathrm{R}}}\,\Big\{e^{-iE_{\boldsymbol{k}}t/\hbar}\,\big[1-f(E_{\boldsymbol{k}})\big] - e^{iE_{\boldsymbol{k}}t/\hbar}\,f(E_{\boldsymbol{k}})\Big\} \\
\big\langle c^\dagger_{\mathrm{L}\,-\boldsymbol{q}\downarrow}(0)\,c^\dagger_{\mathrm{L}\,\boldsymbol{q}\uparrow}(t)\big\rangle &= u_{\boldsymbol{q}}\,v_{\boldsymbol{q}}\,e^{-i\phi_{\mathrm{L}}}\,\Big\{e^{iE_{\boldsymbol{q}}t/\hbar}\,\big[1-f(E_{\boldsymbol{q}})\big] - e^{-iE_{\boldsymbol{q}}t/\hbar}\,f(E_{\boldsymbol{q}})\Big\} \\
\big\langle c_{\mathrm{R}\,-\boldsymbol{k}\downarrow}(0)\,c_{\mathrm{R}\,\boldsymbol{k}\uparrow}(t)\big\rangle &= u_{\boldsymbol{k}}\,v_{\boldsymbol{k}}\,e^{+i\phi_{\mathrm{R}}}\,\Big\{e^{-iE_{\boldsymbol{k}}t/\hbar}\,f(E_{\boldsymbol{k}}) - e^{iE_{\boldsymbol{k}}t/\hbar}\,\big[1-f(E_{\boldsymbol{k}})\big]\Big\}
\end{aligned}
\tag{4.88}
$$

We then have

$$
\begin{aligned}
\mathcal{Y}_{\mathsf{r}}(t) = i\,\Theta(t)\times\tfrac{1}{2}\,g_{\mathrm{L}}\,g_{\mathrm{R}}\,|t|^2 A\,e^{i(\phi_{\mathrm{R}}-\phi_{\mathrm{L}})}\int\limits_{-\infty}^{\infty}\!d\xi\int\limits_{-\infty}^{\infty}\!d\xi'\;u\,v\,u'\,v'\,\times \\
\Big\{\Big[e^{iEt/\hbar}\,f - e^{-iEt/\hbar}\,(1-f)\Big]\times\Big[e^{-iE't/\hbar}\,(1-f') - e^{iE't/\hbar}\,f'\Big] \\
- \Big[e^{iEt/\hbar}\,(1-f) - e^{-iEt/\hbar}\,f\Big]\times\Big[e^{-iE't/\hbar}\,f' - e^{iE't/\hbar}\,(1-f')\Big]\Big\} \quad ,
\end{aligned}
\tag{4.89}
$$

where once again primed and unprimed symbols refer respectively to left (L) and right (R) banks. Recall that the

BCS coherence factors give $uv = \frac{1}{2}\sin(2\vartheta) = \Delta/2E$. Taking the Fourier transform, we have

$$\widetilde{\mathcal{Y}}_{\mathsf{r}}(\omega) = \tfrac{1}{2}\,\hbar\, g_{\mathrm{L}}\, g_{\mathrm{R}}\, |t|^2\, e^{i(\phi_{\mathrm{R}}-\phi_{\mathrm{L}})} A \int\limits_0^\infty \! d\xi \int\limits_0^\infty \! d\xi' \,\frac{\Delta}{E}\,\frac{\Delta'}{E'} \left\{ \frac{f-f'}{\hbar\omega + E - E' + i\epsilon} - \frac{f-f'}{\hbar\omega - E + E' + i\epsilon} \right.$$
$$\left. + \frac{1-f-f'}{\hbar\omega + E + E' + i\epsilon} - \frac{1-f-f'}{\hbar\omega - E - E' + i\epsilon} \right\} \quad . \tag{4.90}$$

Setting $T=0$, we have

$$\widetilde{\mathcal{Y}}_{\mathsf{r}}(\omega) = \frac{\hbar^2 G_{\mathsf{N}}}{2\pi e^2}\, e^{i(\phi_{\mathrm{R}}-\phi_{\mathrm{L}})} \int\limits_0^\infty \! d\xi \int\limits_0^\infty \! d\xi' \,\frac{\Delta\,\Delta'}{E\,E'} \left\{ \frac{1}{\hbar\omega + E + E' + i\epsilon} \right.$$
$$\left. - \frac{1}{\hbar\omega - E - E' + i\epsilon} \right\} \tag{4.91}$$
$$= \frac{\hbar^2 G_{\mathsf{N}}}{2\pi e^2}\, e^{i(\phi_{\mathrm{R}}-\phi_{\mathrm{L}})} \int\limits_\Delta^\infty \! dE\, \frac{\Delta}{\sqrt{E^2-\Delta^2}} \int\limits_{\Delta'}^\infty \! dE'\, \frac{\Delta'}{\sqrt{E'^{\,2}-\Delta'^{\,2}}}$$
$$\times \frac{2\,(E+E')}{(\hbar\omega)^2 - (E+E')^2} \quad . \tag{4.92}$$

There is no general analytic form for this integral. However, for the special case $\Delta = \Delta'$, we have

$$\widetilde{\mathcal{Y}}_{\mathsf{r}}(\omega) = \frac{G_{\mathsf{N}}\hbar^2}{2e^2}\,\Delta\,\mathbb{K}\bigg(\frac{\hbar|\omega|}{4\Delta}\bigg)\, e^{i(\phi_{\mathrm{R}}-\phi_{\mathrm{L}})} \quad , \tag{4.93}$$

where $\mathbb{K}(x)$ is the complete elliptic integral of the first kind. Thus,

$$I_{\mathsf{J}}(t) = G_{\mathsf{N}} \cdot \frac{\Delta}{e}\,\mathbb{K}\bigg(\frac{e|V|}{4\Delta}\bigg)\,\sin\bigg(\phi_{\mathrm{R}} - \phi_{\mathrm{L}} - \frac{2eVt}{\hbar}\bigg) \quad . \tag{4.94}$$

With $V=0$, one finds (at finite T),

$$I_{\mathsf{J}} = G_{\mathsf{N}} \cdot \frac{\pi\Delta}{2e}\,\tanh\bigg(\frac{\Delta}{2k_{\mathrm{B}}T}\bigg)\,\sin(\phi_{\mathrm{R}} - \phi_{\mathrm{L}}) \quad . \tag{4.95}$$

Thus, there is a spontaneous current flow in the absence of any voltage bias, provided the phases remain fixed. The maximum current which flows under these conditions is called the *critical current* of the junction, I_{c}. Writing $R_{\mathsf{N}} = 1/G_{\mathsf{N}}$ for the normal state junction resistance, one has

$$I_{\mathrm{c}} R_{\mathsf{N}} = \frac{\pi\Delta}{2e}\,\tanh\bigg(\frac{\Delta}{2k_{\mathrm{B}}T}\bigg) \quad , \tag{4.96}$$

which is known as the *Ambegaokar-Baratoff relation*. Note that I_{c} agrees with what we found in Eqn. 4.80 for V just above $V^* = 2\Delta$. I_{c} is also the current flowing in a normal junction at bias voltage $V = \pi\Delta/2e$. Setting $I_{\mathrm{c}} = 2eJ/\hbar$ where J is the Josephson coupling, we find our $V=0$ results here in complete agreement with those of Eqn. 4.29 when Coulomb charging energies of the grains are neglected.

Experimentally, one generally draws a current I across the junction and then measures the voltage difference. In other words, the junction is *current-biased*. Varying I then leads to a hysteretic voltage response, as shown in Fig. 4.5. The oscillating current $I(t) = I_{\mathrm{c}}\sin(\phi_{\mathrm{R}} - \phi_{\mathrm{L}} - \Omega t)$ gives no DC average. For a junction of area $A \sim 1\,\mathrm{mm}^2$, one has Ω and $I_{\mathrm{c}} = 1\,\mathrm{mA}$ for a gap of $\Delta \simeq 1\,\mathrm{meV}$. The critical current density is then $j_{\mathrm{c}} = I_{\mathrm{c}}/A \sim 10^3\,\mathrm{A/m}^2$. Current densities in bulk type I and type II materials can approach $j \sim 10^{11}\,\mathrm{A/m}^2$ and $10^9\,\mathrm{A/m}^2$, respectively.

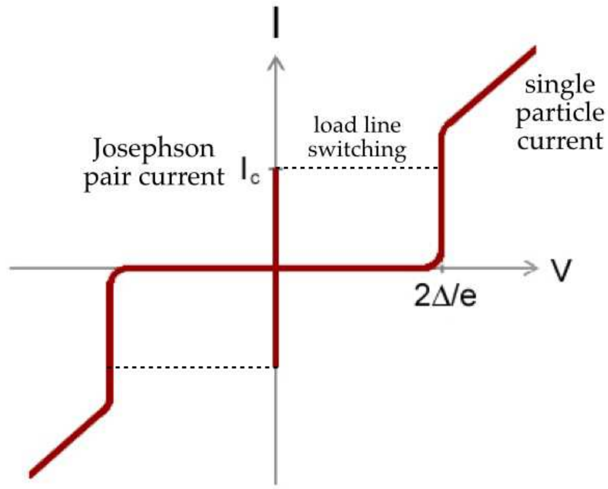

Figure 4.5: Current-voltage characteristics for a current-biased Josephson junction. Increasing current at zero bias voltage is possible up to $|I| = I_c$, beyond which the voltage jumps along the dotted line. Subsequent reduction in current leads to hysteresis.

4.3 The Josephson Effect

4.3.1 Two grain junction

In §4.1 we discussed a model for superconducting grains. Consider now only a single pair of grains, and write

$$\hat{K} = -J\cos(\phi_{\mathrm{L}} - \phi_{\mathrm{R}}) + \frac{2e^2}{C_{\mathrm{L}}}\,M_{\mathrm{L}}^2 + \frac{2e^2}{C_{\mathrm{R}}}\,M_{\mathrm{R}}^2 - 2\mu_{\mathrm{L}} M_{\mathrm{L}} - 2\mu_{\mathrm{R}} M_{\mathrm{R}} \quad , \tag{4.97}$$

where $M_{\mathrm{L,R}}$ is the number of Cooper pairs on each grain in excess of the background charge, which we assume here to be a multiple of $e^* = 2e$. From the Heisenberg equations of motion, we have

$$\dot{M}_{\mathrm{L}} = \frac{i}{\hbar}\,\big[\hat{K}, M_{\mathrm{L}}\big] = \frac{J}{\hbar}\,\sin(\phi_{\mathrm{R}} - \phi_{\mathrm{L}}) \quad . \tag{4.98}$$

Similarly, we find $\dot{M}_{\mathrm{R}} = +\frac{J}{\hbar}\,\sin(\phi_{\mathrm{L}} - \phi_{\mathrm{R}})$. The electrical current flowing from L to R is $I = 2e\dot{M}_{\mathrm{L}}$. The equations of motion for the phases are

$$\begin{aligned} \dot{\phi}_{\mathrm{L}} &= \frac{i}{\hbar}\,\big[\hat{K}\,,\,\phi_{\mathrm{L}}\big] = \frac{4e^2 M_{\mathrm{L}}}{\hbar C_{\mathrm{L}}} - \frac{2\mu_{\mathrm{L}}}{\hbar} \\ \dot{\phi}_{\mathrm{R}} &= \frac{i}{\hbar}\,\big[\hat{K}\,,\,\phi_{\mathrm{R}}\big] = \frac{4e^2 M_{\mathrm{R}}}{\hbar C_{\mathrm{R}}} - \frac{2\mu_{\mathrm{R}}}{\hbar} \quad . \end{aligned} \tag{4.99}$$

Let's assume the grains are large, so their self-capacitances are large too. In that case, we can neglect the Coulomb energy of each grain, and we obtain the *Josephson equations*

$$\frac{d\phi}{dt} = -\frac{2eV}{\hbar} \qquad , \qquad I(t) = I_{\mathrm{c}}\sin\phi(t) \quad , \tag{4.100}$$

where $eV = \mu_{\mathrm{R}} - \mu_{\mathrm{L}}$, $I_{\mathrm{c}} = 2eJ/\hbar$, and $\phi \equiv \phi_{\mathrm{R}} - \phi_{\mathrm{L}}$. When quasiparticle tunneling is accounted for, the second of the Josephson equations is modified to

$$I = I_{\mathrm{c}}\sin\phi + \big(G_0 + G_1\cos\phi\big)V \quad , \tag{4.101}$$

where $G_0 \equiv G_{\mathrm{N}}$ is the quasiparticle contribution to the current, and G_1 accounts for higher order effects.

4.3.2 Effect of in-plane magnetic field

Thus far we have assumed that the effective hopping amplitude t between the L and R banks is real. This is valid in the absence of an external magnetic field, which breaks time-reversal. In the presence of an external magnetic field, t is replaced by $t \to t\,e^{i\gamma}$, where $\gamma = \frac{e}{\hbar c}\int_L^R \boldsymbol{A}\cdot d\boldsymbol{l}$ is the Aharonov-Bohm phase. Without loss of generality, we consider the junction interface to lie in the (x,y) plane, and we take $\boldsymbol{H} = H\hat{\boldsymbol{y}}$. We are then free to choose the gauge $\boldsymbol{A} = -Hx\hat{\boldsymbol{z}}$. Then

$$\gamma = \frac{e}{\hbar c}\int_L^R \boldsymbol{A}\cdot d\boldsymbol{l} = -\frac{e}{\hbar c}\,H\,(\lambda_L + \lambda_R + d)\,x \quad , \tag{4.102}$$

where $\lambda_{L,R}$ are the penetration depths for the two superconducting banks, and d is the junction separatino. Typically $\lambda_{L,R} \sim 100\,\text{Å} - 1000\,\text{Å}$, while $d \sim 10\,\text{Å}$, so usually we may neglect the junction separation in comparison with the penetration depth.

In the case of the single particle current I_N, we needed to compute $\big[\hat{H}^+_T(t), \hat{H}^-_T(0)\big]$ and $\big[\hat{H}^-_T(t), \hat{H}^+_T(0)\big]$. Since $\hat{H}^+_T \propto t$ while $\hat{H}^-_T \propto t^*$, the result depends on the product $|t|^2$, which has no phase. Thus, I_N is unaffected by an in-plane magnetic field. For the Josephson pair tunneling current I_J, however, we need $\big[\hat{H}^+_T(t), \hat{H}^+_T(0)\big]$ and $\big[\hat{H}^-_T(t), \hat{H}^-_T(0)\big]$. The former is proportional to t^2 and the latter to t^{*2}. Therefore the Josephson current density is

$$j_J(x) = \frac{I_c(T)}{A}\,\sin\!\bigg(\phi - \frac{2e}{\hbar c}\,Hd_{\text{eff}}\,x - \frac{2eVt}{\hbar}\bigg), \tag{4.103}$$

where $d_{\text{eff}} \equiv \lambda_L + \lambda_R + d$ and $\phi = \phi_R - \phi_L$. Note that it is $2eHd_{\text{eff}}/\hbar c = \mathsf{arg}(t^2)$ which appears in the argument of the sine. This may be interpreted as the Aharonov-Bohm phase accrued by a tunneling Cooper pair. We now assume our junction interface is a square of dimensions $L_x \times L_y$. At $V=0$, the total Josephson current is then[5]

$$I_J = \int_0^{L_x}\!\!dx\int_0^{L_y}\!\!dy\; j(x) = \frac{I_c\phi_L}{\pi\Phi}\,\sin(\pi\Phi/\phi_L)\,\sin(\gamma - \pi\Phi/\phi_L) \quad , \tag{4.104}$$

where $\Phi \equiv HL_x d_{\text{eff}}$. The maximum current occurs when $\gamma - \pi\Phi/\phi_L = \pm\frac{1}{2}\pi$, where its magnitude is

$$I_{\text{max}}(\Phi) = I_c\left|\frac{\sin(\pi\Phi/\phi_L)}{\pi\Phi/\phi_L}\right| \quad . \tag{4.105}$$

The shape $I_{\text{max}}(\Phi)$ is precisely that of the single slit Fraunhofer pattern from geometrical optics! (See Fig. 4.6.)

4.3.3 Two-point quantum interferometer

Consider next the device depicted in Fig. 4.6(c) consisting of two weak links between superconducting banks. The current flowing from L to R is

$$I = I_{c,1}\,\sin\phi_1 + I_{c,2}\,\sin\phi_2 \quad . \tag{4.106}$$

where $\phi_1 \equiv \phi_{L,1} - \phi_{R,1}$ and $\phi_2 \equiv \phi_{L,2} - \phi_{R,2}$ are the phase differences across the two Josephson junctions. The total flux Φ inside the enclosed loop is

$$\phi_2 - \phi_1 = \frac{2\pi\Phi}{\phi_L} \equiv 2\gamma \quad . \tag{4.107}$$

[5]Take care not to confuse ϕ_L, the phase of the left superconducting bank, with ϕ_L, the London flux quantum $hc/2e$. To the untrained eye, these symbols look identical.

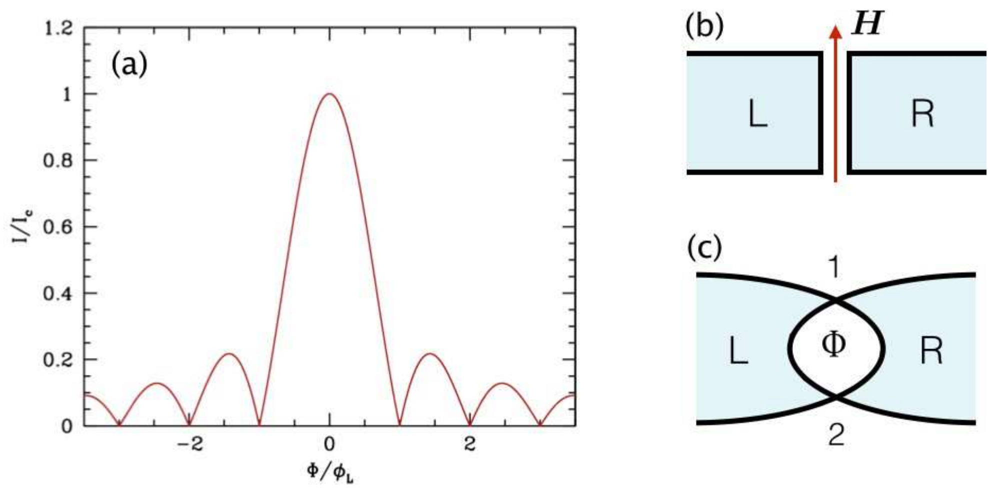

Figure 4.6: (a) Fraunhofer pattern of Josephson current *versus* flux due to in-plane magnetic field. (b) Sketch of Josephson junction experiment yielding (a). (c) Two-point superconducting quantum interferometer.

Writing $\phi_2 = \phi_1 + 2\gamma$, we extremize $I(\phi_1, \gamma)$ with respect to ϕ_1, and obtain

$$I_{\max}(\gamma) = \sqrt{(I_{c,1} + I_{c,2})^2 \cos^2\gamma + (I_{c,1} - I_{c,2})^2 \sin^2\gamma} \quad . \tag{4.108}$$

If $I_{c,1} = I_{c,2}$, we have $I_{\max}(\gamma) = 2I_c\,|\cos\gamma\,|$. This provides for an extremely sensitive measurement of magnetic fields, since $\gamma = \pi\Phi/\phi_L$ and $\phi_L = 2.07 \times 10^{-7}\,\mathrm{G\,cm^2}$. Thus, a ring of area $1\,\mathrm{cm}^2$ allows for the detection of fields on the order of 10^{-7} G. This device is known as a Superconducting QUantum Interference Device, or SQUID. The limits of the SQUID's sensitivity are set by the noise in the SQUID or in the circuit amplifier.

4.3.4 RCSJ Model

In circuits, a Josephson junction, from a practical point of view, is always transporting current in parallel to some resistive channel. Josephson junctions also have electrostatic capacitance as well. Accordingly, consider the *resistively and capacitively shunted Josephson junction* (RCSJ), a sketch of which is provided in Fig. 4.8(c). The equations governing the RCSJ model are

$$\begin{aligned} I &= C\,\dot{V} + \frac{V}{R} + I_c \sin\phi \\ V &= \frac{\hbar}{2e}\,\dot{\phi} \quad , \end{aligned} \tag{4.109}$$

where we again take I to run from left to right. If the junction is *voltage-biased*, then integrating the second of these equations yields $\phi(t) = \phi_0 + \omega_J t$, where $\omega_J = 2eV/\hbar$ is the *Josephson frequency*. The current is then

$$I = \frac{V}{R} + I_c \sin(\phi_0 + \omega_J t) \quad . \tag{4.110}$$

If the junction is *current-biased*, then we substitute the second equation into the first, to obtain

$$\frac{\hbar C}{2e}\,\ddot{\phi} + \frac{\hbar}{2eR}\,\dot{\phi} + I_c \sin\phi = I \quad . \tag{4.111}$$

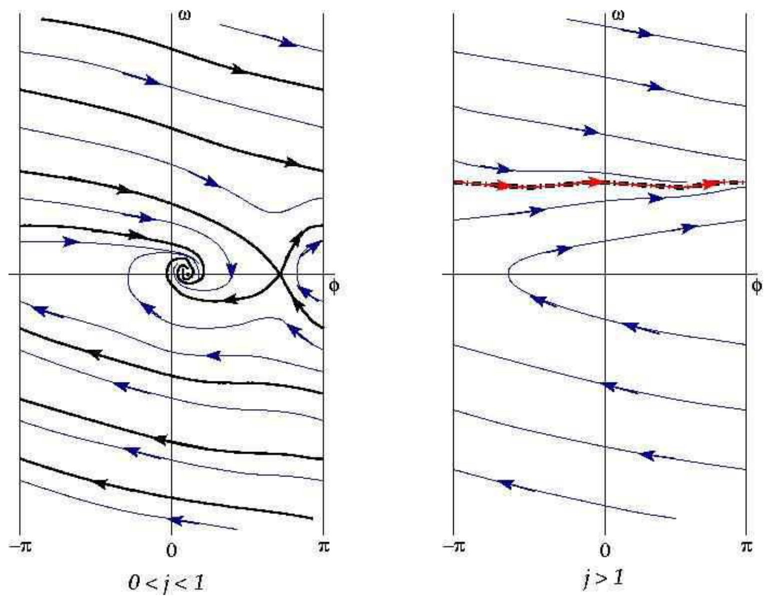

Figure 4.7: Phase flows for the equation $\ddot{\phi} + Q^{-1}\dot{\phi} + \sin\phi = j$. Left panel: $0 < j < 1$; note the separatrix (in black), which flows into the stable and unstable fixed points. Right panel: $j > 1$. The red curve overlying the thick black dot-dash curve is a *limit cycle*.

We adimensionalize by writing $s \equiv \omega_{\rm p} t$, with $\omega_{\rm p} = (2eI_{\rm c}/\hbar C)^{1/2}$ is the *Josephson plasma frequency* (at zero current). We then have

$$\frac{d^2\phi}{ds^2} + \frac{1}{Q}\,\frac{d\phi}{ds} = j - \sin\phi \equiv -\frac{du}{d\phi} \quad , \tag{4.112}$$

where $Q = \omega_{\rm p}\tau$ with $\tau = RC$, and $j = I/I_{\rm c}$. The quantity Q^2 is called the *McCumber-Stewart parameter*. The resistance is $R(T \approx T_{\rm c}) = R_{\rm N}$, while $R(T \ll T_{\rm c}) \approx R_{\rm N}\,\exp(\Delta/k_{\rm B}T)$. The dimensionless potential energy $u(\phi)$ is given by

$$u(\phi) = -j\phi - \cos\phi \tag{4.113}$$

and resembles a 'tilted washboard'; see Fig. 4.8(a,b). This is an $N = 2$ dynamical system on a cylinder. Writing $\omega \equiv \dot{\phi}$, we have

$$\frac{d}{ds}\begin{pmatrix}\phi\\ \omega\end{pmatrix} = \begin{pmatrix}\omega\\ j - \sin\phi - Q^{-1}\omega\end{pmatrix} \quad . \tag{4.114}$$

Note that $\phi \in [0, 2\pi]$ while $\omega \in (-\infty, \infty)$. Fixed points satisfy $\omega = 0$ and $j = \sin\phi$. Thus, for $|j| > 1$, there are no fixed points.

Strong damping : The RCSJ model dynamics are given by the second order ODE,

$$\partial_s^2\phi + Q^{-1}\partial_s\phi = -u'(\phi) = j - \sin\phi \quad . \tag{4.115}$$

The parameter $Q = \omega_{\rm p}\tau$ determines the damping, with large Q corresponding to small damping. Consider the large damping limit $Q \ll 1$. In this case the inertial term proportional to $\ddot{\phi}$ may be ignored, and what remains is a first order ODE. Restoring dimensions,

$$\frac{d\phi}{dt} = \Omega\,(j - \sin\phi) \quad , \tag{4.116}$$

where $\Omega = \omega_{\rm p}^2 RC = 2eI_{\rm c}R/\hbar$. We are effectively setting $C \equiv 0$, hence this is known as the RSJ model. The above equation describes a $N = 1$ dynamical system on the circle. When $|j| < 1$, *i.e.* $|I| < I_{\rm c}$, there are two fixed points,

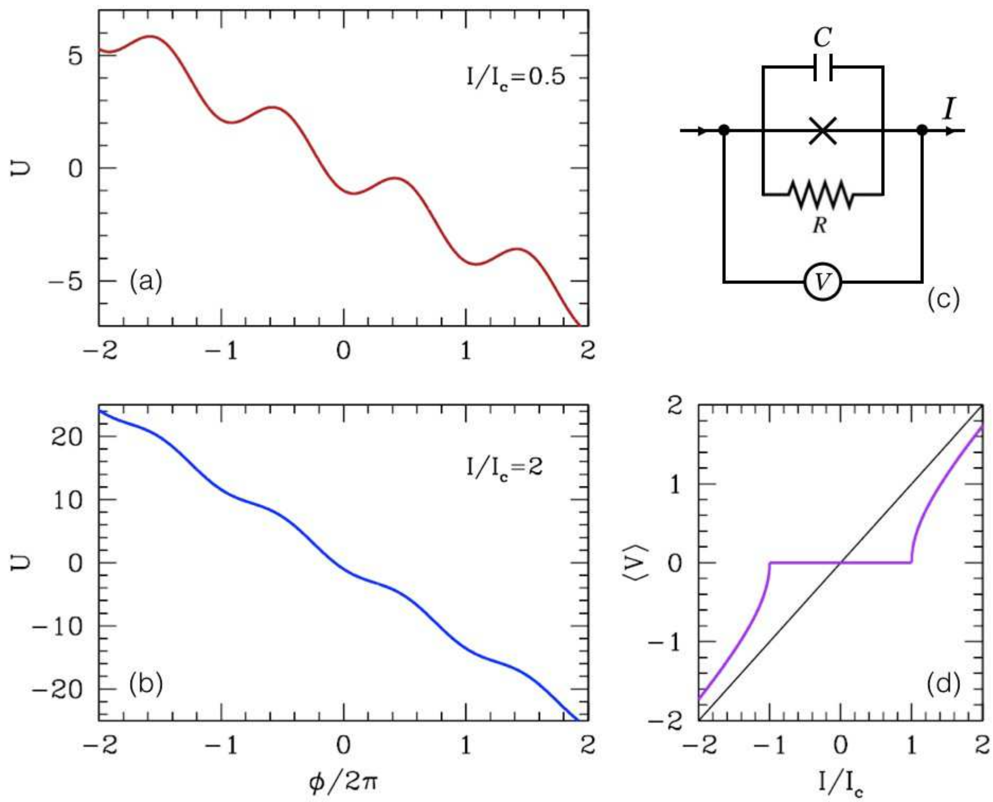

Figure 4.8: (a) Dimensionless washboard potential $u(\phi)$ for $I/I_c = 0.5$. (b) $u(\phi)$ for $I/I_c = 2.0$. (c) The resistively and capacitively shunted Josephson junction (RCSJ). (d) $\langle V\rangle$ *versus* I for the RSJ model.

which are solutions to $\sin\phi^* = j$. The fixed point where $\cos\phi^* > 0$ is stable, while that with $\cos\phi^* < 0$ is unstable. The flow is toward the stable fixed point. At the fixed point, ϕ is constant, which means the voltage $V = \hbar\dot{\phi}/2e$ vanishes. There is current flow with no potential drop.

Consider the case $i > 1$. In this case there is a bottleneck in the ϕ evolution in the vicinity of $\phi = \frac{1}{2}\pi$, where $\dot{\phi}$ is smallest, but $\dot{\phi} > 0$ always. We compute the average voltage

$$\langle V\rangle = \frac{\hbar}{2e}\,\langle\dot{\phi}\rangle = \frac{\hbar}{2e}\cdot\frac{2\pi}{T} \quad , \tag{4.117}$$

where T is the rotational period for $\phi(t)$. We compute this using the equation of motion:

$$\Omega T = \int\limits_0^{2\pi} \frac{d\phi}{j-\sin\phi} = \frac{2\pi}{\sqrt{j^2-1}} \quad . \tag{4.118}$$

Thus,

$$\langle V\rangle = \frac{\hbar}{2e}\sqrt{j^2-1}\cdot\frac{2eI_c R}{\hbar} = R\sqrt{I^2 - I_c^2} \quad . \tag{4.119}$$

This behavior is sketched in Fig. 4.8(d).

<u>*Josephson plasma oscillations*</u> : When $I < I_c$, the phase undergoes damped oscillations in the washboard minima.

Expanding about the fixed point, we write $\phi = \sin^{-1} j + \delta\phi$, and obtain

$$\frac{d^2\delta\phi}{ds^2} + \frac{1}{Q}\,\frac{d\,\delta\phi}{ds} = -\sqrt{1-j^2}\;\delta\phi \quad . \tag{4.120}$$

This is the equation of a damped harmonic oscillator. With no damping ($Q = \infty$), the oscillation frequency is

$$\Omega(I) = \omega_{\rm p}\left(1 - \frac{I^2}{I_{\rm c}^2}\right)^{1/4} \quad . \tag{4.121}$$

When Q is finite, the frequency of the oscillations has an imaginary component, with solutions

$$\omega_{\pm}(I) = -\frac{i\,\omega_{\rm p}}{2Q} \pm \omega_{\rm p}\sqrt{\left(1 - \frac{I^2}{I_{\rm c}^2}\right)^{1/2} - \frac{1}{4Q^2}} \quad . \tag{4.122}$$

Retrapping current in underdamped junctions : The energy of the junction is given by

$$E = \tfrac{1}{2}CV^2 + \frac{\hbar I_{\rm c}}{2e}\,(1-\cos\phi) \quad . \tag{4.123}$$

The first term may be thought of as a kinetic energy and the second as potential energy. Because the system is dissipative, energy is not conserved. Rather,

$$\dot{E} = CV\dot{V} + \frac{\hbar I_{\rm c}}{2e}\,\dot{\phi}\,\sin\phi = V\big(C\dot{V} + I_{\rm c}\sin\phi\big) = V\left(I - \frac{V}{R}\right) \quad . \tag{4.124}$$

Suppose the junction were completely undamped, *i.e.* $R = 0$. Then as the phase slides down the tilted washboard for $|I| < I_{\rm c}$, it moves from peak to peak, picking up speed as it moves along. When $R > 0$, there is energy loss, and $\phi(t)$ might not make it from one peak to the next. Suppose we start at a local maximum $\phi = \pi$ with $V = 0$. What is the energy when ϕ reaches 3π? To answer that, we assume that energy is almost conserved, so

$$E = \tfrac{1}{2}CV^2 + \frac{\hbar I_{\rm c}}{2e}\,(1-\cos\phi) \approx \frac{\hbar I_{\rm c}}{e} \quad \Rightarrow \quad V = \left(\frac{e\hbar I_{\rm c}}{eC}\right)^{1/2}\big|\cos(\tfrac{1}{2}\phi)\big| \quad . \tag{4.125}$$

then

$$\begin{aligned}(\Delta E)_{\rm cycle} &= \int\limits_{-\infty}^{\infty}\!dt\;V\left(I - \frac{V}{R}\right) = \frac{\hbar}{2e}\int\limits_{-\pi}^{\pi}\!d\phi\,\left\{I - \frac{1}{R}\left(\frac{e\hbar I_{\rm c}}{eC}\right)^{1/2}\cos(\tfrac{1}{2}\phi)\right\}\\ &= \frac{\hbar}{2e}\left\{2\pi I - \frac{4}{R}\left(\frac{e\hbar I_{\rm c}}{eC}\right)^{1/2}\right\} = \frac{h}{2e}\left\{I - \frac{4I_{\rm c}}{\pi Q}\right\} \quad .\end{aligned} \tag{4.126}$$

Thus, we identify $I_{\rm r} \equiv 4I_{\rm c}/\pi Q \ll I_{\rm c}$ as the *retrapping current*. The idea here is to focus on the case where the phase evolution is on the cusp between trapped and free. If the system loses energy over the cycle, then subsequent motion will be attenuated, and the phase dynamics will flow to the zero voltage fixed point. Note that if the current I is reduced below $I_{\rm c}$ and then held fixed, eventually the junction will dissipate energy and enter the zero voltage state for any $|I| < I_{\rm c}$. But if the current is swept and $\dot{I}/I$ is faster than the rate of energy dissipation, the retrapping occurs at $I = I_{\rm r}$.

Thermal fluctuations : Restoring the proper units, the potential energy is $U(\phi) = (\hbar I_{\rm c}/2e)\,u(\phi)$. Thus, thermal fluctuations may be ignored provided

$$k_{\rm B}T \ll \frac{\hbar I_{\rm c}}{2e} = \frac{\hbar}{2eR_{\rm N}}\cdot\frac{\pi\Delta}{2e}\,\tanh\!\left(\frac{\Delta}{2k_{\rm B}T}\right) \quad , \tag{4.127}$$

where we have invoked the Ambegaokar-Baratoff formula, Eqn. 4.96. BCS theory gives $\Delta = 1.764\, k_{\rm B}T_{\rm c}$, so we require

$$k_{\rm B}T \ll \frac{h}{8R_{\rm N}e^2} \cdot (1.764\, k_{\rm B}T_{\rm c}) \cdot \tanh\bigg(\frac{0.882\, T_{\rm c}}{T}\bigg) \quad . \tag{4.128}$$

In other words,

$$\frac{R_{\rm N}}{R_{\rm K}} \ll \frac{0.22\, T_{\rm c}}{T}\, \tanh\bigg(\frac{0.882\, T_{\rm c}}{T}\bigg) \quad , \tag{4.129}$$

where $R_{\rm K} = h/e^2 = 25812.8\,\Omega$ is the quantum unit of resistance[6].

We can model the effect of thermal fluctuations by adding a noise term to the RCSJ model, writing

$$C\dot{V} + \frac{V}{R} + I_{\rm c}\sin\phi = I + \frac{V_{\rm f}}{R} \quad , \tag{4.130}$$

where $V_{\rm f}(t)$ is a stochastic term satisfying

$$\big\langle V_{\rm f}(t)\, V_{\rm f}(t')\big\rangle = 2k_{\rm B}TR\,\delta(t-t') \quad . \tag{4.131}$$

Adimensionalizing, we now have

$$\frac{d^2\phi}{ds^2} + \gamma\,\frac{d\phi}{ds} = -\frac{\partial u}{\partial\phi} + \eta(s) \quad , \tag{4.132}$$

where $s = \omega_{\rm p}t$, $\gamma = 1/\omega_{\rm p}RC$, $u(\phi) = -j\phi - \cos\phi$, $j = I/I_{\rm c}(T)$, and

$$\big\langle \eta(s)\,\eta(s')\big\rangle = \frac{2\omega_{\rm p}k_{\rm B}T}{I_{\rm c}^2 R}\,\delta(s-s') \equiv 2\Theta\,\delta(s-s') \quad . \tag{4.133}$$

Thus, $\Theta \equiv \omega_{\rm p}k_{\rm B}T/I_{\rm c}^2R$ is a dimensionless measure of the temperature. Our problem is now that of a damped massive particle moving in the washboard potential and subjected to stochastic forcing due to thermal noise.

Writing $\omega = \partial_s\phi$, we have

$$\begin{aligned} \partial_s\phi &= \omega \\ \partial_s\omega &= -u'(\phi) - \gamma\omega + \sqrt{2\Theta}\,\eta(s) \quad . \end{aligned} \tag{4.134}$$

In this case, $W(s) = \int\limits_0^s ds'\,\eta(s')$ describes a Wiener process: $\big\langle W(s)\,W(s')\big\rangle = \min(s,s')$. The probability distribution $P(\phi,\omega,s)$ then satisfies the Fokker-Planck equation[7],

$$\frac{\partial P}{\partial s} = -\frac{\partial}{\partial\phi}\,(\omega P) + \frac{\partial}{\partial\omega}\Big\{\big[u'(\phi)+\gamma\omega\big]P\Big\} + \Theta\,\frac{\partial^2 P}{\partial\omega^2} \quad . \tag{4.135}$$

We cannot make much progress beyond numerical work starting from this equation. However, if the mean drift velocity of the 'particle' is everywhere small compared with the thermal velocity $v_{\rm th} \propto \sqrt{\Theta}$, and the mean free path $\ell \propto v_{\rm th}/\gamma$ is small compared with the scale of variation of ϕ in the potential $u(\phi)$, then, following the classic treatment by Kramers, we can convert the Fokker-Planck equation for the distribution $P(\phi,\omega,t)$ to the Smoluchowski equation for the distribution $P(\phi,t)$[8]. These conditions are satisfied when the damping γ is

[6] $R_{\rm K}$ is called the *Klitzing* for Klaus von Klitzing, the discoverer of the integer quantum Hall effect.

[7] For the stochastic coupled ODEs $du_a = A_a\,dt + B_{ab}\,dW_b$ where each $W_a(t)$ is an independent Wiener process, *i.e.* $dW_a\,dW_b = \delta_{ab}\,dt$, then, using the Stratonovich stochastic calculus, one has the Fokker-Planck equation $\partial_t P = -\partial_a(A_a P) + \frac{1}{2}\partial_a\big[B_{ac}\,\partial_b(B_{bc}P)\big]$.

[8] See M. Ivanchenko and L. A. Zil'berman, *Sov. Phys. JETP* **28**, 1272 (1969) and, especially, V. Ambegaokar and B. I. Halperin, *Phys. Rev. Lett.* **22**, 1364 (1969).

large. To proceed along these lines, simply assume that ω relaxes quickly, so that $\partial_s \omega \approx 0$ at all times. This says $\omega = -\gamma^{-1} u'(\phi) + \gamma^{-1}\sqrt{2\Theta}\,\eta(s)$. Plugging this into $\partial_s \phi = \omega$, we have

$$\partial_s \phi = -\gamma^{-1} u'(\phi) + \gamma^{-1}\sqrt{2\Theta}\,\eta(s) \quad , \tag{4.136}$$

the Fokker-Planck equation for which is[9]

$$\frac{\partial P(\phi,s)}{\partial s} = \frac{\partial}{\partial\phi}\Big[\gamma^{-1} u'(\phi)\, P(\phi,s)\Big] + \gamma^{-2}\Theta\,\frac{\partial^2 P(\phi,s)}{\partial\phi^2} \quad , \tag{4.137}$$

which is called the Smoluchowski equation. Note that $-\gamma^{-1}u'(\phi)$ plays the role of a local drift velocity, and $\gamma^{-2}\Theta$ that of a diffusion constant. This may be recast as

$$\frac{\partial P}{\partial s} = -\frac{\partial W}{\partial \phi} \qquad , \qquad W(\phi,s) = -\gamma^{-1}\big(\partial_\phi u\big)P - \gamma^{-2}\,\Theta\,\partial_\phi P \quad . \tag{4.138}$$

In steady state, we have that $\partial_s P = 0$, hence W must be a constant. We also demand $P(\phi,s) = P(\phi+2\pi,s)$. To solve, define $F(\phi) \equiv e^{-\gamma\, u(\phi)/\Theta}$. In steady state, we then have

$$\frac{\partial}{\partial\phi}\bigg(\frac{P}{F}\bigg) = -\frac{\gamma^2 W}{\Theta}\cdot\frac{1}{F} \quad . \tag{4.139}$$

Integrating,

$$\begin{aligned}
\frac{P(\phi)}{F(\phi)} - \frac{P(0)}{F(0)} &= -\frac{\gamma^2 W}{\Theta}\int\limits_0^\phi \frac{d\phi'}{F(\phi')}\\
\frac{P(2\pi)}{F(2\pi)} - \frac{P(\phi)}{F(\phi)} &= -\frac{\gamma^2 W}{\Theta}\int\limits_\phi^{2\pi} \frac{d\phi'}{F(\phi')} \quad .
\end{aligned} \tag{4.140}$$

Multiply the first of these by $F(0)$ and the second by $F(2\pi)$, and then add, remembering that $P(2\pi) = P(0)$. One then obtains

$$P(\phi) = \frac{\gamma^2 W}{\Theta}\cdot\frac{F(\phi)}{F(2\pi) - F(0)}\cdot\left\{\int\limits_0^\phi d\phi'\,\frac{F(0)}{F(\phi')} + \int\limits_\phi^{2\pi} d\phi'\,\frac{F(2\pi)}{F(\phi')}\right\} \quad . \tag{4.141}$$

We now are in a position to demand that $P(\phi)$ be normalized. Integrating over the circle, we obtain

$$W = \frac{G(j,\gamma)}{\gamma} \tag{4.142}$$

where

$$\frac{1}{G(j,\gamma/\Theta)} = \frac{\gamma/\Theta}{\exp(\pi\gamma/\Theta) - 1}\left[\int\limits_0^{2\pi} d\phi\, f(\phi)\right]\left[\int\limits_0^{2\pi}\frac{d\phi'}{f(\phi')}\right] + \frac{\gamma}{\Theta}\int\limits_0^{2\pi} d\phi\, f(\phi)\int\limits_\phi^{2\pi}\frac{d\phi'}{f(\phi')} \quad , \tag{4.143}$$

where $f(\phi) \equiv F(\phi)/F(0) = e^{-\gamma\, u(\phi)/\Theta}\, e^{\gamma\, u(0)/\Theta}$ is normalized such that $f(0) = 1$.

It remains to relate the constant W to the voltage. For any function $g(\phi)$, we have

$$\frac{d}{dt}\,\big\langle g\big(\phi(s)\big)\big\rangle = \int\limits_0^{2\pi} d\phi\,\frac{\partial P}{\partial s}\,g(\phi) = -\int\limits_0^{2\pi} d\phi\,\frac{\partial W}{\partial\phi}\,g(\phi) = \int\limits_0^{2\pi} d\phi\, W(\phi)\, g'(\phi) \quad . \tag{4.144}$$

[9]For the stochastic differential equation $dx = v_{\rm d}\,dt + \sqrt{2D}\,dW(t)$, where $W(t)$ is a Wiener process, the Fokker-Planck equation is $\partial_t P = -v_{\rm d}\,\partial_x P + D\,\partial_x^2 P$.

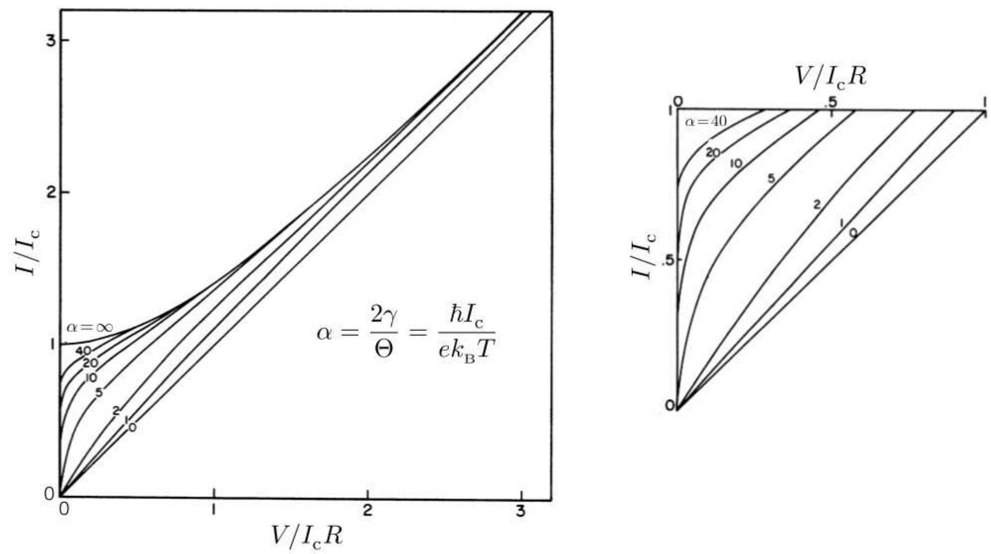

Figure 4.9: Left: scaled current bias $j = I/I_c$ *versus* scaled voltage $v = \langle V \rangle / I_c R$ for different values of the parameter γ/Θ, which is the ratio of damping to temperature. Right: detail of $j(v)$ plots. From Ambegaokar and Halperin (1969).

Technically we should restrict $g(\phi)$ to be periodic, but we can still make sense of this for $g(\phi) = \phi$, with

$$\big\langle \partial_s \phi \big\rangle = \int_0^{2\pi} \! d\phi \, W(\phi) = 2\pi W \quad , \tag{4.145}$$

where the last expression on the RHS holds in steady state, where W is a constant. We could have chosen $g(\phi)$ to be a sawtooth type function, rising linearly on $\phi \in [0, 2\pi)$ then discontinuously dropping to zero, and only considered the parts where the integrands were smooth. Thus, after restoring physical units,

$$v \equiv \frac{\langle V \rangle}{I_c R} = \frac{\hbar \omega_p}{2e I_c R} \, \langle \partial_s \phi \rangle = 2\pi \, G(j, \gamma/\Theta) \quad . \tag{4.146}$$

<u>AC Josephson effect</u> : Suppose we add an AC bias to V, writing

$$V(t) = V_0 + V_1 \sin(\omega_1 t) \quad . \tag{4.147}$$

Integrating the Josephson relation $\dot{\phi} = 2eV/\hbar$, we have

$$\phi(t) = \omega_J \, t + \frac{V_1}{V_0} \frac{\omega_J}{\omega_1} \, \cos(\omega_1 t) + \phi_0 \quad . \tag{4.148}$$

where $\omega_J = 2eV_0/\hbar$. Thus,

$$I_J(t) = I_c \, \sin\!\bigg(\omega_J t + \frac{V_1 \, \omega_J}{V_0 \, \omega_1} \, \cos(\omega_1 t) + \phi_0\bigg) \quad . \tag{4.149}$$

We now invoke the Bessel function generating relation,

$$e^{iz\cos\theta} = \sum_{n=-\infty}^{\infty} J_n(z) \, e^{-in\theta} \tag{4.150}$$

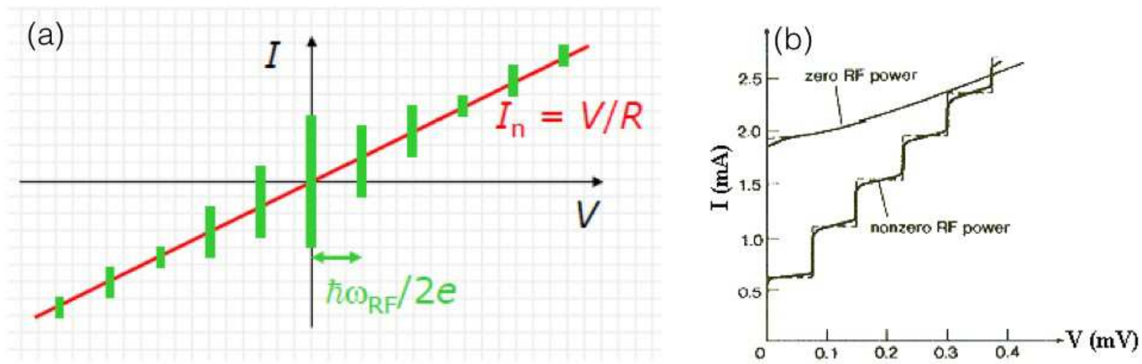

Figure 4.10: (a) Shapiro spikes in the voltage-biased AC Josephson effect. The Josephson current has a nonzero average only when $V_0 = n\hbar\omega_1/2e$, where ω_1 is the AC frequency. From *http://cmt.nbi.ku.dk/student_projects/bsc/heiselberg.pdf*. (b) Shapiro steps in the current-biased AC Josephson effect.

to write

$$I_{\mathrm{J}}(t) = I_{\mathrm{c}} \sum_{n=-\infty}^{\infty} J_n\!\left(\frac{V_1\,\omega_{\mathrm{J}}}{V_0\,\omega_1}\right) \sin\!\big[(\omega_{\mathrm{J}} - n\omega_1)\,t + \phi_0\big] \quad . \tag{4.151}$$

Thus, $I_{\mathrm{J}}(t)$ oscillates in time, except for terms for which

$$\omega_{\mathrm{J}} = n\omega_1 \quad \Rightarrow \quad V_0 = n\,\frac{\hbar\omega_1}{2e} \quad , \tag{4.152}$$

in which case

$$I_{\mathrm{J}}(t) = I_{\mathrm{c}}\, J_n\!\left(\frac{2eV_1}{\hbar\omega_1}\right) \sin\phi_0 \quad . \tag{4.153}$$

We now add back in the current through the resistor, to obtain

$$\begin{aligned} \big\langle I(t) \big\rangle &= \frac{V_0}{R} + I_{\mathrm{c}}\, J_n\!\left(\frac{2eV_1}{\hbar\omega_1}\right) \sin\phi_0 \\ &\in \left[\frac{V_0}{R} - I_{\mathrm{c}}\, J_n\!\left(\frac{2eV_1}{\hbar\omega_1}\right), \frac{V_0}{R} + I_{\mathrm{c}}\, J_n\!\left(\frac{2eV_1}{\hbar\omega_1}\right)\right] \quad . \end{aligned} \tag{4.154}$$

This feature, depicted in Fig. 4.10(a), is known as *Shapiro spikes*.

Current-biased AC Josephson effect : When the junction is current-biased, we must solve

$$\frac{\hbar C}{2e}\,\ddot{\phi} + \frac{\hbar}{2eR}\,\dot{\phi} + I_{\mathrm{c}} \sin\phi = I(t) \quad , \tag{4.155}$$

with $I(t) = I_0 + I_1 \cos(\omega_1 t)$. This results in the *Shapiro steps* shown in Fig. 4.10(b). To analyze this equation, we write our phase space coordinates on the cylinder as $(x_1, x_2) = (\phi, \omega)$, and add the forcing term to Eqn. 4.114, *viz.*

$$\begin{aligned} \frac{d}{dt}\begin{pmatrix} \phi \\ \omega \end{pmatrix} &= \begin{pmatrix} \omega \\ j - \sin\phi - Q^{-1}\omega \end{pmatrix} + \varepsilon \begin{pmatrix} 0 \\ \cos(\nu s) \end{pmatrix} \\ \frac{d\boldsymbol{x}}{ds} &= \boldsymbol{V}(\boldsymbol{x}) + \varepsilon \boldsymbol{f}(\boldsymbol{x}, s) \quad , \end{aligned} \tag{4.156}$$

where $s = \omega_{\mathrm{p}} t$, $\nu = \omega_1/\omega_{\mathrm{p}}$, and $\varepsilon = I_1/I_{\mathrm{c}}$. As before, we have $j = I_0/I_{\mathrm{c}}$. When $\varepsilon = 0$, we have the RCSJ model, which for $|j| > 1$ has a stable limit cycle and no fixed points. The phase curves for the RCSJ model and the limit cycle for $|j| > 1$ are depicted in Fig. 4.7. In our case, the forcing term $\boldsymbol{f}(\boldsymbol{x}, s)$ has the simple form $f_1 = 0$, $f_2 = \cos(\nu s)$, but it could be more complicated and nonlinear in $\boldsymbol{x}$.

The phenomenon we are studying is called *synchronization*[10]. Linear oscillators perturbed by a harmonic force will oscillate with the forcing frequency once transients have damped out. Consider, for example, the equation $\ddot{x} + 2\beta\dot{x} + \omega_0^2 x = f_0 \cos(\Omega t)$, where $\beta > 0$ is a damping coefficient. The solution is $x(t) = A(\Omega)\,\cos\big(\Omega t + \delta(\Omega)\big) + x_{\mathrm{h}}(t)$, where $x_{\mathrm{h}}(t)$ solves the homogeneous equation (*i.e.* with $f_0 = 0$) and decays to zero exponentially at large times. Nonlinear oscillators, such as the RCSJ model under study here, also can be synchronized to the external forcing, but not necessarily always. In the case of the Duffing oscillator, $\ddot{x} + 2\beta\dot{x} + x + \eta x^3$, with $\beta > 0$ and $\eta > 0$, the origin $(x = 0, \dot{x} = 0)$ is still a stable fixed point. In the presence of an external forcing $\varepsilon\, f_0 \cos(\Omega t)$, with β, η, and ε all small, varying the detuning $\delta\Omega = \Omega - 1$ (also assumed small) can lead to hysteresis in the amplitude of the oscillations, but the oscillator is always entrained, *i.e.* synchronized with the external forcing.

The situation changes considerably if the nonlinear oscillator has no stable fixed point but rather a stable limit cycle. This is the case, for example, for the van der Pol equation $\ddot{x} + 2\beta(x^2 - 1)\dot{x} + x = 0$, and it is also the case for the RCSJ model. The limit cycle $\boldsymbol{x}_0(s)$ has a period, which we call T_0, so $\boldsymbol{x}(s + T_0) = \boldsymbol{x}(s)$. All points on the limit cycle (LC) are fixed under the T_0-advance map g_{T_0}, where $g_\tau \boldsymbol{x}(s) = \boldsymbol{x}(s + \tau)$. We may parameterize points along the LC by an angle θ which increases uniformly in s, so that $\dot{\theta} = \nu_0 = 2\pi/T_0$. Furthermore, since each point $\boldsymbol{x}_0(\theta)$ is a fixed point under g_{T_0}, and the LC is presumed to be attractive, we may define the θ*-isochrone* as the set of points $\{\boldsymbol{x}\}$ in phase space which flow to $\boldsymbol{x}_0(\theta)$ under repeated application of g_{T_0}. For an N-dimensional phase space, the isochrones are $(N-1)$-dimensional hypersurfaces. For the RCSJ model, which has $N = 2$, the isochrones are curves $\theta = \theta(\phi, \omega)$ on the (ϕ, ω) cylinder. In particular, the θ-isochrone is a curve which intersects the LC at the point $\boldsymbol{x}_0(\theta)$. We then have

$$\begin{aligned}\frac{d\theta}{ds} &= \sum_{j=1}^{N} \frac{\partial\theta}{\partial x_j}\,\frac{dx_j}{ds} \\ &= \nu_0 + \varepsilon \sum_{j=1}^{N} \frac{\partial\theta}{\partial x_j}\, f_j\big(\boldsymbol{x}(s), s\big) \quad .\end{aligned} \tag{4.157}$$

If we are close to the LC, we may replace $\boldsymbol{x}(s)$ on the RHS above with $\boldsymbol{x}_0(\theta)$, yielding

$$\frac{d\theta}{ds} = \nu_0 + \varepsilon F(\theta, s) \quad , \tag{4.158}$$

where

$$F(\theta, s) = \sum_{j=1}^{N} \frac{\partial\theta}{\partial x_j}\bigg|_{\boldsymbol{x}_0(\theta)} f_j\big(\boldsymbol{x}_0(\theta), s\big) \quad . \tag{4.159}$$

OK, so now here's the thing. The function $F(\theta, s)$ is separately periodic in both its arguments, so we may write

$$F(\theta, s) = \sum_{k,l} F_{k,l}\, e^{i(k\theta + l\nu s)} \quad , \tag{4.160}$$

where $\boldsymbol{f}\big(\boldsymbol{x}, s + \frac{2\pi}{\nu}\big) = \boldsymbol{f}(\boldsymbol{x}, s)$, *i.e.* ν is the forcing frequency. The unperturbed solution has $\dot{\theta} = \nu_0$, hence the forcing term in Eqn. 4.158 is resonant when $k\nu_0 + l\nu \approx 0$. This occurs when $\nu \approx \frac{p}{q}\,\nu_0$, where p and q are relatively prime integers. The resonance condition is satisfied when $k = rp$ and $l = -rq$ for any integer r.

[10]See A. Pikovsky, M. Rosenblum, and J. Kurths, *Synchronization* (Cambridge, 2001).

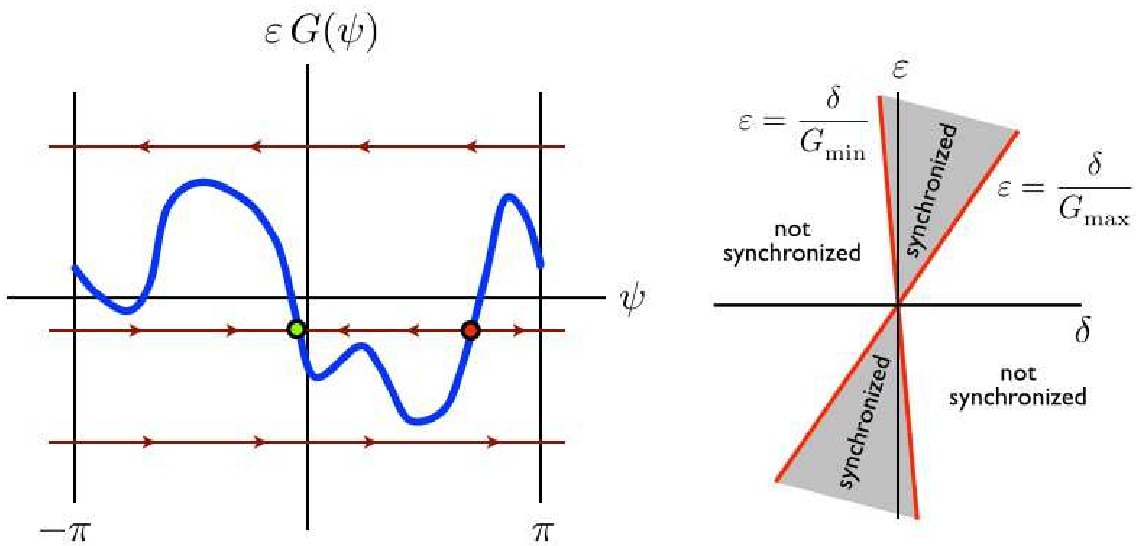

Figure 4.11: Left: graphical solution of $\dot{\psi} = -\delta + \varepsilon\, G(\psi)$. Fixed points are only possible if $-\varepsilon\, G_{\rm min} \le \delta \le G_{\rm max}$. Right: synchronization region, shown in grey, in the (δ, ε) plane.

We now separate the resonant from nonresonant terms in the (k,l) sum, writing

$$\dot{\theta} = \nu_0 + \varepsilon \sum_{r=-\infty}^{\infty} F_{rp,-rq}\, e^{ir(p\theta - q\nu s)} + \text{NRT} \quad , \tag{4.161}$$

where NRT stands for "non-resonant terms". We next average over short time scales to eliminate these nonresonant terms, and focus on the dynamics of the average phase $\langle\theta\rangle$. Defining $\psi \equiv p\,\langle\theta\rangle - q\,\nu s$, we have

$$\begin{aligned}\dot{\psi} &= p\,\langle\dot{\theta}\rangle - q\nu \\ &= (p\nu_0 - q\nu) + \varepsilon p \sum_{r=-\infty}^{\infty} F_{rp,-rq}\, e^{ir\psi} \\ &= -\delta + \varepsilon\, G(\psi) \quad ,\end{aligned} \tag{4.162}$$

where $\delta \equiv q\nu - p\nu_0$ is the detuning, and $G(\psi) \equiv p\sum_r F_{rp,-rq}\, e^{ir\psi}$ is the sum over resonant terms. This last equation is that of a simple $N=1$ dynamical system on the circle! If the detuning δ falls within the range $\big[\varepsilon G_{\rm min}\,,\, \varepsilon G_{\rm max}\big]$, then ψ flows to a stable fixed point where $\delta = \varepsilon\, G(\psi^*)$. The oscillator is then synchronized with the forcing, because $\langle\dot{\theta}\rangle \to \frac{q}{p}\,\nu$. If the detuning is too large and lies outside this range, then there is no synchronization. Rather, $\psi(s)$ increases linearly with the time s, and $\langle\theta(t)\rangle = \theta_0 + \frac{q}{p}\,\nu s + \frac{1}{p}\,\psi(s)$, where

$$dt = \frac{d\psi}{\varepsilon\, G(\psi) - \delta} \qquad \Longrightarrow \qquad T_\psi = \int_0^{2\pi} \frac{d\psi}{\varepsilon\, G(\psi) - \delta} \quad . \tag{4.163}$$

For weakly forced, weakly nonlinear oscillators, resonance occurs only for $\nu = \pm\nu_0$, but in the case of weakly forced, strongly nonlinear oscillators, the general resonance condition is $\nu = \frac{p}{q}\,\nu_0$. The reason is that in the case of weakly nonlinear oscillators, the limit cycle is itself harmonic to zeroth order. There are then only two frequencies in its Fourier decomposition, *i.e.* $\pm\nu_0$. In the strongly nonlinear case, the limit cycle is decomposed into a fundamental frequency ν_0 plus all its harmonics. In addition, the forcing $\boldsymbol{f}(\boldsymbol{x}, s)$ can itself can be a general periodic function of s, involving multiples of the fundamental forcing frequency ν. For the case of the RCSJ, the forcing function is harmonic and independent of $\boldsymbol{x}$. This means that only the $l=\pm 1$ terms enter in the above analysis.

4.4 Ultrasonic Attenuation

Recall the electron-phonon Hamiltonian,

$$\begin{aligned}\hat{H}_{\text{el}-\text{ph}} &= \frac{1}{\sqrt{V}} \sum_{\substack{\boldsymbol{k},\boldsymbol{k}'\\ \sigma,\lambda}} g_{\boldsymbol{k}\boldsymbol{k}'\lambda}\,\big(a^\dagger_{\boldsymbol{k}'-\boldsymbol{k},\lambda} + a_{\boldsymbol{k}-\boldsymbol{k}',\lambda}\big) c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}'\sigma} \\ &= \frac{1}{\sqrt{V}} \sum_{\substack{\boldsymbol{k},\boldsymbol{k}\\ \sigma,\lambda}} g_{\boldsymbol{k}\boldsymbol{k}'\lambda}\big(a^\dagger_{\boldsymbol{k}'-\boldsymbol{k},\lambda} + a_{\boldsymbol{k}-\boldsymbol{k}',\lambda}\big)\big(u_{\boldsymbol{k}}\gamma^\dagger_{\boldsymbol{k}\sigma} - \sigma\, e^{-i\phi}\, v_{\boldsymbol{k}}\,\gamma_{-\boldsymbol{k}\,-\sigma}\big)\big(u_{\boldsymbol{k}'}\gamma_{\boldsymbol{k}'\sigma} - \sigma\, e^{i\phi}\, v_{\boldsymbol{k}'}\,\gamma^\dagger_{-\boldsymbol{k}'\,-\sigma}\big)\ .\end{aligned} \tag{4.164}$$

Let's now compute the phonon lifetime using Fermi's Golden Rule[11]. In the phonon absorption process, a phonon of wavevector $\boldsymbol{q}$ is absorbed by an electron of wavevector $\boldsymbol{k}$, converting it into an electron of wavevector $\boldsymbol{k}'=\boldsymbol{k}+\boldsymbol{q}$. The net absorption rate of $(\boldsymbol{q},\lambda)$ phonons is then is given by the rate of

$$\varGamma^{\text{abs}}_{\boldsymbol{q}\lambda} = \frac{2\pi n_{\boldsymbol{q},\lambda}}{V} \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} \big|g_{\boldsymbol{k}\boldsymbol{k}'\lambda}\big|^2 \big(u_{\boldsymbol{k}}u_{\boldsymbol{k}'} - v_{\boldsymbol{k}}v_{\boldsymbol{k}'}\big)^2 f_{\boldsymbol{k}\sigma}\,\big(1-f_{\boldsymbol{k}'\sigma}\big)\,\delta(E_{\boldsymbol{k}'} - E_{\boldsymbol{k}} - \hbar\omega_{\boldsymbol{q}\lambda})\,\delta_{\boldsymbol{k}',\boldsymbol{k}+\boldsymbol{q}\,\text{mod}\,\boldsymbol{G}}\quad . \tag{4.165}$$

Here $n_{\boldsymbol{q}\lambda}$ is the Bose function and $f_{\boldsymbol{k}\sigma}$ the Fermi function, and we have assumed that the phonon frequencies are all smaller than 2Δ, so we may ignore quasiparticle pair creation and pair annihilation processes. Note that the electron Fermi factors yield the probability that the state $|\boldsymbol{k}\sigma\rangle$ is occupied while $|\boldsymbol{k}'\sigma\rangle$ is vacant. *Mutatis mutandis*, the emission rate of these phonons is[12]

$$\varGamma^{\text{em}}_{\boldsymbol{q}\lambda} = \frac{2\pi (n_{\boldsymbol{q},\lambda}+1)}{V} \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} \big|g_{\boldsymbol{k}\boldsymbol{k}'\lambda}\big|^2 \big(u_{\boldsymbol{k}}u_{\boldsymbol{k}'} - v_{\boldsymbol{k}}v_{\boldsymbol{k}'}\big)^2 f_{\boldsymbol{k}'\sigma}\,\big(1-f_{\boldsymbol{k}\sigma}\big)\,\delta(E_{\boldsymbol{k}'} - E_{\boldsymbol{k}} - \hbar\omega_{\boldsymbol{q}\lambda})\,\delta_{\boldsymbol{k}',\boldsymbol{k}+\boldsymbol{q}\,\text{mod}\,\boldsymbol{G}}\quad . \tag{4.166}$$

We then have

$$\frac{dn_{\boldsymbol{q}\lambda}}{dt} = -\alpha_{\boldsymbol{q}\lambda}\, n_{\boldsymbol{q}\lambda} + s_{\boldsymbol{q}\lambda}\quad , \tag{4.167}$$

where

$$\alpha_{\boldsymbol{q}\lambda} = \frac{4\pi}{V} \sum_{\boldsymbol{k},\boldsymbol{k}'} \big|g_{\boldsymbol{k}\boldsymbol{k}'\lambda}\big|^2 \big(u_{\boldsymbol{k}}u_{\boldsymbol{k}'} - v_{\boldsymbol{k}}v_{\boldsymbol{k}'}\big)^2\,\big(f_{\boldsymbol{k}} - f_{\boldsymbol{k}'}\big)\,\delta(E_{\boldsymbol{k}'} - E_{\boldsymbol{k}} - \hbar\omega_{\boldsymbol{q}\lambda})\,\delta_{\boldsymbol{k}',\boldsymbol{k}+\boldsymbol{q}\,\text{mod}\,\boldsymbol{G}} \tag{4.168}$$

is the attenuation rate, and $s_{\boldsymbol{q}\lambda}$ is due to spontaneous emission.

We now expand about the Fermi surface, writing

$$\frac{1}{V}\sum_{\boldsymbol{k},\boldsymbol{k}'} F(\xi_{\boldsymbol{k}},\xi_{\boldsymbol{k}'})\,\delta_{\boldsymbol{k}',\boldsymbol{k}+\boldsymbol{q}} = \tfrac{1}{4}\,g^2(\mu)\int\limits_{-\infty}^{\infty}\! d\xi \int\limits_{-\infty}^{\infty}\! d\xi'\, F(\xi,\xi')\int\!\frac{d\hat{\boldsymbol{k}}}{4\pi}\int\!\frac{d\hat{\boldsymbol{k}}'}{4\pi}\,\delta(k_{\text{F}}\hat{\boldsymbol{k}}' - k_{\text{F}}\hat{\boldsymbol{k}} - \boldsymbol{q})\ . \tag{4.169}$$

for any function $F(\xi,\xi')$. The integrals over $\hat{\boldsymbol{k}}$ and $\hat{\boldsymbol{k}}'$ give

$$\int\!\frac{d\hat{\boldsymbol{k}}}{4\pi}\int\!\frac{d\hat{\boldsymbol{k}}'}{4\pi}\,\delta(k_{\text{F}}\hat{\boldsymbol{k}}' - k_{\text{F}}\hat{\boldsymbol{k}} - \boldsymbol{q}) = \frac{1}{4\pi k_{\text{F}}^3}\cdot\frac{k_{\text{F}}}{2q}\cdot\Theta(2k_{\text{F}} - q)\quad . \tag{4.170}$$

[11] Here we follow §3.4 of J. R. Schrieffer, *Theory of Superconductivity* (Benjamin-Cummings, 1964).

[12] Note the factor of $n+1$ in the emission rate, where the additional 1 is due to spontaneous emission. The absorption rate includes only a factor of n.

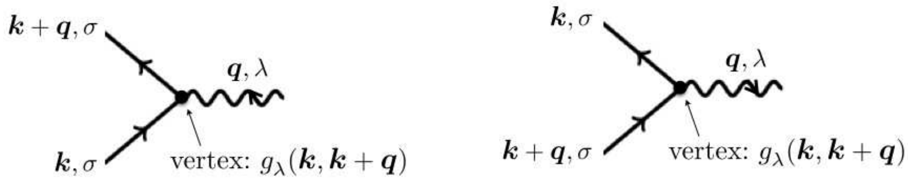

Figure 4.12: Phonon absorption and emission processes.

The step function appears naturally because the constraint $k_{\rm F}\hat{\boldsymbol{k}}' = k_{\rm F}\hat{\boldsymbol{k}} + \boldsymbol{q}$ requires that $\boldsymbol{q}$ connect two points which lie on the metallic Fermi surface, so the largest $|\boldsymbol{q}|$ can be is $2k_{\rm F}$. We will drop the step function in the following expressions, assuming $q < 2k_{\rm F}$, but it is good to remember that it is implicitly present. Thus, ignoring *Umklapp* processes, we have

$$\alpha_{\boldsymbol{q}\lambda} = \frac{g^2(\mu)\,|g_{\boldsymbol{q}\lambda}|^2}{8\,k_{\rm F}^2\,q}\int\limits_{-\infty}^{\infty}\!d\xi\int\limits_{-\infty}^{\infty}\!d\xi'\,(uu'-vv')^2\,(f-f')\,\delta(E'-E-\hbar\omega_{\boldsymbol{q}\lambda}) \quad . \tag{4.171}$$

We now use

$$\begin{aligned}(uu' \pm vv')^2 &= \left(\sqrt{\frac{E+\xi}{2E}}\sqrt{\frac{E'+\xi'}{2E'}} \pm \sqrt{\frac{E-\xi}{2E}}\sqrt{\frac{E'-\xi'}{2E'}}\right)^2 \\ &= \frac{EE'+\xi\xi'\pm\Delta^2}{EE'}\end{aligned} \tag{4.172}$$

and change variables $\big(\xi = E\,dE/\sqrt{E^2-\Delta^2}\,\big)$ to write

$$\alpha_{\boldsymbol{q}\lambda} = \frac{g^2(\mu)\,|g_{\boldsymbol{q}\lambda}|^2}{2\,k_{\rm F}^2\,q}\int\limits_{\Delta}^{\infty}\!dE\int\limits_{\Delta}^{\infty}\!dE'\,\frac{(EE'-\Delta^2)(f-f')}{\sqrt{E^2-\Delta^2}\,\sqrt{E'^{\,2}-\Delta^2}}\,\delta(E'-E-\hbar\omega_{\boldsymbol{q}\lambda}) \quad . \tag{4.173}$$

We now satisfy the Dirac delta function, which means we eliminate the E' integral and set $E' = E + \hbar\omega_{\boldsymbol{q}\lambda}$ everywhere else in the integrand. Clearly the $f - f'$ term will be first order in the smallness of $\hbar\omega_{\boldsymbol{q}}$, so in all other places we may set $E' = E$ to lowest order. This simplifies the above expression considerably, and we are left with

$$\alpha_{\boldsymbol{q}\lambda} = \frac{g^2(\mu)\,|g_{\boldsymbol{q}\lambda}|^2\,\hbar\omega_{\boldsymbol{q}\lambda}}{2\,k_{\rm F}^2\,q}\int\limits_{\Delta}^{\infty}\!dE\left(-\frac{\partial f}{\partial E}\right) = \frac{g^2(\mu)\,|g_{\boldsymbol{q}\lambda}|^2\,\hbar\omega_{\boldsymbol{q}\lambda}}{2\,k_{\rm F}^2\,q}\,f(\Delta) \quad , \tag{4.174}$$

where $q < 2k_{\rm F}$ is assumed. For $q \to 0$, we have $\omega_{\boldsymbol{q}\lambda}/q \to c_\lambda(\hat{\boldsymbol{q}})$, the phonon velocity.

We may now write the ratio of the phonon attenuation rate in the superconducting and normal states as

$$\frac{\alpha_{\rm S}(T)}{\alpha_{\rm N}(T)} = \frac{f(\Delta)}{f(0)} = \frac{2}{\exp\!\left(\frac{\Delta(T)}{k_{\rm B}T}\right)+1} \quad . \tag{4.175}$$

The ratio naturally goes to unity at $T = T_Rc$, where Δ vanishes. Results from early experiments on superconducting Sn are shown in Fig. 4.13.

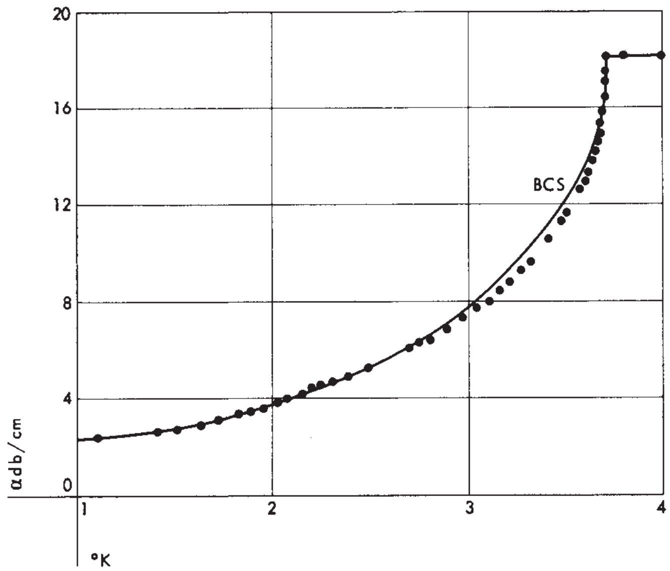

Figure 4.13: Ultrasonic attenuation in tin, compared with predictions of the BCS theory. From R. W. Morse, *IBM Jour. Res. Dev.* **6**, 58 (1963).

4.5 Nuclear Magnetic Relaxation

We start with the hyperfine Hamiltonian,

$$\hat{H}_{\rm HF} = A \sum_{\boldsymbol{k},\boldsymbol{k}'} \sum_{\boldsymbol{R}} \varphi^*_{\boldsymbol{k}}(\boldsymbol{R})\, \varphi_{\boldsymbol{k}'}(\boldsymbol{R}) \Big[J^+_{\boldsymbol{R}}\, c^\dagger_{\boldsymbol{k}\downarrow}\, c_{\boldsymbol{k}'\uparrow} + J^-_{\boldsymbol{R}}\, c^\dagger_{\boldsymbol{k}\uparrow}\, c_{\boldsymbol{k}'\downarrow} + J^z_{\boldsymbol{R}} \big(c^\dagger_{\boldsymbol{k}\uparrow}\, c_{\boldsymbol{k}'\uparrow} - c^\dagger_{\boldsymbol{k}\downarrow}\, c_{\boldsymbol{k}'\downarrow} \big) \Big] \tag{4.176}$$

where $\boldsymbol{J}_{\boldsymbol{R}}$ is the nuclear spin operator on nuclear site $\boldsymbol{R}$, satisfying

$$\big[J^\mu_{\boldsymbol{R}}\, ,\, J^\nu_{\boldsymbol{R}'} \big] = i\, \epsilon_{\mu\nu\lambda}\, J^\lambda_{\boldsymbol{R}}\, \delta_{\boldsymbol{R},\boldsymbol{R}'} \quad , \tag{4.177}$$

and where $\varphi_{\boldsymbol{k}}(\boldsymbol{R})$ is the amplitude of the electronic Bloch wavefunction (with band index suppressed) on the nuclear site $\boldsymbol{R}$. Using

$$c_{\boldsymbol{k}\sigma} = u_{\boldsymbol{k}}\, \gamma_{\boldsymbol{k}\sigma} - \sigma\, v_{\boldsymbol{k}}\, e^{i\phi}\, \gamma^\dagger_{-\boldsymbol{k}\,-\sigma} \tag{4.178}$$

we have for $\boldsymbol{S}_{\boldsymbol{k}\boldsymbol{k}'} = \frac{1}{2}\, c^\dagger_{\boldsymbol{k}\mu}\, \boldsymbol{\sigma}_{\mu\nu}\, c_{\boldsymbol{k}'\nu}$,

$$\begin{aligned}
S^+_{\boldsymbol{k}\boldsymbol{k}'} &= u_{\boldsymbol{k}} u_{\boldsymbol{k}'} \gamma^\dagger_{\boldsymbol{k}\uparrow} \gamma_{\boldsymbol{k}'\downarrow} - v_{\boldsymbol{k}} v_{\boldsymbol{k}'}\, \gamma_{-\boldsymbol{k}\downarrow} \gamma^\dagger_{-\boldsymbol{k}'\uparrow} + u_{\boldsymbol{k}} v_{\boldsymbol{k}'}\, e^{i\phi}\, \gamma^\dagger_{\boldsymbol{k}\uparrow} \gamma^\dagger_{-\boldsymbol{k}'\uparrow} - u_{\boldsymbol{k}} v_{\boldsymbol{k}'}\, e^{-i\phi}\, \gamma_{-\boldsymbol{k}\downarrow} \gamma_{\boldsymbol{k}'\downarrow} \\
S^-_{\boldsymbol{k}\boldsymbol{k}'} &= u_{\boldsymbol{k}} u_{\boldsymbol{k}'} \gamma^\dagger_{\boldsymbol{k}\downarrow} \gamma_{\boldsymbol{k}'\uparrow} - v_{\boldsymbol{k}} v_{\boldsymbol{k}'}\, \gamma_{-\boldsymbol{k}\uparrow} \gamma^\dagger_{-\boldsymbol{k}'\downarrow} - u_{\boldsymbol{k}} v_{\boldsymbol{k}'}\, e^{i\phi}\, \gamma^\dagger_{\boldsymbol{k}\downarrow} \gamma^\dagger_{-\boldsymbol{k}'\downarrow} + u_{\boldsymbol{k}} v_{\boldsymbol{k}'}\, e^{-i\phi}\, \gamma_{-\boldsymbol{k}\uparrow} \gamma_{\boldsymbol{k}'\uparrow} \\
S^z_{\boldsymbol{k}\boldsymbol{k}'} &= \tfrac{1}{2} \sum_\sigma \Big(u_{\boldsymbol{k}} u_{\boldsymbol{k}'}\, \gamma^\dagger_{\boldsymbol{k}\sigma} \gamma_{\boldsymbol{k}'\sigma} + v_{\boldsymbol{k}} v_{\boldsymbol{k}'}\, \gamma_{-\boldsymbol{k}\,-\sigma} \gamma^\dagger_{-\boldsymbol{k}'\,-\sigma} - \sigma\, u_{\boldsymbol{k}} v_{\boldsymbol{k}'}\;\, e^{i\phi}\, \gamma^\dagger_{\boldsymbol{k}\sigma} \gamma^\dagger_{-\boldsymbol{k}'\,-\sigma} - \sigma\, v_{\boldsymbol{k}} u_{\boldsymbol{k}'}\;\, e^{-i\phi}\, \gamma_{-\boldsymbol{k}\,-\sigma} \gamma_{\boldsymbol{k}'\sigma} \Big) \ .
\end{aligned} \tag{4.179}$$

Let's assume our nuclei are initially spin polarized, and let us calculate the rate $1/T_1$ at which the J^z component of the nuclear spin relaxes. Again appealing to the Golden Rule,

$$\frac{1}{T_1} = 2\pi\, |A|^2 \sum_{\boldsymbol{k},\boldsymbol{k}'} |\varphi_{\boldsymbol{k}}(0)|^2\, |\varphi_{\boldsymbol{k}'}(0)|^2\, \big(u_{\boldsymbol{k}} u_{\boldsymbol{k}'} + v_{\boldsymbol{k}} v_{\boldsymbol{k}'}\big)^2 f_{\boldsymbol{k}} \big(1 - f_{\boldsymbol{k}'}\big)\, \delta(E_{\boldsymbol{k}'} - E_{\boldsymbol{k}} - \hbar\omega) \tag{4.180}$$

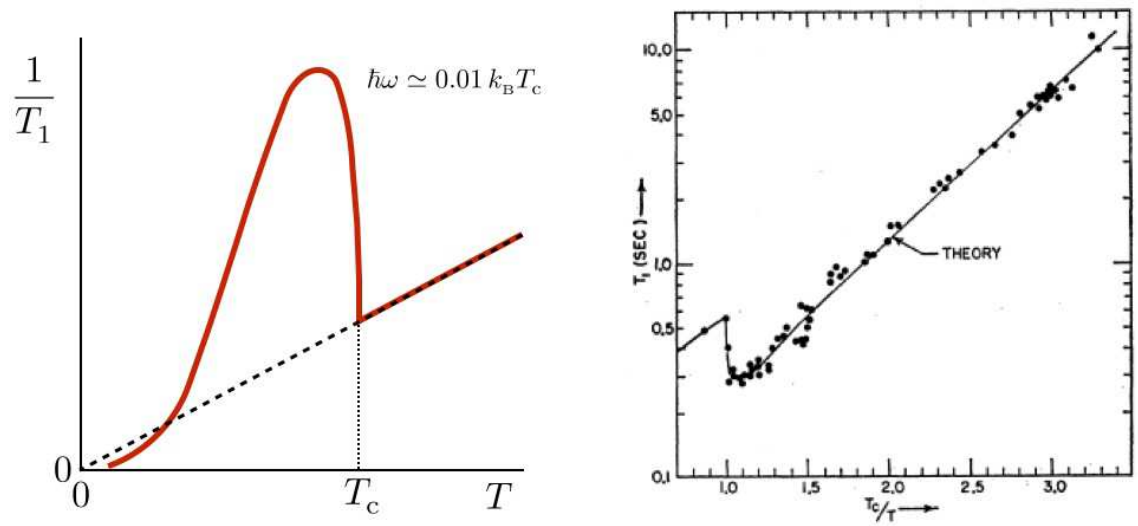

Figure 4.14: Left: Sketch of NMR relaxation rate $1/T_1$ *versus* temperature as predicted by BCS theory, with $\hbar\omega \approx 0.01\,k_{\rm B}T_{\rm c}$, showing the Hebel-Slichter peak. Right: T_1 *versus* $T_{\rm c}/T$ in a powdered aluminum sample, from Y. Masuda and A. G. Redfield, *Phys. Rev.* **125**, 159 (1962). The Hebel-Slichter peak is seen here as a dip.

where ω is the nuclear spin precession frequency in the presence of internal or external magnetic fields. Assuming $\varphi_{\boldsymbol{k}}(\boldsymbol{R}) = C/\sqrt{V}$, we write $V^{-1}\sum_{\boldsymbol{k}} \to \frac{1}{2}g(\mu)\int d\xi$ and we appeal to Eqn. 4.172. Note that the coherence factors in this case give $(uu'+vv')^2$, as opposed to $(uu'-vv')^2$ as we found in the case of ultrasonic attenuation (more on this below). What we then obtain is

$$\frac{1}{T_1} = 2\pi\,|A|^2\,|C|^4\,g^2(\mu)\int\limits_{\Delta}^{\infty}\!dE\,\frac{E(E+\hbar\omega)+\Delta^2}{\sqrt{E^2-\Delta^2}\,\sqrt{(E+\hbar\omega)^2-\Delta^2}}\,f(E)\,\big[1-f(E+\hbar\omega)\big] \quad . \tag{4.181}$$

Let's first evaluate this expression for normal metals, where $\Delta = 0$. We have

$$\frac{1}{T_{1,\rm N}} = 2\pi\,|A|^2\,|C|^4\,g^2(\mu)\int\limits_{0}^{\infty}\!d\xi\,f(\xi)\big[1-f(\xi+\hbar\omega)\big] = \pi\,|A|^2\,|C|^4\,g^2(\mu)\,k_{\rm B}T \quad , \tag{4.182}$$

where we have assumed $\hbar\omega \ll k_{\rm B}T$, and used $f(\xi)\big[1-f(\xi)\big] = -k_{\rm B}T\,f'(\xi)$. The assumption $\omega \to 0$ is appropriate because the nuclear magneton is so tiny: $\mu_{\rm N}/k_{\rm B} = 3.66\times10^{-4}{\rm K/T}$, so the nuclear splitting is on the order of mK even at fields as high as 10 T. The NMR relaxation rate is thus proportional to temperature, a result known as the *Korringa law*.

Now let's evaluate the ratio of NMR relaxation rates in the superconducting and normal states. Assuming $\hbar\omega \ll \Delta$, we have

$$\frac{T_{1,\rm s}^{-1}}{T_{1,\rm N}^{-1}} = 2\int\limits_{\Delta}^{\infty}\!dE\,\frac{E(E+\hbar\omega)+\Delta^2}{\sqrt{E^2-\Delta^2}\,\sqrt{(E+\hbar\omega)^2-\Delta^2}}\left(-\frac{\partial f}{\partial E}\right) \quad . \tag{4.183}$$

We dare not send $\omega \to 0$ in the integrand, because this would lead to a logarithmic divergence. Numerical integration shows that for $\hbar\omega \lesssim \frac{1}{2}k_{\rm B}T_{\rm c}$, the above expression has a peak just below $T = T_{\rm c}$. This is the famous *Hebel-Slichter peak*.

These results for acoustic attenuation and spin relaxation exemplify so-called *case I* and *case II* responses of the superconductor, respectively. In case I, the transition matrix element is proportional to $uu' - vv'$, which vanishes at $\xi = 0$. In case II, the transition matrix element is proportional to $uu' + vv'$.

4.6 General Theory of BCS Linear Response

Consider a general probe of the superconducting state described by the perturbation Hamiltonian

$$\hat{V}(t) = \sum_{\boldsymbol{k},\sigma} \sum_{\boldsymbol{k}',\sigma'} \Big[B\big(\boldsymbol{k}\sigma \,|\, \boldsymbol{k}'\sigma'\big)\, e^{-i\omega t} + B^*\big(\boldsymbol{k}'\sigma' \,|\, \boldsymbol{k}\sigma\big)\, e^{+i\omega t} \Big] c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}'\sigma'} \quad . \tag{4.184}$$

An example would be ultrasonic attenuation, where

$$\hat{V}_{\text{ultra}}(t) = U \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} \phi_{\boldsymbol{k}'-\boldsymbol{k}}(t)\, c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}'\sigma'} \quad . \tag{4.185}$$

Here $\phi(\boldsymbol{r}) = \nabla \cdot \boldsymbol{u}$ is the deformation of the lattice and U is the deformation potential, with the interaction of the local deformation with the electrons given by $U\phi(\boldsymbol{r})\, n(\boldsymbol{r})$, where $n(\boldsymbol{r})$ is the total electron number density at $\boldsymbol{r}$. Another example is interaction with microwaves. In this case, the bare dispersion is corrected by $\boldsymbol{p} \to \boldsymbol{p} + \frac{e}{c}\boldsymbol{A}$, hence

$$\hat{V}_{\mu\text{wave}}(t) = \frac{e\hbar}{2m^* c} \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} (\boldsymbol{k} + \boldsymbol{k}') \cdot \boldsymbol{A}_{\boldsymbol{k}'-\boldsymbol{k}}(t)\, c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}'\sigma'} \quad , \tag{4.186}$$

where m^* is the band mass.

Consider now a general perturbation Hamiltonian of the form

$$\hat{V} = -\sum_i \big(\phi_i(t)\, C_i^\dagger + \phi_i^*(t)\, C_i \big) \tag{4.187}$$

where C_i are operators labeled by i. We write

$$\phi_i(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \hat{\phi}_i(\omega)\, e^{-i\omega t} \quad . \tag{4.188}$$

According to the general theory of linear response formulated in chapter 2, the power dissipation due to this perturbation is given by

$$\begin{aligned} P(\omega) = &-i\omega\, \hat{\phi}_i^*(\omega)\, \hat{\phi}_j(\omega)\, \hat{\chi}_{C_i C_j^\dagger}(\omega) + i\omega\, \hat{\phi}_i(\omega)\, \hat{\phi}_j^*(\omega)\, \hat{\chi}_{C_i^\dagger C_j}(-\omega) \\ &- i\omega\, \hat{\phi}_i^*(\omega)\, \hat{\phi}_j^*(-\omega)\, \hat{\chi}_{C_i C_j}(\omega) + i\omega\, \hat{\phi}_i(\omega)\, \hat{\phi}_j(-\omega)\, \hat{\chi}_{C_i^\dagger C_j^\dagger}(-\omega) \quad . \end{aligned} \tag{4.189}$$

where $\hat{H} = \hat{H}_0 + \hat{V}$ and $C_i(t) = e^{i\hat{H}_0 t/\hbar}\, C_i\, e^{-i\hat{H}_0 t/\hbar}$ is the operator C_i in the interaction representation.

$$\hat{\chi}_{AB}(\omega) = \frac{i}{\hbar} \int_0^\infty dt\, e^{-i\omega t}\, \big\langle \big[A(t)\, ,\, B(0) \big] \big\rangle \tag{4.190}$$

For our application, we have $i \equiv (\boldsymbol{k}\sigma \,|\, \boldsymbol{k}'\sigma')$ and $j \equiv (\boldsymbol{p}\mu \,|\, \boldsymbol{p}'\mu')$, with $C_i^\dagger = c^\dagger_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}'\sigma'}$ and $C_j = c^\dagger_{\boldsymbol{p}'\mu'} c_{\boldsymbol{p}\mu}$, *etc.* So we need to compute the response function,

$$\hat{\chi}_{C_i C_j^\dagger}(\omega) = \frac{i}{\hbar} \int_0^\infty dt\, \Big\langle \Big[c^\dagger_{\boldsymbol{k}'\sigma'}(t)\, c_{\boldsymbol{k}\sigma}(t)\, ,\, c^\dagger_{\boldsymbol{p}\mu}(0)\, c_{\boldsymbol{p}'\mu'}(0) \Big] \Big\rangle\, e^{i\omega t} \quad . \tag{4.191}$$

OK, so strap in, because this is going to be a bit of a bumpy ride.

We evaluate the commutator in real time and then Fourier transform to the frequency domain. Using Wick's theorem for fermions[13],

$$\langle c_1^\dagger\, c_2\, c_3^\dagger\, c_4\rangle = \langle c_1^\dagger\, c_2\rangle\,\langle c_3^\dagger\, c_4\rangle - \langle c_1^\dagger\, c_3^\dagger\rangle\,\langle c_2\, c_4\rangle + \langle c_1^\dagger\, c_4\rangle\,\langle c_2\, c_3^\dagger\rangle \quad , \tag{4.192}$$

we have

$$\begin{aligned}\chi_{C_i C_j^\dagger}(t) &= \frac{i}{\hbar}\Big\langle\Big[c^\dagger_{\boldsymbol{k}'\sigma'}(t)\, c_{\boldsymbol{k}\sigma}(t)\,,\, c^\dagger_{\boldsymbol{p}\mu}(0)\, c_{\boldsymbol{p}'\mu'}(0)\Big]\Big\rangle\,\Theta(t)\\ &= -\frac{i}{\hbar}\Big[F^a_{\boldsymbol{k}'\sigma'}(t)\,F^b_{\boldsymbol{k}\sigma}(t) - F^c_{\boldsymbol{k}\sigma}(t)\,F^d_{\boldsymbol{k}'\sigma'}(t)\Big]\,\delta_{\boldsymbol{p},\boldsymbol{k}}\,\delta_{\boldsymbol{p}',\boldsymbol{k}'}\,\delta_{\mu,\sigma}\,\delta_{\mu',\sigma'}\\ &\qquad + \frac{i}{\hbar}\Big[G^a_{\boldsymbol{k}'\sigma'}(t)\,G^b_{\boldsymbol{k}\sigma}(t) - G^c_{\boldsymbol{k}\sigma}(t)\,G^d_{\boldsymbol{k}'\sigma'}(t)\Big]\,\sigma\sigma'\,\delta_{\boldsymbol{p},-\boldsymbol{k}'}\,\delta_{\boldsymbol{p}',-\boldsymbol{k}}\,\delta_{\mu,-\sigma'}\,\delta_{\mu',-\sigma} \quad ,\end{aligned} \tag{4.193}$$

where, using the Bogoliubov transformation,

$$\begin{aligned} c_{\boldsymbol{k}\sigma} &= u_{\boldsymbol{k}}\,\gamma_{\boldsymbol{k}\sigma} - \sigma\, v_{\boldsymbol{k}}\, e^{+i\phi}\,\gamma^\dagger_{-\boldsymbol{k}\,-\sigma}\\ c^\dagger_{-\boldsymbol{k}\,-\sigma} &= u_{\boldsymbol{k}}\,\gamma^\dagger_{-\boldsymbol{k}\,-\sigma} + \sigma\, v_{\boldsymbol{k}}\, e^{-i\phi}\,\gamma_{\boldsymbol{k}\sigma} \quad ,\end{aligned} \tag{4.194}$$

we find

$$\begin{aligned} F^a_{\boldsymbol{q}\nu}(t) &= -i\,\Theta(t)\,\big\langle c^\dagger_{\boldsymbol{q}\nu}(t)\, c_{\boldsymbol{q}\nu}(0)\big\rangle = -i\,\Theta(t)\,\Big\{u^2_{\boldsymbol{q}}\, e^{iE_{\boldsymbol{q}}t/\hbar}\, f(E_{\boldsymbol{q}}) + v^2_{\boldsymbol{q}}\, e^{-iE_{\boldsymbol{q}}t/\hbar}\big[1-f(E_{\boldsymbol{q}})\big]\Big\}\\ F^b_{\boldsymbol{q}\nu}(t) &= -i\,\Theta(t)\,\big\langle c_{\boldsymbol{q}\nu}(t)\, c^\dagger_{\boldsymbol{q}\nu}(0)\big\rangle = -i\,\Theta(t)\,\Big\{u^2_{\boldsymbol{q}}\, e^{-iE_{\boldsymbol{q}}t/\hbar}\big[1-f(E_{\boldsymbol{q}})\big] + v^2_{\boldsymbol{q}}\, e^{iE_{\boldsymbol{q}}t/\hbar}\, f(E_{\boldsymbol{q}})\Big\}\\ F^c_{\boldsymbol{q}\nu}(t) &= -i\,\Theta(t)\,\big\langle c^\dagger_{\boldsymbol{q}\nu}(0)\, c_{\boldsymbol{q}\nu}(t)\big\rangle = -i\,\Theta(t)\,\Big\{u^2_{\boldsymbol{q}}\, e^{-iE_{\boldsymbol{q}}t/\hbar}\, f(E_{\boldsymbol{q}}) + v^2_{\boldsymbol{q}}\, e^{iE_{\boldsymbol{q}}t/\hbar}\big[1-f(E_{\boldsymbol{q}})\big]\Big\}\\ F^d_{\boldsymbol{q}\nu}(t) &= -i\,\Theta(t)\,\big\langle c_{\boldsymbol{q}\nu}(0)\, c^\dagger_{\boldsymbol{q}\nu}(t)\big\rangle = -i\,\Theta(t)\,\Big\{u^2_{\boldsymbol{q}}\, e^{iE_{\boldsymbol{q}}t/\hbar}\big[1-f(E_{\boldsymbol{q}})\big] + v^2_{\boldsymbol{q}}\, e^{-iE_{\boldsymbol{q}}t/\hbar}\, f(E_{\boldsymbol{q}})\Big\}\end{aligned} \tag{4.195}$$

and

$$\begin{aligned} G^a_{\boldsymbol{q}\nu}(t) &= -i\,\Theta(t)\,\big\langle c^\dagger_{\boldsymbol{q}\nu}(t)\, c^\dagger_{-\boldsymbol{q}\,-\nu}(0)\big\rangle = -i\,\Theta(t)\, u_{\boldsymbol{q}}\, v_{\boldsymbol{q}}\, e^{-i\phi}\Big\{e^{iE_{\boldsymbol{q}}t/\hbar}\, f(E_{\boldsymbol{q}}) - e^{-iE_{\boldsymbol{q}}t/\hbar}\big[1-f(E_{\boldsymbol{q}})\big]\Big\}\\ G^b_{\boldsymbol{q}\nu}(t) &= -i\,\Theta(t)\,\big\langle c_{\boldsymbol{q}\nu}(t)\, c_{-\boldsymbol{q}\,-\nu}(0)\big\rangle = -i\,\Theta(t)\, u_{\boldsymbol{q}}\, v_{\boldsymbol{q}}\, e^{+i\phi}\Big\{e^{-E_{\boldsymbol{q}}t/\hbar}\big[1-f(E_{\boldsymbol{q}})\big] - e^{-iE_{\boldsymbol{q}}t/\hbar}\, f(E_{\boldsymbol{q}})\Big\}\\ G^c_{\boldsymbol{q}\nu}(t) &= -i\,\Theta(t)\,\big\langle c^\dagger_{\boldsymbol{q}\nu}(0)\, c^\dagger_{-\boldsymbol{q}\,-\nu}(t)\big\rangle = -i\,\Theta(t)\, u_{\boldsymbol{q}}\, v_{\boldsymbol{q}}\, e^{-i\phi}\Big\{e^{iE_{\boldsymbol{q}}t/\hbar}\big[1-f(E_{\boldsymbol{q}})\big] - e^{-iE_{\boldsymbol{q}}t/\hbar}\, f(E_{\boldsymbol{q}})\Big\}\\ G^d_{\boldsymbol{q}\nu}(t) &= -i\,\Theta(t)\,\big\langle c^\dagger_{\boldsymbol{q}\nu}(0)\, c^\dagger_{-\boldsymbol{q}\,-\nu}(t)\big\rangle = -i\,\Theta(t)\, u_{\boldsymbol{q}}\, v_{\boldsymbol{q}}\, e^{+i\phi}\Big\{e^{-iE_{\boldsymbol{q}}t/\hbar}\, f(E_{\boldsymbol{q}}) - e^{iE_{\boldsymbol{q}}t/\hbar}\big[1-f(E_{\boldsymbol{q}})\big]\Big\} \quad .\end{aligned} \tag{4.196}$$

Taking the Fourier transforms, we have[14]

$$\hat F^a(\omega) = \frac{u^2 f}{\omega + E + i\epsilon} + \frac{v^2\,(1-f)}{\omega - E + i\epsilon} \quad , \qquad \hat F^c(\omega) = \frac{u^2 f}{\omega - E + i\epsilon} + \frac{v^2\,(1-f)}{\omega + E + i\epsilon} \tag{4.197}$$

$$\hat F^b(\omega) = \frac{u^2\,(1-f)}{\omega - E + i\epsilon} + \frac{v^2 f}{\omega + E + i\epsilon} \quad , \qquad \hat F^d(\omega) = \frac{u^2\,(1-f)}{\omega + E + i\epsilon} + \frac{v^2 f}{\omega - E + i\epsilon} \tag{4.198}$$

and

$$\hat G^a(\omega) = u\,v\,e^{-i\phi}\bigg(\frac{f}{\omega + E + i\epsilon} - \frac{1-f}{\omega - E + i\epsilon}\bigg) \quad , \quad \hat G^c(\omega) = u\,v\,e^{+i\phi}\bigg(\frac{1-f}{\omega - E + i\epsilon} - \frac{f}{\omega + E + i\epsilon}\bigg) \tag{4.199}$$

$$\hat G^b(\omega) = u\,v\,e^{+i\phi}\bigg(\frac{1-f}{\omega + E + i\epsilon} - \frac{f}{\omega - E + i\epsilon}\bigg) \quad , \quad \hat G^d(\omega) = u\,v\,e^{+i\phi}\bigg(\frac{f}{\omega + E + i\epsilon} - \frac{1-f}{\omega - E + i\epsilon}\bigg) \quad . \tag{4.200}$$

[13]Wick's theorem is valid when taking expectation values in Slater determinant states.

[14]Here we are being somewhat loose and have set $\hbar = 1$ to avoid needless notational complication. We shall restore the proper units at the end of our calculation.

Using the result that the Fourier transform of a product is a convolution of Fourier transforms, we have from Eqn. 4.193,

$$\hat{\chi}_{C_i C_j^\dagger}(\omega) = \frac{i}{\hbar}\,\delta_{\boldsymbol{p},\boldsymbol{k}}\,\delta_{\boldsymbol{p}',\boldsymbol{k}'}\,\delta_{\mu,\sigma}\,\delta_{\mu',\sigma'}\int\limits_{-\infty}^{\infty}\!\frac{d\nu}{2\pi}\,\Big[\hat{F}^c_{\boldsymbol{k}\sigma}(\nu)\,\hat{F}^d_{\boldsymbol{k}'\sigma'}(\omega-\nu) - \hat{F}^a_{\boldsymbol{k}'\sigma'}(\nu)\,\hat{F}^b_{\boldsymbol{k}\sigma}(\omega-\nu)\Big]$$
$$+\frac{i}{\hbar}\,\delta_{\boldsymbol{p},-\boldsymbol{k}'}\,\delta_{\boldsymbol{p}',-\boldsymbol{k}}\,\delta_{\mu,-\sigma'}\,\delta_{\mu',-\sigma}\int\limits_{-\infty}^{\infty}\!\frac{d\nu}{2\pi}\,\Big[\hat{G}^a_{\boldsymbol{k}\sigma}(\nu)\,\hat{G}^b_{\boldsymbol{k}'\sigma'}(\omega-\nu) - \hat{G}^c_{\boldsymbol{k}'\sigma'}(\nu)\,\hat{G}^d_{\boldsymbol{k}\sigma}(\omega-\nu)\Big] \quad . \tag{4.201}$$

The integrals are easily done via the contour method. For example, one has

$$i\int\limits_{-\infty}^{\infty}\!\frac{d\nu}{2\pi}\,\hat{F}^c_{\boldsymbol{k}\sigma}(\nu)\,\hat{F}^d_{\boldsymbol{k}'\sigma'}(\omega-\nu) = -\int\limits_{-\infty}^{\infty}\!\frac{d\nu}{2\pi i}\left(\frac{u^2\,f}{\nu-E+i\epsilon}+\frac{v^2\,(1-f)}{\nu+E+i\epsilon}\right)\left(\frac{u'^{\,2}\,(1-f')}{\omega-\nu+E'+i\epsilon}+\frac{v'^{\,2}\,f'}{\omega-\nu-E'+i\epsilon}\right)$$
$$=\frac{u^2\,u'^{\,2}\,(1-f)\,f'}{\omega+E-E'+i\epsilon}+\frac{v^2\,u'^{\,2}\,f f'}{\omega-E-E'+i\epsilon}+\frac{u^2\,v'^{\,2}\,(1-f)(1-f')}{\omega+E+E'+i\epsilon}+\frac{v^2\,v'^{\,2}\,f(1-f')}{\omega-E+E'+i\epsilon} \quad . \tag{4.202}$$

One then finds (with proper units restored),

$$\begin{aligned}\hat{\chi}_{C_i C_j^\dagger}(\omega) &= \delta_{\boldsymbol{p},\boldsymbol{k}}\,\delta_{\boldsymbol{p}',\boldsymbol{k}'}\,\delta_{\mu,\sigma}\,\delta_{\mu',\sigma'}\Bigg(\frac{u^2u'^{\,2}\,(f-f')}{\hbar\omega-E+E'+i\epsilon}-\frac{v^2v'^{\,2}\,(f-f')}{\hbar\omega+E-E'+i\epsilon}\\ &\qquad\qquad+\frac{u^2v'^{\,2}\,(1-f-f')}{\hbar\omega+E+E'+i\epsilon}-\frac{v^2u'^{\,2}\,(1-f-f')}{\hbar\omega-E-E'+i\epsilon}\Bigg)\\ &+\delta_{\boldsymbol{p},-\boldsymbol{k}'}\,\delta_{\boldsymbol{p}',-\boldsymbol{k}}\,\delta_{\mu,-\sigma'}\,\delta_{\mu',-\sigma}\Bigg(\frac{f'-f}{\hbar\omega-E+E'+i\epsilon}-\frac{f'-f}{\hbar\omega+E-E'+i\epsilon}\\ &\qquad\qquad+\frac{1-f-f'}{\hbar\omega+E+E'+i\epsilon}-\frac{1-f-f'}{\hbar\omega-E-E'+i\epsilon}\Bigg)\,uvu'v'\sigma\sigma' \quad .\end{aligned} \tag{4.203}$$

We are almost done. Note that $C_i = c^\dagger_{\boldsymbol{k}'\sigma'}c_{\boldsymbol{k}\sigma}$ means $C^\dagger_i = c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}'\sigma'}$, hence once we have $\hat{\chi}_{C_i C_j^\dagger}(\omega)$ we can easily obtain from it $\hat{\chi}_{C_i^\dagger C_j^\dagger}(\omega)$ and the other response functions in Eqn. 4.189, simply by permuting the wavevector and spin labels.

4.6.1 Case I and case II probes

The last remaining piece in the derivation is to note that, for virtually all cases of interest,

$$\sigma\sigma' B(-\boldsymbol{k}'\,-\sigma'\,|\,-\boldsymbol{k}\,-\sigma) = \eta\,B(\boldsymbol{k}\sigma\,|\,\boldsymbol{k}'\sigma') \quad , \tag{4.204}$$

where $B(\boldsymbol{k}\sigma\,|\,\boldsymbol{k}'\sigma')$ is the transition matrix element in the original fermionic (*i.e.* 'pre-Bogoliubov') representation, from Eqn. 4.184, and where $\eta = +1$ (case I) or $\eta = -1$ (case II). The eigenvalue η tells us how the perturbation Hamiltonian transforms under the combined operations of time reversal and particle-hole transformation. The action of time reversal is

$$\mathcal{T}\,|\,\boldsymbol{k}\,\sigma\,\rangle = \sigma\,|\,-\boldsymbol{k}\,-\sigma\,\rangle \quad \Rightarrow \quad c^\dagger_{\boldsymbol{k}\sigma} \to \sigma\,c^\dagger_{-\boldsymbol{k}\,-\sigma} \tag{4.205}$$

The particle-hole transformation sends $c^\dagger_{\boldsymbol{k}\sigma} \to c_{\boldsymbol{k}\sigma}$. Thus, under the combined operation,

$$\begin{aligned}\sum_{\boldsymbol{k},\sigma}\sum_{\boldsymbol{k}',\sigma'} B(\boldsymbol{k}\sigma\,|\,\boldsymbol{k}'\sigma')\,c^\dagger_{\boldsymbol{k}\sigma}\,c_{\boldsymbol{k}'\sigma'} &\to -\sum_{\boldsymbol{k},\sigma}\sum_{\boldsymbol{k}',\sigma'} \sigma\sigma'\,B(-\boldsymbol{k}'\,-\sigma'\,|\,-\boldsymbol{k}\,-\sigma)\,c^\dagger_{\boldsymbol{k}\sigma}\,c_{\boldsymbol{k}'\sigma'} + \text{const.}\\ &\to -\eta\sum_{\boldsymbol{k},\sigma}\sum_{\boldsymbol{k}',\sigma'} B(\boldsymbol{k}\sigma\,|\,\boldsymbol{k}'\sigma')\,c^\dagger_{\boldsymbol{k}\sigma}\,c_{\boldsymbol{k}'\sigma'} + \text{const.} \quad .\end{aligned} \tag{4.206}$$

If we can write $B(\boldsymbol{k}\sigma\,|\,\boldsymbol{k}'\sigma') = B_{\sigma\sigma'}(\xi_{\boldsymbol{k}},\xi_{\boldsymbol{k}'})$, then, further assuming that our perturbation corresponds to a definite η, we have that the power dissipated is

$$\begin{aligned}P = \tfrac{1}{2}\,g^2(\mu)\sum_{\sigma,\sigma'}\int\limits_{-\infty}^{\infty}\!d\omega\;\omega\int\limits_{-\infty}^{\infty}\!d\xi\int\limits_{-\infty}^{\infty}\!d\xi'\;\big|B_{\sigma\sigma'}(\xi,\xi';\omega)\big|^2\Big\{\big(uu'-\eta vv'\big)^2\,(f-f')\,\Big[\delta(\hbar\omega+E-E')+\delta(\hbar\omega+E'-E)\Big]\\ +\tfrac{1}{2}(uv'+\eta vu')^2\,(1-f-f')\,\Big[\delta(\hbar\omega-E-E')-\delta(\hbar\omega+E+E')\Big]\Big\} \quad .\end{aligned} \tag{4.207}$$

The coherence factors entering the above expression are

$$\begin{aligned}\tfrac{1}{2}(uu'-\eta vv')^2 &= \frac{1}{2}\left(\sqrt{\frac{E+\xi}{2E}}\sqrt{\frac{E'+\xi'}{2E'}} - \eta\sqrt{\frac{E-\xi}{2E}}\sqrt{\frac{E'-\xi'}{2E'}}\right)^2 = \frac{EE'+\xi\xi'-\eta\Delta^2}{2EE'}\\ \tfrac{1}{2}(uv'+\eta vu')^2 &= \frac{1}{2}\left(\sqrt{\frac{E+\xi}{2E}}\sqrt{\frac{E'-\xi'}{2E'}} + \eta\sqrt{\frac{E-\xi}{2E}}\sqrt{\frac{E'+\xi'}{2E'}}\right)^2 = \frac{EE'-\xi\xi'+\eta\Delta^2}{2EE'} \quad .\end{aligned} \tag{4.208}$$

Integrating over ξ and ξ' kills the $\xi\xi'$ terms, and we define the coherence factors

$$F(E,E',\Delta) \equiv \frac{EE'-\eta\Delta^2}{2EE'} \quad , \qquad \widetilde{F}(E,E',\Delta) \equiv \frac{EE'+\eta\Delta^2}{2EE'} = 1 - F \quad . \tag{4.209}$$

The behavior of $F(E,E',\Delta)$ is summarized in Tab. 4.1. If we approximate $B_{\sigma\sigma'}(\xi,\xi';\omega) \approx B_{\sigma\sigma'}(0,0\,;\omega)$, and we define $|\mathcal{B}(\omega)|^2 = \sum_{\sigma,\sigma'}\big|B_{\sigma\sigma'}(0,0\,;\omega)\big|^2$, then we have

$$P = \int\limits_{-\infty}^{\infty}\!d\omega\;|\mathcal{B}(\omega)|^2\,\mathcal{P}(\omega) \quad , \tag{4.210}$$

where

$$\begin{aligned}\mathcal{P}(\omega) \equiv \omega\int\limits_{\Delta}^{\infty}\!dE\int\limits_{\Delta}^{\infty}\!dE'\;\widetilde{n}_{\mathsf{s}}(E)\,\widetilde{n}_{\mathsf{s}}(E')\,\Big\{F(E,E',\Delta)\,(f-f')\,\Big[\delta(\hbar\omega+E-E')+\delta(\hbar\omega+E'-E)\Big]\\ +\widetilde{F}(E,E',\Delta)\,(1-f-f')\,\Big[\delta(\hbar\omega-E-E')-\delta(\hbar\omega+E+E')\Big]\Big\} \quad ,\end{aligned} \tag{4.211}$$

with

$$\widetilde{n}_{\mathsf{s}}(E) = \frac{g(\mu)\,|E|}{\sqrt{E^2-\Delta^2}}\;\Theta(E^2-\Delta^2) \quad , \tag{4.212}$$

which is the superconducting density of states from Eqn. 4.76. Note that the coherence factor for quasiparticle scattering is F, while that for quasiparticle pair creation or annihilation is $\widetilde{F} = 1 - F$.

case	$\hbar\omega \ll 2\Delta$	$\hbar\omega \gg 2\Delta$	$\hbar\omega \approx 2\Delta$	$\hbar\omega \gg 2\Delta$
I ($\eta = +1$)	$F \approx 0$	$F \approx \frac{1}{2}$	$\widetilde{F} \approx 1$	$\widetilde{F} \approx \frac{1}{2}$
II ($\eta = -1$)	$F \approx 1$	$F \approx \frac{1}{2}$	$\widetilde{F} \approx 0$	$\widetilde{F} \approx \frac{1}{2}$

Table 4.1: Frequency dependence of the BCS coherence factors $F(E, E + \hbar\omega, \Delta)$ and $\widetilde{F}(E, \hbar\omega - E, \Delta)$ for $E \approx \Delta$.

4.6.2 Electromagnetic absorption

The interaction of light and matter is given in Eqn. 4.186. We have

$$B(\boldsymbol{k}\sigma \,|\, \boldsymbol{k}'\sigma') = \frac{e\hbar}{2mc}\,(\boldsymbol{k} + \boldsymbol{k}') \cdot \boldsymbol{A}_{\boldsymbol{k}-\boldsymbol{k}'}\,\delta_{\sigma\sigma'} \quad , \tag{4.213}$$

from which we see

$$\sigma\sigma'\,B(-\boldsymbol{k}' \; -\sigma' \,|\, -\boldsymbol{k} \; -\sigma) = -B(\boldsymbol{k}\sigma \,|\, \boldsymbol{k}'\sigma') \quad , \tag{4.214}$$

hence we have $\eta = -1$, *i.e.* case II. Let's set $T = 0$, so $f = f' = 0$. We see from Eqn. 4.211 that $\mathcal{P}(\omega) = 0$ for $\omega < 2\Delta$. We then have

$$\mathcal{P}(\omega) = \tfrac{1}{2}\,g^2(\mu) \int\limits_{\Delta}^{\hbar\omega-\Delta} \! dE \; \frac{E(\hbar\omega - E) - \Delta^2}{\sqrt{(E^2 - \Delta^2)\big((\hbar\omega - E)^2 - \Delta^2\big)}} \quad . \tag{4.215}$$

If we set $\Delta = 0$, we obtain $\mathcal{P}_{\text{N}}(\omega) = \frac{1}{2}\omega^2$. The ratio between superconducting and normal values is

$$\frac{\sigma_{1,\text{s}}(\omega)}{\sigma_{1,\text{N}}(\omega)} = \frac{\mathcal{P}_{\text{s}}(\omega)}{\mathcal{P}_{\text{N}}(\omega)} = \frac{1}{\omega} \int\limits_{\Delta}^{\hbar\omega-\Delta} \! dE \; \frac{E(\hbar\omega - E) - \Delta^2}{\sqrt{(E^2 - \Delta^2)\big((\hbar\omega - E)^2 - \Delta^2\big)}} \quad , \tag{4.216}$$

where $\sigma_1(\omega)$ is the real (dissipative) part of the conductivity. The result can be obtained in closed form in terms of elliptic integrals[15], and is

$$\frac{\sigma_{1,\text{s}}(\omega)}{\sigma_{1,\text{N}}(\omega)} = \bigg(1 + \frac{1}{x}\bigg)\,\mathbb{E}\bigg(\frac{1-x}{1+x}\bigg) - \frac{2}{x}\,\mathbb{K}\bigg(\frac{1-x}{1+x}\bigg) \quad , \tag{4.217}$$

where $x = \hbar\omega/2\Delta$. The imaginary part $\sigma_{2,\text{s}}(\omega)$ may then be obtained by Kramers-Kronig transform, and is

$$\frac{\sigma_{2,\text{s}}(\omega)}{\sigma_{1,\text{N}}(\omega)} = \frac{1}{2}\bigg(1 + \frac{1}{x}\bigg)\,\mathbb{E}\bigg(\frac{2\sqrt{x}}{1+x}\bigg) - \frac{1}{2}\bigg(1 - \frac{1}{x}\bigg)\,\mathbb{K}\bigg(\frac{2\sqrt{x}}{1+x}\bigg) \quad . \tag{4.218}$$

The conductivity sum rule,

$$\int\limits_0^\infty \! d\omega\;\sigma_1(\omega) = \frac{\pi n e^2}{2m} \quad , \tag{4.219}$$

is satisfied in translation-invariant systems[16]. In a superconductor, when the gap opens, the spectral weight in the region $\omega \in (0, 2\Delta)$ for case I probes shifts to the $\omega > 2\Delta$ region. One finds $\lim_{\omega\to 2\Delta^+} \mathcal{P}_{\text{s}}(\omega)/\mathcal{P}_{\text{N}}(\omega) = \frac{1}{2}\pi$. Case II probes, however, lose spectral weight in the $\omega > 2\Delta$ region in addition to developing a spectral gap. The missing spectral weight emerges as a delta function peak at zero frequency. The London equation $\boldsymbol{j} = -(c/4\pi\lambda_{\text{L}})\,\boldsymbol{A}$ gives

$$-i\omega\,\sigma(\omega)\,\boldsymbol{E}(\omega) = -i\omega\,\boldsymbol{j}(\omega) = -\frac{c^2}{4\pi\lambda_{\text{L}}^2}\,\boldsymbol{E}(\omega) \quad , \tag{4.220}$$

[15] See D. C. Mattis and J. Bardeen, *Phys. Rev.* **111**, 412 (1958).
[16] Neglecting interband transitions, the conductivity sum rule is satisfied under replacement of the electron mass m by the band mass m^*.

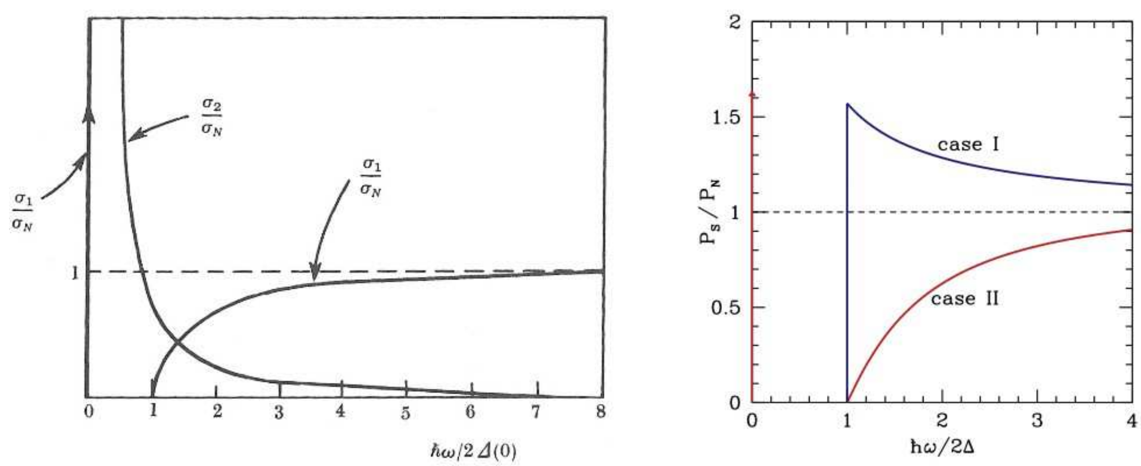

Figure 4.15: Left: real (σ_1) and imaginary (σ_2) parts of the conductivity of a superconductor, normalized by the metallic value of σ_1 just above T_c. From J. R. Schrieffer, *Theory of Superconductivity*. Right: ratio of $\mathcal{P}_s(\omega)/\mathcal{P}_N(\omega)$ for case I (blue) and case II (red) probes.

which says

$$\sigma(\omega) = \frac{c^2}{4\pi\lambda_L^2}\,\frac{i}{\omega} + Q\,\delta(\omega) \quad , \tag{4.221}$$

where Q is as yet unknown[17]. We can determine the value of Q via Kramers-Kronig, *viz.*

$$\sigma_2(\omega) = -\,\mathsf{P}\int\limits_{-\infty}^{\infty}\frac{d\nu}{\pi}\,\frac{\sigma_1(\nu)}{\nu-\omega} \quad , \tag{4.222}$$

where P denotes principal part. Thus,

$$\frac{c^2}{4\pi\lambda_L^2\omega} = -Q\int\limits_{-\infty}^{\infty}\frac{d\nu}{\pi}\,\frac{\delta(\nu)}{\nu-\omega} = \frac{Q}{\pi} \qquad \Rightarrow \qquad Q = \frac{c^2}{4\lambda_L} \quad . \tag{4.223}$$

Thus, the full London $\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)$ may be written as

$$\sigma(\omega) = \lim_{\epsilon\to 0^+}\frac{c^2}{4\lambda_L}\,\frac{1}{\epsilon - i\pi\omega} = \frac{c^2}{4\lambda_L}\left\{\delta(\omega) + \frac{i}{\pi\omega}\right\} \quad . \tag{4.224}$$

Note that the London form for $\sigma_1(\omega)$ includes only the delta-function and none of the structure due to thermally excited quasiparticles ($\omega < 2\Delta$) or pair-breaking ($\omega > 2\Delta$). *Nota bene: while the real part of the conductivity $\sigma_1(\omega)$ includes a $\delta(\omega)$ piece which is finite below 2Δ, because it lies at zero frequency, it does not result in any energy dissipation.* It is also important to note that the electrodynamic response in London theory is purely local. The actual electromagnetic response kernel $K_{\mu\nu}(\boldsymbol{q},\omega)$ computed using BCS theory is $\boldsymbol{q}$-dependent, even at $\omega = 0$. This says that a magnetic field $\boldsymbol{B}(\boldsymbol{x})$ will induce screening currents at positions $\boldsymbol{x}'$ which are not too distant from $\boldsymbol{x}$. The relevant length scale here turns out to be the *coherence length* $\xi_0 = \hbar v_F/\pi\Delta_0$ (at zero temperature).

At finite temperature, $\sigma_1(\omega, T)$ exhibits a Hebel-Slichter peak, also known as the *coherence peak*. Examples from two presumably non-s-wave superconductors are shown in Fig. 4.16.

[17]Note that $\omega\,\delta(\omega) = 0$ when multiplied by any nonsingular function in an integrand.

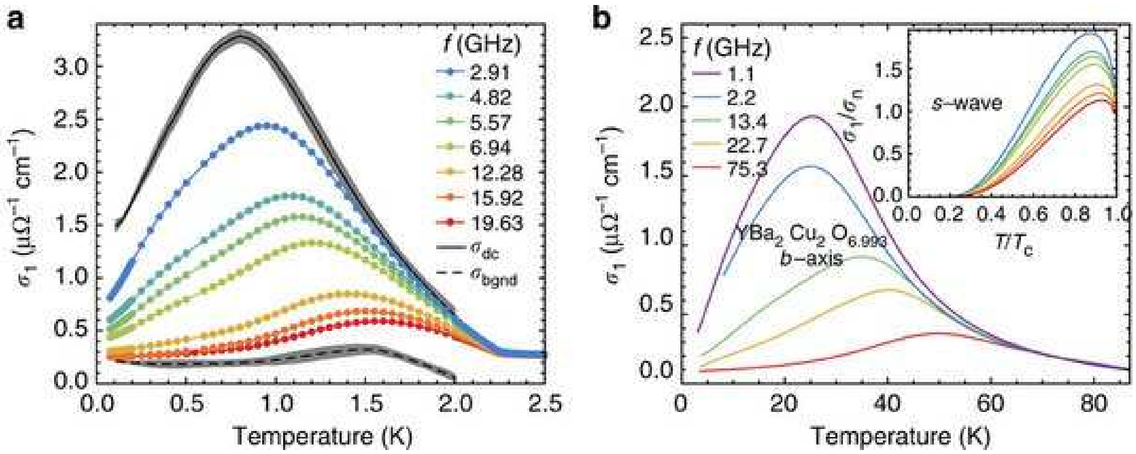

Figure 4.16: Real part of the conductivity $\sigma_1(\omega,T)$ in $\mathrm{CeCoIn_5}$ (left; $T_c = 2.25\,\mathrm{K}$) and in $\mathrm{YBa_2Cu_3O_{6.993}}$ (right; $T_c = 89\,\mathrm{K}$), each showing a coherence peak *versus* temperature over a range of low frequencies. Inset at right shows predictions for s-wave BCS superconductors. Both these materials are believed to involve a more exotic pairing structure. From C. J. S. Truncik *et al.*, *Nature Comm.* **4**, 2477 (2013).

Impurities and translational invariance

Observant students may notice that our derivation of $\sigma(\omega)$ makes no sense. The reason is that $B(\boldsymbol{k}\sigma\,|\,\boldsymbol{k}'\sigma') \propto (\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{A}_{\boldsymbol{k}-\boldsymbol{k}'}$, which is not of the form $B_{\sigma\sigma'}(\xi_{\boldsymbol{k}},\xi_{\boldsymbol{k}'})$. For an electromagnetic field of frequency ω, the wavevector $q=\omega/c$ may be taken to be $q\to 0$, since the wavelength of light in the relevant range (optical frequencies and below) is enormous on the scale of the Fermi wavelength of electrons in the metallic phase. We then have that $\boldsymbol{k}=\boldsymbol{k}'+\boldsymbol{q}$, in which case the coherence factor $u_{\boldsymbol{k}}v_{\boldsymbol{k}'}-v_{\boldsymbol{k}}u_{\boldsymbol{k}'}$ vanishes as $\boldsymbol{q}\to 0$ and $\sigma_1(\omega)$ vanishes as well! This is because in the absence of translational symmetry breaking due to impurities, the current operator $\boldsymbol{j}$ commutes with the Hamiltonian, hence matrix elements of the perturbation $\boldsymbol{j}\cdot\boldsymbol{A}$ cannot cause any electronic transitions, and therefore there can be no dissipation. But this is not quite right, because the crystalline potential itself breaks translational invariance. What is true is this: *with no disorder, the dissipative conductivity $\sigma_1(\omega)$ vanishes on frequency scales below those corresponding to interband transitions*. Of course, this is also true in the metallic phase as well.

As shown by Mattis and Bardeen, if we relax the condition of momentum conservation, which is appropriate in the presence of impurities which break translational invariance, then we basically arrive back at the condition $B(\boldsymbol{k}\sigma\,|\,\boldsymbol{k}'\sigma') \approx B_{\sigma\sigma'}(\xi_{\boldsymbol{k}},\xi_{\boldsymbol{k}'})$. One might well wonder whether we should be classifying perturbation operators by the η parity in the presence of impurities, but provided $\Delta\tau \ll \hbar$, the Mattis-Bardeen result, which we have derived above, is correct.

4.7 Electromagnetic Response of Superconductors

Here we follow chapter 8 of Schrieffer, *Theory of Superconductivity*. In chapter 2 the lecture notes, we derived the linear response result,

$$\big\langle j_\mu(\boldsymbol{x},t)\big\rangle = -\frac{c}{4\pi}\int d^3x'\int dt'\;K_{\mu\nu}(\boldsymbol{x},t\;\;\boldsymbol{x}',t')\,A^\nu(\boldsymbol{x}',t') \quad , \tag{4.225}$$

where $\boldsymbol{j}(\boldsymbol{x},t)$ is the electrical current density, which is a sum of paramagnetic and diamagnetic contributions, *viz.*

$$\begin{aligned}\big\langle j^{\rm p}_\mu(\boldsymbol{x},t)\big\rangle &= \frac{i}{\hbar c}\int\!d^3x'\!\int\!dt'\,\big\langle\big[j^{\rm p}_\mu(\boldsymbol{x},t),j^{\rm p}_\nu(\boldsymbol{x}',t')\big]\big\rangle\,\Theta(t-t')\,A^\nu(\boldsymbol{x}',t')\\ \big\langle j^{\rm d}_\mu(\boldsymbol{x},t)\big\rangle &= -\frac{e}{mc^2}\,\big\langle j^{\rm p}_0(\boldsymbol{x},t)\big\rangle\,A^\mu(\boldsymbol{x},t)\,(1-\delta_{\mu 0})\quad ,\end{aligned}\tag{4.226}$$

with $j^{\rm p}_0(\boldsymbol{x}) = ce\,n(\boldsymbol{x})$. We then conclude[18]

$$\begin{aligned}K_{\mu\nu}(\boldsymbol{x}t;\boldsymbol{x}'t') = \frac{4\pi}{i\hbar c^2}&\Big\langle\big[j^{\rm p}_\mu(\boldsymbol{x},t),j^{\rm p}_\nu(\boldsymbol{x}',t')\big]\Big\rangle\,\Theta(t-t')\\ &+\frac{4\pi e}{mc^3}\,\big\langle j^{\rm p}_0(\boldsymbol{x},t)\big\rangle\,\delta(\boldsymbol{x}-\boldsymbol{x}')\,\delta(t-t')\,\delta_{\mu\nu}\,(1-\delta_{\mu 0})\quad .\end{aligned}\tag{4.227}$$

In Fourier space, we may write

$$K_{\mu\nu}(\boldsymbol{q},t) = \overbrace{\frac{4\pi}{i\hbar c^2}\Big\langle\big[j^{\rm p}_\mu(\boldsymbol{q},t),j^{\rm p}_\nu(-\boldsymbol{q},0)\big]\Big\rangle\,\Theta(t)}^{K^{\rm p}_{\mu\nu}(\boldsymbol{q},t)} + \overbrace{\frac{4\pi n e^2}{mc^2}\,\delta(t)\,\delta_{\mu\nu}\,(1-\delta_{\mu 0})}^{K^{\rm d}_{\mu\nu}(\boldsymbol{q},t)}\quad ,\tag{4.228}$$

where the paramagnetic current operator is

$$\boldsymbol{j}^{\rm p}(\boldsymbol{q}) = -\frac{e\hbar}{m}\sum_{\boldsymbol{k},\sigma}\big(\boldsymbol{k}+\tfrac{1}{2}\boldsymbol{q}\big)\,c^\dagger_{\boldsymbol{k}\sigma}\,c_{\boldsymbol{k}+\boldsymbol{q}\,\sigma}\quad .\tag{4.229}$$

The calculation of the electromagnetic response kernel $K_{\mu\nu}(\boldsymbol{q},\omega)$ is tedious, but it yields all we need to know about the electromagnetic response of superconductors. For example, if we work in a gauge where $A^0=0$, we have $\boldsymbol{E}(\omega) = i\omega\boldsymbol{A}(\omega)/c$ and hence the conductivity tensor is

$$\sigma_{ij}(\boldsymbol{q},\omega) = \frac{i\,c^2}{4\pi\omega}\,K_{ij}(\boldsymbol{q},\omega)\quad ,\tag{4.230}$$

where i and j are spatial indices. Using the results of §4.6, the diamagnetic response kernel at $\omega=0$ is

$$K^{\rm p}_{ij}(\boldsymbol{q},\omega=0) = -\frac{8\pi\hbar e^2}{mc^2}\int\!\frac{d^3k}{(2\pi)^3}\,\big(k_i+\tfrac{1}{2}q_i\big)\big(k_j+\tfrac{1}{2}q_j\big)\,L(\boldsymbol{k},\boldsymbol{q})\quad ,\tag{4.231}$$

where

$$\begin{aligned}L(\boldsymbol{k},\boldsymbol{q}) = &\left(\frac{E_{\boldsymbol{k}}E_{\boldsymbol{k}+\boldsymbol{q}}-\xi_{\boldsymbol{k}}\xi_{\boldsymbol{k}+\boldsymbol{q}}-\Delta_{\boldsymbol{k}}\Delta_{\boldsymbol{k}+\boldsymbol{q}}}{2E_{\boldsymbol{k}}E_{\boldsymbol{k}+\boldsymbol{q}}}\right)\left(\frac{1-f(E_{\boldsymbol{k}})-f(E_{\boldsymbol{k}+\boldsymbol{q}})}{E_{\boldsymbol{k}}+E_{\boldsymbol{k}+\boldsymbol{q}}+i\epsilon}\right)\\ &+\left(\frac{E_{\boldsymbol{k}}E_{\boldsymbol{k}+\boldsymbol{q}}+\xi_{\boldsymbol{k}}\xi_{\boldsymbol{k}+\boldsymbol{q}}+\Delta_{\boldsymbol{k}}\Delta_{\boldsymbol{k}+\boldsymbol{q}}}{2E_{\boldsymbol{k}}E_{\boldsymbol{k}+\boldsymbol{q}}}\right)\left(\frac{f(E_{\boldsymbol{k}+\boldsymbol{q}})-f(E_{\boldsymbol{k}})}{E_{\boldsymbol{k}}-E_{\boldsymbol{k}+\boldsymbol{q}}+i\epsilon}\right)\quad .\end{aligned}\tag{4.232}$$

At $T=0$, we have $f(E_{\boldsymbol{k}}) = f(E_{\boldsymbol{k}+\boldsymbol{q}}) = 0$, and only the first term contributes. As $\boldsymbol{q}\to 0$, we have $L(\boldsymbol{k},\boldsymbol{q}\to 0)=0$ because the coherence factor vanishes while the energy denominator remains finite. Thus, only the diamagnetic response remains, and at $T=0$ we therefore have

$$\lim_{\boldsymbol{q}\to 0} K_{ij}(\boldsymbol{q},0) = \frac{\delta_{ij}}{\lambda^2_{\rm L}}\quad .\tag{4.233}$$

[18]We use a Minkowski metric $g^{\mu\nu} = g_{\mu\nu} = {\rm diag}(-,+,+,+)$ to raise and lower indices.

This should be purely transverse, but it is not – a defect of our mean field calculation. This can be repaired, but for our purposes it suffices to take the transverse part, *i.e.*

$$\lim_{\boldsymbol{q}\to 0} K_{ij}(\boldsymbol{q},0) = \frac{\delta_{ij} - \hat{q}_i\,\hat{q}_j}{\lambda_{\rm L}^2} \quad . \tag{4.234}$$

Thus, as long as $\lambda_{\rm L}$ is finite, the $\omega \to 0$ conductivity diverges.

At finite temperature, we have

$$\lim_{\boldsymbol{q}\to 0} L(\boldsymbol{k},\boldsymbol{q}) = -\frac{\partial f}{\partial E}\bigg|_{E=E_{\boldsymbol{k}}} = \frac{1}{k_{\rm B}T}\, f(E_{\boldsymbol{k}})\big[1-f(E_{\boldsymbol{k}})\big] \quad , \tag{4.235}$$

hence

$$\begin{aligned}\lim_{\boldsymbol{q}\to 0} K^{\rm p}_{ij}(\boldsymbol{q},\omega=0) &= -\frac{8\pi\hbar e^2}{mc^2 k_{\rm B}T}\int\!\frac{d^3\!k}{(2\pi)^3}\, k_i\, k_j\, \frac{e^{E_{\boldsymbol{k}}/k_{\rm B}T}}{\big(e^{E_{\boldsymbol{k}}/k_{\rm B}T}+1\big)^2} \\ &= -\frac{4\pi n e^2}{mc^2\hbar}\left[1-\frac{n_{\rm s}(T)}{n}\right]\delta_{ij} \quad ,\end{aligned} \tag{4.236}$$

where $n = k_{\rm F}^3/3\pi^2$ is the total electron number density, and

$$\frac{n_{\rm s}(T)}{n} = 1 - \frac{\hbar^2\beta}{mk_{\rm F}^3}\int\limits_0^\infty\!\! dk\, k^4\, \frac{e^{\beta E_{\boldsymbol{k}}}}{\big(e^{\beta E_{\boldsymbol{k}}}+1\big)^2} \equiv 1 - \frac{n_{\rm n}(t)}{n} \quad , \tag{4.237}$$

where

$$n_{\rm n}(T) = \frac{\hbar^2}{3\pi^2 m}\int\limits_0^\infty\!\! dk\, k^4 \left(-\frac{\partial f}{\partial E}\right)_{E=E_{\boldsymbol{k}}} \tag{4.238}$$

is the normal fluid density. Expanding about $k = k_{\rm F}$, where $-\frac{\partial f}{\partial E}$ is sharply peaked at low temperatures, we find

$$\begin{aligned} n_{\rm n}(T) &= \frac{\hbar^2}{3m}\cdot 2\!\int\!\frac{d^3\!k}{(2\pi)^3}\, k^2\!\left(-\frac{\partial f}{\partial E}\right) \\ &= \frac{\hbar^2 k_{\rm F}^2}{3m}\, g(\varepsilon_{\rm F})\cdot 2\int\limits_0^\infty\!\! d\xi\,\left(-\frac{\partial f}{\partial E}\right) = 2n\int\limits_0^\infty\!\! d\xi\,\left(-\frac{\partial f}{\partial E}\right) \quad ,\end{aligned} \tag{4.239}$$

which agrees precisely with what we found in Eqn. 3.136. Note that when the gap vanishes at $T_{\rm c}$, the integral yields $\frac{1}{2}$, and thus $n_{\rm n}(T_{\rm c}) = n$, as expected.

There is a slick argument, due to Landau, which yields this result. Suppose a superflow is established at some velocity $\boldsymbol{v}$. In steady state, any normal current will be damped out, and the electrical current will be $\boldsymbol{j} = -en_{\rm s}\boldsymbol{v}$. Now hop on a frame moving with the supercurrent. The superflow in the moving frame is stationary, so the current is due to normal electrons (quasiparticles), and $\boldsymbol{j}' = -en_{\rm n}(-\boldsymbol{v}) = +en_{\rm n}\boldsymbol{v}$. That is, the normal particles which were at rest in the lab frame move with velocity $-\boldsymbol{v}$ in the frame of the superflow, which we denote with a prime. The quasiparticle distribution in this primed frame is

$$f'_{\boldsymbol{k}\sigma} = \frac{1}{e^{\beta(E_{\boldsymbol{k}}+\hbar\boldsymbol{v}\cdot\boldsymbol{k})}+1} \quad , \tag{4.240}$$

since, for a Galilean-invariant system, which we are assuming, the energy is

$$\begin{aligned} E' &= E + \boldsymbol{v}\cdot\boldsymbol{P} + \tfrac{1}{2}M\boldsymbol{v}^2 \\ &= \sum_{\boldsymbol{k},\sigma}\big(E_{\boldsymbol{k}} + \hbar\boldsymbol{k}\cdot\boldsymbol{v}\big)\, n_{\boldsymbol{k}\sigma} + \tfrac{1}{2}M\boldsymbol{v}^2 \quad .\end{aligned} \tag{4.241}$$

Expanding now in $\boldsymbol{v}$,

$$\begin{aligned}\boldsymbol{j}' &= -\frac{e\hbar}{mV}\sum_{\boldsymbol{k},\sigma} f'_{\boldsymbol{k}\sigma}\,\boldsymbol{k} = -\frac{e\hbar}{mV}\sum_{\boldsymbol{k},\sigma}\boldsymbol{k}\left\{ f(E_{\boldsymbol{k}}) + \hbar\boldsymbol{k}\cdot\boldsymbol{v}\,\frac{\partial f(E)}{\partial E}\bigg|_{E=E_{\boldsymbol{k}}} + \ldots\right\} \\ &= \frac{2\hbar^2 e\boldsymbol{v}}{3m}\int\!\frac{d^3\!k}{(2\pi)^3}\,k^2\left(-\frac{\partial f}{\partial E}\right)_{E=E_{\boldsymbol{k}}} = \frac{\hbar^2 e\boldsymbol{v}}{3\pi^2 m}\int\limits_0^\infty\! dk\,k^4\left(-\frac{\partial f}{\partial E}\right)_{E=E_{\boldsymbol{k}}} = \ en_{\rm n}\boldsymbol{v} \quad ,\end{aligned} \tag{4.242}$$

yielding the exact same expression for $n_{\rm n}(T)$. So we conclude that $\lambda_{\rm L}^2 = mc^2/4\pi n_{\rm s}(T)e^2$, with $n_{\rm s}(T=0)=n$ and $n_{\rm s}(T\geq T_{\rm c})=0$. The difference $n_{\rm s}(0)-n_{\rm s}(T)$ is exponentially small in $\Delta_0/k_{\rm B}T$ for small T.

Microwave absorption measurements usually focus on the quantity $\lambda_{\rm L}(T)-\lambda_{\rm L}(0)$. A piece of superconductor effectively changes the volume – and hence the resonant frequency – of the cavity in which it is placed. Measuring the cavity resonance frequency shift $\Delta\omega_{\rm res}$ as a function of temperature allows for a determination of the difference $\Delta\lambda_{\rm L}(T)\propto\Delta\omega_{\rm res}(T)$.

Note that anything but an exponential dependence of $\Delta\ln\lambda_{\rm L}$ on $1/T$ indicates that there are low-lying quasiparticle excitations. The superconducting density of states is then replaced by

$$g_{\rm s}(E) = g_{\rm n}\int\!\frac{d\hat{\boldsymbol{k}}}{4\pi}\,\frac{E}{\sqrt{E^2-\Delta^2(\hat{\boldsymbol{k}})}}\,\Theta\big(E^2-\Delta^2(\hat{\boldsymbol{k}})\big) \quad , \tag{4.243}$$

where the gap $\Delta(\hat{\boldsymbol{k}})$ depends on direction in $\boldsymbol{k}$-space. If $g(E)\propto E^\alpha$ as $E\to 0$, then

$$n_{\rm n}(T)\propto\int\limits_0^\infty\! dE\,g_{\rm s}(E)\left(-\frac{\partial f}{\partial E}\right)\propto T^\alpha \quad , \tag{4.244}$$

in contrast to the exponential $\exp(-\Delta_0/k_{\rm B}T)$ dependence for the s-wave (full gap) case. For example, if

$$\Delta(\hat{\boldsymbol{k}}) = \Delta_0\,\sin^n\!\theta\,e^{in\varphi}\propto\Delta_0\,Y_{nn}(\theta,\varphi) \quad , \tag{4.245}$$

then we find $g_{\rm s}(E)\propto E^{2/n}$. For $n=2$ we would then predict a linear dependence of $\Delta\ln\lambda_{\rm L}(T)$ on T at low temperatures. Of course it is also possible to have *line nodes* of the gap function, *e.g.* $\Delta(\hat{\boldsymbol{k}}) = \Delta_0\,(3\cos^2\theta-1)\propto\Delta_0\,Y_{20}(\theta,\varphi)$.

EXERCISE: Compute the energy dependence of $g_{\rm s}(E)$ when the gap function has line nodes.