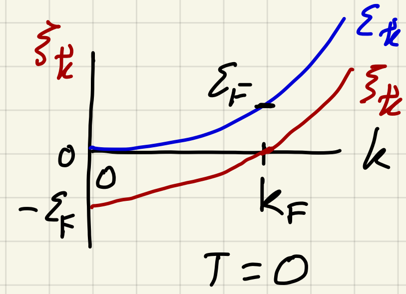
Lecture 17 (Feb. 25)



- **Solution of the mean field Hamiltonian:**

We have, with $\xi_k = \varepsilon_k - \mu$,

$$\hat{K}_{BCS} = \sum_k \underbrace{\begin{pmatrix} c^\dagger_{k\uparrow} & c_{-k\downarrow} \end{pmatrix} \begin{pmatrix} \xi_k & \Delta_k \\ \Delta^*_k & -\xi_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix}}_{\text{to become } \begin{pmatrix} \gamma^\dagger_{k\uparrow} & \gamma_{-k\downarrow} \end{pmatrix} \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma^\dagger_{-k\downarrow} \end{pmatrix}} + K_0$$

where $\xi_k = \varepsilon_k - \mu$ and

$$K_0 = \sum_k \xi_k - \sum_{k,k'} V_{k,k'} \langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \rangle \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle$$

We diagonalize the problem via a unitary transformation,

$$\begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} = \underbrace{\begin{pmatrix} \cos\vartheta_k & -\sin\vartheta_k e^{i\phi_k} \\ \sin\vartheta_k e^{-i\phi_k} & \cos\vartheta_k \end{pmatrix}}_{U_k} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma^\dagger_{-k\downarrow} \end{pmatrix}$$

In order that the $\gamma_{k\sigma}$ operators satisfy Fermi statistics, we must have that U_k is unitary. Then

$$c_{k\sigma} = \cos\vartheta_k \, \gamma_{k\sigma} - \sigma \sin\vartheta_k e^{i\phi_k} \gamma^\dagger_{-k-\sigma}$$

$$\gamma_{k\sigma} = \cos\vartheta_k \, c_{k\sigma} + \sigma \sin\vartheta_k e^{i\phi_k} c^\dagger_{-k-\sigma}$$

The transformed grand canonical Hamiltonian is (dropping k, σ):

$$\tilde{K} = U^\dagger K U = \begin{pmatrix} \cos\vartheta & \sin\vartheta e^{i\phi} \\ -\sin\vartheta e^{-i\phi} & -\cos\vartheta \end{pmatrix} \begin{pmatrix} \xi & \Delta \\ \Delta^* & -\xi \end{pmatrix} \begin{pmatrix} \cos\vartheta & -\sin\vartheta e^{i\phi} \\ \sin\vartheta e^{-i\phi} & -\cos\vartheta \end{pmatrix}$$

Working this out, we obtain

$$\tilde{K}_{11} = (\cos^2\vartheta - \sin^2\vartheta)\,\xi + \sin\vartheta\cos\vartheta(\Delta e^{-i\phi} + \Delta^* e^{i\phi})$$

$$\tilde{K}_{22} = (\sin^2\vartheta - \cos^2\vartheta)\,\xi - \sin\vartheta\cos\vartheta(\Delta e^{-i\phi} + \Delta^* e^{i\phi}) = -\tilde{K}_{11}$$

$$\tilde{K}_{12} = \left[(\Delta e^{-i\phi}\cos^2\vartheta - \Delta^* e^{i\phi}\sin^2\vartheta) - 2\xi\sin\vartheta\cos\vartheta\right] e^{i\phi}$$

$$\tilde{K}_{21} = \tilde{K}_{12}^*$$

We now use our freedom to choose ϑ and ϕ to make the off-diagonal elements vanish. We demand $\phi = \arg(\Delta)$ and

$$2\xi\sin\vartheta\cos\vartheta = |\Delta|\,(\cos^2\vartheta - \sin^2\vartheta)$$

i.e. $\tan(2\vartheta) = |\Delta|/\xi$

We then have

$$\cos(2\vartheta) = \frac{\xi}{E} \quad , \quad \sin(2\vartheta) = \frac{|\Delta|}{E} \quad , \quad E = \sqrt{\xi^2 + |\Delta|^2}$$

The element $\tilde{K}_{11}$ then becomes

$$\tilde{K}_{11} = (\cos^2\vartheta - \sin^2\vartheta)\,\xi - \sin\vartheta\cos\vartheta(\Delta e^{-i\phi} + \Delta^* e^{i\phi})$$

$$= \frac{\xi^2}{E} + \frac{|\Delta|^2}{E} = E$$

and thus

$$\tilde{K} = U^\dagger K U = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$$

This transformation is known as the **Bogoliubov transformation**. Restoring the wavevector subscript, $\phi_{\mathbf{k}} = \arg(\Delta_{\mathbf{k}})$ and

$$\cos(2\vartheta_{\mathbf{k}}) = \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \quad , \quad \sin(2\vartheta_{\mathbf{k}}) = \frac{|\Delta_{\mathbf{k}}|}{E_{\mathbf{k}}} \quad , \quad E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$$

We also have the BCS coherence factors

$$\cos\vartheta_{\mathbf{k}} = \sqrt{\frac{1}{2}\left(1+\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right)} \approx \begin{cases} 0 & \text{if } k<k_F \\ 1 & \text{if } k>k_F \end{cases} \quad , \quad \sin\vartheta_{\mathbf{k}} = \sqrt{\frac{1}{2}\left(1-\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right)} \approx \begin{cases} 1 & \text{if } k<k_F \\ 0 & \text{if } k>k_F \end{cases}$$

In terms of the $\gamma_{\mathbf{k}\sigma}$ fermions, then,

$$\hat{K}_{BCS} = \sum_{\mathbf{k},\sigma} E_{\mathbf{k}}\, \gamma^\dagger_{\mathbf{k}\sigma}\gamma_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} (\xi_{\mathbf{k}} - E_{\mathbf{k}}) - \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \langle c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}\rangle \langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}\rangle$$

What is the ground state $|G\rangle$ in terms of our original $c_{\mathbf{k}\sigma}$ fermions? We must have

$$\gamma_{\mathbf{k}\sigma}|G\rangle = \left(\cos\vartheta_{\mathbf{k}}\, c_{\mathbf{k}\sigma} + \sigma \sin\vartheta_{\mathbf{k}}\, e^{i\phi_{\mathbf{k}}}\, c^\dagger_{-\mathbf{k}-\sigma}\right)|G\rangle = 0$$

for each $\mathbf{k},\sigma$. Therefore,

$$|G\rangle = \prod_{\mathbf{k}} \left(\cos\vartheta_{\mathbf{k}} - \sin\vartheta_{\mathbf{k}}\, e^{i\phi_{\mathbf{k}}}\, c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}\right)|0\rangle$$

This is the famous BCS ground state, first written by J.R. Schrieffer.

To make contact with the familiar consider the case where $\Delta_{\mathbf{k}} = 0$. Note that $\xi_{\mathbf{k}} < 0$ for $|\mathbf{k}| < k_F$ and $\xi_{\mathbf{k}} > 0$ for $|\mathbf{k}| > k_F$. Thus

$$\cos\vartheta_{\mathbf{k}} = \Theta(k-k_F) \quad , \quad \sin\vartheta_k = \Theta(k_F - k)$$

and

$$|G\rangle = \prod_{|\mathbf{k}|<k_F} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}|0\rangle = |F\rangle$$

What are the elementary excitations? We have

$$\gamma^\dagger_{\mathbf{k}\sigma} = \cos\vartheta_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma} + \sigma \sin\vartheta_{\mathbf{k}}\, e^{-i\phi_{\mathbf{k}}}\, c_{-\mathbf{k}-\sigma}$$
$$= \sigma\, \Theta(k_F - k)\, c_{-\mathbf{k}-\sigma} + \Theta(k-k_F)\, c^\dagger_{\mathbf{k}\sigma}$$

The elementary excitations are **particles** above the Fermi surface ($k > k_F$) and **holes** below the Fermi surface ($k_F > k$).

- **Self-consistency**: We now demand two things:

$$N = \sum_{\mathbf{k},\sigma} \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \rangle \quad , \qquad \Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \rangle$$

Work it out:

$$\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \rangle = \langle (\cos\vartheta_{\mathbf{k}}\, \gamma^\dagger_{\mathbf{k}\sigma} - \sigma \sin\vartheta_{\mathbf{k}}\, e^{-i\phi_{\mathbf{k}}}\, \gamma_{-\mathbf{k}-\sigma})(\cos\vartheta_{\mathbf{k}}\, \gamma_{\mathbf{k}\sigma} - \sigma \sin\vartheta_{\mathbf{k}}\, e^{i\phi_{\mathbf{k}}}\, \gamma^\dagger_{-\mathbf{k}-\sigma}) \rangle$$
$$= \cos^2\vartheta_{\mathbf{k}} \langle \gamma^\dagger_{\mathbf{k}\sigma} \gamma_{\mathbf{k}\sigma} \rangle + \sin^2\vartheta_{\mathbf{k}} \langle \gamma_{-\mathbf{k}\sigma} \gamma^\dagger_{-\mathbf{k}\sigma} \rangle$$
$$= \cos^2\vartheta_{\mathbf{k}}\, f_{\mathbf{k}} + \sin^2\vartheta_{\mathbf{k}} (1 - f_{\mathbf{k}}) = \frac{1}{2} - \frac{\xi_{\mathbf{k}}}{2E_{\mathbf{k}}} \tanh\left(\tfrac{1}{2}\beta E_{\mathbf{k}}\right)$$

where $f_{\mathbf{k}} = \langle \gamma^\dagger_{\mathbf{k}\sigma} \gamma_{\mathbf{k}\sigma} \rangle = \dfrac{1}{e^{\beta E_{\mathbf{k}}} + 1} = \frac{1}{2}\left(1 - \tanh\left(\tfrac{1}{2}\beta E_{\mathbf{k}}\right)\right)$.

Next,

$$\langle c_{-\mathbf{k}-\sigma} c_{\mathbf{k}\sigma} \rangle = \langle (\cos\vartheta_{\mathbf{k}}\, \gamma_{-\mathbf{k}-\sigma} + \sigma \sin\vartheta_{\mathbf{k}}\, e^{i\phi_{\mathbf{k}}}\, \gamma^\dagger_{\mathbf{k}\sigma})(\cos\vartheta_{\mathbf{k}}\, \gamma_{\mathbf{k}\sigma} - \sigma \sin\vartheta_{\mathbf{k}}\, e^{i\phi_{\mathbf{k}}}\, \gamma^\dagger_{-\mathbf{k}-\sigma}) \rangle$$
$$= \sigma \sin\vartheta_{\mathbf{k}} \cos\vartheta_{\mathbf{k}}\, e^{i\phi_{\mathbf{k}}} (2 f_{\mathbf{k}} - 1) = -\frac{\sigma \Delta_{\mathbf{k}}}{2E_{\mathbf{k}}} \tanh\left(\tfrac{1}{2}\beta E_{\mathbf{k}}\right)$$

Let's work at $T=0$:

BCS gap equation at $T=0$

$$N = \sum_{\boldsymbol{k}} \left(1 - \frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right) \quad , \quad \Delta_{\boldsymbol{k}} = -\sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'} \frac{\Delta_{\boldsymbol{k}'}}{2E_{\boldsymbol{k}'}}$$

Note that $\Delta_{\boldsymbol{k}} = 0$ is always a solution to the gap equation, just as zero magnetization is always a solution to the mean field theory of an Ising ferromagnet: $m = \tanh(zJm/k_B T)$. In both cases, however, the broken symmetry solution ($\Delta_{\boldsymbol{k}} \neq 0$, $m \neq 0$) is generally of lower energy for $T < T_c$.

To proceed further, we need a model for $V_{\boldsymbol{k},\boldsymbol{k}'}$. Let's take

$$V_{\boldsymbol{k},\boldsymbol{k}'} = \begin{cases} -v/V & \text{if } |\xi_{\boldsymbol{k}}| < \hbar\omega_D \text{ and } |\xi_{\boldsymbol{k}'}| < \hbar\omega_D \\ 0 & \text{otherwise} \end{cases}$$

Here $v > 0$, so the interaction is attractive if $\xi_{\boldsymbol{k}}$ and $\xi_{\boldsymbol{k}'}$ are each within $\hbar\omega_D$ of ε_F and is zero otherwise. We seek a solution of the form

$$\Delta_{\boldsymbol{k}} = \begin{cases} \Delta e^{i\phi} & \text{if } |\xi_{\boldsymbol{k}}| < \hbar\omega_D \\ 0 & \text{otherwise} \end{cases}$$

with Δ real and non-negative. We then have

$$\Delta = +v \int \frac{d^3k}{(2\pi)^3} \frac{\Delta}{2E_{\boldsymbol{k}}} \Theta(\hbar\omega_D - |\xi_{\boldsymbol{k}}|) = \frac{1}{2} v\, g(\varepsilon_F) \int_0^{\hbar\omega_D} d\xi \frac{\Delta}{\sqrt{\xi^2 + \Delta^2}}$$

where we presume $g(\varepsilon_F + \xi) \approx g(\varepsilon_F)$. Thus, we have

$$1 = \frac{1}{2} v g(\varepsilon_F) \int_0^{\hbar\omega_D/\Delta} ds\, (1+s^2)^{-1/2} = \frac{1}{2} v g(\varepsilon_F) \sinh^{-1}(\hbar\omega_D/\Delta)$$

Writing $\Delta_0 \equiv \Delta(T=0)$, then,

$$\Delta_0 = \frac{\hbar\omega_D}{\sinh\left(\frac{2}{g(\varepsilon_F) v}\right)} \approx 2\hbar\omega_D \exp\left(-\frac{2}{g(\varepsilon_F) v}\right)$$

where the latter expression holds for $g(\varepsilon_F) v << 1$. Note that the argument of the exponential is half as large as what we found in the solution of the Cooper problem.

- **Condensation energy** : We have

use gap equation here

$$\langle G|\hat{K}_{BCS}|G\rangle = \sum_{\mathbf{k}} \left(\xi_{\mathbf{k}} - E_{\mathbf{k}} + \frac{|\Delta_{\mathbf{k}}|^2}{2E_{\mathbf{k}}} \right)$$

To compare normal and superconducting ground state energies, we subtract the normal state energy, obtaining

$$E_s - E_n = \sum_{\mathbf{k}} \left(\xi_{\mathbf{k}} - E_{\mathbf{k}} + \frac{|\Delta_{\mathbf{k}}|^2}{2E_{\mathbf{k}}} - 2\xi_{\mathbf{k}} \Theta(k_F - k) \right)$$

$$= 2\sum_{\mathbf{k}} (\xi_{\mathbf{k}} - E_{\mathbf{k}}) \Theta(\xi_{\mathbf{k}}) \Theta(\hbar\omega_D - \xi_{\mathbf{k}}) + \sum_{\mathbf{k}} \frac{\Delta_0^2}{2E_{\mathbf{k}}} \Theta(\hbar\omega_D - |\xi_{\mathbf{k}}|)$$

since

$$\xi_{\mathbf{k}} - E_{\mathbf{k}} - 2\xi_{\mathbf{k}} \Theta(-\xi_{\mathbf{k}}) = \begin{cases} 0 & \text{if } \xi_{\mathbf{k}} > E_{\mathbf{k}} \\ \xi_{\mathbf{k}} - E_{\mathbf{k}} & \text{if } 0 < \xi_{\mathbf{k}} < E_{\mathbf{k}} \\ -\xi_{\mathbf{k}} - E_{\mathbf{k}} & \text{if } -E_{\mathbf{k}} < \xi_{\mathbf{k}} < 0 \\ 0 & \text{if } \xi_{\mathbf{k}} < -E_{\mathbf{k}} \end{cases}$$

We find

$$E_s - E_n = Vg(\varepsilon_F)\Delta_0^2 \int_0^{\hbar\omega_D/\Delta_0} ds \left(s - \sqrt{1+s^2} + \frac{1}{2\sqrt{1+s^2}} \right)$$

$$= \frac{1}{2} Vg(\varepsilon_F)\Delta_0^2 \left\{ \left(\frac{\hbar\omega_D}{\Delta_0}\right)^2 - \left(\frac{\hbar\omega_D}{\Delta_0}\right)\sqrt{1+\left(\frac{\hbar\omega_D}{\Delta_0}\right)^2} \right\}$$

$$\simeq -\frac{1}{4} Vg(\varepsilon_F)\Delta_0^2$$

assuming $\Delta_0 \ll \hbar\omega_D$, which is valid for weak attraction. So the condensation energy density is

$$\Delta g = -\frac{1}{4} g(\varepsilon_F)\Delta_0^2 = -\frac{H_c^2}{8\pi} \Rightarrow H_c(0) = \sqrt{2\pi g(\varepsilon_F)}\,\Delta_0$$

- **Coherence factors:** We found

$$\gamma_{k\sigma}^\dagger = \cos\vartheta_k c_{k\sigma}^\dagger + \sigma \sin\vartheta_k e^{i\phi_k} c_{-k-\sigma}$$

and

$$\cos^2\vartheta_k = \frac{1}{2}\left(1 + \frac{\xi_k}{E_k}\right), \quad \sin^2\vartheta_k = \frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right)$$

with

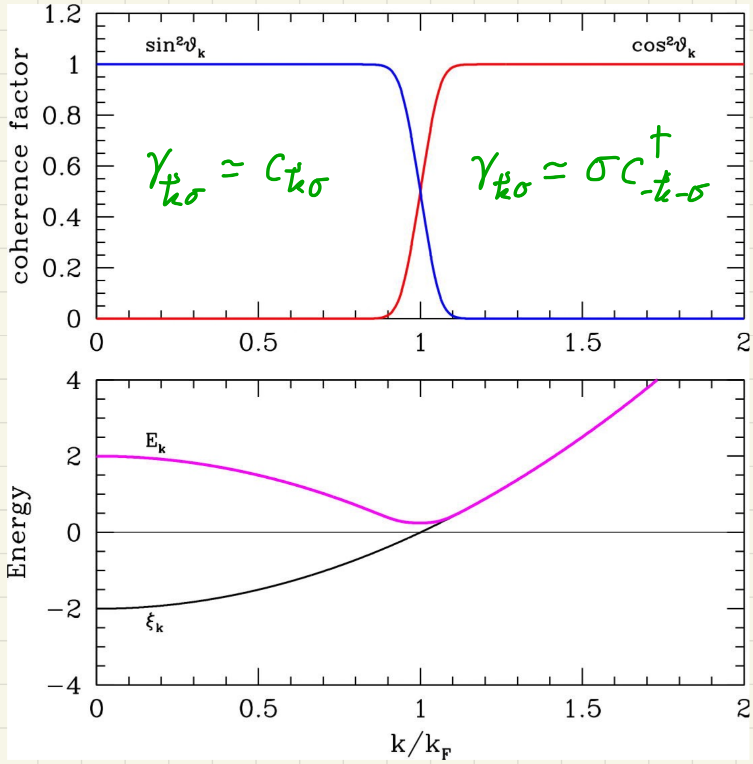
$$\xi_k = \varepsilon_k - \mu, \quad E_k = \sqrt{\xi_k^2 + \Delta_0^2}, \quad \phi_k = 0$$

and where μ and Δ_k are fixed by the conditions

$$N = \sum_k \left(1 - \frac{\xi_k}{E_k}\right), \quad \sum_{k'} V_{k,k'} \frac{1}{2\sqrt{\xi_{k'}^2 + \Delta_0^2}} = 1$$

at $T=0$.

When $\hbar\omega_D \ll \varepsilon_F$, there is a narrow window about $k = k_F$ where $E_{\mathbf{k}}$ differs from $|\xi_{\mathbf{k}}|$. Typically $\Delta_0 \simeq 10^{-4}\varepsilon_F$ in conventional superconductors. So the Bogoliubov operator $\gamma^{\dagger}_{\mathbf{k}\sigma}$ creates a linear combination of electron and hole when $|k-k_F| \lesssim \Delta_0/\hbar v_F \simeq 10^{-3} k_F$.



BCS coherence factors

NB: When $V_{\mathbf{k},\mathbf{k}'} = -v\,\Theta(\hbar\omega_D - |\xi_{\mathbf{k}}|)\,\Theta(\hbar\omega_D - |\xi_{\mathbf{k}'}|)$ the dispersion $E_{\mathbf{k}}$ is discontinuous when $|\xi_{\mathbf{k}}| = \hbar\omega_D \Rightarrow k = k^*_{\pm} = k_F \pm \omega_D/v_F$. However, the magnitude of the discontinuity is tiny:

$$\delta E = \sqrt{(\hbar\omega_D)^2 + \Delta_0^2} - \hbar\omega_D \approx \frac{\Delta_0^2}{2\hbar\omega_D} \Rightarrow \frac{\delta E}{\hbar\omega_D} \simeq 2e^{-4/g(\varepsilon_F)v} \ll 1$$

- **Number and phase**: Consider the state

$$|G(\alpha)\rangle = \prod_{\mathbf{k}} \left(\cos\vartheta_{\mathbf{k}} - e^{i\alpha} e^{i\phi_{\mathbf{k}}} \sin\vartheta_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow}\right) |0\rangle$$

Abbreviate $|G(\alpha)\rangle \equiv |\alpha\rangle$. Consider action of $\hat{N}$ on $|\alpha\rangle$:

$$\hat{N}|\alpha\rangle = \sum_{\mathbf{k}} \left(c^{\dagger}_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} + c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}\downarrow}\right)|\alpha\rangle \qquad \mathbf{k}' \neq \mathbf{k}$$

$$= -2e^{i\alpha} \sum_{\mathbf{k}} \sin\vartheta_{\mathbf{k}}\, e^{i\phi_{\mathbf{k}}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} \prod_{\mathbf{k}'}{}' \left(\cos\vartheta_{\mathbf{k}'} - e^{i\alpha} e^{i\phi_{\mathbf{k}'}} \sin\vartheta_{\mathbf{k}'}\, c^{\dagger}_{\mathbf{k}'\uparrow} c^{\dagger}_{-\mathbf{k}'\downarrow}\right)|0\rangle$$

$$= \frac{2}{i}\frac{\partial}{\partial\alpha}|\alpha\rangle$$

$\hat{M} = \frac{1}{2}\hat{N}$ = # Cooper pairs $\Rightarrow$ $\hat{M} \leftrightarrow \frac{1}{i}\frac{\partial}{\partial\alpha}$

Project onto state of definite particle number $N = 2M$:

$$|M\rangle = \int_{-\pi}^{\pi} \frac{d\alpha}{2\pi}\, e^{-iM\alpha}\, |\alpha\rangle$$

Number fluctuations:

$$\frac{\langle\alpha|\hat{N}^2|\alpha\rangle - \langle\alpha|\hat{N}|\alpha\rangle^2}{\langle\alpha|\hat{N}|\alpha\rangle} = \frac{2\int d^3k\, \sin^2\vartheta_k \cos^2\vartheta_k}{\int d^3k\, \sin^2\vartheta_k}$$

Thus, $\Delta N_{RMS} \propto \sqrt{\langle N\rangle}$