PHYSICS 239.c : CONDENSED MATTER PHYSICS
FINAL EXAMINATION
Instructions: Do problem 0 and any three of problems 1 through 4.

(0) Provide brief but accurate answers to each of the following questions:

(a) What is the Hohenberg-Mermin-Wagner theorem, and what is Goldstone's theorem?

(b) In the context of the Boltzmann equation, what is meant by the term, "collisional invariant"? What are two examples of collisional invariants in the case of (single band) electron transport?

(c) The point group D_8, describing the symmetries of a planar octagon, is relevant to molecular chemistry, but is not among the 32 crystallographic point groups. Why not?

(d) What is the Mössbauer effect?

(e) What is a Wannier state? What quantum numbers are necessary to specify a Wannier state? What completeness and orthonormality conditions to the Wannier states satisfy?

(1) The hexagonal close packed (hcp) structure is a simple hexagonal (sh) Bravais lattice with a two-element basis. The three elementary direct lattice vectors of the sh structure are

$$\boldsymbol{a}_1 = a(\tfrac{1}{2}\hat{\boldsymbol{x}} - \tfrac{\sqrt{3}}{2}\hat{\boldsymbol{y}}) \qquad , \qquad \boldsymbol{a}_2 = a(\tfrac{1}{2}\hat{\boldsymbol{x}} + \tfrac{\sqrt{3}}{2}\hat{\boldsymbol{y}}) \qquad , \qquad \boldsymbol{a}_3 = c\hat{\boldsymbol{z}}$$

The two basis vectors are **0** and $\boldsymbol{\delta} = \frac{1}{3}\boldsymbol{a}_1 + \frac{2}{3}\boldsymbol{a}_2 + \frac{1}{2}\boldsymbol{a}_3$.

(a) The hcp lattice is close-packed, which means that $|\boldsymbol{\delta}| = a$. Find the value of c in terms of the in-plane lattice spacing a.

(b) What is the coordination number z (*i.e.* the number of nearest neighbors of any given site) of the hcp lattice? Write down the positions of all z neighbors of the lattice site **0** in terms of $\boldsymbol{a}_{1,2,3}$ and $\boldsymbol{\delta}$.

(c) What are the three elementary reciprocal lattice vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$?

(d) The space group of the hcp structure ($P63/mmc$) is nonsymmorphic (it contains a twofold screw operation). Consider the Bragg peaks located at wavevectors $\boldsymbol{G} = n_1\,\boldsymbol{b}_1 + n_2\,\boldsymbol{b}_2 + n_3\,\boldsymbol{b}_3$. What is the condition on $\{n_1, n_2, n_3\}$ for there to be an extinction in the diffraction pattern at $\boldsymbol{G}$?

(2) Consider the tight binding Hamiltonian for s-orbitals on the railroad trestle lattice, depicted in Fig. 1. The hopping amplitude along each rail is t and the hopping amplitude between the rails is t'. Both t and t' are positive.

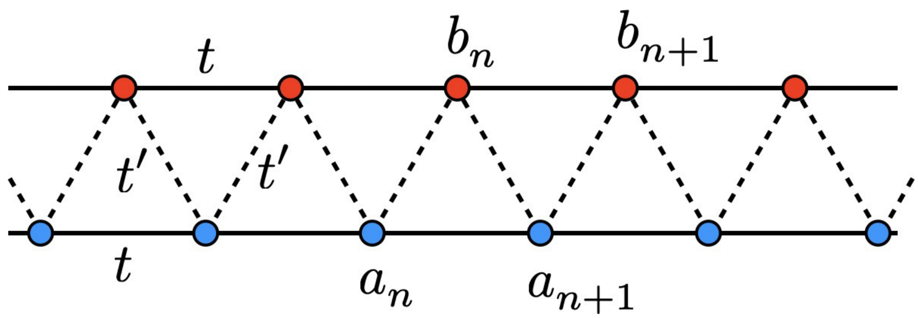

Figure 1: Railroad trestle lattice

(a) Write the tight-binding Hamiltonian in real space. You may use either braket notation with local orthonormal orbitals $|\, n, a \,\rangle$ and $|\, n, b \,\rangle$ or fermionic second quantized operators a_n and b_n and their conjugates.

(b) Write the tight-binding Hamiltonian in crystal momentum space, *i.e.* using the Fourier transformed states $|\, k, a \,\rangle$ and $|\, k, b \,\rangle$ or the second quantized operators a_k and b_k (and their conjugates).

(c) Solve for the electronic energy bands $E_j(\theta)$, where $\theta = ka$ and a is the lattice spacing along either rail. How many bands are there? Sketch their dispersion.

(3) Consider an infinite one-dimensional chain of atoms, each of mass m, located at positions $x_n = na + u_n$, with potential energy

$$V = \tfrac{1}{2} \sum_{n<n'} K_{nn'}\, (u_n - u_{n'})^2 \quad .$$

Thus, each pair of atoms (n, n') is connected by a spring of spring constant $K_{nn'}$ whose unstretched length is $|n-n'|a$, where a is the lattice constant. You may assume the potential has the lattice translation symmetry, *i.e.* $K_{nn'} = K(n-n') = K(n'-n)$ is an even function of the difference $n - n'$.

(a) Find the equation of motion for the Fourier modes $\hat{u}_k \equiv N^{-1/2} \sum_n u_n\, e^{-ikna}$, where $N \to \infty$ is the number of unit cells.

(b) Find an expression for the phonon dispersion $\omega(k)$.

(c) Write down an expression for the ground state wavefunction $\Psi_0\big(\{u_n\}\big)$.

(d) Suppose $K(\ell) = K_0\, \ell^{-2}$. Compute the phonon frequency $\omega(k)$ and the zero temperature quantum fluctuation $\langle\, \Psi_0 \,|\, u_n^2 \,|\, \Psi_0 \,\rangle$ of the atomic positions. It may interest you to know that for $\theta \in [0, 2\pi]$, it is a True Fact that

$$\mathsf{Re}\,\mathsf{Li}_2(e^{i\theta}) = \sum_{n=1}^{\infty} \frac{\cos(n\theta)}{n^2} = \tfrac{1}{6}\pi^2 - \tfrac{1}{4}\theta\,(2\pi - \theta) \quad ,$$

where

$$\mathsf{Li}_k(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^k} \quad .$$

is the polylogarithm function.

(e) For $K(\ell) = K_0\,(\delta_{\ell,1} + \delta_{\ell,-1})$, we found $\omega_k = 2(K_0/m)^{1/2}\,\big|\sin(\frac{1}{2}ka)\big|$, hence $\omega(k) = c|k|$ at long wavelengths. The zero temperature fluctuations $\Psi_0\big(\{u_n\}\big)$ then diverge. Yet your result for the fluctuations in part (d) should have been finite. Why do you suppose this might be the case?

(4) Consider the currents

$$\begin{aligned}
\boldsymbol{j} &= -2e \int\limits_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\, \boldsymbol{v}\,\delta f \\
\boldsymbol{J} &\equiv 2 \int\limits_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\, (\varepsilon - \mu)^2\, \boldsymbol{v}\,\delta f \quad .
\end{aligned}$$

Define the response coefficients ρ, Q, ω, and υ by the relations

$$\begin{aligned}
\boldsymbol{\mathcal{E}} &= \rho\,\boldsymbol{j} + Q\,\boldsymbol{\nabla} T \\
\boldsymbol{J} &= \omega \boldsymbol{j} - \upsilon\,\boldsymbol{\nabla} T \quad .
\end{aligned}$$

For a system with cubic symmetry, find expressions for the transport coefficients ρ, Q, ω, and υ in terms of the integrals

$$\begin{aligned}
\mathcal{K}_n &= \frac{\tau}{12\pi^3\hbar} \int\limits_{-\infty}^{\infty} d\varepsilon\, (\varepsilon - \mu)^n \left(-\frac{\partial f^0}{\partial \varepsilon}\right) \int dS_\varepsilon\, |\boldsymbol{v}| \\
&= \frac{\sigma_0}{e^2}\, \varepsilon_{\mathrm{F}}^{-3/2}\, \mathcal{S}\left[\varepsilon^{3/2}(\varepsilon - \mu)^n\right]\bigg|_{\varepsilon=\mu} \quad ,
\end{aligned}$$

where

$$\mathcal{S} = \pi\mathcal{D} \csc \pi\mathcal{D} = 1 + \frac{\pi^2}{6}\,\mathcal{D}^2 + \frac{7\pi^4}{360}\,\mathcal{D}^4 + \ldots \quad ,$$

with $\mathcal{D} = k_{\mathrm{B}} T\,\partial_\varepsilon$.