NATIONAL UNIVERSITY OF SINGAPORE

PC5203 – ADVANCED SOLID STATE PHYSICS

(Semester II: AY 2020-21)

Via Zoom on Wednesday 5 May 5:00-7:00pm; Time Allowed: 2 Hours

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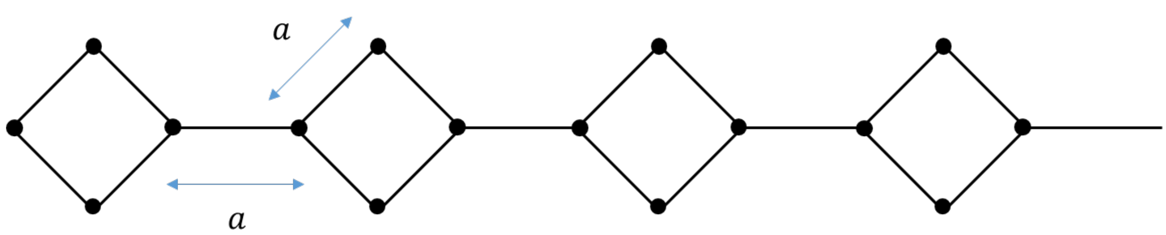
INSTRUCTIONS TO STUDENTS

1. This assessment paper contains FOUR questions and comprises FOUR printed pages (including this cover page).
2. Students are required to answer ALL questions.
3. Students should write the answers for each question on a new page. Scanned or soft copies should be uploaded to LumiNUS as a single PDF file before 7:30pm.
4. This is an OPEN BOOK examination.
5. Calculators or software packages are allowed.

1. Consider a quasi-one-dimensional lattice consisting of connected squares of side length a as shown below. Each vertex of the square denotes a site that (at most one) electron can hop to.
    a. Based on the geometry given, define the unit cell. Give the real space lattice vectors $\boldsymbol{R}_l$ and specify the Brillouin zone in reciprocal $\mathbf{k}$ space.
    b. Consider N repeating unit cells with periodic boundary condition defined in part a, specify the group elements A_j that characterize the symmetry of the system. For each group element, also write down the character $\chi(A_j)$ of all the irreducible representations.
    c. Consider the tight-binding model defined on the 1D lattice, with hopping parameter t between nearest neighbor sites of distance a and zero otherwise. Write down the many-body Hamiltonian $\widehat{H} = c^{\dagger}Hc$ with (spinless) creation and annihilation fermionic operators defined on each site. Specify your naming convention clearly.
    d. The single particle wave function is determined by the Schrödinger equation $H\psi = \epsilon\psi$. Without actually solving it, based on the Bloch theorem, what is the form of the wave function, specifically for the quasi-1D square model?
    e. Determine the Hamiltonian $H(k)$ in wave-vector k space. What is the matrix dimension of the Hamiltonian $H(k)$?
    f. Determine the dispersion relation of the system, $\epsilon_n(k)$. How many bands do we have? From the dispersion relation, determine the transmission function, $T(E)$, in a ballistic electron transport in a Landauer formula. Draw a qualitative plot of $T(E)$ vs energy E.



2. The Dyson equation $G = g + g\Sigma G$ defined on the Keldysh contour is, more explicitly,

$$G_{jk}(\tau,\tau') = g_{jk}(\tau,\tau') + \sum_{l,m}\iint d\tau_1 d\tau_2\, g_{jl}(\tau,\tau_1)\Sigma_{lm}(\tau_1,\tau_2)G_{mk}(\tau_2,\tau').$$

Here the contour time integrals are convolutions, and matrices are multiplied.
    a. What is the equivalent form of the Dyson equation in real time t and branch indices $\sigma = \pm$?

b. Given that we have $G^r = G^t - G^<$, assumed to be true also for g and Σ, as well as other relations valid for the Green's functions, show that the retarded Green's function satisfies $G^r = g^r + g^r\Sigma^r G^r$.
c. Is it also true that $G^t = g^t + g^t\Sigma^t G^t$ for the time-ordered Green's function?
d. Derive an equation that $G^<$ must satisfy. Solve it and show it is the Keldysh equation $G^< = G^r\Sigma^< G^a$, under certain assumption about small g. Specify this assumption explicitly.

3. Consider the single mode constant relaxation-time approximation for the Boltzmann equation for electrons.

$$\frac{\partial f}{\partial t} + \mathbf{v}(\mathbf{k}) \cdot \frac{\partial f}{\partial \mathbf{r}} + \mathbf{F} \cdot \frac{\partial f}{\partial (\hbar \mathbf{k})} = -\frac{f - f^0}{\tau}$$

where $\mathbf{v}(\mathbf{k})$ is electron group velocity, $\mathbf{F} = -e\mathbf{E}$ is external applied force, $\mathbf{k}$ is electron wave vector, and τ is electron relaxation time, f^0 is the equilibrium Fermi distribution at energy $\epsilon_{\mathbf{k}}$ and chemical potential μ. We consider the case that the system is homogenous in space so that the distribution f will be independent of the position $\mathbf{r}$. Consider the electrons in a metal driven under a high frequency electric field in *x* direction, $\mathbf{E} = \hat{\boldsymbol{x}}Ee^{-i\omega t}$. Due to this sinusoidal external drive, the time-dependent solution of the Boltzmann equation in steady state also has the same frequency, i.e., $f \to fe^{-i\omega t}$. We assume the field amplitude E is small so that the first order perturbation in E is valid.

a. Show that the AC conductivity is given by the Drude model $\sigma(\omega) = e^2 C \frac{1}{\frac{1}{\tau} - i\omega}$, where

$$C = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\, v_x(\boldsymbol{k})^2 \left(-\frac{\partial f^0}{\partial \epsilon_{\boldsymbol{k}}}\right).$$

Here the integration is within the first Brillouin zone.

b. The above integral for C can be performed if we take the low-temperature limit so that the Fermi function becomes a step function. For a free particle with the dispersion $\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}$, assuming the Fermi sphere fits inside the first Brillouin zone, show that the constant $C = \frac{n}{m}$, where n is electron density and m is electron mass.

4. Let $H(\mathbf{k})$ be a $\mathbf{k}$-space Hamiltonian of an *N* by *N* Hermitian matrix, *N* > 1. Here the vector $\mathbf{k} = (k_x, k_y)$ is assumed two dimensional. Let the set of orthonormal eigenvectors be $\Psi_n(\mathbf{k})$ with eigenvalues $E_n(\mathbf{k})$ such that $H(\mathbf{k})\Psi_n(\mathbf{k}) = E_n(\mathbf{k})\Psi_n(\mathbf{k})$.
   a. Define the Berry phase $d\gamma_n$ of band n between two nearby points, $\mathbf{k}$ and $\mathbf{k} + d\mathbf{k}$, using eigenstates $\Psi_n(\mathbf{k})$ of the Hamiltonian, remembering that $\mathbf{k}$ is two-dimensional. This defines the Berry connection.
   b. From the expression in part a, using the Stokes theorem, define the Berry curvature $\Omega_n(\mathbf{k})$ (in z direction only).
   c. The expression in part b uses the partial derivatives of the wave functions. Using the fact that the normalized wave function also satisfies the time-independent Schrödinger equation, show that we can express the Berry curvature, alternatively, as

$$\Omega_n(\mathbf{k}) = -\mathrm{Im} \sum_{m \neq n} \frac{\Psi_n^\dagger(\mathbf{k}) \dfrac{\partial H(\mathbf{k})}{\partial k_x} \Psi_m(\mathbf{k})\, \Psi_m^\dagger(\mathbf{k}) \dfrac{\partial H(\mathbf{k})}{\partial k_y} \Psi_n(\mathbf{k})}{\left(E_m(\mathbf{k}) - E_n(\mathbf{k})\right)^2} - (x \leftrightarrow y).$$

   Here the second term is the same as the first except the role of k_x and k_y are swapped.

---- End ---- [WJS]