PC5203 Advanced Solid State Physics

Weeks 10-13, due Thursday 18 Nov 2021

[main concepts to cover: Boltzmann equation, Berry curvature, superconductivity.]

1. Consider the electron-electron Coulomb interaction of the form $H' = \frac{1}{2}\sum_{jl} c_j^\dagger c_l^\dagger v_{jl} c_l c_j$ on a simple cubic lattice of lattice constant a, so that the site j or l is defined on lattice sites on a system of $N = L^3$ sites. The noninteracting part takes the standard form of $c^+ H c = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \tilde{c}_{\mathbf{k}}^+ \tilde{c}_{\mathbf{k}}$ with a single band. (a) Transform the Coulomb interaction into $\mathbf{k}$ space, by $c_j = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} \tilde{c}_{\mathbf{k}} e^{i\mathbf{k}\cdot\boldsymbol{R}_j}$, assuming v is translationally invariant, i.e., $v_{jl} = v(\boldsymbol{R}_j - \boldsymbol{R}_l)$, determine the interaction H' in $\mathbf{k}$ space. Here $\boldsymbol{R}_j$ is the real space lattice vector for the site j and $\mathbf{k}$ varies over the first Brillouin zone of the simple cubic lattice. (b) Using H' as the small perturbation in the Fermi golden rule, determine the form of the collision rate $\left(\frac{\partial f}{\partial t}\right)_{\rm colli}$ for the Boltzmann equation under Coulomb scattering potential. [Hint: this is formally very similar to the original Boltzmann equation for classical particles, except that we have to take the Pauli exclusion principle into account for the fermionic electrons]. (c) Show that the collision rate is zero when the distribution f is given by the equilibrium Fermi distribution $f^0 = 1/(e^{\beta(\epsilon_{\mathbf{k}}-\mu)} + 1)$.

2. Consider the phonon Hall model Hamiltonian given as $H = \frac{1}{2}(p - Au)^2 + \frac{1}{2}u^T K u$, where u is a column vector of displacements relative to the equilibrium positions, p is the conjugate momentum, K is a symmetric force constant matrix, and A is an antisymmetric matrix. *T* stands for matrix transpose. p^2 means $p^T p$ for brevity.
    a. Derive the classical Hamilton equations of motion from the Hamiltonian given.
    b. Assuming periodicity of a two-dimensional crystal lattice, we can rewrite the vector u as $u_{\boldsymbol{l},j}$, where $\boldsymbol{l} = (l_1, l_2)$ is pair of integers such that real space lattice vector is given as $\mathrm{R}_{\boldsymbol{l}} = l_1\boldsymbol{a}_1 + l_2\boldsymbol{a}_2$. The unit cell is described by the two $\boldsymbol{a}$ vectors. The index j specifies the degrees of freedom in a unit cell, e.g., for graphene, $j = 1$ to 6 as there are two atoms per unit cell, and each atom can move in x, y, z directions. Because of lattice periodicity, both the matrix A and K is a function of the difference in $\boldsymbol{l}$. Derive the equation of motion in $\mathbf{q}$ space, that is, the Fourier transform in index $\boldsymbol{l}$, with the usual convention. Give the relation of the Dynamic matrix D to the real space force constant matrix K, and also define the **q** space A in terms of the real space one.

c. Assuming all the atoms move in one single frequency ω in the normal mode, derive the eigenvalue problem $H_{\text{eff}}\Psi = \omega\Psi$ (that is, give the expression for the effective Hamiltonian H_{eff}. Here Ψ is a column vector consisting of position u and velocity v in **q** space).

d. From the definition of Berry connection $d\gamma = -\text{Im}\,\bar{\Psi}\,d\Psi$, derive the Berry curvature formula (for each fixed **q**)

$$\Omega_n = -\text{Im}\sum_{m\neq n}\frac{\bar{\Psi}_n\,\partial_x H_{\text{eff}}\Psi_m\;\bar{\Psi}_m\partial_y H_{\text{eff}}\Psi_{\text{n}}}{(\omega_n-\omega_m)^2} - (x\leftrightarrow y).$$

Here we sum over m excluding the case of $m=n$, for a fixed n. And $\bar{\Psi} = \Psi^\dagger\begin{bmatrix} D & 0 \\ 0 & I\end{bmatrix}$, $D = D(\mathbf{q})$ is the usual dynamic matrix, and I is the identity matrix (all in space of site index j). We assume the modes are normalized according to $\bar{\Psi}\,\Psi = 1$. The index m or n labelled the eigenmodes, the partial derivative is with respect to q_x for ∂_x and similar for y component. The second subtraction term is obtained by swapping x with y.

[Read Sun Kangtai's PhD. Thesis]

3. The energy of the electrons and magnetic field in a conventional superconductor is $F = \int\frac{1}{2}m\mathbf{v}^2 n\,d^3\mathbf{r} + \int\frac{1}{2\mu_0}\mathbf{B}^2 d^3\mathbf{r} + \text{const.}$

   a. By minimizing the energy F, together with the definition of current, $\mathbf{j} = (-e)n\mathbf{v}$, and Ampere's law, $\nabla\times\mathbf{B} = \mu_0\mathbf{j}$, derive the London equation

   $$\mathbf{j} = -\frac{ne^2}{m}\mathbf{A}\,.$$

   Here the vector potential $\mathbf{A}$ is transverse, i.e., $\nabla\cdot\mathbf{A} = 0$. $\mathbf{B} = \nabla\times\mathbf{A}$. We treat the electron density n as a constant.

   b. Why the London equation (in another form) implies the Meissner effect, that is, the magnetic induction $\mathbf{B}$ is zero inside a superconductor body?

   [Read P.-G. de Gennes book on superconductivity]

4. The (spinless, one-dimensional) BCS ground state is postulated to be

   $$|\text{BCS}\rangle = \prod_{p>0}\left(u_p + v_p c_p^\dagger c_{-p}^\dagger\right)|0\rangle,$$

   here $|0\rangle$ is the electron vacuum state, u_p and v_p are complex numbers. This wave function represents zero, one, or any number of Cooper pairs with opposite momenta.

a. Determine the condition needed on the coefficient u and v if $\langle \mathrm{BCS} | \mathrm{BCS} \rangle = 1$, that is, the many-particle state is normalized to one.

b. Compute the expectation value of BCS Hamiltonian in the ground state, $E_g = \langle \mathrm{BCS} \,|\, \hat{H}^{\mathrm{BCS}} \,|\, \mathrm{BCS} \rangle$, here

$$\hat{H}^{\mathrm{BCS}} = \sum_{p} (\epsilon_p - \mu)\, c_p^{\dagger} c_p + \sum_{p,q>0} V_{pq} c_p^{\dagger} c_{-p}^{\dagger} c_{-q} c_q$$

(This is actually a K-miltonian, $\hat{K} = \hat{H} - \mu \hat{N}$, because we subtracted a chemical potential term). We assume the interaction matrix V is symmetric with respect to the index p and q.

c. By minimizing the ground state energy, E_g in part b, derive the solution of u and v to be, for each wavevector p, $u^2 = \frac{1}{2}(1 + \frac{\xi}{E})$, $v^2 = \frac{1}{2}(1 - \frac{\xi}{E})$, $\xi = \epsilon - \mu$, and the quasi-particle energy $E = \sqrt{\xi^2 + \Delta^2}$, and $\Delta_p = -\sum_{q>0} V_{pq} u_q v_q$. This is the gap equation in BCS theory.

[Hint. Read Feynman's book on statistical mechanics]