PH320: Condensed Matter Physics - II.

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Mon - Wed - Fri : 11·00 - 12·00.
Venue : Lecture Hall 4.

Marks Distributions : Home work - 20 %.
Mid term - 25 %.
Term paper + Presentation - 25 %.
End term - 30 %.

References :

This is a course to learn various approximate methods to solve a many-body electronic system in a lattice. Before we make any approximation, the full system we want to solve is made of $N = N_x N_y N_z$ lattice sites on three dimension (with N_μ are the lattice sites along the $\mu = x, y, z$ direction). At each site an atom of atomic mass sitting here and here we consider an monoatomic lattice to start with and later it will be trivial to generalize to multiple atoms per unit cell.

In condensed matter, we consider the nucleus a point charge $+Ze$, and mass M, whose coordinate is $\vec{R}_I$, $I = 1, \cdots, N$. Then there are Z electrons in each atom having mass m and coordinates $\vec{r}_i$, $i = 1, \cdots, ZN$. Then the many body Hamiltonian we want to solve is

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{ZN} \nabla_i^2 - \frac{\hbar^2}{2M}\sum_{I=1}^{N} \nabla_I^2 + \frac{(Ze)^2}{2}\sum_{I,J=1}^{N} \frac{1}{|\vec{R}_I - \vec{R}_J|} - Ze^2 \sum_{i,I} \frac{1}{|\vec{r}_i - \vec{R}_I|}$$

$$+ \frac{e^2}{2}\sum_{i,j} \frac{1}{|\vec{r}_i - \vec{r}_j|} . \qquad --- (1).$$

$$= H_e + H_N + H_{NN} + H_{Ne} + H_{ee}$$

All these terms have their usual meanings. Our ultimate goal is to solve this entire Hamiltonian, which does not have an exact solution. So, at various stages in this course, we will consider different pieces of this Hamiltonian.

Chapter I : Review of Condensed matter physics-I (CMP-I) course.

- In CMP-I couse, we have studied the following Hamiltonian.

(i) The electron-electron interaction (H_{ee}) is completely ignored.

(ii) The nucleons is assumed to be completely stationary, i.e., $R_I(t) = R_I(t=0)$. Hence, $H_N = 0$. Since, R_I are just fixed coordinates, H_{NN} is simply a fixed-in-time background potential which gives an overall shift to the eigenenergies and hence are ignored. Then H_{Ne} becomes a single particle potential for the electron.

(iii) <u>Born-Oppenheimer Approximation</u>: Born and Oppenheimer realized that for the case of $R_I(t) = R_I(0)$, and in the limit of $H_{Ne} \to 0$, the atomic wavefunction can be written as a product wave function of the electron $\psi(r_i)$ & that of the nucleus $\Phi(R_I)$ as

$$\psi_{Atom}(\vec{R}_I, \vec{r}_i) \sim \Phi(\vec{R}_I)\,\psi(\vec{r}_i).$$

This is an exact statement for $H_{Ne} = 0$. Born-Oppenheimer argued that this approximation is still a good approximation for most of the real materials and greatly simplies the problem.

→ Later on, the 'H_{Ne}' term is included perturbatively, giving rise to the so-called electron-phonon coupling that we will study in chapter-7.

Appendix :

→ There are also modern geometric method to improve the Born-Oppenheimer Approximation, in which one includes the effect of 'H_{Ne}' term as a "phase" and "metric" term in the wave function $\psi_{Atom}(\vec{R}, \vec{r})$ which are called Berry curvature and Quantum metric. This will be studied in a term paper as a project.

- With the Born-Oppenheimer Approximation, the electronic Hamiltonian we want to study is

$$\mathcal{H} = H_e + H_{Ne} = \sum_{r_i} H(r_i) = \sum_{r_i} h_e(r_i) + h_{Ne}(r_i),$$

under the periodic boundary condition that $h(r_i + \vec{R}_I) = h(r_i)$. The Hamiltonian can be fully diagonalized / solved by the Bloch states $\psi_{n\vec{k}}(\vec{r}) = u_{nk}(r)\, e^{i\vec{k}\cdot\vec{r}}$

where $u_{nk}(\vec{r} + \vec{R}) = u_{nk}(\vec{r})$.

Note that n is the eigenstate index (not site index 'i' or atomic orbital index).

- The discrete Fourier transformation of the Bloch eigenstate to the periodic lattice $\vec{R}$ is called the "wannier orbitals" (which are distinct from the atomic orbitals).

- We are often interested in energy states around the Fermi-level to study the low-energy & low-temparature properties of materials. To model them effectively, we develop tight-binding model. There are also other effective lattice model (such as the t-J model) and effective field theory (such as the Fermi-liquid) model that we will discuss in subsequent chapters.

Chapter II : Second Quantization

In this chapter, we take a diversion to learn a powerful technique in quantum theory called the second quantization method. The method is general and used in all branches of quantum theory. Its a generalization of the creation and destruction operators introduced for the Quantum Harmonic oscillator, or the ladder operators defined for the angular momentum operators. This is a very powerful method in which the incorporation of the quantum statistics (fermion's/boson's odd/even parity wavefunction) of many particle wavefunction. We will study the reminder of this course in second quantization method and hence this is a no-miss chapter.

We will first review the concept of identical particles, and the associated quantum statistics for exchanging two or more identical particles. We will review the fermion, boson and anyon cases in 3, 2+1 dimensions. We will discuss the Correlation between identical particles introduced by quantum statistics without even any interaction term in the Hamiltonian between the particles.

In this chapter, we will first start with writing many-body wavefunction in first quantization method, followed by the same in second quantization methods. We will introduce the concept of Fock space, as opposed to the Hilbert space in first quantization. We will also learn to express physical operators in second quantization method. We will draw some Feynmann diagrams for each operators. Finally we will define the Field operators.

Appendix : Supersymmetric Quantum Theory in Second Quantization.

Chapter 3 : Hartree - Fock Theory :

Essentially, here we introduce the electron - electron interaction part (H_{ee}) to the Born - Oppenheimer approximation Hamiltonian and study this Hamiltonian :

$$H = H_e + H_{Ne} + H_{ee}$$

- The Hartree - Fock approximation is a very interesting type of variational approximation in which we map an N - body interacting electronic system to an N - independent quasiparticles systems, traversing in the lattice on a mean or average potential term provided by all other quasiparticles.

- Therefore, the Hartree - Fock method is somewhat a manifestation of the Mean - Field Theory, that we will formally introduced here, but used in various other forms throughout this course.

→ Jellium Model : We assume $H_{Ne}(\vec{r_i}) = H_{Ne}(0) \equiv$ uniform positive charge density.

→ We will implement the Hartree - Fock method for electron - liquid case, where the wavevector / momentum of the electrons are very small, i.e., the wavelength of the electrons are very large compared to the unit cell length. Therefore, the unit cell lengthscale negligible for the Bloch wavefunctions and we call them electron liquid. We will identify two main term of $\langle \Psi_{HF} | H_{ee} | \Psi_{HF} \rangle \sim E_H + E_F$, where E_H is called the Hartree or Direct term and E_F is called the Fock or Exchange term. The direct term is like the classical Coulomb interaction between two quasi-particles charge densities. The exchange term is the true quantum mechanical term arising due to the exchange statistics of identical particles. (Due to the exchange term we have magnetism in real material).

→ We will also find that the exchange energy can be written in terms of a function $F(x)$. This function will appear throughout this course in all chapters for $x = k/k_F$ for single electron's case occupying states up to the Fermi momenta k_F, or $x = q/2k_F$ for electron-hole scattering or interaction channel with scattering momentum q. The function $F(x)$ has logarithmic singularity at $x=1$. This is the main source of instability / singularity of the Fermi-surface to all sorts of interactions, disorder, and electron phonon couplings. For example, the breakdown of the uniform positive charge density of the Jellium model, the Friedel oscillation, Stoner instability for interaction, or Kohn anomaly for electron-phonon coupling.

→ Next we consider the strong coupling limit where $H_{ee} \gg H_e$, where the potential energy dominates over the kinetic energy of electrons. Here, of course, the Hartree-Fock theory, which is a momentum space picture, breaks down and the potential energy dominates. Potential energy localizes the electrons, and one obtains the "Wigner Crystal" phase.

Appendix The Density Functional Theory (DFT).

Chapter 4: The Linear Response Theory

There are several important general lessons / messages in this chapter. First is the shortcomings of the variational / mean-field theory in the quantum many-body systems. Because, in this approach we are calculating a variational (also called saddle point or classical) ground state, which is not an eigenstate of the many-body Hamiltonian. This means, the energy (and particle number) is not conserved in this ground state. Due to uncertainty principle (which is also called the quantum fluctuation), the energy and particle numbers are changing / fluctuating in this ground state. This quantum fluctuations are also called low-energy (gapless) excitation spectrum. They can modify or even destroy the variational / mean-field ground state. Therefore, we have to study these excitations / fluctuations to determine the robustness of the variational / mean-field ground state. We will generally find two sets of resolutions to the ground state after including the fluctuations. First, the fluctuation spectrum can adiabatically modify the variational ground state, by shifting the energy, modifying the quasiparticle's effective mass, and/or screening of the charge density. Secondly, the fluctuations can produce singularity (non-analyticity) in the ground state, which says the variational solution is unstable to a phase transition to a new phase. Some of the instabilities we will learn are Stoner instability, Friedel oscillation, Kohn Anomaly, etc.

In this chapter, we will learn how to evaluate the fluctuation or excitation spectrum in some ground state. The method we will learn to evaluate the excitation spectrum is called the Linear Response Theory or Kubo formula. We calculate it using first-order time-dependent perturbation theory (hence called linear), in the interaction picture. Roughly speaking, it computes the response in some quantity such as charge or spin density at some position, due to a small disturbance in the same charge or spin density at some other position. The quantity that captures this response function is called the correlation function (mainly density-density correlation function or susceptibility). There are mainly two reasons (or three) why the disturbace to a particle at one position is felt by a particle at another position in a many body system. One reason is the quantum correlation due to quantum statistics (related to uncertainty) which is active even for non-interacting particles. The second one is the interaction (Hee) term between the particles. (The third one is the entangement between particles which can be due to different reasons and will not be discussed in this course).

The response function is a complex function, whose imaginary part gives the absorption/emission spectrum of energy/particle. In the case of conserved (isolated) system, the absorbed energy must be dissipated at a later time and somewhere else giving rise to fluctuation-dissipation theorems. This leads to Kramer's - Kronig relation, f-sum rules, causality. These theorems are the test of the analyticity or non-singularity of the response/correlation function. We will test the non-analyticity in all sorts of limit of $q\to 0$, $q\to 2k_F$, long-time, instantaneous responses.

We will see that the excitation spectrum of the non-interacting electrons on a Fermi surface (defined by only $H_e + H_{Ne}$), called the particle-hole excitation or Lindhard function, are singular. This singularity is due to purely quantum correlation on a Fermionic system. The singularity depends on the dimension of the lattice.

Next we will study the response function in the presence of the electron-electron interaction (H_{ee}). To compute the response function, i.e, the fluctuation/excitation spectrum with H_{ee}, we will introduce an approximation called the time-dependent mean-field theory, which is popularly known as the Random Phase Approximation (RPA). The interacting correlation function also turn out to be singular at various limit. These results suggests the concept of screening. Roughly speaking, screening means, in many body systems, the effective charge density and the Coulomb interaction between them are not really like those of bare electrons. Rather, as one electron moves in a positive potential background, it effectively change the local charge density and hence the Coulomb interaction it exerts on another charge density is reduced. This reduction factor of the Coulomb potential is called the dielectric constant

ε, which is essentially evaluated from the interacting density-density correlation function. We will study here static screening (called the Thomas-Fermi Screening), Friedal oscillation of quasiparticle charge density due to Fermi-surface singularity in the dielectric function. Then we will study finite frequency screening and the Plasma oscillation or Plasma mode from the imaginary part of the correlation function. We will study why metals absorb photon energy below the plasma frequency.

Finally we will learn various tests and consequences of the analyticity of the response functions such as the Kramer's-Kronig Relation, Spectral / Lehmann representation, Causality, Fermi-golden rule, Dissipation-Fluctuation Theorem, and the so-called f-sum rule of the spectral weight.

Chapter 5: The Fermi-Liquid Theorem

One of the remarkable properties of quantum metals is that despite all the singularities and instabilities described in the previous chapter, the metallic state is stable. This means, experimentally we do observe metallic state. Landau showed that this is due to the Fermi statistics of electrons which resists electrons to interact near the Fermi-level. Landau proposed a low-energy theory to effectively model the H_{ee} term in terms of electron and hole density around the fermi level - which is called the Fermi-liquid theory.

Band structure and Fermi surfaces are defined for $\hat{H}_e + \hat{H}_{Ne}$ as we studied in Condensed Matter Physics-I course. We ask what does '$\hat{H}_{ee}$' do to the electrons sitting on well-defined momentum states, i.e., on the band structure. Generally, we say, '$\hat{H}_{ee}$' or any perturbation term, does two things: (i) It changes the energy dispersion $\epsilon_k \to \epsilon_k'$ (assuming adiabaticity, i.e., electron retains). The corresponding energy shift $\Sigma_k = \epsilon_k' - \epsilon_k$ is called the self-energy. We will learn how to manipulate Σ_k to define how this energy shift essentially renormalize the band velocity and band mass - which is called mass renormalization. (ii) The second thing it does is to scatter the electron from its initial k-state to some other k' state. In another language, we say the electron's lifetime 'τ' in the k-state is finite. We can compute τ

using the Fermi's Golden rule, or it is calculated in more sophisticated procedure by the imaginary part of the self-energy $\Sigma_k'' \sim \hbar/\tau$.

Landau showed that as long as the interaction term is density-density interaction, as the Coulomb interaction, H_{ee}, is, the lifetime of the electrons (or quasiparticles) is infinite on the Fermi surface and decreases as $|\varepsilon_k|^2$ as we move away from the Fermi level. The reason the lifetime of the electrons on the Fermi surface is infinite, i.e., the electrons do not interact on the Fermi-surface is due to the Pauli exclusion principle. More specifically, as all the momentum states are filled on the Fermi surface, the electrons do not have any available state to scatter to. This simple and remarkable quantum property protects the metallic state.

The Fermi-Liquid Theory is also our first introduction to the "field theory" - as an effective theory to describe the electrons behavior for states near the Fermi-level only, which the full lattice model such as Density Functional Theory or Tight binding model describe energy states at all momenta quantum states.

Appendix: We will introduce the Green's function formalism and self-energy either as an Appendix to this chapter or as a new chapter or as a term paper in a project.

Chapter 6: The Hubbard Model

We learned in chapter 4 that the screenings, ei, correlation effects of many body system, make the Coulomb interaction exponentially decaying in real space (c.f. Thomas-Fermi Screening). Therefore, the Coulomb interaction becomes short-ranged. The Hubbard model is the shortest possible ranged or onsite interaction between an up & down spin electron. The interaction term is written as $H_{ee} \sim U n_\uparrow n_\downarrow$ at each lattice site. This simple looking interaction offers rich physics that we study in this chapter, and infact govern most of the interacting physics that we observe in correlated material.

The model cannot be solved exactly except in some special cases (ei, 1D). There are two obvious limit of $U \to 0$ & $U \to \infty$, where we can solve the problem perturbatively. At $U \to 0$, limit, we introduce U term perturbatively on the H_e term, and solve the ground state, excitation spectrum that we studied in Chapter 4 for long-range Coulomb interaction. Because $H_e + H_{NE}$ is the kinetic energy term, and we start from the momentum space picture and introduce U-term perturbatively, or within the mean field theory. We will study Stoner instability, Ferromagnetism, Spin and charge density waves.

Next, we will stude the $U \to \infty$ limit. Since its a potential energy term, we will study it from the real space picture, and introduce the $H_e + H_{NE}$, i.e., the kinetic energy term as perturbation. This problem has interesting solution at and near the half-filling. We get an effective Heisenberg like term - called the t-J-model. We get Mott insulator, Nagaoka FM, strong coupling anti-ferromagnetism, spin-liquid like phases.

Appendix :

We will also extend the above discussions to a related model called the Kondo model, and the mixed-valence model, appropriate for heavy-fermion materials. This will be taught as an Appendix or home work or term paper.

Chapter 7 : Phonons, Electron-Phonon Coupling and superconductivity.

In this chapter we are essentially going to relax the Born-Oppenheimer approximation and study the vibration of the nucleons in the $H_{NN} + H_N$ term. The nucleons vibration are simply computed by $R_I(t) = R_I(0) + \delta R_I(t)$, which gives a problem of N-coupled quantum Harmonic oscillator. The problem will be solved via Fourier transformation, which gives dispersion relation to the normal modes that we have otherwise studied in classical mechanics. They are called phonon modes.

Next we will include the H_{Ne} term for $\vec{R}_I \to \vec{R}_I + \delta \vec{R}$, which gives the electron-phonon coupling term. We will study the band/mass renormalization and quasiparticle lifetime of electrons and phonons due to the electron-phonon coupling. In otherwords, we will study the complex self-energy correction to both electronic and phonon spectrum. Notable physics of interests are the Kohn anomaly, Ultrasound attenuation in the phonon's spectrum, and Peierels instability, charge density wave in the electronic spectrum due to the electron-phonon coupling. Interestingly, most of these instabilities are related to the singularity in the F(x) function at the Fermi-momenta that we will introduce in chapter 2.

The other interesting physics to study here is the effective attractive electron-electron interaction mediated by the electron-phonon coupling. The method to be used to derive this interaction is similar to the effective model derivation for the t-J or Kondo model that is already introduced in the previous chapter.

We will first show that while the Fermi-liquid theory shows that the Fermi surface is robust to any repulsive (short-range) density-density interaction, but this is not true for attractive interaction. This is called the Cooper instability. Cooper showed that any Fermi surface is unstable to cooper pair formation and superconductivity for any infinitesimally small attractive interaction. In other words, all metals must superconduct at low-temperature.

We will study the famous BCS Theory, and the so-called Bogoliubov-de-Gennes (BdG) mean-field Hamiltonian for superconductivity.

Appendix: Superfluid density, Meissner effect.

Chapter 8: Boltzmann Transport Equation

In this last chapter of this convse, we will study a semi-classical Boltzmann trasport phenomena in the phase-space. We studied effective fluctuation of the occupation density around the fermi surface in the momentum state (adiabatic approximation for k-being good quantum number). In this chapter, we will study the fluctuation of the occupation density in both momentum and real space, ie, the phase space. We will introduce a very useful and popular relaxation time approximation, or transport life time of quasiparticle, which is generally different from the quasiparticle lifetime introduce in chapter 4, but occasionally they coincide. The semi-classical apprach to compute the relaxation time will be derived. Finally, we will use this relaxation time approximation to compute electrical and thermal conductivity of material. We will study this problem for three main cases of impurity scattering, electron-phonon scattering and electron-electron scattering.