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Band structure theory: a story about the fountain of youth.

A few remarks

- Very old theory. The fundimental problems was clarified in 20s-30s.
- Very simple. Basically free fermions.
- We had thought that we understood it.
- But it gives us a big surprise in the last 30 years, especially in the last 5 years.

1.1. Born– Oppenheimer approximation

Wavefunction (N_e electrons and N_i ions)

$$\psi_e(r_1,\, r_2,\, r_3\, ... \mathrm{r}_{N_e}) = \psi_e(\{r_i\}) \tag{1.1}$$

$$\psi_i(R_1,\, R_2,\, R_3\, ... \mathrm{R}_{N_i}) = \psi_i(\{R_i\}) \tag{1.2}$$

$$H = H_e + H_i + H_{\mathrm{ee}} + H_{\mathrm{ie}} + H_{\mathrm{ii}} \tag{1.3}$$

$$H_e = -\frac{1}{2\,m_e}\left(\partial_{r_1}{}^2 + \partial_{r_2}{}^2 + ... \,\partial_{r_N}{}^2\right) \tag{1.4}$$

$$H_i = -\frac{1}{2\,M_i}\left(\partial_{R_1}{}^2 + \partial_{R_2}{}^2 + ... \,\partial_{R_N}{}^2\right) \tag{1.5}$$

$$H_{\mathrm{ee}} = \sum_{i<j}\frac{e^2}{|\,r_i - r_j\,|} \tag{1.6}$$

$$H_{\mathrm{ii}} = \sum_{i<j}\frac{n^2\,e^2}{|\,R_i - R_j\,|} \tag{1.7}$$

$$H_{\mathrm{ie}} = \sum_{i,j}\frac{n\,e^2}{|\,R_i - r_j\,|} \tag{1.8}$$

Ion mass are much larger than electrons.

So Ions moves much slower (if $K.E._{\cdot i} = K.E._{\cdot e}$)

For electrons, ions are "stationary", so we can treat ions as a static background.

$$H = H_e + V_i + H_{\mathrm{ee}} \tag{1.9}$$

Ignore H_{ee} for now,

$$H = H_e + V_i \tag{1.10}$$

Without interactions between electrons. The question here is: How does one electron move in the presence of lattice background?

A few remarks

- Born– Oppenheimer approximation is an assumption. So does the assumption that one can ignore electron-electron interactions. There is no solid theortical proof it must be valid. It is just a simple point to start from, but whether it is correct or not need to be examined by experirments.
- Philosophy: Start from something simple (not necessarily well-justified theortically) and see if it can produce the correct results, wich agrees with experiments. If yes, we say that the simple assumption captures the fundimental physics here. If not, we need more sophisciated assumptions to understand this system.

1.2. Why free fermion?

1. Simple: a good starting point

2. In many metal or insulators, free electron theory works very well

- Free fermion theory can explain lots of phenomena
- On the quantitative level, it gives more accurate results than a naive interacting theory (the mean-field approximation)
- Landau fermion liquid theory. (Will be discussed latter)

1.3. Free fermions in vacuum

$$-\frac{1}{2\,m}\,\nabla^2\,\psi\!\left(\vec{r}\right) = \epsilon\,\psi\!\left(\vec{r}\right) \tag{1.11}$$

(Continuous) translational symmetry: the system (H) is invariant when we change $\vec{r}$ to $\vec{r} + \vec{a}$. Here $\vec{a}$ is an arbitrary vector.

A continuous symmetry implies a conservation law. Here, it is the momentum conservation $\left[\vec{p},\,H\right] = 0$. So we can find common eigenstates for $\vec{p}$ and H.

Eigenstates of $\vec{p}$: plane waves

$$\psi_k = \exp\!\left(i\,\vec{k}\cdot\vec{r}\right) \tag{1.12}$$

so,

$$-\frac{1}{2\,m}\,\nabla^2\,\psi_k = \frac{k^2}{2\,m}\,\psi_k \tag{1.13}$$

Eigen-energy:

$$\epsilon_k = \frac{k^2}{2\,m} \tag{1.14}$$

1.4. Free fermions in a crystal

Crystal: atoms form a periodic structure (a lattice).

Fermions in a crystal: they will see a periodic potential.

$$\left[-\frac{1}{2\,m}\,\nabla^2 + V\!\left(\vec{r}\right)\right]\psi\!\left(\vec{r}\right) = \epsilon\,\psi\!\left(\vec{r}\right) \tag{1.15}$$

with

$$V\!\left(\vec{r}\right) = V\!\left(\vec{r} + \vec{a}_i\right) \tag{1.16}$$

Symmetry: discrete translational symmetry: the system (H) is invariant when we move the system by one lattice spacing $\vec{a}_i$

- Q: What is the eigenstate of this Hamiltonian?
- A: Bloch waves

(Here, I consider a 1D system for simplicity. All the conclusions discussed here can be generalized to other dimensions easily.)

$$\psi_{n,k}(r) = u_{n,k}(r) \exp(i \, k \, r) \tag{1.17}$$

Here $u_{n,k}$ is a periodic function of r with the same periodicity as the lattice

$$u_{n,k}(r + a) = u_{n,k}(r) \tag{1.18}$$

n is an integer (the band index) and k is a real number (the momentum).

Remarks:

- although k is called a "momentum". It is NOT the momentum of the Bloch wave. $k \neq \langle \psi_{n,k} | -i \, \partial_r | \psi_{n,k} \rangle$
- $-\frac{\pi}{a} < k < \frac{\pi}{a}$, where a is the lattice spacing. The region between $-\frac{\pi}{a}$ and $\frac{\pi}{a}$ is called the Brillouin zone
  - Q: Why k is confined to the BZ between $-\frac{\pi}{a}$ and $\frac{\pi}{a}$? What if $k > \frac{\pi}{a}$
  - A: $k + 2\pi/a$ is the same as k, if we redefine u

$$\psi_{n,k+2\pi/a}(r) = u_{n,k+2\pi/a}(r) \exp[i(\,k + 2\pi/a)\,r] = u_{n,k+2\pi/a}(r) \exp\left(i\,\frac{2\pi}{a}\,r\right) \exp(i\,k\,r) \tag{1.19}$$

Notice that both $u_{n,k}(r)$ and $\exp(i\,2\pi\,r/a)$ are periodic functions of r with periodicity a (a lattice spacing), we can combine them together and define their product as $\tilde{u}(r)$ a new periodic function with the same periodicity.

$$\psi_{n,k+2\pi/a}(r) = u_{n,k}(r) \exp(i\,k\,r) = \psi_{n,k}(r) \tag{1.20}$$

Bottom line: $k + 2\pi/a$ is the same as k. So we just need the region between $-\frac{\pi}{a}$ and $\frac{\pi}{a}$.

How about the eigennergy ϵ?

Define eigen-energy of the state $\psi_{n,k}(r)$: $\epsilon_n(k)$

For each n, $\epsilon_n(k)$ as a function of k is called an energy band.

- $\epsilon_n(k)$ is a smooth function of k
  - Why?
  - A: $\partial_k \psi_{n,k}(r)$ has no singularity.
    - This was a major question of solid state physics. We understood it in the 20s-30s. Now we took it as granted, so this discussion almost totally disappeared from modern literature and textbooks (until recently!)
    - The study about $\partial_k \psi_{n,k}(r)$ created the foundation for topological insulators. We will see how important $\partial_k \psi_{n,k}$ is for TIs, later when we discuss about TIs.
    - It is also useful for graphene
- $\epsilon_n(k)$ usually don't cross with each other: (que to avoided level crossing. For more information, please refer to your favorate quantum mechanics textbook on "degenerate perturbation").
  - Different k may have the same energy $\epsilon_n(k) = \epsilon_m(k')$. These degeneracy is protected by the discrete translational symmetry. $H_{\text{hyber}} = | \psi_{n,k} \rangle \langle \psi_{m,k'} |$ is not allowed, because it breaks the translational symmetry.
  - But for same k, the energies of different bands cannot be the same.
- But! there are exceptions (sometimes exceptions usually lead to Noble Prize): Very famous example, graphene

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1.5. Band structure theory and transport: metal, insulator, and semi-metal

Fermi statistics: At low T, fermions occupies all the states below the chemical potential. Two possibilities:

1. chemical potential cross with some of the bands

2. chemical potential doesn't cross with any band (μ is located inside the energy gap)

For case 1:

- Some bands are fully filled: valence bands
- Some bands are empty: empty bands

- Some bands are partially filled: conducting bands----- these bands give us conductivity

Apply a electric field (increase μ on one side and reduce the chemical potential on the other side), what will happen?

The side with a larger μ has a more electrons (higher density). The side with smaller μ has less electrons (lower density).

Density difference gives current! j=σ E

It is a metal.

- Fermi surface: Fermi surface controls all low energy physics.

For case 2:

- Some bands are fully filled: valence bands
- Some bands are empty: empty bands
- no partially filled: no conducting bands----- no conductivity

Apply a electric field (increase μ on one side and reduce the chemical potential on the other side), what will happen?

Number of electrons doesn't change (unless electric potential μ is tooooo large) no matter how one increases or decreases μ.

No density difference. No currents. j=0

It is an insulator.

- No Fermi surface

Case 3: semi-metal: the band structure has a band crossing point and the Fermi energy is located at the band crossing point (graphene)

- Same as an insulator: no conducting bands
- Same as a metal: it is a conductor

Bottom line: a metal with no Fermi surface

No Fermi surface is a big deal. Because the size of the Fermi surface (k_F) appears almost everywhere (heat capacity, magnetic susceptibility, density of the state ...). Not k_F is zero! One cannot just apply old knowledge on a metal with finite k_F to graphene. Everything needs to be recalculated. Some of them question are still under debating today in the study of graphene.

Case 4: Topological insulator: insulator inside, but metal outside.

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Topological insulator part I: Phenomena

(Part II and Part III discusses how to understand a topological insluator based band-structure theory and gauge theory)

(Part IV discusses more complicated T-reversal invariance topological insulators)

One phenomena: bulk insulator: surface/edge is metallic.

Example: integer quantum Hall effect

2.1. Quantum Hall effect

Hall effect:
- Electrons moving in a 2D plane (2D electron gas or 2DEG): Apply an electric field E, we get some current j. Typically, $E \ // \ J$. Let's assume they are in the x direction E_x and j_x. Resistivity $\rho_{xx} = E_x / j_x$
- Apply a B field perpendicular to the 2D plane. Lorentz force leads to charge accumulation for the top and bottom edge. This gives a E field perpendicular to the current (E_y). Hall resistivity: $\rho_{xy} = E_y / j_x$
- Rotational symmetry: $\rho_{xx} = \rho_{yy}$ and $\rho_{xy} = \rho_{yx}$
- Classical mechanics: $\rho_{xy} = B$

$$e \, E_y = e \, v \, B \tag{2.1}$$

$$j_x = e \, v \, n \tag{2.2}$$

$$\rho_{xy} = E_y / j_x = \frac{v \, B}{e \, v \, n} = \frac{B}{e \, n} \tag{2.3}$$

Remark: very useful experimental technique. It determines the carrier density.

Integer Quantum Hall effect

ρ_{xy}: plateaus. $\sigma_{xy} = \frac{1}{\rho_{xy}}$ is quantized: $\nu \, e^2 / h$ (ν is an integer, known as the filling factor or filling fraction). In the same time, $\rho_{xx} = 0$ at these plateaus.

Between two plateaus, not universal (sample dependent).

σ_{xy} quantization. Very accurate. The second best way to measure the fine structure constant

The fine structure constant is one of the key fundamental constants. In CGS unit

$$\alpha = \frac{e^2}{\hbar \, c} \tag{2.4}$$

c is the speed of light, whose value is exactly known (no error). Quantum Hall effect gives e^2 / h, so we can get α.

The most accurate way to determine α comes from g-2