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# Research Note

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## Abstract

The note presents my gains in the first two weeks research, including states in 1-D periodic potentials, crystal structures, Sommerfeld Free-electron theory and the one-electron approximation. I just show some A brief group meeting review is also being presented in the note. In the end of note, I list some problems which I encountered early in the project.

## Learning

### 1-D periodic potentials

In the early days of solid-state physics, just this desire for technical simplicity was the motivation for the studies on one-dimensional periodic potentials.

The most important theory is Bloch Theory, which shows that the wavefunction of eigenstate in 1-D periodic potential can be write as:

$$\Phi_k(x) = e^{ikx}u_k(x), u_k(x+a) = u_k(x) \quad (1)$$

$$\Phi_k(x+t_n) = e^{ikt_n}\Phi_k(x) \quad (2)$$

From this point of view, we consider a simplest periodic potential, the finite energy walls, to show the conception of energy band in periodic potential. After that, the general periodic potential and a phenomenological conception of mine will be discussed.

Consider this kind of periodic potential,

$$V(x+a) = V(x) = \begin{cases} V_0, & 0 \leq x < b \\ 0, & b \leq x \leq a \end{cases} \quad (3)$$

After applied the Bloch boundary condition into Schrödinger Equation and neglected some unnecessary terms (here we consider that  $b$  is small enough but  $V_0b$  is constant), one can easily derive,

$$P \frac{\sin qa}{qa} + \cos qa = \cos ka \quad (4)$$

Where P is a constant depends on  $V_0$  and q is a function of E. One can easily finds that *for some energy, the right side can be greater than 1 and lead to a complex k, which imply a damping wave.* We call those energy levels forbidden level.

The energy bands structure of more general periodic potential can be expressed by introducing translation constant.

$$\text{Re} \left[ \frac{1}{t^*[E]} e^{iq[E]x} \right] = \cos ka \quad (5)$$

A phenomenological explain of forbidden bonds can be discovered from Equation (5) that the gap of energy could dependent on the translation constant. Since the translation constants is less than 1, some energy does not relate to a real wave. It looks like the energy band was formed because the boundary of potential “kick out” some waves whose wave vector contents an imagery part.

## Crystal structures and Reciprocal vector

Analyzing the crystal structure is a basis skill for a researcher majors in condensed matter physics. Variety structures of crystal make the materials completely deferent in many aspects, precisely, face-centered-cubic irons are not ferromagnetic while body-centered cubic irons are.

The lattices structure can be determined by translation vectors and basis vectors. The lattices are some periodic arrangement of points in space, and there is a cell on each point. The translation vectors begin from a lattice to another while the basis vectors are in the cells and imply the internal structure of a cell on a lattice.

We can use the fundamental translation vectors base to express all the translation vectors by integer numbers  $n_1, n_2, n_3$ .

$$\mathbf{t} = n_1 \mathbf{t}_1 + n_2 \mathbf{t}_2 + n_3 \mathbf{t}_3 \quad (6)$$

The volume spanned by fundamental translation vectors is call primitive cells. There is no lattice inside the primitive cells, which inspires us to introduce another kind of primitive cells, known as Wigner-Seitz Primitive Cells.

Wigner-Seitz cell about a reference lattice is defined by a property that any point of the cell is closer to that lattice point than to any other. Precisely, we find mid-vertical planes of the reference lattices and its nearest, second nearest and so on. Those planes span a volume around the reference lattices and can be easily checked that it is Wigner-Seitz cell.

Now we introduce reciprocal space and reciprocal vectors by Fourier transform. For a periodic function, we have

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$$n(\mathbf{x}) = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} \quad (7)$$

Introduce a set of vectors  $\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3$ .

$$\begin{cases} \mathbf{g}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\Omega} \\ \mathbf{g}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\Omega} \\ \mathbf{g}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\Omega} \\ \Omega = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) \end{cases} \quad (8)$$

The significance of the set is that the Fourier the  $\mathbf{G}$  in equation (7) is spanned by  $\mathbf{g}$ , which imply those  $\mathbf{g}$  are the bases of Fourier transform space. We call them reciprocal space and reciprocal vectors.

## Free-electron theory and Fermi-Dirac distributions

This theory is introduced by Sommerfeld. The most fundamental hypothesis of the model is the dispersion of energy for conduction electrons inside the metal takes this form

$$E(\vec{k}) = E_c + \frac{\hbar^2 k^2}{2m} \quad (9)$$

Where  $E_c$  donate the bottom energy level of the conduction band. I emphasize that conduction electrons are those electrons in the most external shell.

The most important result of this dispersion is the density of state take this form by introduce the Fermi level  $E_F$  and number  $N$  of electrons.

$$D(E) = \frac{3N}{2E_F} \left( \frac{E}{E_F} \right)^{\frac{1}{2}} \quad (10)$$

Fermi-Dirac distribution gives the occupation probability of a one-particle quantum state of energy  $E$ .

$$f(\mu, T, E) = \frac{1}{e^{(E-\mu)/(k_B T)} + 1} \quad (11)$$

where  $\mu$  is the chemical potential,  $k$  is the Boltzmann constant, and  $T$  is the absolute temperature.

The trick to determine the chemical potential in Sommerfeld model is called Sommerfeld expansion. I do not want to introduce it but just outline its fundamental

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ideas.

We already knew this integration shows the total number of electrons.

$$N = \int_{-\infty}^{\infty} D(E)f(E)dE \quad (12)$$

Since  $D(E)f(E)dE$  means how many states were occupied around E and undistinguishable Fermions occupy different states.

We can solve the chemical potential, from equation (10) and equation (12). Sommerfeld gave a great approach to calculate this integration and show that chemical potential takes this form

$$\mu(T) = E_F \left[ 1 - \frac{\pi^2}{12} \left( \frac{T}{T_F} \right)^2 \right] \quad (13)$$

## One electron approximation and Density Functional Theory.

One electron approximation tries to approach the real material with many body effects by an electron in potential. However, I meet some problems and not clear with these chapter. I report the outline of one electron approximation and density functional theory and list my problems in the end of the note.

Hartree-Fock Theory suggested that the N-electrons states take this form

$$|\Phi(r_1\sigma_1, r_2\sigma_2, \dots, r_N\sigma_N)\rangle = \frac{1}{\sqrt{N!}} \sum_i (-1)^{p_i} P_i |\Phi(r_1\sigma_1)\Phi(r_1\sigma_1), \dots, \Phi(r_N\sigma_N)\rangle \quad (14)$$

And the Hartree-Fock equation told us

$$\left[ \frac{p^2}{2m} + V_{nucl} + V_{coul} + V_{exch} \right] \phi = E\phi \quad (15)$$

The density functional theory suggests that any properties of many-body system can be determined by the ground state density. That's is to say, if we find the ground state density, we will know everything of the state, including the energy band structure, density of state, and even the complex properties of materials. This theory is the fundamental of first-principles calculate, radiate the chemistry, material science, biology and other different subject.

## Some problems

Meanwhile, I also meet some problems.

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1. The derivation of Hartree-Fock equation is quite confused, and the book omitted some part and just told me: “not hard to check”. However I do not understand the derivation and physical meanings of exchange energy term.
  2. Should I understand every thing contented in books like I always did in my education, or just take the outline of the book and quickly put myself into research and read papers?