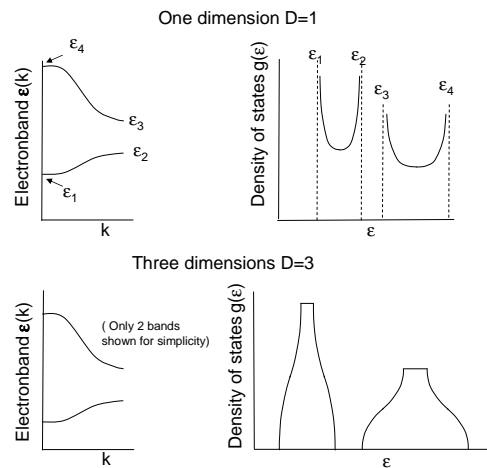


Physics 489 S 04 Lecture 12

Independent Electrons in Crystals: General Theory (A&M chapter 8)

1. Review of Course up to now
 - (a) Electron Liquid in Condensed Matter; Homogeneous “Jellium”; Drude theory for transport
 - (b) Structure of crystals: Periodicity, Elastic scattering
 - (c) Vibrations of nuclei in crystals; Dispersion curves; quantization; heat capacity; transport
2. Part IV: Electrons in Crystals: Independent Electrons
 Schrödinger Eq. $H\psi(\mathbf{r}) = (-\frac{1}{2}\nabla^2 + V(\mathbf{r}))\psi(\mathbf{r}) = \epsilon\psi(\mathbf{r})$
 Key point: $V(\mathbf{r} + \mathbf{R}) = V(\mathbf{r})$ for any lattice translation vector \mathbf{R} .
3. Bloch Theorem (first proof, A&M p 134)
 Define the translation operator: $T_{\mathbf{R}}f(\mathbf{r}) = f(\mathbf{r} + \mathbf{R})$
 Since $T_{\mathbf{R}}$ commutes with H , we can construct simultaneous eigenfunctions of H and all the $T_{\mathbf{R}}$.
 Simple to construct eigenstates of $T_{\mathbf{R}}$, since $T_{\mathbf{R}_1+\mathbf{R}_2} = T_{\mathbf{R}_1}T_{\mathbf{R}_2}$
 Thus if $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, then $T_{\mathbf{R}} = (T_{\mathbf{a}_1})^{n_1}(T_{\mathbf{a}_2})^{n_2}(T_{\mathbf{a}_3})^{n_3}$
 Eigenfunctions vary from one cell to another only by a phase: $\psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = \exp(i\mathbf{k} \cdot \mathbf{R})\psi_{\mathbf{k}}(\mathbf{r})$
4. Eigenstates of H can be chosen as $\psi_{\mathbf{k},n}(\mathbf{r})$, with eigenvalues $\epsilon_{\mathbf{k},n}$, $n = 1, 2, 3, \dots$
 Equivalently, $\psi_{\mathbf{k},n}(\mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{r})u_{\mathbf{k},n}(\mathbf{r})$, where $u_{\mathbf{k},n}(\mathbf{r})$ is periodic.
 All possible $\psi_{\mathbf{k},n}(\mathbf{r})$ can be constructed in the way with \mathbf{k} restricted to one primitive cell of reciprocal lattice
 For \mathbf{k} outside the primitive cell, we can choose $\psi_{\mathbf{k}+\mathbf{G}}(\mathbf{r}) = \psi_{\mathbf{k}}(\mathbf{r})$.
5. Boundary condition: Born-von Karman condition gives \mathbf{k} real with $\mathbf{k} = (m_1/N_1)\mathbf{b}_1 + (m_2/N_2)\mathbf{b}_2 + (m_3/N_3)\mathbf{b}_3$
6. Construction of eigenstates (second proof of Bloch theorem).
 Starting with the definition $\psi_{\mathbf{k},n}(\mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{r})u_{\mathbf{k},n}(\mathbf{r})$, expand $u(\mathbf{r})$ in Fourier components.
 It is straightforward to express the Schrödinger equation in Fourier components.
 Leads to separate matrix equation for the Hamiltonian for each \mathbf{k} , independent of other \mathbf{k} inside one primitive cell.
 The solution is that u is a periodic function $u_{\mathbf{k},n}(\mathbf{r}) = \sum_{\mathbf{G}} u_{\mathbf{k},n}(\mathbf{G})\exp(i\mathbf{G} \cdot \mathbf{r})$, which proves the Bloch theorem and provides an explicit way to solve for the eigenvalues $\epsilon_{\mathbf{k},n}$ and eigenfunctions $\psi_{\mathbf{k},n}(\mathbf{r})$.
7. Bands
 For each integer n , the eigenvalue $\epsilon_{\mathbf{k},n}$ is a continuous function of \mathbf{k} which forms a “band” of allowed energies.
 Between bands there can be ranges on energies where no states are allowed. These are called “band gaps”.

Figure 1: Electron bands and density of states in 1 dimension and 3 dimensions. In 3 dimensions there may be overlapping bands but this is not shown for simplicity.



8. Band counting

Each band has exactly one \mathbf{k} state per cell

If we assume that the electrons in the crystal are independent - except that they must obey the Pauli exclusion principle - then each \mathbf{k} state can hold 1 electron of each spin. Then each band can hold 1 electron of each spin per cell.

There is an infinite number of bands, $n = 1, 2, 3, \dots, \infty$

(unlike phonons for which there are $3S$ bands for S atoms per cell in three dimensions.)

The lowest energy state of the crystal is for the electrons to fill the lowest energy states up to the Fermi energy leaving all states above the Fermi energy empty.

Leads to the basic description of metals and insulators - MORE LATER.

9. Density of states

$$g(\epsilon) = (1/2\pi)^D \int d^D k \delta(\epsilon_n(\mathbf{k}) - \epsilon)$$

The ideas are the same as for the eigenvalues $\omega_{\mathbf{k},n}^2$ for phonons. Note that electron bands have quadratic variation near the edges of the band, $\epsilon_{\mathbf{k},n} = \epsilon_n^0 + A_x k_x^2 + A_y k_y^2 + A_z k_z^2$.