Condensed Matter Physics

Condensed Matter Physics – Michael P. Marder

Density-Functional Theory of Atoms and Molecules – Robert G. Parr and Weitao Yang

Introduction To Solid State Physics – Charles Kittel

The Free Fermi Gas and Single Electron Model

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Chapter 6

Much of condensed matter physics lies within a Hamiltonian that one easily can write down in a single line. It is

$$\hat{\mathcal{H}} = \sum_l \frac{\hat{P}_l^2}{2M_l} + \frac{1}{2} \sum_{l \neq l'} \frac{q_l q_{l'}}{|\hat{R}_l - \hat{R}_{l'}|}.$$

The *single-electron* model

$$\sum_{l=1}^{N}\left(\frac{-\hbar^2\nabla_l^2}{2m}+U(\vec{r}_l)\right)\Psi(\vec{r}_1\ldots\vec{r}_N)=\mathcal{E}\Psi(\vec{r}_1\ldots\vec{r}_N)$$

$$\left(\frac{-\hbar^2\nabla^2}{2m}+U(\vec{r})\right)\psi_l(\vec{r})=\mathcal{E}_l\psi_l(\vec{r})$$

The *free Fermi* gas

$$\frac{-\hbar^2}{2m}\sum_{l=1}^{N}\nabla_l^2\Psi(\vec{r}_1\ldots\vec{r}_N)=\mathcal{E}\Psi(\vec{r}_1\ldots\vec{r}_N)$$

To simplify further we imposes periodic boundary conditions

$$\Psi(x_1+L, y_1, z_1\ldots, z_N)=\Psi(x_1, y_1, z_1\ldots z_N)$$
$$\Psi(x_1, y_1+L, z_1\ldots, z_N)=\Psi(x_1, y_1, z_1\ldots z_N)$$
$$\vdots$$

One Free Fermion

$$\psi_{\vec{k}} = \frac{1}{\sqrt{\mathcal{V}}} e^{i\vec{k}\cdot\vec{r}}$$

$$L^3 = \mathcal{V}$$

$$\vec{k} = \frac{2\pi}{L}\,(l_x, l_y, l_z)$$

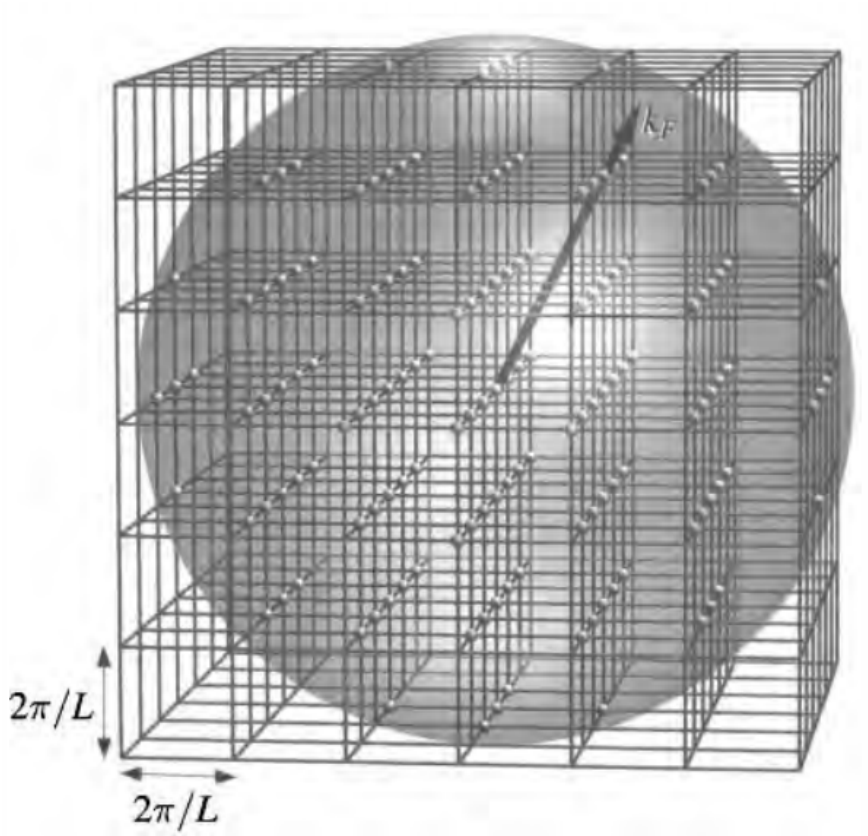
l_x, l_y, and l_z are integers ranging from $-\infty$ to ∞

$$\mathcal{E}^0_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$$

Many Free Fermions

The ground state of electrons obeying free Fermi gas assumption is constructed from products of the one-electron wave functions. The Pauli exclusion principle forbids any given state from being occupied more than once, and therefore any given state indexed by $\vec{k}$ is able to host no more than two electrons, one for each value of spin.

Many Free Fermions



$$\vec{k} = \frac{2\pi}{L}\,(l_x,\, l_y,\, l_z)$$

l_x, l_y, and l_z are integers ranging from $-\infty$ to ∞

Densities of States

$$D_{\vec{k}} = 2\frac{1}{(2\pi)^3}$$

For each wave vector Pauli's exclusion principle allows two electrons, one with spin up and the other with spin down.

$$\int [d\vec{k}] \equiv \frac{2}{\mathcal{V}} \sum_{\vec{k}} = \int d\vec{k}\, D_{\vec{k}} = \frac{2}{(2\pi)^3} \int d\vec{k}$$

Energy Density of States

$$D(\mathcal{E}) = \int [d\vec{k}]\ \delta(\mathcal{E} - \mathcal{E}_{\vec{k}})$$

The units of densities of states are able to change without much warning. Often they are expressed in units of 1/[eV atom], which means they are related to the function defined by above equation by a factor of density *n*.

Energy Density of States

$$D(\mathcal{E}) = \int [d\vec{k}]\ \delta(\mathcal{E} - \mathcal{E}^0_{\vec{k}})$$

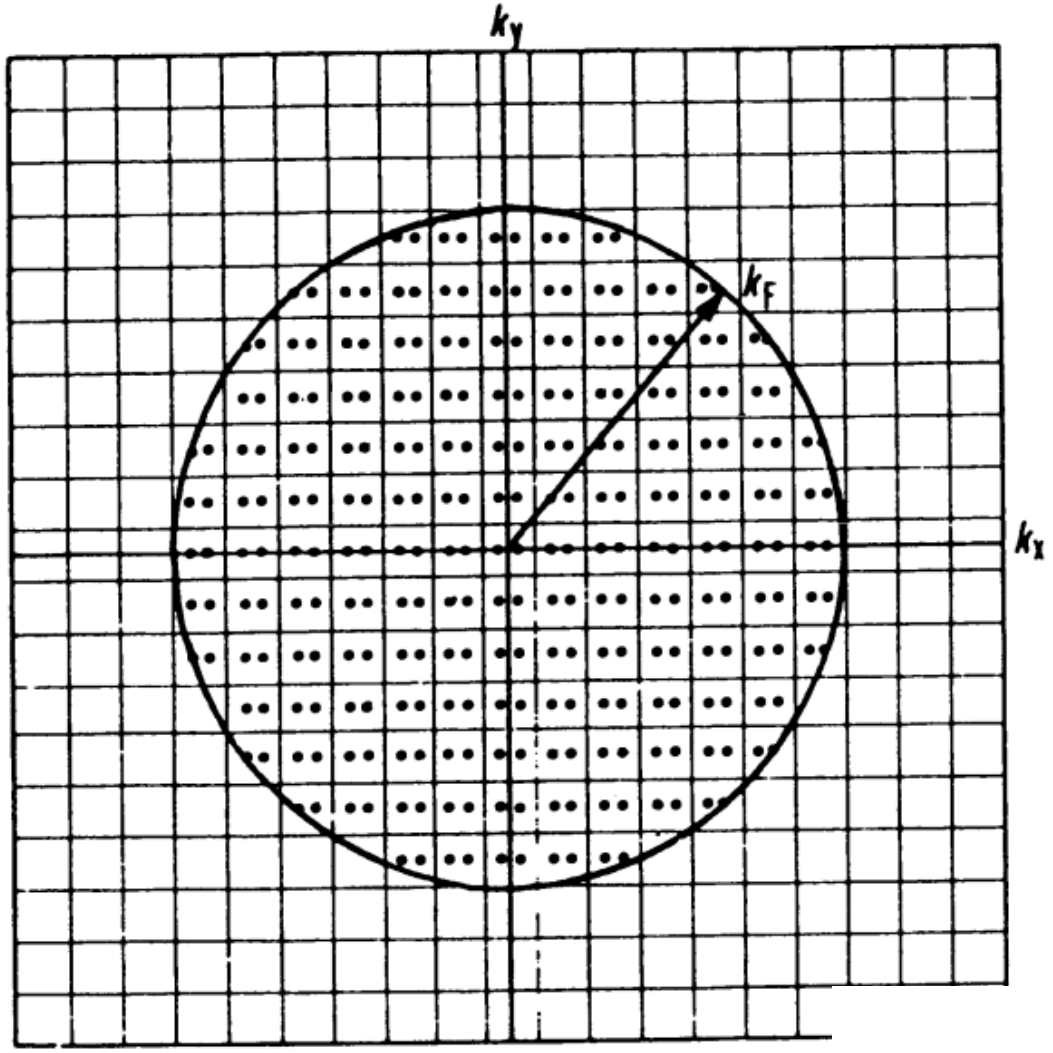
$$= 4\pi \frac{2}{(2\pi)^3} \int_0^\infty dk\ k^2 \delta(\mathcal{E} - \mathcal{E}^0_{\vec{k}})$$

For the free Fermi gas

$$= \frac{1}{\pi^2} \int_0^\infty \frac{d\mathcal{E}^0}{|d\mathcal{E}^0/dk|} \frac{2m\mathcal{E}^0}{\hbar^2} \delta(\mathcal{E} - \mathcal{E}^0)$$

$$= \frac{m}{\hbar^3 \pi^2} \sqrt{2m\mathcal{E}}$$

$$= 6.812 \cdot 10^{21}\ \sqrt{\mathcal{E}/\mathrm{eV}}\ \mathrm{eV}^{-1}\ \mathrm{cm}^{-3}.$$



$$4\pi \int_0^{k_F} g(k) k^2 dk = \frac{N}{V_g} = n$$

$$k_F = (3\pi^2 n)^{1/3}, \qquad E_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

For the free Fermi gas

$$k_F = (3\pi^2 n)^{1/3} = 3.09\ [n \cdot \text{Å}^3]^{1/3}\,\text{Å}^{-1}$$

$$\mathcal{E}_F = \frac{\hbar^2 k_F^2}{2m} = 36.46\ [n \cdot \text{Å}^3]^{2/3}\,\text{eV}$$

$$v_F = \hbar k_F / m = 3.58\ [n \cdot \text{Å}^3]^{1/3} \cdot 10^8\ \text{cm s}^{-1}$$

$$D(\mathcal{E}_F) = \frac{3}{2}\frac{n}{\mathcal{E}_F} = 4.11 \cdot 10^{-2}\ [n \cdot \text{Å}^3]\ \text{eV}^{-1}\ \text{Å}^{-3}$$

Non-Interacting Electrons in a Periodic Potential

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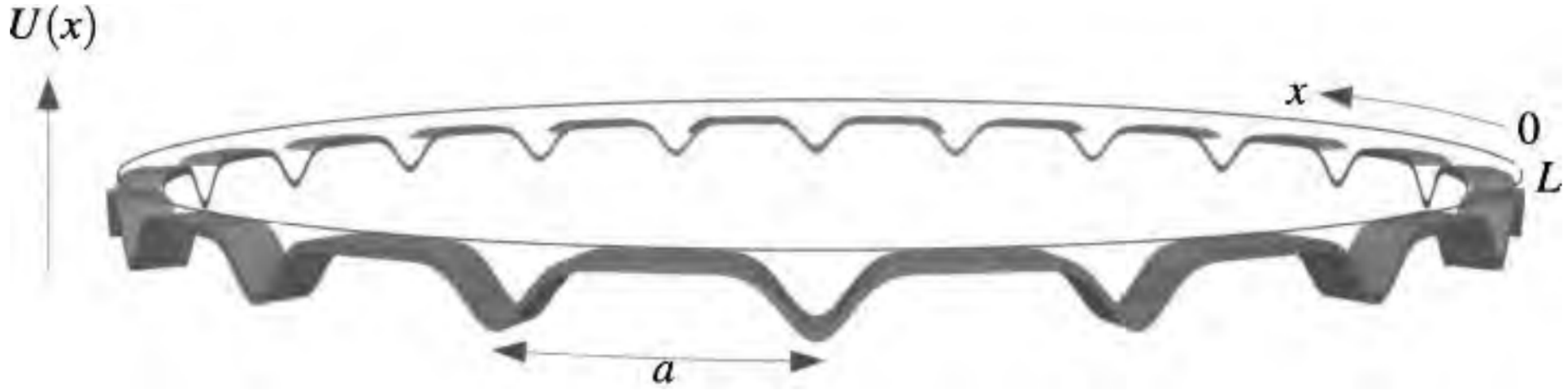
Chapter 7

Bloch's Theorem in One Dimension

Bloch proposed that the electron move in a periodic potential $U(\vec{r})$, making the problem nearly interactable, which obeys

$$U(\vec{r}+\vec{R}) = U(\vec{r})$$

For all $\vec{R}$ in a Bravais lattice.



The setting for Bloch's theorem in one dimension is a potential $U(x)$ of period a on a periodic domain of length L

The Hamiltonian is

$$\hat{\mathcal{H}} = \frac{\hat{P}^2}{2m} + U(\hat{R}).$$

Schrödinger equation in one dimension

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)+U(x)\psi(x)=\mathcal{E}\psi(x)$$

Boundary condition $\psi(x+L)=\psi(x)$

Suppose that the potential $U(x)$ was just $U(x) = 0$.
Then the solutions would be

$$\psi_k(x) = \frac{e^{ikx}}{\sqrt{L}}$$

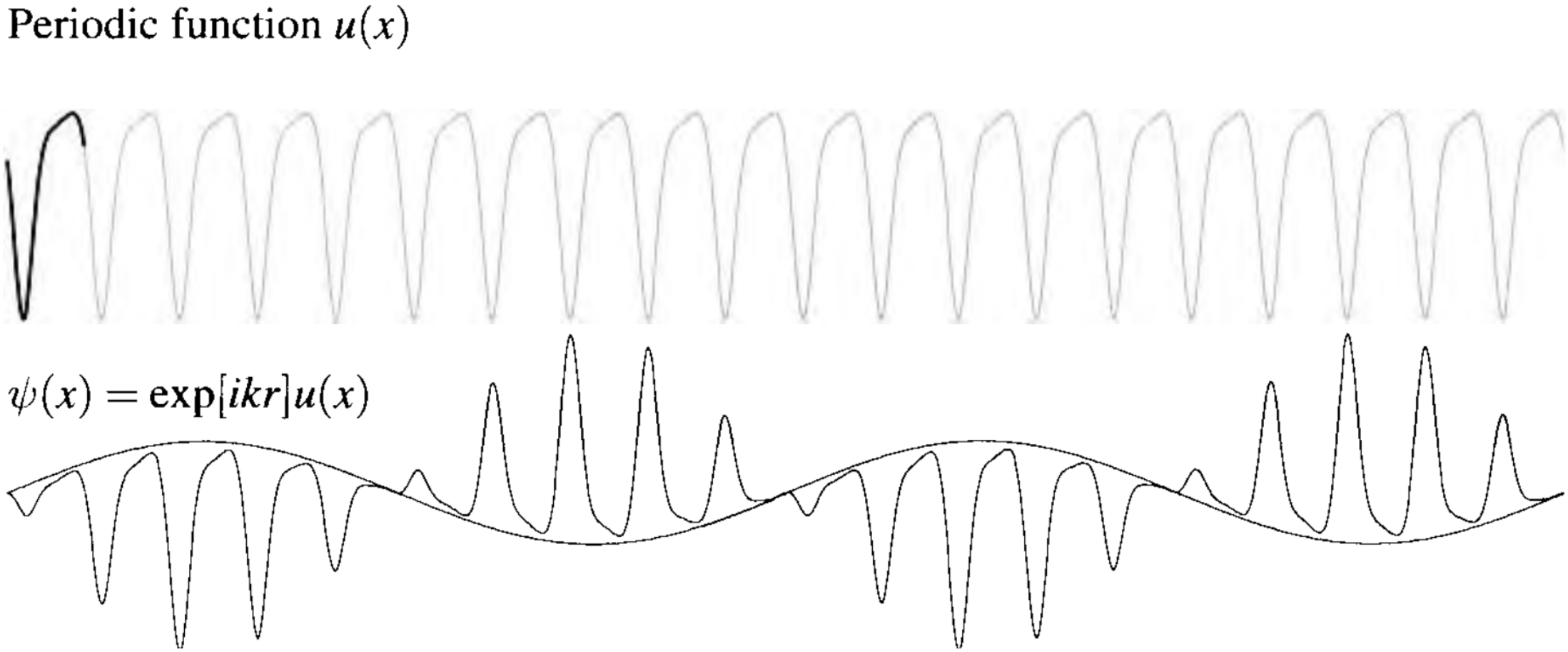
When the potential $U(x)$ is not zero, the solutions retain the same basic structure, but change to

$$\psi_k(x) = \frac{e^{ikx}u(x)}{\sqrt{N}}$$

$$\psi_k(x) = \frac{e^{ikx}u(x)}{\sqrt{N}}$$

ψ is normalized over the whole system, u is normalized over a single unit cell

Where $u(x)$ is a function that like $U(x)$ is periodic with period a, and where $N = L/a$ is the number of cells in the full periodic system. That is, the solutions are plane waves $\exp[ikx]$ modulated by a periodic function $u(x)$.



Bloch wave functions are periodic functions $u(r)$ modulated by a plane wave of longer period. The lower portion of the figure displays the real part of $\psi(x)$