Condensed Matter Physics

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References

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

Condensed Matter Physics – Michael P. Marder

Chapter 6

The Hamiltonian

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

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

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

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

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

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

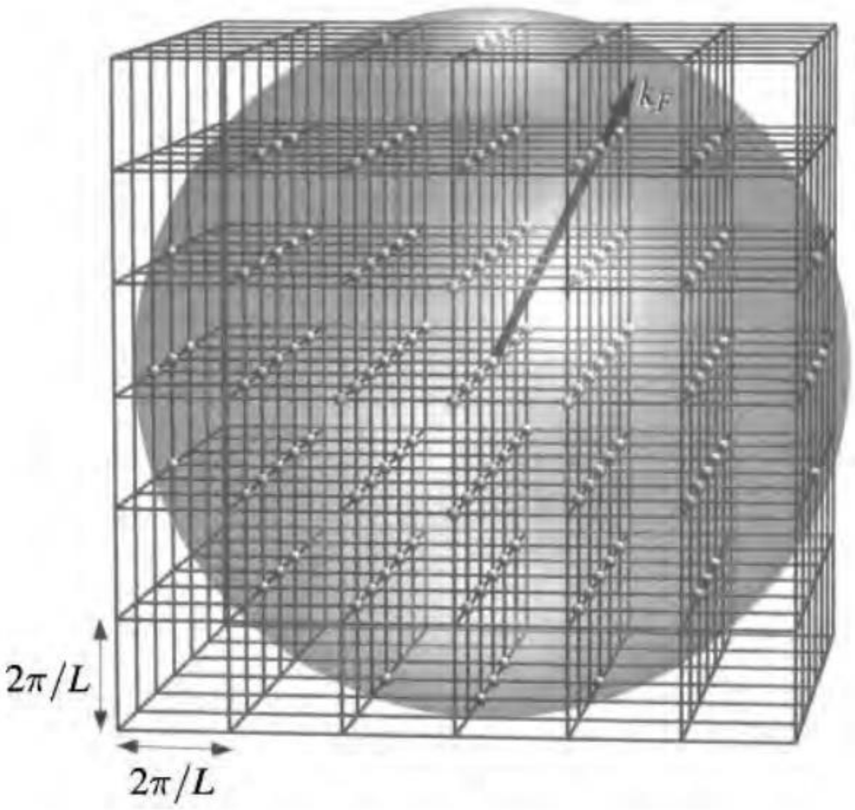
l_x, l_y, and l_z are integers ranging from $-\infty$ to ∞

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

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



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

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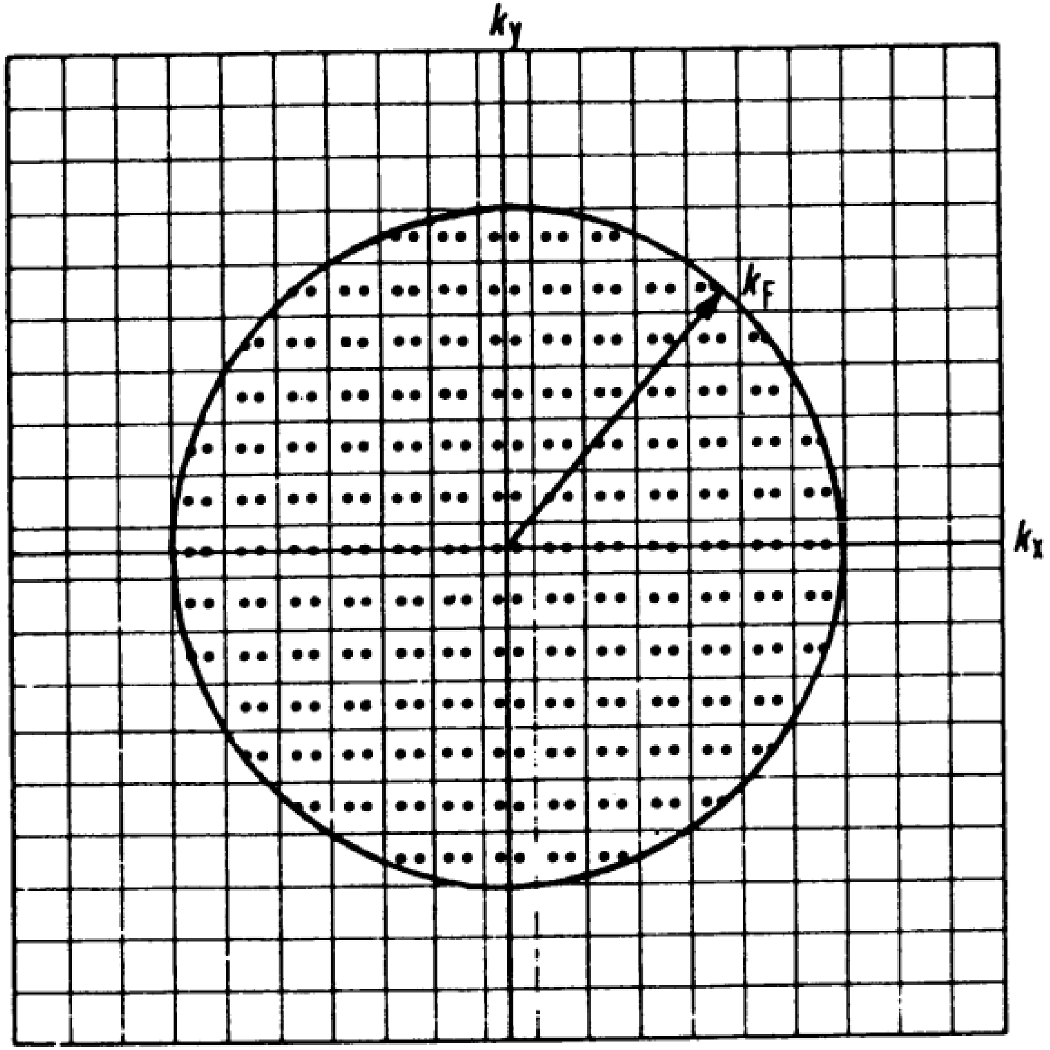


k_y
k_F
k_x

Density 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.

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

Energy Density of States

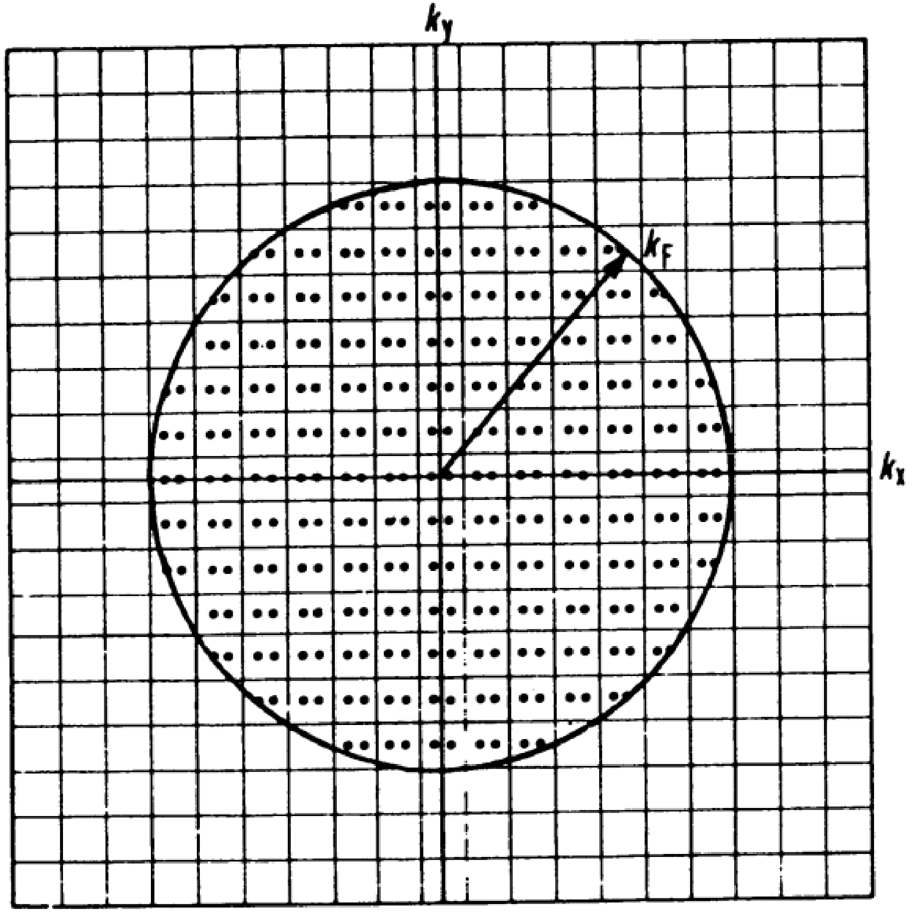
$$D(\mathcal{E}) = \int [d\vec{k}]\ \delta(\mathcal{E} - \mathcal{E}_{\vec{k}})$$

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

For the free Fermi gas

$$
\begin{aligned}
D(\mathcal{E}) &= \int [d\vec{k}]\ \delta(\mathcal{E} - \mathcal{E}^0_{\vec{k}}) \\
&= 4\pi \frac{2}{(2\pi)^3} \int_0^\infty dk\ k^2 \delta(\mathcal{E} - \mathcal{E}^0_{\vec{k}}) \\
&= \frac{1}{\pi^2} \int_0^\infty \frac{d\mathcal{E}^0}{|d\mathcal{E}^0/dk|} \frac{2m\mathcal{E}^0}{\hbar^2} \delta(\mathcal{E} - \mathcal{E}^0) \\
&= \frac{m}{\hbar^3 \pi^2} \sqrt{2m\mathcal{E}} \\
&= 6.812 \cdot 10^{21}\ \sqrt{\mathcal{E}/\mathrm{eV}}\ \mathrm{eV}^{-1}\ \mathrm{cm}^{-3}.
\end{aligned}
$$



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

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

For the free Fermi gas

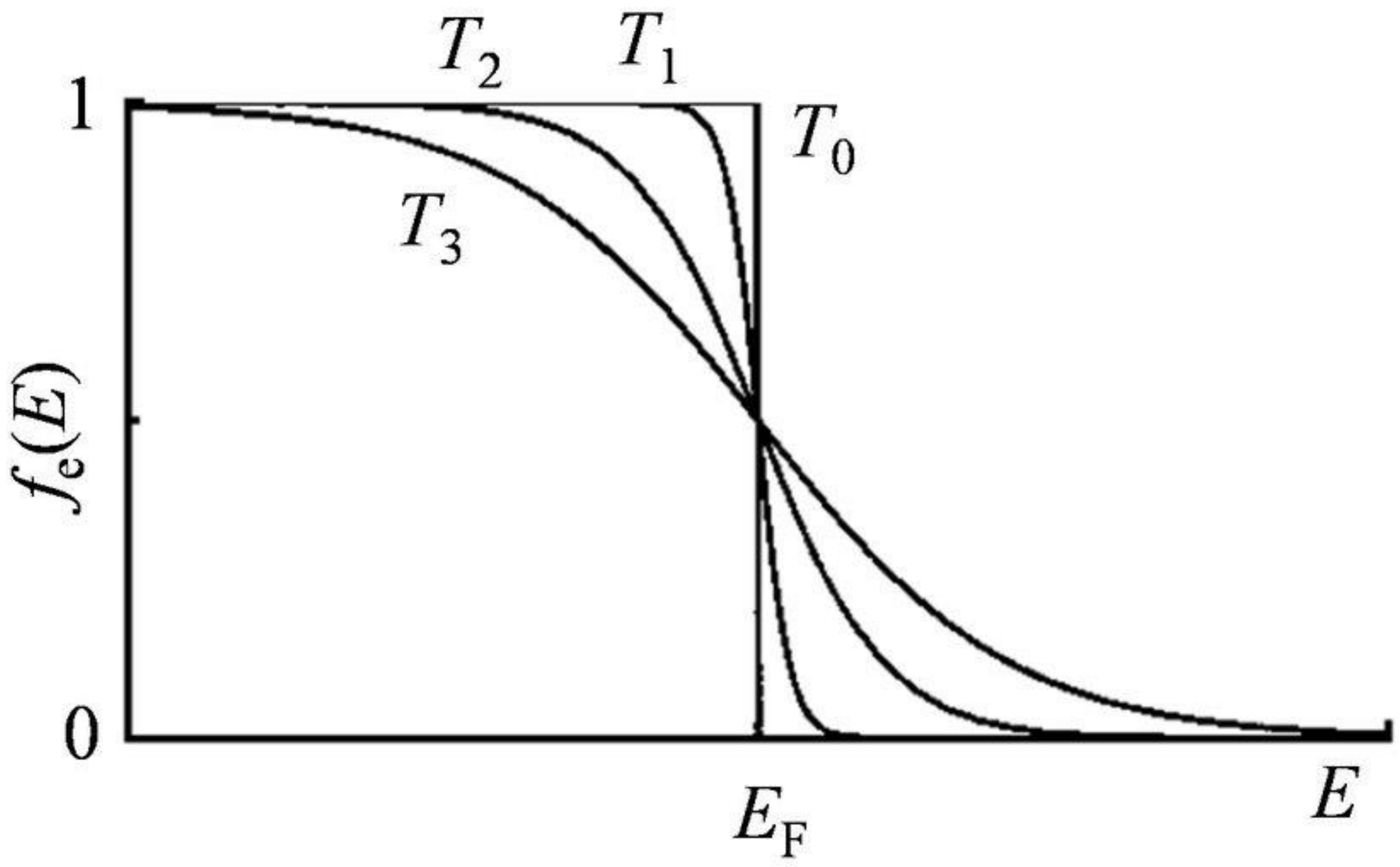
$$k_F = (3\pi^2 n)^{1/3} = 3.09\ [n \cdot \text{Å}^3]^{1/3}\,\text{Å}^{-1}$$

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

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

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

Fermi Distribution Function



Fermi Distribution Function

$$f(\mathcal{E}) = \frac{1}{e^{\beta(\mathcal{E}-\mu)}+1}$$