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

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

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

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

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

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

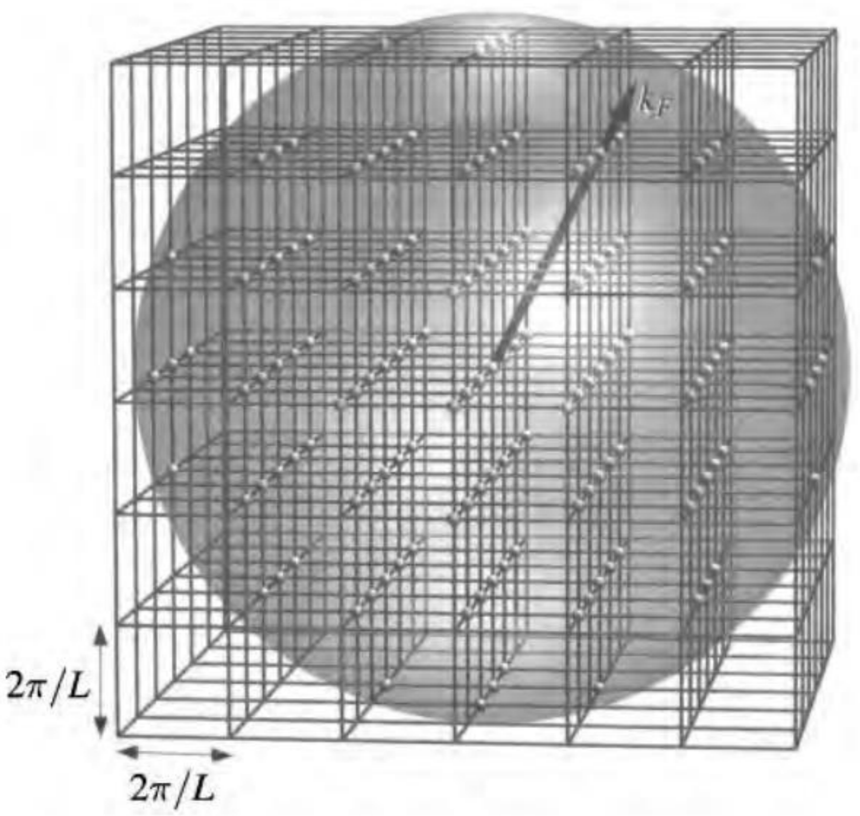
l_x, l_y, and l_z are integers ranging from $-\infty$ to ∞

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

Many Free Fermions

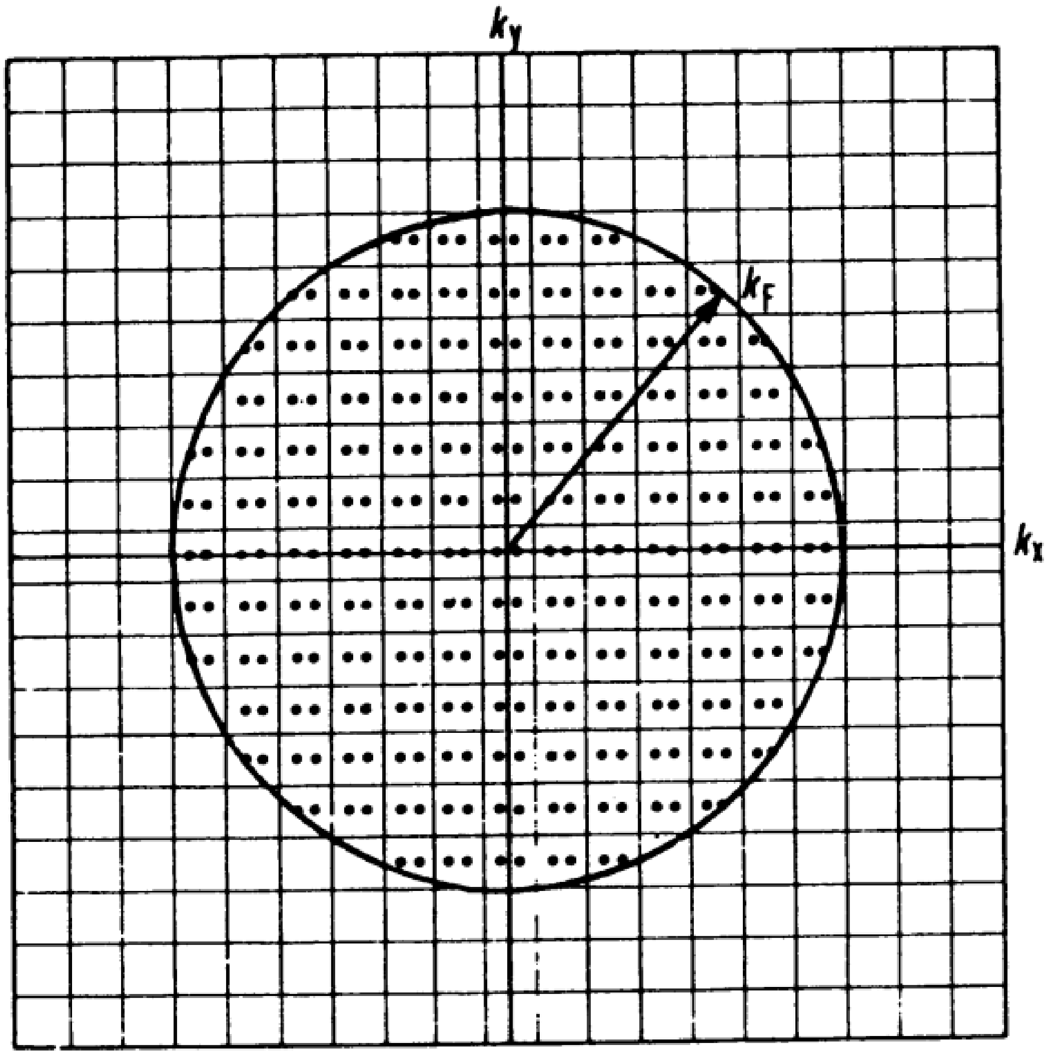
The ground state of electrons obeying free Fermi gas assumption is constructed from products of the one-electron wave functions. The Pauli exclusion principle forbids any given state from being occupied more than once, and therefore any given state indexed by $\vec{k}$ is able to host no more than two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



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

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

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

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

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

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

Electron density

The number of electrons that can fit into a sphere of radius k_F is

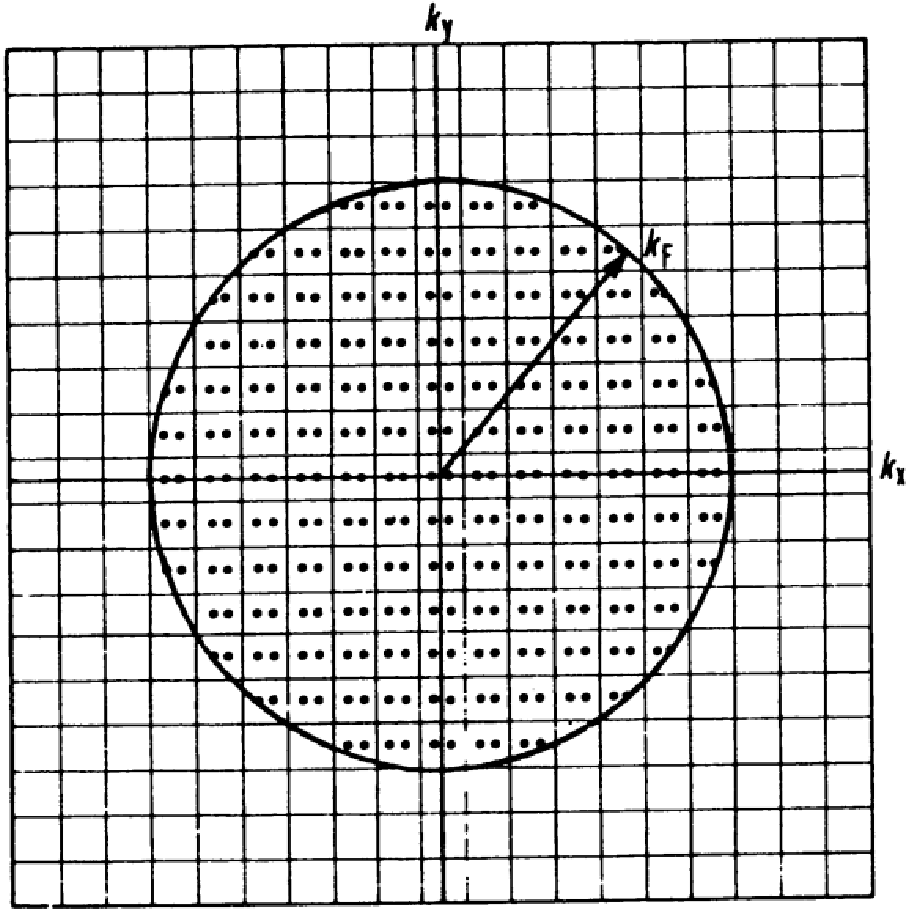
$$N = \sum_{\vec{k}\sigma} f_{\vec{k}}$$

Because $f_{\vec{k}}$ is 1 only if the state is occupied.

$$= \mathcal{V} \int [d\vec{k}] \, f_{\vec{k}},$$

$$= \frac{\mathcal{V}}{4\pi^3} \frac{4\pi}{3} k_F^3 = \frac{\mathcal{V} k_F^3}{3\pi^2},$$

$$\boxed{n = N/\mathcal{V}}$$



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

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

For the free Fermi gas

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

$$\mathcal{E}_F = \frac{\hbar^2 k_F^2}{2m} = 36.46\ [n \cdot \mathring{A}^3]^{2/3} \mathrm{eV}$$

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

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

Grand Partition Function

$$Z_{\mathrm{gr}} = \sum_{\text{states}} e^{\beta(\mu N - \mathcal{E})}$$

$$= \sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \sum_{n_3=0}^{1} \ldots e^{\beta \sum_l n_l(\mu - \mathcal{E}_l)}$$

$$= \prod_l \left\{ \sum_{n_l=0}^{1} e^{\beta\, n_l[\mu - \mathcal{E}_l]} \right\}$$

$$= \prod_l \left[1 + e^{\beta[\mu - \mathcal{E}_l]} \right].$$

$$\boxed{\sum_{n_1=0}^{N} \sum_{n_2=0}^{N} \cdots \sum_{n_M=0}^{N} \prod_{l=1}^{M} A_{n_l} = \prod_{l=1}^{M} \left\{ \sum_{n_l=0}^{N} A_{n_l} \right\}}$$

Grand Potential

$$\Pi \equiv -k_B T \ln \mathrm{Z}_{\mathrm{gr}}$$

$$= -k_B T \sum_l \ln\left[1 + e^{\beta[\mu - \mathcal{E}_l]}\right].$$

$$= -k_B T \mathcal{V} \int d\mathcal{E}\, D(\mathcal{E}) \ln\left[1 + e^{\beta[\mu - \mathcal{E}]}\right].$$

Fermi Distribution Function

$$N = -\frac{\partial \Pi}{\partial \mu}$$

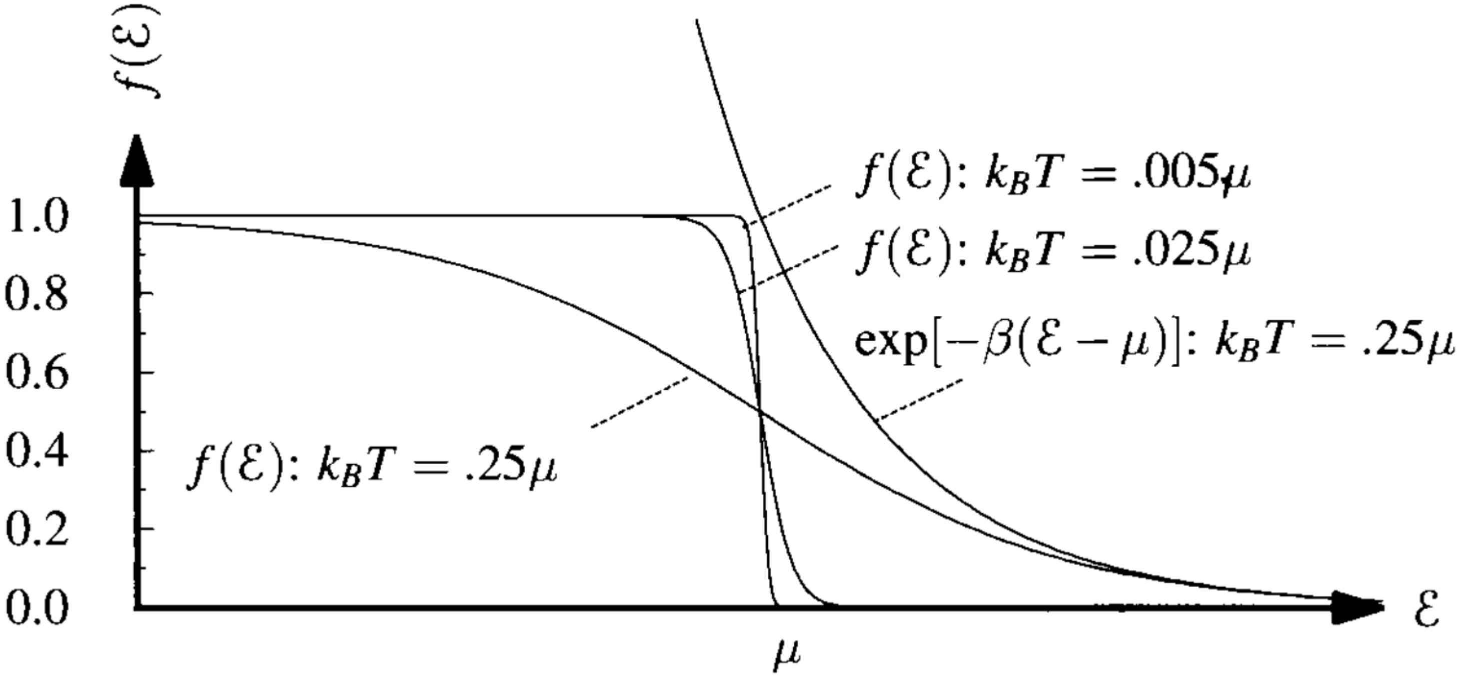
$$= \mathcal{V} \int d\mathcal{E}' \, D(\mathcal{E}') \frac{e^{\beta\mu - \beta\mathcal{E}'}}{1 + e^{\beta\mu - \beta\mathcal{E}'}}$$

$$\Rightarrow n = \frac{N}{\mathcal{V}} = \int d\mathcal{E}' \, D(\mathcal{E}') f(\mathcal{E}'),$$

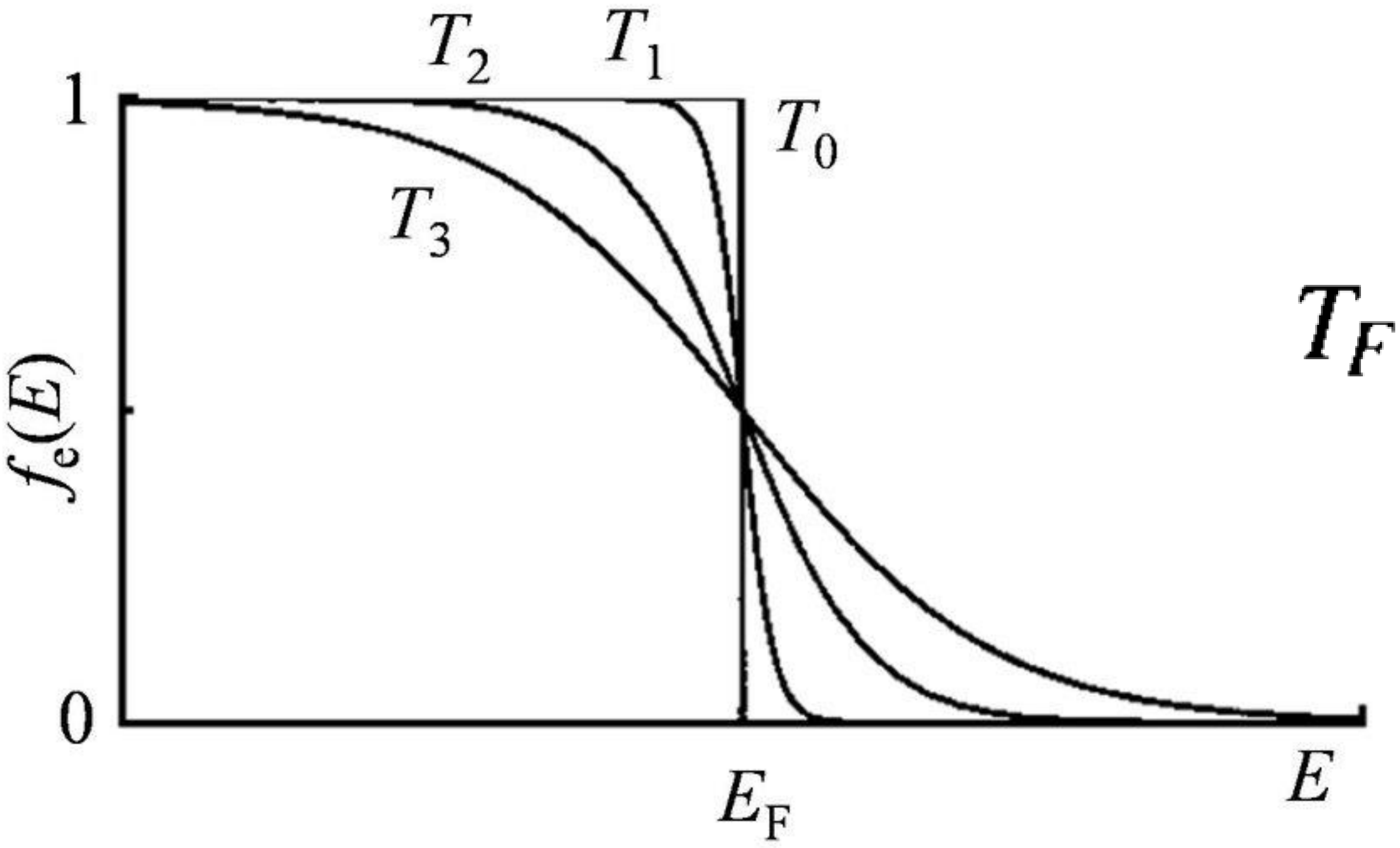
$$\boxed{f(\mathcal{E}) = \frac{1}{e^{\beta(\mathcal{E} - \mu)} + 1}}$$

Fermi Distribution Function

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



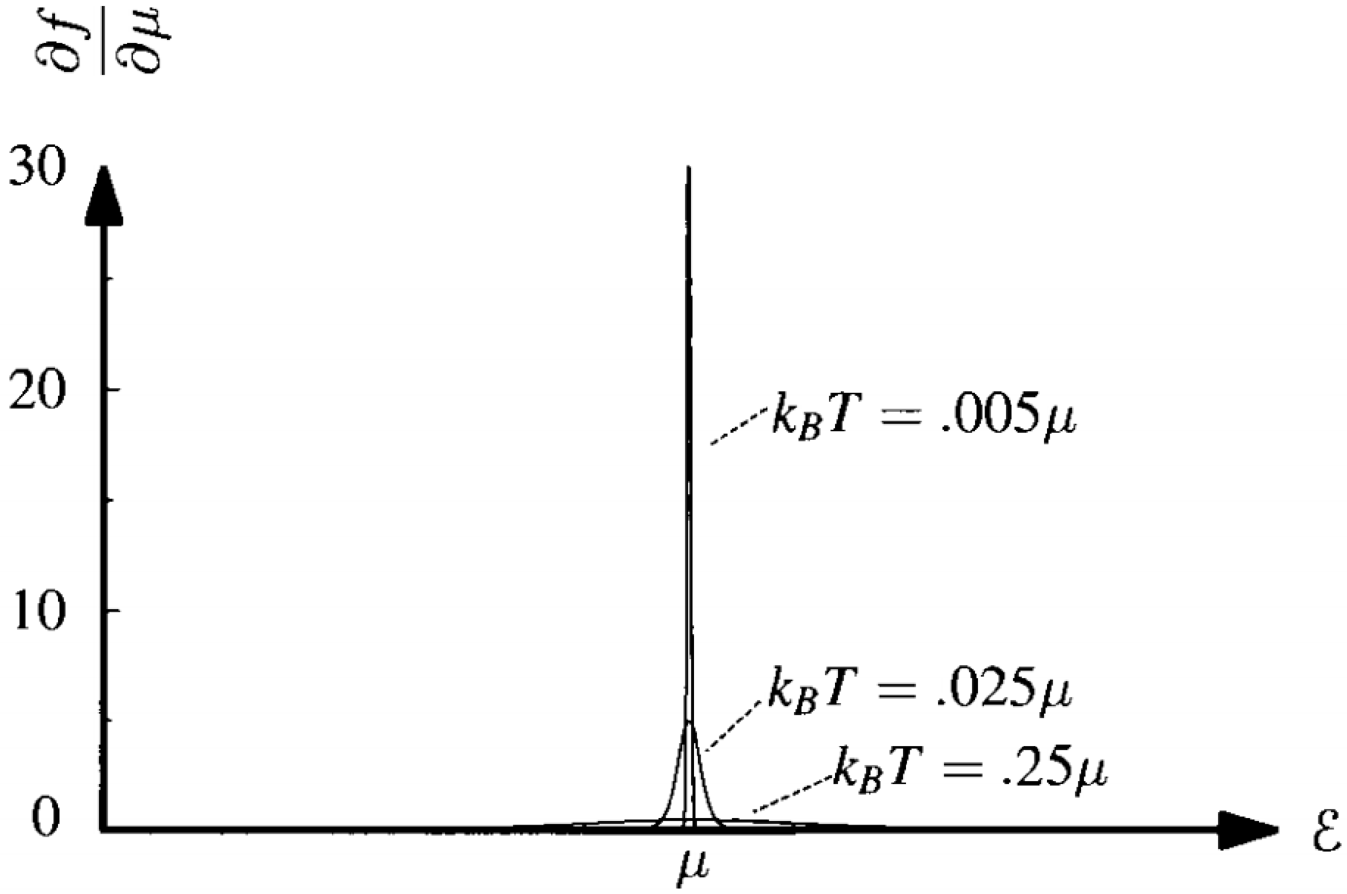
Fermi Distribution Function



$$T_F = \mathcal{E}_F / k_B ,$$

Element	Z	n (10^{22} cm^{-3})	k_F (10^8 cm^{-1})	$\mathcal{E}_F$ (eV)	T_F (10^4 K)	v_F (10^8 cm s^{-1})	r_s/a_0
Li	1	4.60	1.11	4.68	5.43	1.28	3.27
Na	1	2.54	0.91	3.15	3.66	1.05	3.99
K	1	1.32	0.73	2.04	2.37	0.85	4.95
Rb	1	1.08	0.68	1.78	2.06	0.79	5.30
Cs	1	0.85	0.63	1.52	1.76	0.73	5.75
Cu	1	8.49	1.36	7.04	8.17	1.57	2.67
Ag	1	5.86	1.20	5.50	6.38	1.39	3.02
Au	1	5.90	1.20	5.53	6.42	1.39	3.01
Be	2	24.72	1.94	14.36	16.67	2.25	1.87
Mg	2	8.62	1.37	7.11	8.26	1.58	2.65
Ca	2	4.66	1.11	4.72	5.48	1.29	3.26
Sr	2	3.49	1.01	3.89	4.52	1.17	3.59

The derivative of the Fermi function



Specific Heat of Noninteracting Electrons at Low T

$$c_V = \frac{1}{V}\frac{\partial \mathcal{E}}{\partial T}\Big|_{NV}$$

$$c_V = \frac{\pi^2}{3}k_B^2 T D(\mathcal{E}_F)$$