Solutions

PHY 831: Statistical Mechanics
Exam 1

October 18, 2021

25 1. (10 ~~points~~) Consider a one-dimensional solid of length L at temperature T containing N atoms in a chain. Each atom has one spin-half conduction electron (so the rest of the electrons can effectively be neglected). Model excitations of the lattice using a one-dimensional version of the Debye model, so that the density of states in frequency space is given by $g(\omega) = L/(2\pi c_s)$, where c_s is the sound speed, $k = \omega/c_s$ is the wavenumber, and the energy of a phonon is given by $\epsilon = \hbar\omega$. Since motion is only possible in the x-direction, the waves can have only one polarization. Treat the electrons as a free, non-relativistic gas confined to move in one-dimension.

   5 (a) What is the electron chemical potential of this system at zero temperature (i.e., what is the Fermi energy ϵ_F, expressed in terms of the electron density)?

   5 (b) What is the electron contribution to the energy of the system at zero temperature?

   5 (c) What is the Debye frequency for the lattice, expressed in terms of N, L, and c_s?

   10 (d) What is the phonon contribution to the energy for T small compared to the Debye temperature?

25 2. For free bosons in a D-dimensional box with an energy-momentum relation $\epsilon = ap^s$, where a and s are positive constants, what is the dimension at which Bose-Einstein condensation begins to occur at low temperatures, in terms of D and s?

25 3. Consider a gas of N spin-1/2 non-relativistic electrons of mass m (non-interacting) confined to a two dimensional area A.

   10 (a) Compute the single particle density of states and derive an expression for the Fermi energy ϵ_F in terms of the matter density.

   5 (b) At $T = 0$, compute the average energy, expressed in terms of N and the Fermin energy.

   5 (c) Calculate the force per unit length exerted by the system (i.e., the 2d-analog of pressure) at $T = 0$.

   5 (d) Now consider $T > 0$ but $k_B T << \epsilon_F$. What is the average energy to $\mathcal{O}(T^2)$ in the Sommerfeld expansion?

25 4. Consider a gas of spinless bosons with a pairwise hard core interaction $u(r < a) = \infty$.

12 (a) Treating the system as a classical gas, compute the b_2 coefficient in the virial cluster expansion.

13 (b) Treating the system as a quantum gas, compute the b_2 coefficient to leading non-vanishing order in a/l_Q.

$\boxed{1}$

a.) use $N_e = 2 \sum_k \Theta(k_F - |k|) \xrightarrow[\text{to int}]{\text{convert}} 2L \int_{-k_F}^{k_F} \frac{dk}{2\pi}$

$$= \frac{2L \; 2k_F}{2\pi} = \frac{2Lk_F}{\pi}$$

$$\therefore \quad \frac{N_e}{L} = \rho_e = \frac{2k_F}{\pi}$$

$$\text{or} \quad k_F = \frac{\pi}{2}\rho_e$$

$$\boxed{\therefore \; \epsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\frac{\pi^2}{4}\rho_e^2 = \frac{\hbar^2\pi^2\rho_e^2}{8m}}$$

<u>NOTE</u>: Other paths to the answer are fine.

E.g., use

$N_e = \int_0^{\epsilon_F} g(\epsilon)\, d\epsilon$ + plug in 1d $g(\epsilon)$ for NR energies

+ you get the same result.

b.) $E_e = 2\sum_k \Theta(k_F - |k|)\frac{\hbar^2 k^2}{2m} \longrightarrow \frac{2L}{2\pi}\cdot\frac{2\hbar^2}{2m}\int_0^{k_F} dk\, k^2$

$$\boxed{E_e = \frac{L\hbar^2}{\pi m}\frac{k_F^3}{3}}$$

or, writing in terms of ϵ_F several equivalent ways (I should have been more precise as to what variables to express E_e in terms of)

$$\boxed{E_e = \frac{2L}{3\pi} k_F \epsilon_F = \frac{2L}{3\pi}\frac{\pi}{2}\rho_e \epsilon_F}$$

but $L\rho_e = N_e$

$$\boxed{\therefore\ E_e = \frac{N}{3}\epsilon_F}$$

(any of these forms will get full credit.)

Same comment as in part a). Other paths to the answer are fine.

E.g., use $E_e = \int_0^{\epsilon_F} d\epsilon\, g(\epsilon)\,\epsilon$

using 1d NR $g(\epsilon)$.

c.) You're given $g(\omega) = \frac{L}{2\pi c_s}$ for the phonon DOS.

Recall, ω_D defined as

$$\int_0^{\omega_D} g(\omega)\, d\omega = N \quad (\text{for 1d})$$

$$\Downarrow$$

$$\frac{L}{2\pi c_s}\omega_D = N \Rightarrow \boxed{\omega_D = \frac{N}{L}\cdot 2\pi c_s}$$

d.) $$E_{phonon} = \int_0^{\omega_D} d\omega\, g(\omega) \frac{\hbar\omega}{e^{\beta\hbar\omega}-1}$$

let $\beta\hbar\omega = x \rightarrow d\omega = \frac{1}{\beta\hbar} dx$

$$E_{phonon} = \frac{1}{(\beta\hbar)^2}\cdot\frac{L}{2\pi c_s}\cdot\hbar \int_0^{\beta\hbar\omega_D} \frac{dx\, x}{e^x - 1}$$

for $k_B T \ll \hbar\omega_D$, $\beta\omega_D \gg 1$ so extend upper limit to ∞. (Note, Debye Temp $\Theta_D = \frac{\hbar\omega_D}{k_B}$)

$$\boxed{\therefore E_{phonon} \overset{T \ll \Theta_D}{\approx} \frac{L(k_B T)^2}{2\pi c_s \hbar} \int_0^{\infty} \frac{dx\, x}{e^x - 1} = \frac{L\pi (k_B T)^2}{12\hbar c_s}}$$

mathematica $= \zeta(2) = \frac{\pi^2}{6}$

$\boxed{2.}$ $\epsilon = ap^s$ bosons, $a + s > 0$ (take spin-0 since not specified)

$$\langle N \rangle \equiv N = \int d\epsilon \, g(\epsilon) \, n(\epsilon)$$

$$= \int d\epsilon \, g(\epsilon) \frac{1}{e^{\beta(\epsilon-\mu)} - 1}$$

$$g(\epsilon) = \frac{L^D}{(2\pi\hbar)^D} \int d^D p \; \delta(\epsilon - \epsilon(p))$$

$$= \frac{L^D}{(2\pi\hbar)^D} S_D \int p^{D-1} dp \; \delta(\epsilon - \epsilon(p))$$

$$= \frac{L^D}{(2\pi\hbar)^D} S_D \int p^{D-1} dp \; \frac{\delta(p - p_0)}{\left| \frac{\partial \epsilon(p)}{\partial p} \right|_{p_0}}$$

where $\epsilon(p_0) = \epsilon$

Now for $\epsilon(p) = ap^s$, $\frac{\partial \epsilon}{\partial p} = s a p^{s-1}$

and $a p_0^s = \epsilon \Rightarrow p_0 = \left(\frac{1}{a}\epsilon\right)^{1/s}$

$$\Rightarrow g(\epsilon) = \frac{L^D}{(2\pi\hbar)^D} S_D \cdot \frac{1}{s a p_0^{s-1}} \cdot p_0^{D-1} = \frac{L^D S_D}{(2\pi\hbar)^D} \cdot \frac{1}{sa} p_0^{D-s}$$

$$\therefore\ g(\epsilon) = \frac{L_1^D S_D}{(2\pi\hbar)^D} \cdot \frac{1}{sa} \left(\frac{\epsilon}{a}\right)^{\frac{D-s}{s}}$$

$$= \alpha\, \epsilon^{\frac{D-s}{s}}$$ (lump all non-ϵ dep. ~~in~~ the prefactor α)

$$\Rightarrow N = \alpha \int \frac{d\epsilon\ \epsilon^{\frac{D-s}{s}}}{z^{-1} e^{\beta\epsilon} - 1} \qquad z = e^{\beta\mu}$$

let $x = \beta\epsilon \qquad d\epsilon = \frac{1}{\beta} dx$

$$\Rightarrow N = \frac{\alpha}{\beta^{\left(\frac{D-s}{s}+1\right)}} \int_0^\infty \frac{dx\ x^{\frac{D-s}{s}}}{z^{-1}e^{x} - 1}$$

* Recall, to check if BEC occurs we set $\mu = 0^-$ + see if the expression for N diverges

1) If $N \to \infty$ for $\mu = 0^-$ $\Rightarrow$ NO BEC

2) If $N \to$ finite for $\mu = 0^-$ $\Rightarrow$ BEC occurs

$\therefore$ Need to study $I = \int_0^\infty \frac{dx\ x^{\frac{D}{s}-1}}{e^x - 1}$; any ∞ will come from the blowing up of integrand near $x \to 0$.

$\therefore$ Near $x = 0$, the integrand behaves as

$$\frac{x^{\frac{D}{s}-1}}{e^x - 1} \simeq \frac{x^{\frac{D}{s}-1}}{1+x-1} \sim x^{\frac{D}{s}-2}$$

$\therefore$ $I = \infty$ if $\frac{D}{s} - 2 \leq -1$

$I = \text{finite}$ if $\frac{D}{s} - 2 > -1$

$\therefore$ BEC occurs for $\frac{D}{s} > 1$

BEC does NOT occur if $\frac{D}{s} \leq 1$

$\boxed{3}$ NR 2d fermi gas

a) Find $g(\epsilon)$ + $\epsilon_F = \epsilon_F(\rho)$ $\quad \rho = \frac{N}{A}$

$$g(\epsilon) = \underbrace{2}_{\text{spin deg.}} \times \frac{L^2}{(2\pi\hbar)^2} \underbrace{(2\pi)}_{S_D \; D=2} \int p\,dp\, \delta(\epsilon - \epsilon(p)) \qquad \epsilon(p) = \frac{p^2}{2m}$$

$$= \frac{4\pi L^2}{4\pi^2 \hbar^2} \int p\,dp \frac{\delta(p-p_0)}{\left| \frac{\partial \epsilon(p)}{\partial p} \right|} \qquad \text{where } \epsilon(p_0) = \epsilon \text{ defines } p_0.$$

$$= \frac{L^2}{\pi\hbar^2} \int \cancel{p}\,dp \frac{\delta(p-p_0)}{\frac{\cancel{p}}{m}}$$

$$\boxed{g(\epsilon)_{2d,NR} = \frac{L^2 m}{\pi \hbar^2}}$$

Now, $N = \int_0^{\epsilon_F} g(\epsilon)\,d\epsilon = \frac{Am}{\pi\hbar^2} \epsilon_F$

$$\Rightarrow \boxed{\epsilon_F = \frac{\hbar^2 \pi}{m} \frac{N}{A} = \frac{\hbar^2 \pi}{m} \rho}$$

b) $E = \int_0^{\epsilon_F} g(\epsilon)\epsilon \, d\epsilon$

$$= \frac{Am}{\pi\hbar^2}\frac{\epsilon_F^2}{2}$$

$$= \frac{A\cancel{m}}{\cancel{\pi\hbar^2}}\frac{\cancel{\hbar^2\pi}}{\cancel{m}}\rho\frac{\epsilon_F}{2}$$

but $A \cdot \rho = N$

$$\boxed{\therefore E = \frac{N}{2}\epsilon_F}$$

c.) $P = -\left(\frac{\partial E}{\partial A}\right)_N = -\frac{N}{2}\frac{\partial \epsilon_F}{\partial A}$

$$= -\frac{N}{2}\frac{\partial \rho}{\partial A}\frac{\partial \epsilon_F}{\partial \rho}$$

$\frac{\partial \rho}{\partial A} = \frac{-N}{A^2} = -\frac{1}{A}\rho$

$$= \frac{N}{2A}\rho\frac{\partial}{\partial \rho}\epsilon_F$$

but $\rho\frac{\partial}{\partial \rho}\epsilon_F = \epsilon_F$

$$\boxed{\therefore P = \frac{N}{2A}\epsilon_F = \frac{E}{A}}$$

(should have been more precise about what variables to write P in terms of.)

d.) Recall, the Sommerfeld expansion is the same for any dimension d (and is indep. of whether we use NR, Relativistic, UR ϵ's) since we express everything in terms of $g(\epsilon)$.

$\Downarrow$

$\therefore$ Simply use results from class (see p. 9 of L22 in the boxed equation) for a general quantity written as

$$I(\mu, T) = \int d\epsilon\, \phi(\epsilon)\, f(\epsilon) \qquad \text{where } f(\epsilon) = \text{F.D. dist} = \frac{1}{e^{\beta(\epsilon-\mu)}+1}$$

$$\approx \underbrace{\int_0^{\epsilon_F} d\epsilon\, \phi(\epsilon)}_{T=0 \text{ result}} + \underbrace{\left[\phi'(\epsilon_F) - \phi(\epsilon_F)\left(\frac{g'}{g}\right)_{\epsilon_F}\right]\frac{\pi^2}{6}(kT)^2}_{\text{finite } T \text{ corrections}}$$

For energy, $\phi(\epsilon) = \epsilon\, g(\epsilon)$

$\therefore \quad \phi'(\epsilon_F) = g(\epsilon_F) + \epsilon_F\, g'(\epsilon_F)$

$-\phi(\epsilon_F)\left(\frac{g'}{g}\right)_{\epsilon_F} = -\epsilon_F\, g'(\epsilon_F)$

$$\boxed{\delta E = g(\epsilon_F)\,\frac{\pi^2}{6}(k_B T)^2}$$

plug in $g(\epsilon_F)$

$\boxed{4}$

a) $b_2 = \frac{1}{2v_a V}\left(Q_2 - Q_1^2\right)$

$$Q_1 = \int d\vec{r} = V$$

$$Q_2 = \int d\vec{r}_1 d\vec{r}_2 \, e^{-\beta u(|\vec{r}_1 - \vec{r}_2|)}$$

$$= \int d\vec{r}_1 d\vec{r}_2 \left(1 + f_{12}\right) \qquad f_{12} = e^{-\beta u(r_{12})} - 1$$

$$= V^2 + \int d\vec{r}_1 d\vec{r}_2 \, f_{12}$$

$$\therefore \; b_2 = \frac{1}{2v_a V} \int d\vec{r}_1 d\vec{r}_2 \, f(\vec{r}_1 - \vec{r}_2)$$

Now, if $u(r) = \infty \quad r < a$

$\qquad\qquad = 0 \quad r > 0$

$$\Rightarrow \quad f(r) = -1 \quad r < a$$

$$\qquad\quad = 0 \quad r > a$$

$$\therefore \; b_2 = \frac{1}{2v_a V} \cancel{\int d\vec{R}}^{\,V} \int d\vec{r} \, f(\vec{r}) = \frac{1}{2v_a} \int d\vec{r} \, \Theta(a - |\vec{r}|)$$

$$= \frac{1}{2v_a} \cdot \frac{4}{3}\pi a^3$$

$$\therefore \boxed{b_2 = \frac{2}{3}\pi \left(\frac{a}{l_\alpha}\right)^3}$$

used $v_\alpha = l_\alpha^3$

classical calc.

b.) Quantum calc.

use result from class (see p.12 L 27)

$$b_2 = b_2^0 + 2^{3/2} \frac{l_\alpha^2}{\pi^2} \int_0^\infty k\,dk \sum_l{}' (2l+1)\, \delta_l(k)\, e^{-\beta \hbar^2 k^2 / m}$$

where $b_2^0 = 2^{-5/2}$ for bosons

$$\sum_l{}' = \sum_{l=0,2,4..} \quad \text{" "}$$

Now, since this was a take-home exam, I don't expect you to solve from scratch the QM scattering result that

$$\tan \delta_l(k) = \frac{j_l(ka)}{n_l(ka)} \qquad \delta_0 = -ka$$

The $\delta_{\ell=2}$ + higher is in terms of the j_ℓ + n_ℓ spherical bessel + neumann functions. The point is that their leading behavior ~~of~~ is

$$\delta_\ell(k) \sim \mathcal{O}((ka)^{2\ell+1}),$$

so $\ell = 2, 4, \ldots$ are subleading compared to $\ell = 0$.

$$\therefore \; b_2 \simeq 2^{-5/2} - 2^{3/2}\frac{\ell_Q^2}{\pi^2} a \underbrace{\int_0^\infty dk\, k^2 e^{-\beta\frac{\hbar^2 k^2}{m}}}_{\text{elementary integral } I}$$

$$I = \frac{1}{2}\int_{-\infty}^{\infty} dk\, k^2 e^{-\alpha k^2} \qquad \alpha = \frac{\beta\hbar^2}{m}$$

$$= \frac{\sqrt{\pi}}{4}\frac{1}{\alpha^{3/2}} = \frac{\sqrt{\pi}}{4}\left(\frac{m}{\beta\hbar^2}\right)^{3/2}$$

$$= \frac{\sqrt{\pi}}{4}\left(\frac{k_B T m}{\hbar^2}\right)^{3/2}$$

recall $\ell_Q = \sqrt{\frac{2\pi\hbar^2}{m k_B T}} \Rightarrow \frac{\ell_Q^2}{2\pi} = \frac{\hbar^2}{m k_B T}$

$$\therefore \; I = \left(\frac{2\pi}{\ell_Q^2}\right)^{3/2}\cdot\frac{\sqrt{\pi}}{4} = \frac{2^{3/2}\cdot\pi^2}{\ell_Q^3\, 4}$$

$\therefore\ b_2 = 2^{-5/2} - 2^{3/2} \frac{l_\alpha^2}{\cancel{\pi^2}} \frac{a\sqrt{2}\,\cancel{\pi^2}}{l_\alpha^3 \cdot 2}$

$$\boxed{b_2 = 2^{-5/2} - \frac{2a}{l_\alpha}}$$

QM result