

QUALIFYING EXAMINATION, Part 2

Solutions

Problem 1: Quantum Mechanics I

(a) We assume the vector potential \vec{A} to point along the ring with a constant magnitude A . A is found by applying Stokes' theorem along the ring

$$A(2\pi R) = \Phi = \pi R_0^2 B ,$$

where Φ is the total magnetic flux through the ring. Thus

$$\vec{A} = \frac{R_0^2 B}{2R} \hat{\varphi} ,$$

where $\hat{\varphi}$ is polar-coordinate unit vector pointing along the ring.

(b) The Hamiltonian is given by

$$H = \frac{1}{2m} \left(\vec{p} - \frac{e}{c} \vec{A} \right)^2 ,$$

where \vec{p} is the canonical momentum of the electron.

(c) Since the electron is confined to the ring, $\vec{p} = p_\varphi \hat{\varphi}$ where φ is the polar angle and p_φ is the magnitude of the momentum along the ring.

Therefore

$$H = \frac{1}{2m} \left(p_\varphi - \frac{eR_0^2 B}{2Rc} \right)^2 = \frac{1}{2m} \left(\frac{L_z}{R} - \frac{eR_0^2 B}{2Rc} \right)^2 ,$$

where L_z is the angular momentum of the electron along the z-axis. The eigenfunctions of H are the eigenfunctions of L_z

$$\Psi_n(\varphi) = \frac{1}{\sqrt{2\pi}} e^{in\varphi} .$$

The corresponding eigenvalues of L_z are given by $n\hbar$ where $n = \dots, -3, -2, -1, 0, 1, 2, 3, \dots$. Thus the eigenvalues of H are

$$E_n = \frac{\hbar^2}{2mR^2} \left(n - \frac{eR_0^2 B}{2\hbar c} \right)^2 .$$

These can also be written as

$$E_n = \frac{\hbar^2}{2mR^2} \left(n - \frac{\Phi}{\Phi_0} \right)^2 ,$$

where $\Phi_0 = hc/e$.

(d)

$$V = -E\vec{x} = -ER \cos \varphi .$$

With the condition in (d), the unperturbed levels are non-degenerate. Therefore, non-degenerate perturbation theory can be used. In first-order perturbation theory

$$\delta E_n^{(1)} = \langle n|V|n \rangle = -ER \langle n| \cos \varphi |n \rangle = 0 .$$

The above matrix element vanishes since the perturbation $\cos \varphi = (e^{i\varphi} + e^{-i\varphi})/2$ can only connect state n to states $n \pm 1$.

Problem 2: Quantum Mechanics II

(a) Labeling the two particles by 1, 2, the two-particle Hamiltonian is

$$\hat{H} = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} + \frac{1}{2}k\hat{x}_1^2 + \frac{1}{2}k\hat{x}_2^2.$$

The eigenstates of \hat{H} for two distinguishable particles are specified by two non-negative integer quantum numbers j, k (one for each particle), and the total energy is the sum of the two energies

$$E_{j,k} = \hbar\omega(j + 1/2) + \hbar\omega(k + 1/2) = \hbar\omega(j + k + 1).$$

For bosons, the total wave function must be symmetric under particle exchange, and without spin this means $\Psi(x_1, x_2) = \Psi(x_2, x_1)$. The lowest possible total energy is for $j = k = 0$ which is symmetric: if $\phi_n(x)$ are the harmonic oscillator eigenfunctions, $\Psi_0(x_1, x_2) = \phi_0(x_1)\phi_0(x_2)$ is clearly symmetric. The first excited state for bosons is the symmetric combination of $j = 1, k = 0$ and $j = 0, k = 1$: $\Psi_1(x_1, x_2) = (\phi_1(x_1)\phi_0(x_2) + \phi_0(x_1)\phi_1(x_2))/\sqrt{2}$, and its energy is $2\hbar\omega$.

(b) For spinless fermions, the spatial wave function must be antisymmetric $\Psi(x_1, x_2) = -\Psi(x_2, x_1)$. Thus the $j = k = 0$ solution is not allowed (you can't put two fermions in the same state). The first allowed state is the antisymmetric combination of $j = 1, k = 0$ and $j = 0, k = 1$: $\Psi_0(x_1, x_2) = [\phi_1(x_1)\phi_0(x_2) - \phi_0(x_1)\phi_1(x_2)]/\sqrt{2}$. Thus $E_0 = 2\hbar\omega$. The excited state is the antisymmetric combination of $j = 2, k = 0$ and $j = 0, k = 2$ with energy $3\hbar\omega$.

(c) For two spin-1/2 electrons, the total wave function can be written a spatial part times a spin part and must be antisymmetric. If we add the two spins, the total allowed spin is either $S = 0$ or $S = 1$. An $S = 0$ state ($|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle)/\sqrt{2}$ is antisymmetric in spin space while the $S = 1$ state is symmetric.

The ground state is obtained by putting both particles in the lowest oscillator orbital (symmetric in space) and is thus an $S = 0$ state with energy $E_0 = \hbar\omega$. This situation correspond to part (a) where the spatial wave function is symmetric.

The first excited level is obtained by putting one electron in oscillator level 0 and another electron in oscillator level 1, each one with either spin up or spin down. Its energy is $E_1 = 2\hbar\omega$. Now both $S = 0$ and $S = 1$ are allowed. In particular the $S = 1, S_z = 1$ state with both electron spin up is symmetric in spin space is antisymmetric in space and is therefore analogous to the spatial state in part (b).

The $S = 0$ ground-state is non-degenerate. However, the excited level has both $S = 0$ (one state) and $S = 1$ (three states $S_z = -1, 0, +1$) and is therefore four-fold degenerate.

Note (Y.A.): this problem can also be solved without coupling the spins.

(d) The Hamiltonian

$$\hat{H} = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} + \frac{k\hat{x}_1^2}{2} + \frac{k\hat{x}_2^2}{2} - \alpha k\hat{x}_1\hat{x}_2$$

can be written using ladder operators as

$$\hat{H} = \hbar\omega(\hat{a}_1^\dagger\hat{a}_1 + \hat{a}_2^\dagger\hat{a}_2 + 1) - \frac{\alpha k\hbar}{2m\omega}(\hat{a}_1 + \hat{a}_1^\dagger)(\hat{a}_2 + \hat{a}_2^\dagger).$$

We use the notation $|j, k\rangle$ to label the unperturbed states with oscillators in states j, k (see part (a)). The unperturbed ground state is $|0, 0\rangle$.

The first-order shift of the ground-state energy $\delta E_0^{(1)} = \langle 0, 0 | \hat{V}_{int} | 0, 0 \rangle$ vanishes since the interaction term modifies the number of oscillator quanta of each particle separately by ± 1 .

It is thus necessary to go to second order

$$\delta E_0^{(2)} = \sum_{q \neq 0} \frac{|\langle q | \hat{V}_{int} | 0 \rangle|^2}{E_0 - E_q}.$$

The energy denominator is $E_{0,0} - E_{1,1} = -2\hbar\omega$ and the matrix element is

$$\begin{aligned} \langle 1, 1 | \hat{V}_{int} | 0, 0 \rangle &= -\frac{\alpha k\hbar}{2m\omega} \langle 1, 1 | (\hat{a}_1 + \hat{a}_1^\dagger)(\hat{a}_2 + \hat{a}_2^\dagger) | 0, 0 \rangle \\ &= -\frac{\alpha k\hbar}{2m\omega} \langle 1, 1 | \hat{a}_1^\dagger \hat{a}_2^\dagger | 0, 0 \rangle = -\frac{\alpha k\hbar}{2m\omega} \langle 1, 1 | 1, 1 \rangle \\ &= -\frac{\alpha k\hbar}{2m\omega} = -\frac{\alpha\hbar\omega}{2}. \end{aligned}$$

Thus the second-order shift is

$$\delta E_0^{(2)} = \frac{(\alpha\hbar\omega/2)^2}{-2\hbar\omega} = -\frac{\alpha^2\hbar\omega}{8}.$$

(e) The potential part of the Hamiltonian is quadratic in x_1 and x_2 so one can change coordinates linearly to create two decoupled oscillators, i.e. transform to normal coordinates. The kinetic part remains invariant since the particles have the same mass. The normal coordinates are the symmetric and antisymmetric combinations

$$u = \frac{x_1 + x_2}{\sqrt{2}}, \quad v = \frac{x_1 - x_2}{\sqrt{2}}.$$

The Hamiltonian becomes

$$\hat{H} = \frac{\hat{p}_u^2 + \hat{p}_v^2}{2m} + \frac{k}{2} [(1 - \alpha)\hat{u}^2 + (1 + \alpha)\hat{v}^2],$$

and is the sum of two independent oscillators. Its energies and wave functions are labeled by two non-negative integers r, s and are given by

$$E_{r,s} = \hbar\omega\sqrt{1-\alpha}(r+1/2) + \hbar\omega\sqrt{1+\alpha}(s+1/2) ,$$

and

$$\Psi_{r,s}(u, v) = \phi_r(u)\phi_s(v) .$$

To impose Bose-Einstein statistics, we notice that $u \rightarrow u$ and $v \rightarrow -v$ under the interchange of x_1 and x_2 . Also the oscillator states $\phi_n(x)$ are even or odd following the number parity of n . Thus for $\Psi_{r,s}$ to be even under interchange s must be even (i.e., odd oscillator states s are not allowed) and there is no restriction on r .

The ground state is then $r = s = 0$ and the first excited state is $r = 1, s = 0$. The energies are

$$E_0 = \frac{\hbar\omega}{2}(\sqrt{1-\alpha} + \sqrt{1+\alpha}) , \quad E_1 = \frac{\hbar\omega}{2}(3\sqrt{1-\alpha} + \sqrt{1+\alpha}) .$$

E_0 is even in α so its Taylor series starts at order α^2 , while E_1 is neither odd or even so its series generically starts at order α . We also notice that the exact energies $E_{r,s}$ are dimensionless numbers multiplying $\hbar\omega$. This must be true since there is only one energy scale $\hbar\omega$ in the problem and the perturbation did not introduce a new energy scale.

Problem 3: Statistical Mechanics I

(a) The partition function for a single oscillator is

$$\begin{aligned} Z_1 &= \sum_{n=0}^{\infty} e^{-\beta E_n} = \sum_{n=0}^{\infty} e^{-(n+\frac{1}{2})\hbar\omega\beta} \\ &= e^{-\frac{1}{2}\hbar\omega\beta} \sum_{n=0}^{\infty} (e^{-\hbar\omega\beta})^n \\ &= \frac{e^{-\frac{1}{2}\hbar\omega\beta}}{1 - e^{-\hbar\omega\beta}} = \frac{1}{2 \sinh(\hbar\omega\beta/2)}. \end{aligned}$$

(b) The average canonical energy of a single oscillator is

$$\langle E \rangle = -\frac{\partial \ln Z_1}{\partial \beta} = \frac{\partial}{\partial \beta} \ln \left(2 \sinh \frac{\hbar\omega\beta}{2} \right) = \frac{\hbar\omega}{2} \frac{1}{\tanh(\hbar\omega\beta/2)}.$$

Therefore, the total internal energy of $3N$ independent oscillators is

$$U = \frac{3N\hbar\omega}{2 \tanh(\hbar\omega\beta/2)}.$$

(c) The heat capacity for the whole solid is

$$C_V = \frac{\partial U}{\partial T} = -k\beta^2 \frac{\partial U}{\partial \beta} = 3Nk \left(\frac{\beta\hbar\omega}{2} \right)^2 \frac{1}{\sinh(\hbar\omega\beta/2)^2}.$$

(d) To sketch $C_V(T)$, plot $\frac{C_V}{3Nk}$ vs. $\frac{kT}{\hbar\omega} = T/\theta_e$, where $\theta_e = \frac{\hbar\omega}{k}$ is defined as the Einstein temperature. We can rewrite

$$\frac{C_V}{3Nk} = \frac{(\theta_e/2T)^2}{\sinh(\theta_e/2T)^2}$$

To study the behavior at the limits, it is convenient to express C_V as

$$C_V = 3Nk \left(\frac{\beta\hbar\omega}{2} \right)^2 \frac{4}{(e^{\hbar\omega\beta/2} - e^{-\hbar\omega\beta/2})^2} = 3Nk (\beta\hbar\omega)^2 \frac{e^{\hbar\omega\beta}}{(e^{\hbar\omega\beta} - 1)^2}.$$

For low temperatures (high β), $\beta\hbar\omega \gg 1$, and

$$C_V \approx 3Nk (\beta\hbar\omega)^2 e^{-\hbar\omega\beta}.$$

The Einstein's model predicts that the specific heat approaches zero exponentially fast at low temperatures, because all the oscillations have one common frequency. The correct

behavior is provided by the Debye Model (1912), which properly takes into account the fact that the frequencies of the waves are not all the same and leads to a T^3 power law for the specific heat (as is verified by the experiments).

For high temperatures (low β), $\beta\hbar\omega \ll 1$, and $e^{\hbar\omega\beta/2} - e^{-\hbar\omega\beta/2} \approx \beta\hbar\omega$. The heat capacity is then

$$C_V \approx 3Nk.$$

This is the Dulong-Petit law (1819), and it states that the specific heat of solids should be independent of temperature.

This high temperature limit can also be derived by equipartition theorem, which states that in a classical system each quadratic degree of freedom contributes an average energy of $kT/2$. The harmonic oscillator has two quadratic terms in the Hamiltonian - kinetic energy and potential energy - and in equipartition the average oscillator energy is kT . The internal energy of the 3D solid is then given by $U = 3NkT$, leading to $C_V = 3Nk$. This holds even when the oscillators have different frequencies.

Problem 4: Statistical Mechanics II

(a) The density of single-particle states in momentum space is given by $g(\mathbf{k}) = (2s + 1)A/(2\pi)^2$. We have

$$(2s + 1) \frac{A}{(2\pi)^2} d^2\vec{k} = (2s + 1) \frac{A}{(2\pi)^2} 2\pi k dk = (2s + 1) \frac{A}{2\pi} \frac{m}{\hbar^2} d\epsilon,$$

where we have used $d\epsilon = \frac{\hbar^2}{m} k dk$. Therefore

$$g(\epsilon) = (2s + 1) \frac{A}{2\pi} \frac{m}{\hbar^2}.$$

(b) The Fermi energy is determined from the total number of particles

$$N = \int_0^{\epsilon_F} d\epsilon g(\epsilon) = (2s + 1) \frac{A}{2\pi} \frac{m}{\hbar^2} \epsilon_F.$$

We find

$$\epsilon_F = \frac{1}{2s + 1} \frac{2\pi\hbar^2}{m} \rho.$$

where $\rho = N/A$.

(c) The total energy E at $T = 0$ is given by

$$E = \int_0^{\epsilon_F} d\epsilon \epsilon g(\epsilon) = (2s + 1) \frac{A}{2\pi} \frac{m}{\hbar^2} \frac{1}{2} \epsilon_F^2 = A \frac{1}{2s + 1} \frac{\pi\hbar^2}{m} \rho^2 = \frac{1}{2s + 1} \frac{\pi\hbar^2}{m} \frac{N^2}{A}.$$

Thus

$$\frac{E}{A} = \frac{1}{2s + 1} \frac{\pi\hbar^2}{m} \rho^2.$$

[The total energy per particle can be more easily derived from $E/A = \int_0^{\epsilon_F} d\epsilon \epsilon g(\epsilon) / \int_0^{\epsilon_F} d\epsilon g(\epsilon) = \int_0^{\epsilon_F} d\epsilon \epsilon / \int_0^{\epsilon_F} d\epsilon = \epsilon_F/2$].

(d) At $T = 0$ the pressure is given by $P = -\partial E / \partial A$ (the partial derivative is at fixed entropy S but at $T = 0$, this is equivalent to a derivative at fixed T since according to the third law $S = 0$ at $T = 0$). We find

$$P = -\frac{\partial E}{\partial A} = \frac{1}{2s + 1} \frac{\pi\hbar^2}{m} \frac{N^2}{A^2} = \frac{1}{2s + 1} \frac{\pi\hbar^2}{m} \rho^2.$$

(e) The equilibrium condition at $T = 0$ is $P_1 = P_2$, where P_1 and P_2 are the pressures on the left and right sides of the piston, respectively. Since $P \propto \rho^2/(2s + 1)$, we find

$$\rho_1^2/2 = \rho_2^2/4 ,$$

or

$$\frac{\rho_1}{\rho_2} = \frac{1}{\sqrt{2}} .$$