QUALIFYING EXAMINATION, Part 2

Solutions

Problem 1: Quantum Mechanics I

(a)

$$[a, a^\dagger] = \left[\sqrt{\frac{m\omega}{2\hbar}}x + \frac{i}{\sqrt{2m\omega\hbar}}p, \sqrt{\frac{m\omega}{2\hbar}}x - \frac{i}{\sqrt{2m\omega\hbar}}p\right] = -\frac{i}{2\hbar}[x,p] + \frac{i}{2\hbar}[p,x] = 1 \ ,$$

where we have used $[x,x] = [p,p] = 0$ and $[x,p] = -[p,x] = i\hbar$.

(b) For a we have

$$a|0\rangle = 0 \ , \ \ a|1\rangle = |0\rangle \ , \ \ a|2\rangle = \sqrt{2}|1\rangle \ .$$

In a matrix form

$$a = \begin{pmatrix} 0 & 1 & 0 & \dots \\ 0 & 0 & \sqrt{2} & \dots \\ 0 & 0 & 0 & \dots \\ \dots & & & \end{pmatrix} \ .$$

Similarly for $a^\dagger$

$$a^\dagger|0\rangle = |1\rangle \ , \ \ a^\dagger|1\rangle = \sqrt{2}|2\rangle \ , \ \ a^\dagger|2\rangle = \sqrt{3}|3\rangle \ .$$

In a matrix form

$$a^\dagger = \begin{pmatrix} 0 & 0 & 0 & \dots \\ 1 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & \dots \\ \dots & & & \end{pmatrix} \ .$$

(c) Using $H = (a^\dagger a + 1/2)\hbar\omega$ and $a^\dagger a|n\rangle = n|n\rangle$, we find

$$\langle H\rangle = (n + 1/2)\hbar\omega \ .$$

Using the expressions for a and $a^\dagger$, we have

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \ ; \quad p = -i\sqrt{\frac{m\hbar\omega}{2}}(a - a^\dagger) \ .$$

We find

$$\langle x\rangle \propto \langle a + a^\dagger\rangle = 0 \ ; \quad \langle p\rangle \propto \langle a - a^\dagger\rangle = 0 \ ,$$

since a and $a^\dagger$ cannot connect $|n\rangle$ to itself.

$$\langle x^2\rangle = \frac{\hbar}{2m\omega}\langle (a+a^\dagger)^2\rangle = \frac{\hbar}{2m\omega}\langle aa^\dagger + a^\dagger a\rangle = \frac{\hbar}{2m\omega}\langle 2a^\dagger a + 1\rangle = (n+1/2)\frac{\hbar}{m\omega} \ ,$$

where we have used $\langle a^2\rangle = \langle {a^\dagger}^2\rangle = 0$ and $aa^\dagger = a^\dagger a + 1$ from the commutation relation. Similarly

$$\langle p^2\rangle = -\frac{m\hbar\omega}{2}\langle (a-a^\dagger)^2\rangle = \frac{m\hbar\omega}{2}\langle aa^\dagger + a^\dagger a\rangle = \frac{m\hbar\omega}{2}\langle 2a^\dagger a + 1\rangle = (n+1/2)m\hbar\omega \ .$$

Another method is to use the virial theorem

$$\left\langle \frac{p^2}{2m} \right\rangle = \left\langle \frac{1}{2}m\omega^2 x^2 \right\rangle = \frac{1}{2}\langle H\rangle \ ,$$

from which we obtain the same expressions for $\langle x^2\rangle$ and $\langle p^2\rangle$.

(d) The time evolution of the wave function is given by

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left(e^{-iHt/\hbar}|0\rangle + e^{-iHt/\hbar}|1\rangle\right) = \frac{1}{\sqrt{2}}\left(e^{-i\omega t/2}|0\rangle + e^{-3i\omega t/2}|1\rangle\right) \ .$$

To calculate the time dependence of $\langle x\rangle$ and $\langle x^2\rangle$, we can use either operator or matrix algebra.

Method I:

$$\langle x\rangle(t) = \sqrt{\frac{\hbar}{2m\omega}}\langle\psi(t)|a+a^\dagger|\psi(t)\rangle = \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}\left(e^{-i\omega t}\langle 0|a|1\rangle + e^{i\omega t}\langle 1|a^\dagger|0\rangle\right) = \sqrt{\frac{\hbar}{2m\omega}}\cos\omega t \ ,$$

or

$$\langle x\rangle(t) = x_0\cos\omega t \ , \quad \text{where} \quad x_0 = \sqrt{\frac{\hbar}{2m\omega}} \ .$$

$$\begin{aligned}\langle x^2\rangle &= \frac{\hbar}{2m\omega}\langle\psi(t)|(a+a^\dagger)^2|\psi(t)\rangle = \frac{1}{2}\frac{\hbar}{2m\omega}\left(\langle 0|aa^\dagger + a^\dagger a|0\rangle + \langle 1|aa^\dagger + a^\dagger a|1\rangle\right) \\ &= \frac{1}{2}\frac{\hbar}{2m\omega}\left(\langle 0|2a^\dagger a + 1|0\rangle + \langle 1|2a^\dagger a + 1|1\rangle\right) = \frac{\hbar}{m\omega} = 2x_0^2 \ .\end{aligned}$$

Method II (Dan):

Using $x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$ and the matrix representation of a and $a^\dagger$ in part (b), we find the matrix representation of x

$$x = \sqrt{\frac{\hbar}{2m\omega}} \begin{pmatrix} 0 & 1 & 0 & \dots \\ 1 & 0 & \sqrt{2} & \dots \\ 0 & \sqrt{2} & 0 & \dots \\ \dots & & & \end{pmatrix} .$$

The wave function $|\psi(t)\rangle$ is represented by the vector $\frac{1}{\sqrt{2}} e^{-i\omega t/2} \begin{pmatrix} 1 \\ e^{-i\omega t} \\ 0 \\ \dots \end{pmatrix}$. Therefore

$$\begin{aligned} \langle x \rangle(t) &= \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}} \begin{pmatrix} 1 & e^{i\omega t} & 0 & \dots \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & \dots \\ 1 & 0 & \sqrt{2} & \dots \\ 0 & \sqrt{2} & 0 & \dots \\ \dots & & & \end{pmatrix} \begin{pmatrix} 1 \\ e^{-i\omega t} \\ 0 \\ \dots \end{pmatrix} \\ &= \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}} \begin{pmatrix} 1 & e^{i\omega t} & 0 & \dots \end{pmatrix} \begin{pmatrix} e^{-i\omega t} \\ 1 \\ \sqrt{2}e^{-i\omega t} \\ \dots \end{pmatrix} = \sqrt{\frac{\hbar}{2m\omega}} \cos \omega t \, . \end{aligned}$$

The matrix x^2 is given by

$$x^2 = x_0^2 \begin{pmatrix} 1 & 0 & \sqrt{2} & \dots \\ 0 & 3 & 0 & \dots \\ \sqrt{2} & 0 & 5 & \dots \\ \dots & & & \end{pmatrix} .$$

Therefore

$$\begin{aligned} \langle x^2 \rangle(t) &= \frac{1}{2} x_0^2 \begin{pmatrix} 1 & e^{i\omega t} & 0 & \dots \end{pmatrix} \begin{pmatrix} 1 & 0 & \sqrt{2} & \dots \\ 0 & 3 & 0 & \dots \\ \sqrt{2} & 0 & 5 & \dots \\ \dots & & & \end{pmatrix} \begin{pmatrix} 1 \\ e^{-i\omega t} \\ 0 \\ \dots \end{pmatrix} \\ &= \frac{1}{2} x_0^2 \begin{pmatrix} 1 & e^{i\omega t} & 0 & \dots \end{pmatrix} \begin{pmatrix} 1 \\ 3e^{-i\omega t} \\ \sqrt{2} \\ \dots \end{pmatrix} = 2x_0^2 \, . \end{aligned}$$

(e) The coordinate $x \propto a + a^\dagger$. Since a and $a^\dagger$ do not connect $|0\rangle$ and $|2\rangle$, we have

$$\langle x \rangle(t) = 0 \, .$$

Problem 2: Quantum Mechanics II

(a) Since there is no interaction and no spin-dependence in the Hamiltonian, the energy eigenvalues are determined solely by the spatial degree of freedom x, and the many-body states will be appropriately antisymmetrized combinations of the single-particle states.

The boundary conditions for the single-particle wave function $\psi(x)$ in an infinite square well between $x = -L/2$ and $x = L/2$ are $\psi(-L/2) = \psi(L/2) = 0$. The normalized single-particle eigenstates are given by

$$\psi_n(x) = \sqrt{\frac{2}{L}} \begin{cases} \cos\left(\frac{\pi n x}{L}\right) & n \text{ odd} \\ \sin\left(\frac{\pi n x}{L}\right) & n \text{ even} \end{cases} .$$

The corresponding eigenvalues are $\epsilon_n = \hbar^2 k_n^2/2m = \hbar^2\pi^2 n^2/2mL^2$.

We label these single-particle eigenstates as $|n\rangle_i$, where $i = 1, 2$ labels the particle. The two-particle wave function can be expressed as a product of a spatial wave function and a spin wave function. The total wave function must be antisymmetric under the exchange of the two particles. Thus, when the spatial wave function is symmetric, the spin wave function must be antisymmetric and vice versa.

The lowest two-particle eigenstate corresponds to both particles in the lowest spatial single-particle state $n = 1$ and its energy is $E = 2\epsilon_1 = \hbar^2\pi^2/mL^2$. The corresponding spatial wave function $|1\rangle_1|1\rangle_2$ is symmetric, hence the spin wave function must be antisymmetric (i.e., a singlet). The complete normalized ground-state wave function is

$$(|1\rangle_1|1\rangle_2)\ \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right) .$$

The next lowest two-particle states will involve particles in the spatial single-particle states $n = 1$ and $n = 2$ with total energy of $E = \epsilon_1 + \epsilon_2 = 5\hbar^2\pi^2/2mL^2$. These could be combined into a symmetric spatial wave function, which would require an antisymmetric (i.e., singlet) spin wave function

$$\frac{1}{\sqrt{2}}\left(|1\rangle_1|2\rangle_2 + |2\rangle_1|1\rangle_2\right)\ \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right) ,$$

or they could be combined into an antisymmetric spatial wave function, which would require a symmetric (i.e., triplet) spin wave function. Note that there are three symmetric spin wave functions giving three two-particle eigensates

$$\begin{gathered} \tfrac{1}{\sqrt{2}}\left(|1\rangle_1|2\rangle_2 - |2\rangle_1|1\rangle_2\right)\ \left(|\uparrow\rangle_1|\uparrow\rangle_2\right) , \\ \tfrac{1}{\sqrt{2}}\left(|1\rangle_1|2\rangle_2 - |2\rangle_1|1\rangle_2\right)\ \tfrac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2\right) , \\ \tfrac{1}{\sqrt{2}}\left(|1\rangle_1|2\rangle_2 - |2\rangle_1|1\rangle_2\right)\ \left(|\downarrow\rangle_1|\downarrow\rangle_2\right) . \end{gathered}$$

These last four states all have the same energy $E = \epsilon_1 + \epsilon_2$. The next lowest energy state will have both particles in $n = 2$ giving an energy of $2\epsilon_2 > \epsilon_1 + \epsilon_2$. Thus the five states listed above are the five lowest energy eigenstates.

(b) The additional spin-dependent interaction term in the Hamiltonian will cause the energy eigenvalues to depend upon the spin state. To determine this depedence, we we can rewrite the interaction as

$$H_{\rm ex} = A\vec{\sigma}_1 \cdot \vec{\sigma}_2 = A\left(\vec{S}^2 - \vec{\sigma}_1^2 - \vec{\sigma}_2^2\right)/2 = A\left(\vec{S}^2 - 3/2\right)/2 \ ,$$

where $\vec{S} = \vec{\sigma}_1 + \vec{\sigma}_2$ is the total spin of the two particles and we have used $\vec{\sigma}_1^2 = \vec{\sigma}_1^2 = 3/4$.

The spin wave functions used in the solution of part (a) are eigenstates of $\vec{S}^2$ with eigenvalues $S(S+1)$ and therefore also eigenstates of the interaction term with eigenvalues $A[S(S+1)-3/2]/2$. The antisymetric spin wave function is an $S = 0$ state with eigenvalue $-3A/4$ of $H_{\rm ex}$, while the three symmetric spin wave functions are $S = 1$ states with degenerate eigenvalue $A/4$ of $H_{\rm ex}$.

Thus the five states found in the solution to part (a) remain eigenstates but their energies are shifted. Since $A \ll \epsilon_1$, these five eigenstates also remain the five eigenstates with the lowest energies.

The two-particle ground state is antisymmetric in spin space and thus its energy is $2\epsilon_1 - 3A/4 = \hbar^2\pi^2/mL^2 - 3A/4$.

The lowest two-particle excited state is the one which is antisymmetric in spin space and its energy is $\epsilon_1 + \epsilon_2 - 3A/4 = 5\hbar^2\pi^2/2mL^2 - 3A/4$.

The second two-particle excited level is three-fold degenerate and corresponds to the three eigenfunctions which are symmetric in spin space with energy $\epsilon_1 + \epsilon_2 + A/4 = 5\hbar^2\pi^2/2mL^2 + A/4$.

(c) The conditions described in the problem indicate that the transition rates could be calculated by Fermi's golden rule

$$R_{i\to f} \propto \langle f|B|i\rangle^2 \delta(\hbar\omega - (E_f - E_i)) \ .$$

where i and f label the initial and final energy eigenstates. Since B is a real number, we can rewrite the previous expression as

$$R_{i\to f} \propto \langle f|i\rangle^2 \delta(\hbar\omega - (E_f - E_i)) \ ,$$

which vanishes for all $i \neq f$ by virtue of the orthogonality of eigenfunctions. Thus this perturbation generates no transitions.

(d) For this perturbation

$$R_{i\to f} \propto \langle f|\hat{x}|i\rangle^2 \delta(\hbar\omega - (E_f - E_i)) \ ,$$

or using the wave functions in coordinate space (for a square well between $x = -L/2$ and $x = L/2$)

$$R_{i\to f} \propto \left|\int_{-L/2}^{L/2} dx \psi_f(x)\, x\, \psi_i(x)\right|^2 \delta(\hbar\omega - (E_f - E_i)) \ .$$

The eigenfunctions in the interval $[-L/2, L/2]$ have definite parity (under reflection $x \to -x$). Since x is odd under reflection, it can connect only eigenstates of opposite parity. Thus only transitions between eigenstates with n even and n odd (or vice versa) are allowed (i.e., non-zero).

The delta function term in the expression for $R_{i\to f}$ sets an additional resonance condition on the frequency ω

$$\hbar\omega = E_f - E_i \ .$$

Statistical Mechanics I - solution

(a) Since the particles are distinguishable

$$\Omega = \frac{N!}{n_0!\, n_1!\, n_2!} \ .$$

The entropy is given by $k \ln \Omega$. Using Stirling's formula for $N, n_i \gg 1$, we find

$$S = k \ln \Omega \approx k \left(N \ln N - n_1 \ln n_1 - n_2 \ln n_2 - n_3 \ln n_3 \right) = -k \sum_i n_i \ln \left(\frac{n_i}{N} \right) \ .$$

(b) The entropy is maximized in an isolated system.

(c) Using the expression in (a), the entropy per particle is

$$\frac{S}{N} = -k \sum_i \frac{n_i}{N} \ln \left(\frac{n_i}{N} \right) \ .$$

Interpreting $p_i = \frac{n_i}{N}$ to be the probability of finding the particle in state i

$$\frac{S}{N} = -k \sum_i p_i \ln p_i$$

is just the usual entropy of the single-particle ensemble $\{p_i\}$.

(d)

$$E = \sum_i \epsilon_i n_i = \epsilon_1 n_1 + \epsilon_2 n_2 + \epsilon_3 n_3 \ ,$$

$$N = \sum_i n_i = n_1 + n_2 + n_3 \ .$$

(e) In an equilibrium of the isolated system, the entropy is maximized holding E and N fixed. Using the method of Lagrange multipliers, we introduce Lagrange multipliers λ and α for the two constraints E and N, respectively, and maximize (with no constraints)

$$S' \equiv S - \lambda E - \alpha N = -k \sum_i n_i \ln \left(\frac{n_i}{N} \right) - \lambda \sum_i \epsilon_i n_i - \alpha \sum_i n_i \ .$$

We have

$$0 = \frac{\partial S'}{\partial n_i} = -k \left[\ln \left(\frac{n_i}{N} \right) + 1 \right] - \lambda \epsilon_i - \alpha \ .$$

$$\frac{n_i}{N} = C e^{-\frac{\lambda}{k} \epsilon_i} \ ,$$

where C is a constant related to α. The constant C is determined by the particle-number equation $\sum n_i = N$ to be

$$C = [\sum_j e^{-\frac{\lambda}{k}\epsilon_i}]^{-1} \ .$$

We then have

$$\frac{n_i}{N} = \frac{e^{-\frac{\lambda}{k}\epsilon_i}}{\sum_j e^{-\frac{\lambda}{k}\epsilon_i}} \ .$$

The Lagrange multiplier λ is determined by the energy constraint

$$E = \sum n_i \epsilon_i = N \sum_i \epsilon_i e^{-\frac{\lambda}{k}\epsilon_i} \ ,$$

or

$$\sum_i \epsilon_i e^{-\frac{\lambda}{k}\epsilon_i} = \frac{E}{N} \ .$$

The probabilities $p_i = n_i/N \propto e^{-\frac{\lambda}{k}\epsilon_i}$ have the form of the canonical ensemble and λ can be interpreted as an effective inverse temperature $\lambda = 1/T$. While the many-particle ensemble is micro-canonical, the effective single-particle ensemble is canonical since all the other particles act as a heat bath.

Problem 4: Statistical Mechanics II

(a) The density of single-particle states in momentum space is given by $g(\mathbf{k}) = A/(2\pi)^2$. We have $\frac{A}{(2\pi)^2} d^2\mathbf{k} = \frac{A}{(2\pi)^2} 2\pi k\, dk = \frac{A}{2\pi} \frac{m}{\hbar^2} d\epsilon$, where we have used $d\epsilon = \frac{\hbar^2}{m} k\, dk$. Thus

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

(b) μ is determined from the particle-number equation

$$N = \int_0^\infty d\epsilon g(\epsilon) \frac{1}{1 + e^{\beta(\epsilon - \mu)}} \; .$$

For $\zeta \equiv e^{\beta\mu} \ll 1$, we have $e^{\beta(\epsilon-\mu)} = e^{\beta\epsilon}\zeta^{-1} \geq \zeta^{-1} \gg 1$ for any $\epsilon \geq 0$. In this limit $\frac{1}{1+e^{\beta(\epsilon-\mu)}} \approx e^{-\beta(\epsilon-\mu)} = \zeta e^{-\beta\epsilon}$ and

$$N \approx \zeta \int_0^\infty d\epsilon g(\epsilon) e^{-\beta\epsilon} = \zeta A \left(\frac{mkT}{2\pi\hbar^2} \right) \equiv \zeta N_c \quad \text{or} \quad \zeta \approx N/N_c \; .$$

(c) The occupation of a single-particle bound state with energy $-\epsilon_0$ is given by the Fermi-Dirac distribution $[1 + e^{\beta(-\epsilon_0 - \mu)}]^{-1}$. Since there are N bound states with energy $-\epsilon_0$

$$N_b = \frac{N}{1 + e^{-\beta(\epsilon_0 + \mu)}} \; .$$

The average number of free particles is given by an expression similar to the one in (a)

$$N_f = \int_0^\infty d\epsilon g(\epsilon) \frac{1}{1 + e^{\beta(\epsilon - \mu)}} \; .$$

In the limit $\zeta \ll 1$, we use the same approximation as in part (a) to obtain

$$N_f \approx \zeta N_c \; .$$

(d) μ is determined by the total number of particles

$$N = N_b + N_f = \frac{N}{1 + e^{-\beta(\epsilon_0 + \mu)}} + \int_0^\infty d\epsilon g(\epsilon) \frac{1}{1 + e^{\beta(\epsilon - \mu)}}$$

or

$$\frac{N}{1 + e^{\beta(\epsilon_0 + \mu)}} = \int_0^\infty d\epsilon g(\epsilon) \frac{1}{1 + e^{\beta(\epsilon - \mu)}} = N_f \; .$$

In the limit $\zeta \ll 1$, we can use the approximation in (c) for N_f to obtain

$$\frac{N}{1+\zeta e^{\beta\epsilon_0}} = \zeta N_c \ .$$

This leads to a quadratic equation for ζ

$$e^{\beta\epsilon_0}\zeta^2 + \zeta - N/N_c = 0 \ .$$

We find

$$\zeta = \frac{1}{2}e^{-\beta\epsilon_0}\left[\sqrt{4e^{\beta\epsilon_0}N/N_c + 1} - 1\right] \ ,$$

where the solution is chosen by the condition that $\zeta > 0$. N_f is given by

$$N_f \approx \zeta N_c = \frac{1}{2}e^{-\beta\epsilon_0}N_c\left[\sqrt{4e^{\beta\epsilon_0}N/N_c + 1} - 1\right] \ .$$