

QUALIFYING EXAMINATION, Part 2

Solutions

Problem 1: Quantum Mechanics I

(a) We may decompose the Hamiltonian into two parts:

$$H = H_1 + H_2 ,$$

where $H_j = \frac{1}{2m}p_j^2 + \frac{1}{2}m\omega^2x_j^2 = \hbar\omega \left(a_j^\dagger a_j + 1/2 \right)$ with eigenenergies $\hbar\omega \left(n_j + \frac{1}{2} \right)$ for integers $n_j \geq 0$ and $j = 1, 2$. Since $[a_j, a_k^\dagger] = \delta_{j,k}$, $[a_j, a_k] = 0$, and $[a_j^\dagger, a_k^\dagger] = 0$, we have $[H_1, H_2] = (\hbar\omega)^2 [a_1^\dagger a_1, a_2^\dagger a_2] = 0$. Hence, we can find simultaneous eigenstates of the H_j .

(b) For non-negative integers n_j , the quantum number $n = n_1 + n_2$ can take all possible non-negative integers $n = 0, 1, 2, \dots$. The eigenenergy is

$$E_n = \hbar\omega (n_1 + n_2 + 1) = \hbar\omega (n + 1) .$$

We may have $n + 1$ possible solutions for $n = n_1 + n_2$, with

$$(n_1, n_2) = (0, n), (1, n - 1), \dots, \text{ or } (n, 0) .$$

Hence the degeneracy of the level associated with quantum number n is $n + 1$.

(c) The operator $A_{jk} = a_j^\dagger a_k$ annihilates one quantum in oscillator i and creates another quantum in oscillator j . Hence the total number of quanta $n = n_1 + n_2$ is preserved and all A_{jk} commute with H . In particular, any linear combination of the A_{jk} commutes with H .

The other two hermitian combinations are $A_{12} + A_{21}$ and $i(A_{21} - A_{12})$.

(d) Expressing x_j and p_j as linear combination of a_j^\dagger and a_j , we find

$$\hbar L \equiv x_1 p_2 - x_2 p_1 = \hbar i (a_2^\dagger a_1 - a_1^\dagger a_2) = \hbar i (A_{21} - A_{12}) .$$

(e) We first use $[A, BC] = [A, B]C + B[A, C]$ to compute the commutators of A_{jk} :

$$[A_{jk}, A_{lm}] = [a_j^\dagger a_k, a_l^\dagger a_m] = [a_j^\dagger a_k, a_l^\dagger] a_m + a_l^\dagger [a_j^\dagger a_k, a_m] = \delta_{kl} a_j^\dagger a_m - \delta_{jm} a_l^\dagger a_k .$$

Defining

$$J_x = (A_{11} - A_{22})/2 , \quad J_y = (A_{12} + A_{21})/2 , \quad J_z = L/2 = i(A_{21} - A_{12})/2$$

and using the above commutation relations, we find

$$\begin{aligned}
[J_x, J_y] &= \frac{1}{4} [A_{11} - A_{22}, A_{12} + A_{21}] \\
&= \frac{1}{4} ([A_{11}, A_{12}] + [A_{11}, A_{21}] - [A_{22}, A_{12}] - [A_{22}, A_{21}]) \\
&= \frac{1}{4} (a_1^\dagger a_2 - a_2^\dagger a_1 + a_1^\dagger a_2 - a_2^\dagger a_1) = iJ_z.
\end{aligned}$$

Similarly, we can verify $[J_y, J_z] = iJ_x$ and $[J_z, J_x] = iJ_y$, which are the same as for a three-dimensional angular momentum.

(f) We can compute (no need to do that)

$$\begin{aligned}
\mathbf{J}^2 &= (J_x^2 + J_y^2 + J_z^2) \\
&= \frac{1}{4} \left[(a_1^\dagger a_1 - a_2^\dagger a_2)^2 + (a_1^\dagger a_2 + a_2^\dagger a_1)^2 + (-i)^2 (a_1^\dagger a_2 - a_2^\dagger a_1)^2 \right] \\
&= \frac{1}{4} (a_1^\dagger a_1 + a_2^\dagger a_2) (a_1^\dagger a_1 + a_2^\dagger a_2 + 2) = j(j+1),
\end{aligned}$$

where in the last step we have restricted the operator \mathbf{J}^2 to eigenstates with quantum number n for which $a_1^\dagger a_1 + a_2^\dagger a_2 = n$ and define $j = n/2$.

The degeneracy associated with quantum number j is $2j + 1 = n + 1$, which is consistent with the result from part (b).

Since for a given j the allowed values of J_z are $-j, -j + 1, \dots, j$ and $L = 2J_z$, we find that the allowed values of L for level with quantum number n are

$$L = -n, -n + 2, \dots, n.$$

(g) The symmetry group responsible for the degeneracy is the one generated by J_x, J_y, J_z , which is $\text{SO}(3)$ [isomorphic to $\text{SU}(2)$]. The $\text{SO}(2)$ generated by the physical angular momentum $L = 2J_z$ is a subgroup of the above $\text{SO}(3)$.

Problem 2: Quantum Mechanics II

(a) For real $\Omega_1 = \Omega_2 = \Omega$, the Hamiltonian can be represented by a 3×3 matrix:

$$H = \begin{pmatrix} 0 & 0 & \Omega \\ 0 & 0 & \Omega \\ \Omega & \Omega & 0 \end{pmatrix}$$

in the basis of $|g_1\rangle$, $|g_2\rangle$ and $|e\rangle$. By solving

$$\det [H - \lambda I] = -\lambda^3 + 2\lambda\Omega^2 = 0,$$

we have the eigenenergies

$$\lambda = 0, \pm\sqrt{2}\Omega.$$

The associated eigenstates are

$$|\phi_0\rangle = \frac{|g_1\rangle - |g_2\rangle}{\sqrt{2}}$$

$$|\phi_{\pm}\rangle = \frac{|g_1\rangle + |g_2\rangle}{2} \pm \frac{|e\rangle}{\sqrt{2}}.$$

We can verify that $H|\phi_0\rangle = \Omega(|e\rangle - |e\rangle) = 0$ and $H|\phi_{\pm}\rangle = \pm\sqrt{2}\Omega|\phi_{\pm}\rangle$.

(b) The initial state can be expressed in the eigenbasis of the Hamiltonian:

$$|\psi(0)\rangle = |g_1\rangle = \frac{1}{\sqrt{2}}|\phi_0\rangle + \frac{1}{2}|\phi_+\rangle + \frac{1}{2}|\phi_-\rangle.$$

With the Hamiltonian evolution, we have

$$\begin{aligned} |\psi(t)\rangle &= e^{-iHt/\hbar} |\psi(0)\rangle \\ &= \frac{1}{\sqrt{2}}|\phi_0\rangle + \frac{1}{2}e^{-i\sqrt{2}\Omega t}|\phi_+\rangle + \frac{1}{2}e^{i\sqrt{2}\Omega t}|\phi_-\rangle \\ &= \frac{1}{2}\left(1 + \cos\sqrt{2}\Omega t\right)|g_1\rangle + \frac{1}{2}\left(1 - \cos\sqrt{2}\Omega t\right)|g_2\rangle - i\frac{1}{\sqrt{2}}\sin\sqrt{2}\Omega t|e\rangle. \end{aligned}$$

For $t = T = \frac{\pi}{\sqrt{2}\Omega}$, we have $|\psi(T)\rangle = |g_2\rangle$ with all its population evolved into state $|g_2\rangle$.

(c) Method I: Similar to part (a), we can solve the 3×3 matrix and find the zero energy eigenstate.

Method II: We expand the zero-energy eigenstate as $|\phi_0\rangle = c_1|g_1\rangle + c_2|g_2\rangle + c_e|e\rangle$. For zero-energy eigenstate, we have

$$H|\phi_0\rangle = (\Omega_1 c_1 + \Omega_2 c_2)|e\rangle + \Omega_1^* c_e |g_1\rangle + \Omega_2^* c_e |g_2\rangle = 0,$$

which implies $c_e = 0$ and $\Omega_1 c_1 + \Omega_2 c_2 = 0$. Hence, we find

$$|\phi_0\rangle = \frac{1}{\sqrt{|\Omega_1|^2 + |\Omega_2|^2}} (\Omega_2 |g_1\rangle - \Omega_1 |g_2\rangle)$$

for the zero-energy eigenstate.

(d) Method I: Expand the zero-energy eigenstate as

$$|\phi\rangle = \sum_{j=1}^{n-1} c_j |g_j\rangle + c_e |e\rangle .$$

It satisfies

$$H |\phi\rangle = \left(\sum_{j=1}^{n-1} \Omega_j c_j \right) |e\rangle + c_e \sum_{j=1}^{n-1} \Omega_j^* |g_j\rangle = 0 .$$

Hence, we have $c_e = 0$ and

$$\sum_{j=1}^{n-1} \Omega_j c_j = 0 .$$

The last equation expresses the orthogonality of the vector c_j to the vector Ω_j^* in an $(n-1)$ -dimensional space. There are $(n-2)$ such orthogonal vectors, corresponding to the $n - 2$ zero-energy eigenstates.

More explicitly, we can find these eigenstates by having

$$|\phi_l\rangle = \frac{1}{\sqrt{|\Omega_l|^2 + |\Omega_{l+2}|^2}} (\Omega_{l+2} |g_l\rangle - \Omega_l |g_{l+2}\rangle)$$

for $l = 0, \dots, n - 3$. Note that part (c) is just the special case with $n = 3$.

Method II: We may rewrite the Hamiltonian as

$$\begin{aligned} \frac{H}{\hbar} &= \Omega_{tot} |e\rangle \Omega_{tot} \left(\sum_{j=1}^{n-1} \frac{\Omega_j}{\Omega_{tot}} \langle g_j| \right) + \Omega_{tot} \left(\sum_{j=1}^{n-1} \frac{\Omega_j^*}{\Omega_{tot}} |g_j\rangle \right) \langle e| \\ &= \Omega_{tot} (|e\rangle \langle \phi_B| + |\phi_B\rangle \langle e|) \end{aligned}$$

with $\Omega_{tot} = \sqrt{\sum_{j=1}^{n-2} |\Omega_j|^2}$ and normalized state $|\phi_B\rangle = \sum_{j=1}^{n-1} \frac{\Omega_j^*}{\Omega_{tot}} |g_j\rangle$. Any superposition of $\{|g_j\rangle\}_{j=1, \dots, n-1}$ orthogonal to $|\phi_B\rangle$ has zero energy. For example, we can explicitly find $n - 2$ such linearly independent zero energy eigenstates:

$$H |\phi_l\rangle = 0$$

with

$$|\phi_l\rangle = \frac{1}{\sqrt{|\Omega_l|^2 + |\Omega_{l+2}|^2}} (\Omega_{l+2} |g_l\rangle - \Omega_l |g_{l+2}\rangle),$$

for $l = 0, \dots, n - 3$, which span the $n - 2$ dimensional zero energy eigenspace.

Statistical Mechanics I

(a) In classical statistical mechanics the statistical distribution in phase space is given by $\rho(\mathbf{p}, \mathbf{x}) \propto e^{-\beta H(\mathbf{p}, \mathbf{x})}$ where $\beta = 1/kT$ and H is the Hamiltonian as a function of momenta \mathbf{p} and cartesian coordinates \mathbf{x} . Since the kinetic energy is independent of the coordinates, we can integrate over the momenta and find that the probability density is given by a Boltzmann factor

$$P(\mathbf{x}) = \int d\mathbf{p} \rho(\mathbf{p}, \mathbf{x}) \propto \int d\mathbf{p} e^{-\beta H(\mathbf{p}, \mathbf{x})} \propto e^{-\beta V(\mathbf{x})}.$$

The normalized distribution is

$$P(\mathbf{x}) = \frac{e^{-\frac{V(\mathbf{x})}{kT}}}{\int d\mathbf{x}' e^{-\frac{V(\mathbf{x}')}{kT}}}.$$

(b) In normal coordinates, the potential matrix is diagonal and the potential is given by

$$V(\mathbf{y}) = \frac{1}{2} \sum_m \lambda_m y_m^2.$$

Using the result in (a), the distribution of the normal coordinates is then given by

$$P(\mathbf{y}) \propto e^{-\frac{\sum_m \lambda_m y_m^2}{2kT}}.$$

The distribution of a normal coordinate y_m is obtained by integrating all other normal coordinates and is a Gaussian

$$P(y_m) = \left(\frac{\lambda_m}{2\pi kT} \right)^{1/2} e^{-\frac{\lambda_m y_m^2}{2kT}}.$$

(c) According to the equipartition theorem, the thermal average of each separated quadratic term in the Hamiltonian is $kT/2$. Thus

$$\left\langle \frac{1}{2} \lambda_m y_m^2 \right\rangle = \frac{kT}{2}.$$

We find

$$\langle y_m^2 \rangle = \frac{kT}{\lambda_m} = \frac{kT}{2\kappa \left[1 - \cos\left(\frac{p\pi}{N+1}\right) \right]}.$$

We can also calculate $\langle y_m^2 \rangle$ directly from the Gaussian distribution found in part (b), leading to the same result.

(d) Since $P(\mathbf{y}) = \prod_m P(y_m)$, the variables y_m are uncorrelated, i.e.,

$$\langle y_m y_n \rangle = \langle y_m \rangle \langle y_n \rangle = 0$$

for $m \neq n$.

(e) The original coordinate are related to the normal coordinates by $\mathbf{x} = \mathbf{R}^{-1}\mathbf{y}$. Since R is orthogonal and symmetric $\mathbf{R}^{-1} = \mathbf{R}^T = \mathbf{R}$ and $\mathbf{x} = \mathbf{R}\mathbf{y}$. We then have $x_n = \sum_m R_{nm}y_m$. Using the results in (c), we find

$$\langle x_n^2 \rangle = \sum_{m,k} R_{nm}R_{nk} \langle y_m y_k \rangle = \sum_m R_{nm}^2 \langle y_m^2 \rangle .$$

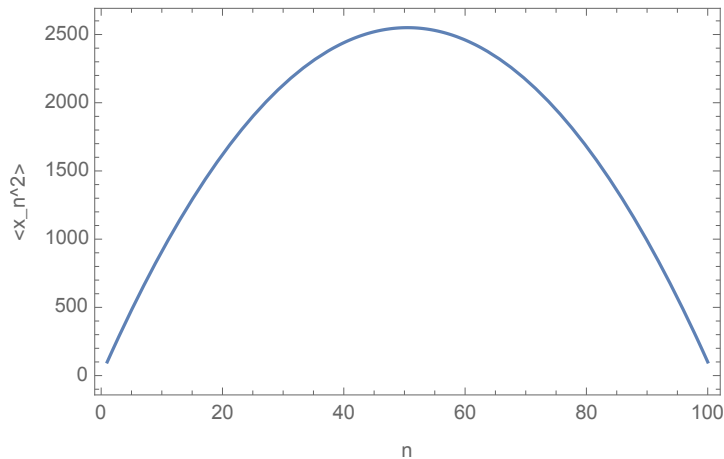
Substituting the expression for $\langle y_m^2 \rangle$ from part (b) and R_{mn} , we find

$$\langle x_n^2 \rangle = \frac{kT}{(N+1)\kappa} \sum_{m=1}^N \sin^2 \left(\frac{\pi nm}{N+1} \right) \frac{1}{1 - \cos \left(\frac{m\pi}{N+1} \right)} .$$

Using the formula for the sum given in the problem, we have

$$\langle x_n^2 \rangle = \frac{kT}{\kappa} n \left(1 - \frac{n}{N+1} \right) .$$

A sketch of $\langle x_n^2 \rangle$ versus n is shown in the figure below for $N = 100$.



Problem 4: Statistical Mechanics II

(a) The average occupation of each adsorption site is given by the Fermi-Dirac distribution $1/[e^{\beta(-\Delta-\mu)} + 1]$. Thus

$$\langle N_a \rangle = \frac{N_0}{z^{-1}e^{-\beta\Delta} + 1},$$

where $\beta = \frac{1}{kT}$ and $z = e^{\beta\mu}$ is the fugacity.

(b) Since the kinetic energy is $\frac{p^2}{2m}$, we have

$$\langle N_f \rangle = 2V \int \frac{d^3p}{(2\pi\hbar)^3} \frac{1}{z^{-1}e^{\beta p^2/2m} + 1} = \frac{2V}{(2\pi\hbar)^3} \int_0^\infty \frac{4\pi p^2 dp}{z^{-1}e^{\beta p^2/2m} + 1}.$$

For convenience in the following parts, it is useful to change variables $x = \sqrt{\frac{\beta}{2m}}p$ and obtain

$$\langle N_f \rangle = 2V \left(\frac{m}{2\pi\hbar^2}\right)^{\frac{3}{2}} (kT)^{\frac{3}{2}} \frac{4}{\sqrt{\pi}} \int_0^\infty dx \frac{x^2}{z^{-1}e^{x^2} + 1} = c(kT)^{\frac{3}{2}} f_{3/2}(z),$$

where $c = 2V \left(\frac{m}{2\pi\hbar^2}\right)^{\frac{3}{2}}$.

(c) At zero temperature, the state must be in the ground state consistent with the Pauli exclusion principle. Thus, all N_0 adsorption sites are occupied at $T = 0$ and the remaining $N - N_0$ atoms are free. Thus

$$\langle N_a \rangle = N_0, \quad \langle N_f \rangle = N - N_0.$$

The Fermi energy is the highest occupied single-particle level at $T = 0$, i.e., in the ground state. There are $N - N_0$ fermions occupying the levels in the box of volume V and

$$N - N_0 = \frac{2V}{(2\pi\hbar)^3} \int_0^{p_F} 4\pi p^2 dp = \frac{V}{3\pi^2\hbar^3} p_F^3 = \frac{V}{3\pi^2\hbar^3} (2m\epsilon_F)^{3/2}.$$

The Fermi energy is thus given by

$$\epsilon_F = 3\pi^2 \left(\frac{\hbar^2}{2m}\right) \left(\frac{N - N_0}{V}\right)^{2/3}.$$

(d) At sufficiently large T , z is small and we can approximate $f_{3/2}(z) \approx z$. Hence, $\langle N_f \rangle \approx c(kT)^{\frac{3}{2}}z$. Since $N > N_0$ some number of atoms must be free. To get a finite number of free atoms, it must be that $z \propto (kT)^{-\frac{3}{2}}$. Using this results in the probability for adsorption sites being occupied, we conclude that

$$\langle N_a \rangle \approx \frac{N_0}{\text{const}(kT)^{3/2}e^{-\beta\Delta} + 1} \rightarrow 0, \quad \langle N_f \rangle \rightarrow N$$

at large temperatures.

(e) The Fermi energy is the highest occupied level at $T = 0$. Since $N = N_0$ all atoms occupy the adsorption sites and the Fermi energy is $-\Delta$.