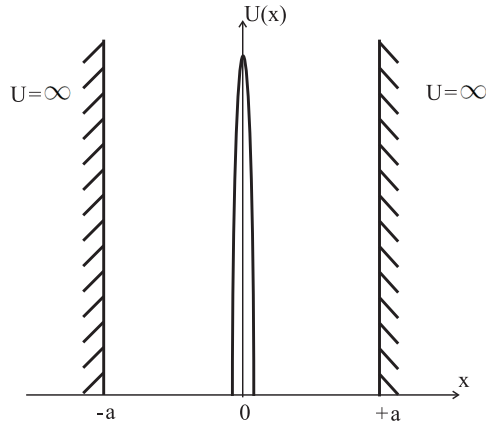**Problem II.1**

Consider a quantum particle of mass m confined within a one-dimensional infinite square-well potential in the presence of an additional repulsive delta-potential in the middle of the well:

$$U(x) = \begin{cases} \beta\,\delta(x), & \text{if } -a < x < a; \\ \infty, & \text{if } |x| > a, \end{cases} \tag{1}$$

where $\delta(x)$ is the Dirac δ-function and $\beta \geq 0$. The potential $U(x)$ is illustrated below.

(a) [**2 points**] Consider the parity (reflection) operator $\hat{P}$, whose action on an arbitrary function $\psi(x)$ is defined as follows:

$$\hat{P}\,\psi(x) = \psi(-x)\,.$$

Explain (briefly) why the eigenstates of the potential $U(x)$, given by Eq. (1), should also be eigenstates of the parity operator.

Since the potential $U(x)$ is an even function, the Hamiltonian commutes with the parity operator, and therefore both the parity and energy are good quantum numbers, which can be determined simultaneously.

(b) [**4 points**] Consider the stationary Schrödinger equation with the energy E corresponding to the potential (1). What boundary conditions must the wave function satisfy at $x = \pm a$? Also, prove that the wave function satisfies the following matching condition at $x = 0$:

$$\psi'(0^+) - \psi'(0^-) = \frac{2m\beta}{\hbar^2}\psi(0), \tag{2}$$

where the left-hand side represents the difference of the derivatives $\psi' = d\psi/dx$ taken in the limit $x \to 0$ from the positive side ($x > 0$) and from the negative side ($x < 0$).

See, for instance,
http://physicspages.com/pdf/Griffiths%20QM/Griffiths%20Problems%2002.44.pdf .
The wave functions must satisfy the boundary conditions $\psi(\pm a) = 0$.

To find the matching condition at $x = 0$, integrate the Schrödinger equation with $U(x) = \beta\,\delta(x)$ within an infinitesimally small vicinity of the point $x = 0$ and use the continuity of the wave function, $\psi(0^-) = \psi(0^+)$, and the properties of the Dirac δ-function.

1

(c) [**3 points**] Show that the odd-parity $(-)$ and even-parity $(+)$ wave function forms below both satisfy the Schrödinger equation everywhere that the potential is finite, and determine a relationship between the parameters $k_{\pm}$ and the energy E.

$$\psi_-(x) = \sin\left[k_-\, x\right] \tag{3}$$
$$\psi_+(x) = \sin\left[k_+\left(|x| - a\right)\right] \tag{4}$$

For $|x| < a$ and $x \neq 0$, the potential $U = 0$, so the wave functions must satisfy the Schrödinger equation for a free particle

$$-\frac{\hbar^2}{2m}\,\psi''(x) = E\psi(x). \tag{5}$$

Substituting (3) and (4) into (5), we find that these wave functions do satisfy the Schrödinger equation, and $E_{\pm} = \hbar^2 k_{\pm}^2/(2m)$.

(d) [**4 points**] Apply the boundary conditions formulated above to the odd-parity wave function $\psi_-(x)$ from Eq. (3) and determine the allowed values of k_- and the corresponding eigenenergies E_-. How are the eigenenergies E_- affected by the presence of the δ-function potential in the middle of the well?

Because the odd-parity states $\psi_-(x)$ vanish at $x = 0$, they always satisfy the matching condition (2) and are unaffected by the presence of the δ-function potential. The boundary condition $\psi(\pm a) = 0$ gives $k_- a = n\pi$ and

$$E_-^{(n)} = \frac{\pi^2 \hbar^2 n^2}{2ma^2}, \ \text{ with } n = 1, 2, 3, \ldots. \tag{6}$$

Eq. (6) corresponds to the energies $E = \pi^2 \hbar^2 N^2/2m(2a)^2$ for a particle in a box of the width $2a$ for the even values of $N = 2n$, which corresponds to the odd wave functions.

(e) [**4 points**] Prove that the even-parity wave function $\psi_+(x)$ from Eq. (4) is an eigenfunction of the Schrödinger equation if the wave vector k_+ satisfies the following equation:

$$\tan(k_+ a) = -\frac{k_+ a}{\xi}, \quad \text{where} \quad \xi = \frac{ma\beta}{\hbar^2}. \tag{7}$$

From Eqs. (1) and (7), determine the dimensionality of β and ξ.

Eq. (4) satisfies the boundary conditions $\psi(\pm a) = 0$ by construction.

Substituting (4) into (2), we obtain (7).

ξ is dimensionless, and β has the dimensionality of Energy*Length.

(f) [**4 points**] Examine Eq. (7) in the limit $\xi \to 0$, which corresponds to a vanishingly weak δ-function potential. Determine the allowed values of k_+ and the corresponding even-parity energy levels E_+ in this case. Compare your result with the well-known spectrum of an infinite potential well without δ-function potential $(\beta = 0)$.

2

When $\xi = 0$, Eq. (7) gives $\tan(k_+ a) = \infty$, so $k_+ a = N\pi/2$, where N is odd. The corresponding energies are

$$E_+^{(N)} = \frac{\pi^2 \hbar^2 N^2}{2m(2a)^2}, \text{ with } N = 1, 3, 5 \ldots. \tag{8}$$

Eq. (8) corresponds to the energies of a particle in a box of the width $2a$ for the odd values of N, which corresponds to the even wave functions.

(g) [**4 points**] Now consider the limit of a very strong δ-function potential: $\xi \to \infty$. Determine the allowed values of k_+ and the corresponding energy levels E_+ from Eq. (7) in this limit. How does this energy spectrum of even-parity eigenstates compare with the energy spectrum of the odd-parity eigenstates found in part (d)?

When $\xi = \infty$, Eq. (7) gives $\tan(k_+ a) = 0$, so $k_+ a = n\pi$. The corresponding energies are

$$E_+^{(n)} = \frac{\pi^2 \hbar^2 n^2}{2ma^2}, \text{ with } n = 1, 2, 3, \ldots. \tag{9}$$

The energies (9) are the same as in Eq. (6).

Problem II.2

A diatomic molecule with moment of inertia I is constrained to rotate freely in the xy plane with angular momentum L_z. The molecule has a permanent electric dipole moment $\mathcal{P}$ along the molecule axis, whose magnitude $\mathcal{P}_0$ is independent of the rotational motion or external conditions. The Hamiltonian for the quantum system is

$$\hat{H} = \frac{(\hat{L}_z)^2}{2I} . \tag{1}$$
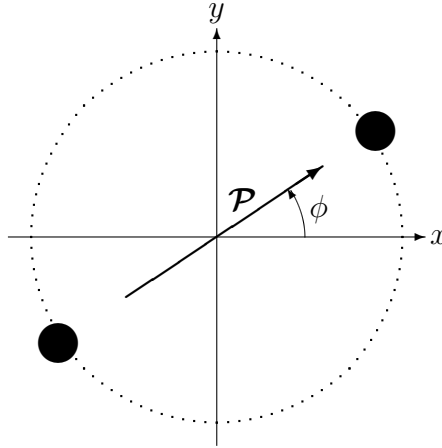
(a) [**6 points**] The orientation of the dipole moment $\mathcal{P}$ relative to the x axis is specified by the angle ϕ as shown in the figure. Write down the Hamiltonian (1) in the ϕ representation and obtain the energy eigenvalues E_n and eigenfunctions $\psi_n(\phi)$. What is the degeneracy of each eigenstate?

The $\hat{L}_z$ operator is $i\hbar\frac{\partial}{\partial\phi}$, so $\hat{H} = \frac{-\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2}$.

The time-independent Schrödinger equation is $\hat{H}\psi = E\psi$, which in this case becomes the differential equation

$$\frac{-\hbar^2}{2I}\frac{\partial^2\psi}{\partial\phi^2} = E\psi . \tag{2}$$

This is immediately recognizable as a wave equation, with solutions of the form $\psi(\phi) = Ae^{ib\phi}$, with $A = 1/\sqrt{2\pi}$ to normalize. The solutions are all the wavefunctions which are azimuthally periodic, i.e. $\psi(\phi+2\pi) = \psi(\phi)$. That implies that b must be an integer n (positive, zero, or negative). Substituting, we find that n must satisfy

$$\frac{\hbar^2 n^2}{2I} = E . \tag{3}$$

Therefore, the energy eigenvalues are

$$E_n = \frac{n^2\hbar^2}{2I} . \tag{4}$$

The $n = 0$ state (with zero energy) is not degenerate, but all other energy levels have twofold degeneracy (n and $-n$).

(b) [**5 points**] Now a weak uniform electric field $\boldsymbol{\mathcal{E}} = \mathcal{E}_0 \, \hat{e}_x$ is applied to the system along the x axis, adding a term $-\boldsymbol{\mathcal{P}} \cdot \boldsymbol{\mathcal{E}}$ to the Hamiltonian. Write down the new Hamiltonian for the system in terms of ϕ, then use perturbation theory to calculate the shifts of the energy eigenvalues to first order in $\mathcal{E}_0$. Does the perturbation lift the degeneracy to first order in $\mathcal{E}_0$?

The new Hamiltonian is

$$\hat{H} = \hat{H}_0 + V(\phi) = \frac{-\hbar^2}{2I} \frac{\partial^2}{\partial \phi^2} - \mathcal{P}_0 \mathcal{E}_0 \cos \phi \,. \tag{5}$$

The perturbation that was added to the Hamiltonian is $\Delta \hat{H} = -\mathcal{P}_0 \mathcal{E}_0 \cos \phi$. The simplest version of perturbation theory assumes that the states are not degenerate, in which case the energy shifts are given by $\Delta E_n = \langle n | \Delta \hat{H} | n \rangle$ (where the $|n\rangle$ states are the eigenstates of the unperturbed Hamiltonian). The fact that we have degenerate states here could complicate things... but it turns out it doesn't, because the matrix elements between the degenerate states are all zero:

$$\langle -n | \Delta \hat{H} | n \rangle = \int_0^{2\pi} d\phi \, \frac{1}{\sqrt{2\pi}} e^{-i(-n)\phi} \left(-\mathcal{P}_0 \mathcal{E}_0 \cos \phi \right) \frac{1}{\sqrt{2\pi}} e^{in\phi} \tag{6}$$

$$= \frac{-\mathcal{P}_0 \mathcal{E}_0}{2\pi} \int_0^{2\pi} d\phi \, e^{i2n\phi} \cos \phi = 0 \,. \tag{7}$$

Anyway, that just goes to justify that the energy shifts are given by the simple form:

$$\Delta E_n = \langle n | \Delta \hat{H} | n \rangle = \int_0^{2\pi} d\phi \, \frac{1}{\sqrt{2\pi}} e^{-in\phi} \left(-\mathcal{P}_0 \mathcal{E}_0 \cos \phi \right) \frac{1}{\sqrt{2\pi}} e^{in\phi} \tag{8}$$

$$= \frac{-\mathcal{P}_0 \mathcal{E}_0}{2\pi} \int_0^{2\pi} d\phi \, \cos \phi \quad = 0 \,. \tag{9}$$

So there are *no* energy level shifts to first order, and the degeneracy is not lifted.

(c) [**6 points**] Use perturbation theory to calculate the corresponding perturbed wave functions to first order in $\mathcal{E}_0$.

Perturbation theory tells us that the perturbed wavefunctions are given in terms of the unperturbed ones $\psi_n^{(0)}$ by

$$\psi_n = \psi_n^{(0)} + \sum_{k \neq n} \frac{\langle k | \Delta \hat{H} | n \rangle}{E_n^{(0)} - E_k^{(0)}} \, \psi_k^{(0)} \tag{10}$$

with

$$\langle k | \Delta \hat{H} | n \rangle = \int_0^{2\pi} d\phi \, \frac{1}{\sqrt{2\pi}} e^{-i(k)\phi} \left(-\mathcal{P}_0 \mathcal{E}_0 \cos \phi \right) \frac{1}{\sqrt{2\pi}} e^{in\phi} \tag{11}$$

$$= \frac{-\mathcal{P}_0 \mathcal{E}_0}{2\pi} \int_0^{2\pi} d\phi \, e^{i(n-k)\phi} \frac{e^{i\phi} + e^{-i\phi}}{2} \tag{12}$$

$$= \frac{-\mathcal{P}_0 \mathcal{E}_0}{4\pi} \int_0^{2\pi} d\phi \, \left(e^{i(n-k+1)\phi} + e^{i(n-k-1)\phi} \right) \tag{13}$$

$$= \frac{-\mathcal{P}_0 \mathcal{E}_0}{2} \left(\delta_{n-k+1} + \delta_{n-k-1} \right) \,. \tag{14}$$

In other words, this picks out two terms that give nonzero contributions, with $k = n+1$ and $k = n-1$. So the perturbed wavefunction is

$$\psi_n = \psi_n^{(0)} - \frac{-\mathcal{P}_0 \mathcal{E}_0}{2} \left[\frac{1}{E_n^{(0)} - E_{n+1}^{(0)}} \psi_{n+1}^{(0)} + \frac{1}{E_n^{(0)} - E_{n-1}^{(0)}} \psi_{n-1}^{(0)} \right]. \tag{15}$$

Those energy factors involve

$$E_n^{(0)} - E_{n+1}^{(0)} = \left(n^2 - (n+1)^2 \right) \frac{\hbar^2}{2I} = (-2n-1) \frac{\hbar^2}{2I} = -(2n+1) \frac{\hbar^2}{2I} \tag{16}$$

$$E_n^{(0)} - E_{n-1}^{(0)} = \left(n^2 - (n-1)^2 \right) \frac{\hbar^2}{2I} = (2n-1) \frac{\hbar^2}{2I} \tag{17}$$

and inserting the wavefunctions $\psi_n^{(0)} = e^{in\phi}/\sqrt{2\pi}$,

$$\psi_n = \frac{e^{in\phi}}{\sqrt{2\pi}} - \frac{\mathcal{P}_0 \mathcal{E}_0}{2} \frac{2I}{\hbar^2} \left[\frac{-1}{2n+1} \frac{e^{i(n+1)\phi}}{\sqrt{2\pi}} + \frac{1}{2n-1} \frac{e^{i(n-1)\phi}}{\sqrt{2\pi}} \right] \tag{18}$$

$$= \frac{e^{in\phi}}{\sqrt{2\pi}} \left[1 + \frac{\mathcal{P}_0 \mathcal{E}_0 I}{\hbar^2} \left(\frac{e^{i\phi}}{2n+1} - \frac{e^{-i\phi}}{2n-1} \right) \right]. \tag{19}$$

(d) **[5 points]** Evaluate the expectation value $\langle \mathcal{P}_x \rangle$ of the x component of the dipole moment operator $\mathcal{P}$ in each energy eigenstate; denote the expectation value for state ψ_n by $\langle \mathcal{P}_x \rangle_n$. From that, deduce the electric polarizability

$$\alpha_n = \langle \mathcal{P}_x \rangle_n / \mathcal{E}_0 \tag{20}$$

of each state.

The expectation value for the nth eigenstate is

$$\langle \mathcal{P}_x \rangle_n = \langle n | \mathcal{P} \cos \phi | n \rangle \tag{21}$$

$$= \int_0^{2\pi} d\phi \, \psi_n^*(\phi) \left(\mathcal{P}_0 \cos \phi \right) \psi_n(\phi) \tag{22}$$

$$= \frac{\mathcal{P}_0}{2\pi} \int_0^{2\pi} d\phi \left[1 + \frac{\mathcal{P}_0 \mathcal{E}_0 I}{\hbar^2} \left(\frac{e^{-i\phi}}{2n+1} - \frac{e^{i\phi}}{2n-1} \right) \right] \tag{23}$$

$$\times \left(\frac{e^{i\phi} + e^{-i\phi}}{2} \right) \left[1 + \frac{\mathcal{P}_0 \mathcal{E}_0 I}{\hbar^2} \left(\frac{e^{i\phi}}{2n+1} - \frac{e^{-i\phi}}{2n-1} \right) \right]. \tag{24}$$

Expanding the integrand gives us 18 terms, but only the ones without any $e^{i\phi}$ factor give a nonzero integral. There are four such terms in two identical pairs. They give:

$$\langle \mathcal{P}_x \rangle_n = \frac{\mathcal{P}_0}{2\pi} \frac{\mathcal{P}_0 \mathcal{E}_0 I}{2\hbar^2} 2\pi \left(\frac{2}{2n+1} - \frac{2}{2n-1} \right) \tag{25}$$

$$= \frac{\mathcal{P}_0^2 \mathcal{E}_0 I}{2\hbar^2} \frac{(-4)}{(2n+1)(2n-1)} \tag{26}$$

$$= \frac{-2\mathcal{P}_0^2 \mathcal{E}_0 I}{\hbar^2 \left(4n^2 - 1 \right)}. \tag{27}$$

So the polarizability is

$$\alpha_n \equiv \langle \mathcal{P}_x \rangle_n / \mathcal{E}_0 = \frac{-2\mathcal{P}_0^2 I}{\hbar^2 \left(4n^2 - 1\right)} \, . \tag{28}$$

(e) [**3 points**] Provide a physical explanation for the difference in the signs of α for the lowest energy eigenstate versus the other states. (Hint: Classically, would the dipole spend more time aligned or anti-aligned with the applied field?)

The polarizability is positive for $n = 0$ and negative for all $n \neq 0$. For the $n = 0$ state, there is no rotation so the dipole is free to align with the applied electric field. For any $n \neq 0$ state, the dipole is rotating; conservation of energy implies that it rotates faster when the potential energy is lower (aligned with the field) and slower when the potential energy is higher (anti-aligned). That means it will spend *less* time aligned with the field, so on average it will be slightly anti-aligned, which is what negative polarizability means.

Problem II.3

The differential cross-section $d\sigma/d\Omega$ for the elastic scattering of a particle of mass m from a target characterized by a potential $V(\boldsymbol{r})$ is

$$\frac{d\sigma}{d\Omega} = |f(\boldsymbol{k}, \boldsymbol{k}')|^2, \tag{1}$$

where $\hbar\boldsymbol{k}$ and $\hbar\boldsymbol{k}'$ are the incident and scattered momenta of the particle, with $|\boldsymbol{k}| = |\boldsymbol{k}'|$. In the first-order Born approximation, the scattering amplitude $f(\boldsymbol{k}, \boldsymbol{k}')$ can be written as

$$f(\boldsymbol{k}, \boldsymbol{k}') = -\frac{1}{4\pi}\frac{2m}{\hbar^2} \int d^3r \; e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} \; V(\boldsymbol{r}) \; . \tag{2}$$

The first-order Born approximation is valid if

$$\left| \frac{2m}{\hbar^2}\frac{1}{4\pi} \int d^3r \; \frac{e^{ikr}}{r} V(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \right| \ll 1 \; . \tag{3}$$

(a) **[2 points]** Show that $q \equiv |\boldsymbol{k} - \boldsymbol{k}'|$ can be written as

$$q = 2|\boldsymbol{k}|\sin(\theta/2), \tag{4}$$

where θ is the angle between $\boldsymbol{k}$ and $\boldsymbol{k}'$ (the scattering angle).

This can be shown, for instance, using the law of cosines and the trig identity $\sin^2(\theta/2) = \frac{1}{2}(1 - \cos\theta)$.

(b) **[5 points]** For a spherically symmetric potential $V(r)$, show that Eq. (2) reduces to

$$f(\theta) = -\frac{2m}{\hbar^2}\frac{1}{q} \int_0^\infty dr \, r \, V(r) \sin(qr) \tag{5}$$

expressed using the direct correspondence between q and θ.

See, for example, section 7.2 of Sakurai (Modern Quantum Mechanics), or Hitoshi Murayama's notes online at http://hitoshi.berkeley.edu/221b/scattering2.pdf .

(c) **[5 points]** Let $V(r)$ be the Yukawa potential

$$V(r) = \frac{V_0}{\mu}\frac{e^{-\mu r}}{r}. \tag{6}$$

Show that in this case, the scattering amplitude is

$$f(\theta) = \frac{2mV_0}{\hbar^2\mu}\frac{1}{q^2 + \mu^2}. \tag{7}$$

(d) [**5 points**] Recall the Coulomb potential

$$V_C(r) = \frac{ZZ'e^2}{4\pi r},$$
(8)

and the Rutherford formula for Coulomb scattering

$$\frac{d\sigma_C}{d\Omega} = \frac{4m^2 Z^2 Z'^2 e^4}{\hbar^4} \frac{1}{16\,k^4 \sin^4(\theta/2)},$$
(9)

where Ze is the electric charge of the scattered particle and $Z'e$ is the electric charge of the target. Find the appropriate limit on μ and V_0/μ such that the Yukawa potential (6) reduces to the Coulomb potential and show that the scattering amplitude (7) produces the Rutherford formula in this limit.

(e) [**4 points**] Consider the Yukawa potential (6) and very low scattering momenta such that $|\mathbf{k}| \ll \mu$. Under what condition (in terms of V_0, μ and m) is the first-order Born approximation valid?

(f) [**4 points**] Consider the Yukawa potential (6) and very high scattering momenta such that $|\mathbf{k}| \gg \mu$. Under what condition (in terms of V_0, μ, m and $|\mathbf{k}|$) is the first-order Born approximation valid?

Possibly useful:

$\int_{-1}^{1} dx \int_{0}^{\infty} e^{iar(1+x)-br} = \frac{1}{a} \log(1 - \frac{2ia}{b})$ for real and positive a and b

$\log(1+x) \approx x$ for $x \ll 1$

$\log(1+x) \approx \log(x)$ for $x \gg 1$

Problem II.4

Consider a system consisting of two particles, A and B, each of spin 1. The two particles may form a bound state, which we treat as a composite particle C. The states of the particles are represented in the basis $|j, m\rangle_{A,B,C}$, where j and m are the quantum numbers of the angular momentum and its projection on the z axis, and the index A, B, or C indicates the particle. In this problem, assume conservation of angular momentum. Consider only the spin angular momentum of the particles and ignore the orbital angular momentum and the spatial part of the wave functions.

The particles A and B are bosons. Consider two cases: (i) the particles A and B are distinguishable (i.e. different), (ii) the particles A and B are indistinguishable (i.e. identical).

(a) [**5 points**] Given that $j_A = 1$ and $j_B = 1$, what are the possible values of the angular momentum j_C of the composite particle C? Answer the question in the two cases (i) and (ii). In the latter case, discuss the symmetry of the composite wave function with respect to interchange of the particles A and B to argue that one certain j_C value is forbidden.

Given that $j_A = 1$ and $j_B = 1$, the possible values of j_C are 0, 1, and 2. This is the answer in the case (i), where the particles are distinguishable.

In the case (ii), where the particles A and B are indistinguishable bosons, the wavefunction must be symmetric with respect to interchange of the particles A and B. The permitted values of j_C in this case are 0 and 2. They have symmetric wavefunctions, whereas the wavefunction for $j_C = 1$ is antisymmetric. A way to see that mathematically is to note that in the symmetric combination

$$(|1, 1\rangle|1, -1\rangle + |1, -1\rangle|1, 1\rangle) , \tag{1}$$

referring to the Clebsch-Gordan table, the $|j_C = 1, m_C = 0 >$ amplitudes cancel to zero.

(b) [**5 points**] Suppose the Hamiltonian of the system is

$$\hat{H} = a\, (\hat{J}_{z,C})^2,$$

where $\hat{J}_{z,C} = \hat{J}_{z,A} + \hat{J}_{z,B}$ is the z component of the angular momentum operator of the composite particle C, and a is a coefficient.

What are the eigenvalues of the Hamiltonian, and what are their degeneracies? Answer the question in the two cases (i) and (ii).

The eigenvalues of the Hamiltonian are $E = a\, m_C^2$, where m_C^2 takes the values 0, 1, and 4, corresponding to $m_C = 0$, $m_C = \pm 1$, and $m_C = \pm 2$. In the case (i), taking into account the values of $j_C = 0, 1, 2$, the degeneracies of these eigenvalues are 3, 4, and 2. In the case (ii), we have $j_C = 0$ and 2, so the degeneracies of these eigenvalues are 2, 2, and 2.

(c) [**6 points**] Suppose initially one of the particles A and B is in the state $|1, 1\rangle$ and another in the state $|1, -1\rangle$. Then, these particles combine to form the particle C. What are the possible states $|j, m\rangle_C$ of the composite particle C in this case? What are the probabilities of finding the particle C in these states?

Answer the question in the two cases (i) and (ii). In the latter case, write down the properly symmetrized wavefunction of the initial state of the particles A and B.

In the case (i), the possible states $|j, m\rangle_C$ are $|2, 0\rangle$, $|1, 0\rangle$, and $|1, 0\rangle$. They all have $m_C = m_A + m_B = 0$ and different values of j_C. From the Clebsch-Gordan coefficients, the probabilities of these states are $1/6$, $1/2$, and $1/3$.

In the case (ii), the state with $j_C = 1$ is not permitted, because it is antisymmetric. So, the permitted states are $|2, 0\rangle$ and $|1, 0\rangle$ with the probabilities $1/3$ and $2/3$. The wavefunction of the initial state must be symmetric for indistinguishable bosons:

$$\frac{1}{\sqrt{2}}(|1, 1\rangle_A|1, -1\rangle_B + |1, -1\rangle_A|1, 1\rangle_B) = \sqrt{\frac{1}{3}}|2, 0\rangle + \sqrt{\frac{2}{3}}|0, 0\rangle.$$

(d) [**5 points**] Suppose the particle C is in the state $|0, 0\rangle_C$. Suppose it is a metastable state, and the particle C decays to particles A and B. Write down the wavefunction of the two-particle system $|\psi\rangle_{AB}$ in the basis of the states $|1, m_1\rangle_A|1, m_2\rangle_B$. For each case [(i) and (ii)], what are the permitted combinations of the numbers m_1 and m_2, and what are the probabilities of finding the particles A and B in these states?

$$|0, 0\rangle_C = \sqrt{\frac{1}{3}}|1, 1\rangle_A|1, -1\rangle_B - \sqrt{\frac{1}{3}}|1, 0\rangle_A|1, -0\rangle_B + \sqrt{\frac{1}{3}}|1, -1\rangle_A|1, 1\rangle_B$$

The permitted combinations of the numbers m_1 and m_2 are $(1, -1)$, $(0, 0)$, and $(-1, 1)$. Their probabilities are $1/3$, $1/3$, and $1/3$. When the particles are indistinguishable, the probability is $2/3$ for finding one particle with $m = 1$ and another with $m = -1$.

(e) [**4 points**] Considering the composite particle C from the previous part, suppose that a measurement finds the particle A in the state $|1, 1\rangle_A$. Then, what are the possible states $|1, m\rangle_B$ of the particle B? Justify your answer.

It is not possible to write the wavefunction $|\psi\rangle_{AB}$ as a product $|\psi\rangle_A|\psi\rangle_B$, so this is an entangled state. The final eigenstate has $m_C = 0$, so m_A and m_B must add up to that. If a measurement finds the particle A with $m = 1$, then $m = -1$ for the particle B with probability 1. Once the state of the particle A has been measured, the state of the particle B is completely certain.

Information about selected Clebsch-Gordan coefficients is below:

$$|1,1\rangle|1,-1\rangle = \sqrt{\frac{1}{6}}\,|2,0\rangle + \sqrt{\frac{1}{2}}\,|1,0\rangle + \sqrt{\frac{1}{3}}\,|0,0\rangle \tag{2}$$

$$|1,0\rangle|1,0\rangle = \sqrt{\frac{2}{3}}\,|2,0\rangle \qquad\qquad - \sqrt{\frac{1}{3}}\,|0,0\rangle \tag{3}$$

$$|1,-1\rangle|1,1\rangle = \sqrt{\frac{1}{6}}\,|2,0\rangle - \sqrt{\frac{1}{2}}\,|1,0\rangle + \sqrt{\frac{1}{3}}\,|0,0\rangle \tag{4}$$

$$|2,0\rangle = \sqrt{\frac{1}{6}}\,|1,1\rangle|1,-1\rangle + \sqrt{\frac{2}{3}}\,|1,0\rangle|1,0\rangle + \sqrt{\frac{1}{6}}\,|1,-1\rangle|1,1\rangle \tag{5}$$

$$|1,0\rangle = \sqrt{\frac{1}{2}}\,|1,1\rangle|1,-1\rangle \qquad\qquad - \sqrt{\frac{1}{2}}\,|1,-1\rangle|1,1\rangle \tag{6}$$

$$|0,0\rangle = \sqrt{\frac{1}{3}}\,|1,1\rangle|1,-1\rangle - \sqrt{\frac{1}{3}}\,|1,0\rangle|1,0\rangle + \sqrt{\frac{1}{3}}\,|1,-1\rangle|1,1\rangle \tag{7}$$

Problem II.5

In this problem you will compare noninteracting boson gases in three dimensions ($d = 3$) and in two dimensions ($d = 2$). Some interesting statistical properties are qualitatively different depending on the dimensionality.

For both cases ($d = 3, 2$), consider N noninteracting spinless bosons of mass m in a volume $V = L^d$. Assume periodic boundary conditions so that the single-particle energy levels are eigenstates of momentum $\hbar\mathbf{k}$ with energy $\epsilon(k) = \hbar^2 k^2/2m$. Also assume that the system size is large so that it is safe to calculate in the continuous (not discrete) limit.

(a) [**6 points**] Find the density of states as a function of energy, $\nu_d(\epsilon)$. (Hint: first calculate the total number of states with energy $\leq \epsilon$, then determine the density of states from that.)

Let $N_d(\epsilon)$ be the the number of states with energy $\leq \epsilon$ in the dimensionality-d case. The available states are uniform in $\mathbf{k}$ phase space, so

$$N_d(\epsilon) = \sum_{\epsilon(k) \leq \epsilon} = \frac{L^d}{(2\pi)^d} \int_{k \leq \sqrt{2m\epsilon/\hbar^2}} d^d k$$

The volume integral is $\frac{4\pi}{3} k_{\max}^3$ in 3 dimensions and $\pi k_{\max}^2$ in 2 dimensions, so

$$N_3(\epsilon) = \frac{L^3}{8\pi^3} \frac{4\pi}{3} \left(\frac{2m\epsilon}{\hbar^2}\right)^{3/2} = \frac{L^3 \sqrt{2m^3}}{3\pi^2 \hbar^3} \epsilon^{3/2} \tag{1}$$

$$N_2(\epsilon) = \frac{L^2}{4\pi^2} \pi \left(\frac{2m\epsilon}{\hbar^2}\right) = \frac{L^2 m}{2\pi \hbar^2} \epsilon \tag{2}$$

The density of states is the derivative: $\nu_d(\epsilon) = \frac{d}{d\epsilon} N_d(\epsilon)$. Explicitly,

$$\nu_3(\epsilon) = \frac{L^3 \sqrt{2m^3}}{2\pi^2 \hbar^3} \epsilon^{1/2} \tag{3}$$

$$\nu_2(\epsilon) = \frac{L^2 m}{2\pi \hbar^2} \tag{4}$$

(b) [**2 points**] Having found $\nu_3(\epsilon)$ and $\nu_2(\epsilon)$, what is the qualitative difference between them as $\epsilon \to 0$?

$\nu_3(\epsilon) \propto \epsilon^{1/2}$ so it goes to zero as $\epsilon \to 0$, while $\nu_2(\epsilon)$ remains constant.

(c) [**2 points**] Now assume a grand canonical ensemble with a given *average* number density of particles, $\langle N \rangle / V$. For an arbitrary d, write down an expression equating the average number density, $n \equiv \langle N \rangle / V$, to an integral that involves $\nu_d(\epsilon)$ and the Bose-Einstein distribution function

$$n_{BE}(\epsilon) = \frac{1}{e^{(\epsilon - \mu)/k_B T} - 1}, \tag{5}$$

where μ the chemical potential. (Do not try to evaluate the integral at this time.)

$$n = \frac{1}{L^d} \int_0^\infty d\epsilon \; \nu_d(\epsilon) \; n_{BE}(\epsilon) = \frac{1}{L^d} \int_0^\infty d\epsilon \; \frac{\nu_d(\epsilon)}{e^{(\epsilon-\mu)/k_B T} - 1}$$

(d) [**3 points**] We assert (without asking you to prove it here) that μ must be < 0. Assuming that the temperature is fixed, explain how you can tell from the integral that $n(\mu)$ increases as $\mu \to 0^-$.

For $\mu < 0$, the exponential term is always > 1, so the denominator of the integrand is positive for all ϵ. Increasing μ (approaching zero but still < 0) makes the exponential term smaller, so the denominator of the integrand is smaller, so the integral is larger. In other words, $n(\mu)$ increases as $\mu \to 0$.

(e) [**6 points**] For $d = 3$, show that at fixed temperature T, $n(\mu)$ increases to a finite value as $\mu \to 0^-$. Invert the relationship to obtain an expression for the critical temperature, T_c, as a function of n.

In the limit $\mu \to 0^-$,

$$n(\mu \to 0^-) = \frac{\sqrt{2m^3}}{2\pi^2 \hbar^3} \int_0^\infty d\epsilon \; \frac{\epsilon^{1/2}}{e^{\epsilon/k_B T} - 1}$$

To do this integral, define $x^2 = (\epsilon/k_B T)$, implying that $\epsilon^{1/2} = \sqrt{k_B T}\, x$ and $d\epsilon = 2k_B T x \, dx$. Then the integral becomes

$$n(\mu \to 0^-) = \frac{\sqrt{2m^3}}{2\pi^2 \hbar^3} \, 2(k_B T)^{3/2} \int_0^\infty dx \; \frac{x^2}{e^{x^2} - 1} \tag{6}$$

$$= \frac{\sqrt{2}}{\pi^2 \hbar^3} \, (mk_B T)^{3/2} \, \frac{\sqrt{\pi}}{4} \zeta(3/2) \tag{7}$$

$$= \left(\frac{mk_B T}{2\pi \hbar^2} \right)^{3/2} \zeta(3/2) \tag{8}$$

which is finite since $\zeta(3/2) \approx 2.612$.

Inverting this relationship,

$$T_c = \frac{2\pi \hbar^2}{mk_B} \left(\frac{n_c}{\zeta(3/2)} \right)^{2/3} \tag{9}$$

(f) [**2 points**] For a $d = 3$ Bose gas, what happens when $n > n_c$ for a given T, or $T < T_c$ for a given n? What is the experimental signature in the momentum distribution when the critical value is exceeded?

Bose-Einstein condensation! There is a peak in the momentum distribution around zero momentum, as the "excess" particles bunch up there.

(g) [**4 points**] For $d = 2$, prove that the integral relation for n can increase without bound as $\mu \to 0^-$. That means that there is no critical temperature in the two-dimensional Bose gas—an important qualitative difference from the three-dimensional case.

We have already established that $n(\mu)$ increases as μ increases toward zero. In the limit $\mu \to 0^-$, for $d = 2$,

$$n(\mu \to 0^-) = \frac{m}{2\pi\hbar^2} \int_0^\infty d\epsilon \, \frac{1}{e^{\epsilon/k_B T} - 1} \, .$$

We can show that the integral diverges. Let $x = (\epsilon/k_B T)$ so that the integral is

$$\int_0^\infty dx \, \frac{1}{e^x - 1}$$

times a constant. For the small-x part of the integration region, $e^x \approx 1 + x$, so the integral can be approximated as

$$\approx \int_0^{\text{small}} dx \, \frac{1}{x} + \int_{\text{small}}^\infty dx \, \frac{1}{e^x - 1} \, .$$

The first part diverges since it involves a $\ln 0$. In other words, $n(\mu)$ can become arbitrarily large as $\mu \to 0^-$.

Possibly useful:

$$\zeta(3/2) = \frac{4}{\sqrt{\pi}} \int_0^\infty dx \frac{x^2}{\exp(x^2) - 1} = 2.612...$$