



Soluton to final exam
FY2045 Quantum Mechanics I
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Problem 1 Multiple choice problems

a) The general rule when adding two spins is that the total spin quantum number can take the values

$$s = s_1 + s_2, s_1 + s_2 - 1, \dots, |s_1 - s_2|.$$

When adding more than two spins, we have to repeat this procedure. For $\frac{1}{2} + \frac{1}{2}$ we get

$$s = \frac{1}{2} + \frac{1}{2}, \frac{1}{2} - \frac{1}{2} = 1, 0.$$

For $\frac{1}{2} + \frac{1}{2} + \frac{1}{2}$,

$$s = 1 + \frac{1}{2}, 1 - \frac{1}{2}, 0 + \frac{1}{2} \Rightarrow s = \frac{3}{2}, \frac{1}{2}.$$

Adding the fourth spin, $\frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2}$, we get

$$s = \frac{3}{2} + \frac{1}{2}, \frac{3}{2} - \frac{1}{2}, \frac{1}{2} + \frac{1}{2}, \frac{1}{2} - \frac{1}{2} \Rightarrow s = 2, 1, 0.$$

Hence, alternative **E** is the correct one.

b) The dual vector of $|n\rangle$ is $\langle n|$. For a general vector $|\psi\rangle = \sum_n c_n |n\rangle$, the dual vector is given by $\langle\psi| = \sum_n c_n^* \langle n|$. In this case we therefore get

$$\langle\psi| = \frac{1}{3} [(1 - 2i)^* \langle 1| + (2i)^* \langle 2|] = \frac{1}{3} [(1 + 2i) \langle 1| - 2i \langle 2|]. \quad (1)$$

This is option **C**.

c) We require

$$1 = \langle \psi | \psi \rangle = |A|^2 [\langle 1 | - \langle 2 | + \sqrt{3} \langle 3 |] [|1\rangle - |2\rangle + \sqrt{3} |3\rangle] = |A|^2 [1 + 1 + 3] = 5|A|^2. \quad (2)$$

Choosing A real and positive, we get $A = \frac{1}{\sqrt{5}}$ — option **A** is correct.

d) The probabilities associated with each energy is $P_n = |c_n|^2$, where $c_1 = A$, $c_2 = -A$ and $c_3 = \sqrt{3}A$. Hence,

$$\langle E \rangle_\psi = |A|^2 [E_1 + E_2 + 3E_3] = \epsilon \frac{1 + 4 + 3 \cdot 9}{5} = \frac{32}{5} \epsilon. \quad (3)$$

Option **E** is the correct answer.

e) Since the total spin is non-zero, the particles cannot have spin $s = 0$, thus excluding option **A**. Moreover, since there is an even number of particles, a total spin of 1 can occur for four particles with any spin $s \geq \frac{1}{2}$, which excludes option **D**.

Since $E_{\text{tot}} = 7\epsilon < E_3$, only states with energies $E_1 = \epsilon$ and $E_2 = 4\epsilon$ can be occupied. The only way of getting 7ϵ is if three particles have energies E_1 and one has E_2 . This means the particles can be bosons, such that there is no restriction on the number of particles in each state, *or* they can be fermions with spin $s > \frac{1}{2}$, since for spin quantum number s there are $2s + 1$ possible values for the projection quantum number m . Hence, we have excluded options **B** and **C**.

This leaves only option **E** — how can we be sure the system is not in the ground state? If the particles are bosons, all could be in the state with energy E_1 , giving a ground state energy of 4ϵ . For fermions with $s > \frac{1}{2}$ we have at least 4 possible values of m , meaning that also all fermions could have energy E_1 . Since the measured energy is larger than 4ϵ , we conclude that the system is in an excited state. Hence, **E** is the correct option.

f) Since electrons are fermions, the total system state has to be antisymmetric and the electrons cannot occupy the same single-particle state. However, since electrons have two possible spin states, they can be in the same single-particle energy state if they are in the spin-singlet configuration. The states with lowest energy are therefore:

$$\begin{aligned} \psi_1(x_1)\psi_1(x_2) \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} &\Rightarrow E = 2E_1 = 2\epsilon, \\ \frac{\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1)}{\sqrt{2}} \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} &\Rightarrow E = E_1 + E_2 = 5\epsilon, \\ \frac{\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)}{\sqrt{2}} \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} &\Rightarrow E = E_1 + E_2 = 5\epsilon, \\ \frac{\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)}{\sqrt{2}} [|\uparrow\uparrow\rangle \text{ or } |\downarrow\downarrow\rangle] &\Rightarrow E = E_1 + E_2 = 5\epsilon \text{ for both.} \end{aligned}$$

Since we have four different states all with the same energy, the energies of the three states with lowest energy are $2E_1, 5E_1$ and $5E_1$, making **B** the correct option.

However: The wording of the problem is ambiguous, and it is reasonable to give the three lowest (degenerate) energies rather than the energies of the three states of the system with lowest energy. Hence, full points have also been given to those choosing option **C**.

g) Since the particles are fermions, they cannot all be in the same single-particle state. However, two particles can occupy each single-particle energy state due to the two possible spin directions. Hence, to minimize the total system energy we need to (partly) fill the three lowest energy states, which have quantum numbers $(1, 1, 1)$, $(2, 1, 1)$ and $(1, 2, 1)$. The state $(1, 1, 2)$ is not occupied since the reduced length in the z direction leads to a larger energy increase when increasing n_z compared to n_x and n_y . Hence, **B** is the correct answer.

h) With the inclusion of the magnetic field, we get the energy eigenvalues

$$\begin{aligned} E_{111,\sigma} &= \frac{17E_0}{4} - \sigma H, \\ E_{211,\sigma} = E_{121,\sigma} &= \frac{29E_0}{4} - \sigma H, \\ E_{221,\sigma} &= \frac{41E_0}{4} - \sigma H, \\ E_{112,\sigma} &= 11E_0 - \sigma H, \end{aligned}$$

ordered by their value when $H = 0$, with $E_0 \equiv \frac{\hbar^2 \pi^2}{2mL^2}$. In order for the state $(1, 1, 2)$ to be occupied, this state has to be one of the five single-particle states with lowest energy for either spin up or down. Since $E_{111,\sigma}$, $E_{211,\sigma}$, $E_{121,\sigma}$ and $E_{221,\sigma}$ always are lower than $E_{112,\sigma}$, we have to find the values of H for which $E_{112,\sigma} < E_{211,-\sigma}$:

$$\begin{aligned} 11E_0 - \sigma H &< \frac{29E_0}{4} + \sigma H \Rightarrow 2\sigma H > \frac{15E_0}{4} \\ &\Rightarrow |H| > H_c \equiv \frac{15}{8}E_0. \end{aligned}$$

Hence, **D** is the correct answer.

Problem 2 Short answer questions

a) Since $\langle H \rangle_\psi \geq E_0$, the variational method turns the estimation of the ground state energy into a minimization problem. By using trial functions (states) ψ ($|\psi\rangle$) with many free parameters, it is possible to achieve very good estimates for the ground state of a system.

b) The bra-ket $\langle a|b\rangle$ is the probability amplitude of measuring a system in state $|a\rangle$ when it is in state $|b\rangle$. $|\langle a|b\rangle|^2$ gives the probability.

c) The Fermi energy E_F is the energy of the highest filled single-particle state in a system of fermions. The Fermi momentum p_F is the corresponding momentum, the radius in momentum-space separating filled and unfilled states, related by

$$E_F = \frac{p_F^2}{2m}.$$

Problem 3 Spin in a magnetic field

a) We want to solve the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi = \hat{H} \psi. \quad (4)$$

Since $\hat{H}$ is independent of time, we try a separable solution

$$\psi = \chi e^{-iEt/\hbar}, \quad (5)$$

where χ is a spinor. Inserted into Eq. (4) we get

$$E\chi e^{-iEt/\hbar} = e^{-iEt/\hbar} \hat{H} \chi, \quad (6)$$

meaning that we are left to solve the eigenvalue equation

$$\hat{H} \chi = -\mu_B B \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \chi = E \chi. \quad (7)$$

This matrix equation is already diagonal, and we therefore directly get the eigenvalues

$$E_{\pm} = \mp \mu_B B, \quad (8)$$

with stationary eigenvectors

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (9a)$$

$$\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (9b)$$

Hence, the general solution is

$$\chi(t) = a_+ \chi_+ e^{i\mu_B B t/\hbar} + a_- \chi_- e^{-i\mu_B B t/\hbar}. \quad (10)$$

b) We begin by calculating the expectation value of the Pauli matrices:

$$\langle \sigma_x \rangle = \chi^\dagger \sigma_x \chi = \frac{1}{3} \begin{pmatrix} 1 & i\sqrt{2} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ -i\sqrt{2} \end{pmatrix} = 0, \quad (11a)$$

$$\langle \sigma_y \rangle = \chi^\dagger \sigma_y \chi = \frac{1}{3} \begin{pmatrix} 1 & i\sqrt{2} \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ -i\sqrt{2} \end{pmatrix} = -\frac{2\sqrt{2}}{3}, \quad (11b)$$

$$\langle \sigma_z \rangle = \chi^\dagger \sigma_z \chi = \frac{1}{3} \begin{pmatrix} 1 & i\sqrt{2} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ -i\sqrt{2} \end{pmatrix} = -\frac{1}{3}. \quad (11c)$$

Using $\mathbf{S} = S_x \hat{e}_x + S_y \hat{e}_y + S_z \hat{e}_z = \frac{\hbar}{2} \boldsymbol{\sigma}$, we get

$$\langle \mathbf{S} \rangle = -\frac{\hbar}{6} [2\sqrt{2} \hat{e}_y + \hat{e}_z], \quad (12)$$

meaning that the spin points mostly in the y direction at $t = 0$. For $\langle H \rangle$ we get

$$\langle H \rangle = -\mu_B B \langle \sigma_z \rangle = \frac{\mu_B B}{3}. \quad (13)$$

c) A general, time-dependent solution for the system is

$$\chi(t) = a_+ \chi_+ e^{i\mu_B B t / \hbar} + a_- \chi_- e^{-i\mu_B B t / \hbar}. \quad (14)$$

From the state at $t = 0$ we identify the coefficients

$$a_+ = \frac{1}{\sqrt{3}}, \quad (15a)$$

$$a_- = -i\sqrt{\frac{2}{3}}. \quad (15b)$$

At $t > 0$ we therefore have the state

$$\chi(t) = \frac{1}{\sqrt{3}} \left[\chi_+ e^{i\mu_B B t / \hbar} - i\sqrt{2} \chi_- e^{-i\mu_B B t / \hbar} \right] = \frac{1}{\sqrt{3}} \begin{pmatrix} e^{i\mu_B B t / \hbar} \\ -i\sqrt{2} e^{-i\mu_B B t / \hbar} \end{pmatrix}. \quad (16)$$

Problem 4 Variational principle

a) The expectation value is

$$\langle H \rangle = \frac{\langle \phi | \hat{H} | \phi \rangle}{\langle \phi | \phi \rangle} = \frac{-\frac{\hbar^2}{2m} [-2\alpha I_1(2\alpha) + \alpha^2 I_2(2\alpha)] + \gamma I_3(2\alpha)}{I_2(2\alpha)}, \quad (17)$$

where $I_n(\beta) \equiv \beta^{-n-1}n!$. Hence, we get¹

$$\langle H \rangle = \frac{-\frac{\hbar^2}{2m} \left[-2\frac{\alpha}{4\alpha^2} + \frac{2\alpha^2}{8\alpha^3} \right] + \frac{6\gamma}{16\alpha^4}}{\frac{2}{8\alpha^3}} = \frac{\hbar^2}{2m}\alpha^2 + \frac{3\gamma}{2\alpha}. \quad (18)$$

b) The trial wavefunction is a good trial function because it normalizable, is zero for $x \leq 0$ where the potential is infinite, and it goes to zero when the potential increases for large x .

c) We minimize $\langle H \rangle$ with respect to α :

$$\frac{\partial \langle H \rangle}{\partial \alpha} = \frac{\hbar^2}{m}\alpha - \frac{3\gamma}{2\alpha^2} = 0 \quad \Rightarrow \quad \alpha = \left(\frac{3\gamma m}{2\hbar^2} \right)^{1/3}, \quad (19)$$

where we only keep real and positive solutions.² Hence, the upper bound for the ground state energy is

$$\begin{aligned} E_0 \leq \langle H \rangle \Big|_{\alpha = \left(\frac{3\gamma m}{2\hbar^2} \right)^{1/3}} &= \frac{\hbar^2}{2m} \left(\frac{3\gamma m}{2\hbar^2} \right)^{2/3} + \frac{3\gamma}{2} \left(\frac{2\hbar^2}{3\gamma m} \right)^{1/3} = \left(\frac{9\hbar^2\gamma^2}{4m} \right)^{1/3} \left[\frac{1}{2} + 1 \right] \\ &\leq \frac{9}{4} \left(\frac{2\hbar^2\gamma^2}{3m} \right)^{1/3} \end{aligned} \quad (20)$$

Problem 5 3D isotropic harmonic oscillator

a) The Hamiltonian separates into three parts for each spatial direction,

$$\hat{H} = \hat{H}_x + \hat{H}_y + \hat{H}_z,$$

where $\hat{H}_i$ with $i \in \{x, y, z\}$ is the Hamiltonian for a one-dimensional harmonic oscillator. Since the Hamiltonian is separable, and $[H_i, H_j] = 0$ for $i \neq j$, the eigenvectors of $\hat{H}$ should be products of the eigenvectors of $\hat{H}_i$, namely $|n_x, n_y, n_z\rangle \equiv |n_x\rangle|n_y\rangle|n_z\rangle$, where we use n_i to label the energy eigenstate in direction i . Inserting this ansatz in to the Schrödinger equation we get

$$\begin{aligned} \hat{H}|n_x, n_y, n_z\rangle &= [\hat{H}_x|n_x\rangle]|n_y\rangle|n_z\rangle + |n_x\rangle[\hat{H}_y|n_y\rangle]|n_z\rangle + |n_x\rangle|n_y\rangle[\hat{H}_z|n_z\rangle] \\ &= \hbar\omega \left[\left(n_x + \frac{1}{2} \right) |n_x\rangle|n_y\rangle|n_z\rangle + |n_x\rangle \left(n_y + \frac{1}{2} \right) |n_y\rangle|n_z\rangle + |n_x\rangle|n_y\rangle \left(n_z + \frac{1}{2} \right) |n_z\rangle \right] \\ &= \hbar\omega \left(n_x + n_y + n_z + \frac{3}{2} \right) |n_x, n_y, n_z\rangle \equiv E_{n_x n_y n_z} |n_x, n_y, n_z\rangle, \end{aligned}$$

¹Dimensional analysis is a great way to check if this expression is reasonable. Since the argument of the exponential function has to be dimensionless, we must have $[\alpha] = \text{m}^{-1}$. Hence, the expectation values of the kinetic and potential energy should be proportional to $\hbar^2\alpha^2/m$, and γ/α , respectively. Moreover, the probability density $[\psi(x)^2] = [|A|^2 x^2] = \text{m}^{-1}$, that is $[|A|^2] = \text{m}^{-3}$. Hence, $|A|^2 \propto \alpha^{-3}$.

²Again, we could have used dimensional analysis to check if the expression for α seems reasonable.

showing that $|n_x, n_y, n_y\rangle$ indeed are energy eigenstates of the total system Hamiltonian with the energy eigenvalues given in the problem text. Since $n = 0, 1, 2, \dots$ for the 1D case, we must have $n_i = 0, 1, 2, \dots$.

b) We calculate the commutator between the Hamiltonian and $\hat{L}_z$:

$$[\hat{H}, \hat{L}_z] = \sum_i \left[\frac{\hat{p}_i^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}_i^2, \hat{x}_i \hat{p}_y - \hat{y} \hat{p}_x \right].$$

Since operators along different directions commute, the above simplifies to

$$\begin{aligned} [\hat{H}, \hat{L}_z] &= \frac{1}{2m}[\hat{p}_x^2, \hat{x}_i \hat{p}_y] + \frac{1}{2m}[\hat{p}_y^2, -\hat{y} \hat{p}_x] + \frac{m\omega^2}{2}[\hat{x}^2, -\hat{y} \hat{p}_x] + \frac{m\omega^2}{2}[\hat{y}^2, \hat{x} \hat{p}_y] \\ &= \frac{i\hbar}{m}[-\hat{p}_y \hat{p}_x + \hat{p}_x \hat{p}_y] + i\hbar m\omega^2[-\hat{y} \hat{x} + \hat{x} \hat{y}] = 0 + 0. \end{aligned}$$

The Hamiltonian is unchanged when interchanging x, y and z , meaning that we also have $[\hat{H}, \hat{L}_i] = 0$ for $i = x, y$. Therefore,

$$[\hat{H}, \hat{\mathbf{L}}^2] = \sum_i [\hat{H}, \hat{L}_i^2] = \sum_i \left\{ [\hat{H}, \hat{L}_i] \hat{L}_i + \hat{L}_i [\hat{H}, \hat{L}_i] \right\} = \sum_i (0 + 0) = 0. \quad \square$$

c) By adding and subtracting the expressions for the ladder operators, we get

$$\begin{aligned} a_j + a_j^\dagger &= \sqrt{\frac{2m\omega}{\hbar}} \hat{x}_j, \\ a_j - a_j^\dagger &= i\sqrt{\frac{2}{\hbar m\omega}} \hat{p}_j. \end{aligned}$$

Rearranging these expressions, we get

$$\hat{x}_j = \sqrt{\frac{\hbar}{2m\omega}} (a_j^\dagger + a_j), \quad (21)$$

$$\hat{p}_j = i\sqrt{\frac{\hbar m\omega}{2}} (a_j^\dagger - a_j). \quad (22)$$

Inserting into the given definition for $\hat{L}_z$, we get

$$\hat{L}_z = \frac{i\hbar}{2} \left[(a_x^\dagger + a_x)(a_y^\dagger - a_y) - (a_y^\dagger + a_y)(a_x^\dagger - a_x) \right] = i\hbar(a_x a_y^\dagger - a_x^\dagger a_y). \quad \square \quad (23)$$

Here, we have used the fact that the ladder operators in different directions commute, such that $a_x^{(\dagger)} a_y^{(\dagger)} - a_y^{(\dagger)} a_x^{(\dagger)} = 0$.

d) The energy $\frac{5}{2}\hbar\omega$ corresponds to the first excited states, meaning $|1, 0, 0\rangle$, $|0, 1, 0\rangle$ and $|0, 0, 1\rangle$. These three states are orthonormal, and it is possible to construct sets of three other orthonormal energy eigenvectors with the same energy using these as a basis:

$$|n = 1, r\rangle = c_{100}^r|1, 0, 0\rangle + c_{010}^r|0, 1, 0\rangle + c_{001}^r|0, 0, 1\rangle,$$

where r labels the three orthonormal vectors. Operating with $\hat{L}_z$, we get

$$\begin{aligned}\hat{L}_z|1, r\rangle &= i\hbar(a_x a_y^\dagger - a_x^\dagger a_y)[c_{100}|1, 0, 0\rangle + c_{010}|0, 1, 0\rangle + c_{001}|0, 0, 1\rangle] \\ &= i\hbar[c_{100}(|0, 1, 0\rangle - |0, 1, 0\rangle) + c_{010}(0 - |1, 0, 0\rangle) + c_{001}(0 + 0)] \\ &= i\hbar[c_{100}|0, 1, 0\rangle - c_{010}|1, 0, 0\rangle + 0 \cdot c_{001}|0, 0, 1\rangle],\end{aligned}$$

which we require to be equal to $\hbar m|1, r\rangle$. Hence, we get the set of equations

$$\begin{aligned}m c_{100}^r &= -i c_{010}^r, \\ m c_{010}^r &= i c_{100}^r, \\ m c_{001}^r &= 0,\end{aligned}$$

or

$$\begin{pmatrix} m & i & 0 \\ -i & m & 0 \\ 0 & 0 & m \end{pmatrix} \begin{pmatrix} c_{100}^r \\ c_{010}^r \\ c_{001}^r \end{pmatrix} = 0.$$

To find the nontrivial solutions, we require that the determinant of the above matrix is zero:

$$m(m^2 + i^2) = 0 \quad \Rightarrow \quad m = 0, \pm 1.$$

Inserting these values in the above system of equations, and requiring normalization, we find the simultaneous eigenstates of $\hat{H}$ and $\hat{L}_z$ with energy $\frac{5}{2}\hbar\omega$ and angular momentum projection quantum numbers $m = -1, 0, 1$:

$$|1, m = \pm 1\rangle = \frac{|1, 0, 0\rangle \pm i|0, 1, 0\rangle}{\sqrt{2}}, \quad \text{with } \hat{L}_z|1, m = \pm 1\rangle = \pm\hbar|1, m = \pm 1\rangle, \quad (24)$$

$$|1, m = 0\rangle = |0, 0, 1\rangle, \quad \text{with } \hat{L}_z|1, m = 0\rangle = 0 \cdot \hbar|1, m = 0\rangle. \quad (25)$$

Problem 6 Anisotropic harmonic oscillator

a) From the expression for the raising and lowering operators given in the previous problem, we find

$$\hat{z} = \sqrt{\frac{\hbar}{2m\omega}}(a_z^\dagger + a_z), \quad (26)$$

such that we get the first-order correction to the ground state

$$E_0^{(1)} = \frac{\kappa\hbar}{2m\omega}\langle 0, 0, 0|(a_z^\dagger + a_z)^2|0, 0, 0\rangle = \frac{\kappa\hbar}{2m\omega}\langle 0, 0, 0|a_z a_z^\dagger|0, 0, 0\rangle = \frac{\kappa\hbar}{2m\omega}. \quad (27)$$

b) The first excited state is three-fold degenerate, and we should generally use degenerate perturbation theory. However, in the previous problem, we saw that we could find energy eigenstates which are also eigenstates of $\hat{L}_z$ with unique eigenvalues. Since $\hat{L}_z$ commutes with the perturbation, we can use non-degenerate perturbation theory if we use these states as our unperturbed states. We then get

$$E_{1,\pm 1}^{(1)} = \frac{\kappa \hbar}{2m\omega} \langle 1, \pm 1 | (a_z^\dagger + a_z)^2 | 1, \pm 1 \rangle. \quad (28)$$

Both $|1, \pm 1\rangle$ are proportional to $|n_z = 0\rangle$, and we therefore get the same correction as for the ground state:

$$E_{1,\pm 1}^{(1)} = \frac{\kappa \hbar}{4m\omega} [\langle 1_x | \langle 0_y | \pm i \langle 0_x | \langle 1_y |] [| 1_x \rangle | 0_y \rangle \pm i | 0_x \rangle | 1_y \rangle] \langle 0_z | (a_z^\dagger + a_z)^2 | 0_z \rangle = \frac{\kappa \hbar}{2m\omega}. \quad (29)$$

For the remaining state, we find

$$\begin{aligned} E_{1,0}^{(1)} &= \frac{\kappa \hbar}{2m\omega} \langle 1, 0 | (a_z^\dagger + a_z)^2 | 1, 0 \rangle = \frac{\kappa \hbar}{2m\omega} \langle 0_x | 0_x \rangle \langle 0_y | 0_y \rangle \langle 1_z | (a_z^\dagger + a_z)^2 | 1_z \rangle \\ &= \frac{\kappa \hbar}{2m\omega} \langle 1_z | a_z^\dagger a_z + a_z a_z^\dagger | 1_z \rangle = \frac{3\kappa \hbar}{2m\omega}. \end{aligned} \quad (30)$$

The first excited states to first order in κ are therefore

$$E_{1,\pm 1} = \hbar\omega \left[\frac{5}{2} + \frac{\kappa}{2m\omega^2} \right], \quad (31)$$

$$E_{1,0} = \hbar\omega \left[\frac{5}{2} + \frac{3\kappa}{2m\omega^2} \right], \quad (32)$$

which means that the degeneracy is partially lifted for the first excited state.

Even though we used the angular momentum eigenstates in the above calculations, it would have been just as efficient to use $|1, 0, 0\rangle$, $|0, 1, 0\rangle$ and $|0, 0, 1\rangle$ directly: Since the perturbation only affects the z part of the states, matrix elements between states that have orthogonal x and y parts are zero, reducing the matrix to a diagonal matrix.

c) The exact solution can be found by rewriting the z dependent part of the Hamiltonian,

$$\hat{H}_z = \frac{\hat{p}_z^2}{2m} + \left[\frac{1}{2}m\omega^2 + \kappa \right] \hat{z}^2 \equiv \frac{\hat{p}_z^2}{2m} + \frac{1}{2}m\omega_z^2 \hat{z}^2, \quad (33)$$

where $\omega_z = \sqrt{\omega^2 + 2\kappa/m}$. This is just a harmonic oscillator with $\omega \rightarrow \omega_z$, and the eigenenergies are given by $E_{n_z} = \hbar\omega_z(n_z + \frac{1}{2})$. Hence, the exact eigenenergies of the 3D harmonic oscillator are

$$E_{n_x n_y n_z} = \hbar\omega(n_x + n_y + 1) + \hbar\omega_z \left(n_z + \frac{1}{2} \right). \quad \square \quad (34)$$

To compare with the results from perturbation theory, we expand the exact solution to first order in κ . Using

$$\omega_z \approx \omega + \frac{\kappa}{m\omega}, \quad (35)$$

we get

$$E_{n_x, n_y, n_z} \approx \hbar\omega \left(n_x + n_y + n_z + \frac{3}{2} \right) + \frac{\hbar\kappa}{m\omega} \left(n_z + \frac{1}{2} \right), \quad (36)$$

which is in perfect agreement with the results from perturbation theory to first order in κ , i.e. when κ is small.