

UNIVERSITETET I OSLO

Det matematisk-naturvitenskapelige fakultet

Exam in: FYS3110, Quantum mechanics

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Problem 1

A hermitian operator $\hat{A}$ operates on the orthonormal energy eigenkets $|1\rangle$ and $|2\rangle$ with energies E_1 and E_2 respectively in the following way

$$\hat{A}|1\rangle = |2\rangle, \quad \hat{A}|2\rangle = |1\rangle$$

1.1 (6 points) Find the eigenvalues and eigenvectors (as combinations of $|1\rangle$ and $|2\rangle$) of $\hat{A}$.

Solution: Adding and subtracting the two equations one finds

$$\hat{A}(|1\rangle + |2\rangle) = (|1\rangle + |2\rangle)$$

$$\hat{A}(|1\rangle - |2\rangle) = -(|1\rangle - |2\rangle)$$

Therefore the normalized eigenvectors and corresponding eigenvalues are

$$\frac{1}{\sqrt{2}}(|1\rangle + |2\rangle), \quad \text{eigenvalue} = +1$$
$$\frac{1}{\sqrt{2}}(|1\rangle - |2\rangle), \quad \text{eigenvalue} = -1$$

No reasoning is required here. It is enough to just write down the eigenstates and their corresponding eigenvalues. For full score the eigenvectors must be normalized.

1.2 (6 points) A measurement of $\hat{A}$ at time $t = 0$ gives as the result one of the eigenvalues of $\hat{A}$. Show that the probability of getting the *other* eigenvalue of $\hat{A}$ when measuring $|A\rangle$ again at time $t > 0$ is given by $P(t) = \sin^2[(E_2 - E_1)t/2\hbar]$.

Solution: Let us assume that the eigenvalue gotten by the first measurement is $+1$.

Then the initial state is $|+\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$. The time-evolution of this state is

$$|t\rangle = e^{-i\hat{H}t/\hbar}|+\rangle = \frac{1}{\sqrt{2}}(e^{-iE_1t/\hbar}|1\rangle + e^{-iE_2t/\hbar}|2\rangle)$$

The probability amplitude for measuring the other eigenvalue of $\hat{A}$ is

$$\begin{aligned}\langle -|t\rangle &= \frac{1}{2}(e^{-iE_1t/\hbar} - e^{-iE_2t/\hbar}) = \frac{i}{2i}e^{-i(E_1+E_2)t/2\hbar}(e^{-i(E_1-E_2)t/2\hbar} - e^{i(E_1-E_2)t/2\hbar}) \\ &= -ie^{-i(E_1+E_2)t/2\hbar}\sin\left(\frac{E_1-E_2}{2\hbar}\right)\end{aligned}$$

Thus the probability of measuring the other eigenvalue at time t is

$$P(t) = \left| -ie^{-i(E_1+E_2)t/2\hbar}\sin\left(\frac{E_1-E_2}{2\hbar}\right) \right|^2 = \sin^2\left(\frac{E_1-E_2}{2\hbar}\right), \quad q.e.d.$$

One gets exactly the same result if the initial measurement was -1 .

For full score the final expression must be convincingly explained. Partial credit will be given for the correct time-dependent state. Partial credit will also be given for a correct (intermediate) expression for the probability.

Problem 2

Two stationary spin-1 particles interact with the following Hamiltonian operator

$$\hat{H} = J \left[\frac{1}{\hbar^2} \vec{S}_1 \cdot \vec{S}_2 \right]^p.$$

J is a real non-zero constant with units of energy, and $\vec{S}_i$ is the spin operator (spin-1) of particle i , ($i \in \{1, 2\}$). p is a positive integer. Only consider the spin degrees of freedom in this problem.

2.1(6 points) Find all the energy eigenvalues of $\hat{H}$ for general p and J . For what values of J and p will the ground state have total spin zero?

Solution: Defining the total spin operator $\vec{S}_{tot} = \vec{S}_1 + \vec{S}_2$ we have the following relation

$$\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}(S_{tot}^2 - S_1^2 - S_2^2) = \frac{\hbar^2}{2}(s_{tot}(s_{tot} + 1) - 4)$$

where we have replaced S_1^2 and S_2^2 with their values $s(s+1)\hbar^2 = 2\hbar^2$ for spin-1s ($s = 1$).

The total spin $s_{tot} \in \{0, 1, 2\}$ which follows from the rules of adding angular momenta. Thus

the Hamiltonian takes the form

$$\hat{H} = J \left[\frac{1}{2} (s_{tot} (s_{tot} + 1) - 4) \right]^p$$

The energy eigenvalues are therefore

s_{tot}	E_p
0	$J(-2)^p$
1	$J(-1)^p$
2	$J(+1)^p$

From the table it follows that the ground state has $s_{tot} = 0$ if either $J > 0$ and p is odd, or $J < 0$ and p is even.

For full score, all the energy eigenvalues must be stated. And the correct condition for the ground state having spin zero.

2.2 (6 points) Show that the Hamiltonian can be written

$$\hat{H} = J \left[\frac{1}{2\hbar^2} (S_1^+ S_2^- + S_1^- S_2^+ + 2S_1^z S_2^z) \right]^p$$

where $S_i^\pm = S_i^x \pm iS_i^y$.

Solution: Inverting we see that $S_i^x = \frac{1}{2} (S_i^+ + S_i^-)$ and $S_i^y = \frac{1}{2i} (S_i^+ - S_i^-)$. Then writing out the operator scalar product, we have

$$\begin{aligned} \frac{1}{\hbar^2} (S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z) &= \frac{1}{\hbar^2} \left[\frac{1}{4} (S_1^+ + S_1^-) (S_2^+ + S_2^-) - \frac{1}{4} (S_1^+ - S_1^-) (S_2^+ - S_2^-) + S_1^z S_2^z \right] \\ &= \frac{1}{\hbar^2} \left[\frac{1}{2} (S_1^+ S_2^- + S_1^- S_2^+) + S_1^z S_2^z \right] \\ &= \frac{1}{2\hbar^2} (S_1^+ S_2^- + S_1^- S_2^+ + 2S_1^z S_2^z) \end{aligned}$$

and the only thing left to do is to multiply by J and raise the operator to the p 'th power:

$$H = J \left[\frac{1}{2\hbar^2} (S_1^+ S_2^- + S_1^- S_2^+ + 2S_1^z S_2^z) \right]^p, \quad \text{q.e.d.}$$

To get points on this "Show that" problem, one must in fact show the algebraic steps involving the ladder operators and their relation to the cartesian components of the spin

operators. No credit is given for just stating without any algebra: "It is easy to see" or similar. It is ok to do the proof "in reverse".

For spin-1 the ladder operators act on the S^z eigenstates $|m\rangle$, $m \in \{-1, 0, 1\}$ in the following way:

$$\begin{aligned} S^+|-1\rangle &= \hbar\sqrt{2}|0\rangle & S^-|-1\rangle &= |null\rangle \\ S^+|0\rangle &= \hbar\sqrt{2}|1\rangle & S^-|0\rangle &= \hbar\sqrt{2}|-1\rangle \\ S^+|1\rangle &= |null\rangle & S^-|1\rangle &= \hbar\sqrt{2}|0\rangle \end{aligned}$$

where $|null\rangle$ is the null ket with zero norm.

In the following set $p = 1$ and assume that J is such that the ground state has total spin zero.

2.3(6 points) Calculate $\hat{H}|1, -1\rangle$ and $\hat{H}|0, 0\rangle$. Here the notation $|m_1, m_2\rangle$ indicates the S_z quantum numbers (m_1 and m_2) of the two spins.

Solution: Using the expression in **2.2** we have

$$\begin{aligned} \hat{H}|1, -1\rangle &= \frac{J}{2\hbar^2} (S_1^+ S_2^- + S_1^- S_2^+ + 2S_1^z S_2^z) |1, -1\rangle \\ &= \frac{J}{2\hbar^2} \left(\underbrace{S_1^+ S_2^- |1, -1\rangle}_{|null\rangle} + \underbrace{S_1^- S_2^+ |1, -1\rangle}_{2\hbar^2|0,0\rangle} + \underbrace{2S_1^z S_2^z |1, -1\rangle}_{-2\hbar^2|1,-1\rangle} \right) \\ &= \underline{J(|0, 0\rangle - |1, -1\rangle)} \end{aligned}$$

and

$$\begin{aligned} \hat{H}|0, 0\rangle &= \frac{J}{2\hbar^2} (S_1^+ S_2^- + S_1^- S_2^+ + 2S_1^z S_2^z) |0, 0\rangle \\ &= \frac{J}{2\hbar^2} \left(\underbrace{S_1^+ S_2^- |0, 0\rangle}_{2\hbar^2|1,-1\rangle} + \underbrace{S_1^- S_2^+ |0, 0\rangle}_{2\hbar^2|-1,1\rangle} + \underbrace{2S_1^z S_2^z |0, 0\rangle}_{|null\rangle} \right) \\ &= \underline{J(|1, -1\rangle + |-1, 1\rangle)} \end{aligned}$$

For full score here the results must be correct. Partial credit will be given for partially correct results.

2.4(6 points) Use the variational method with the trial state $|\psi\rangle = \alpha|1, -1\rangle + \beta|0, 0\rangle + \alpha|-1, 1\rangle$, where α, β are real to find an upper bound on the ground state energy of $\hat{H}$. (Hint: It can help to parameterize $\alpha = \frac{1}{\sqrt{2}} \cos \theta$, and you may also need the identity $\cos^2(2\theta) = \frac{1}{1+\tan^2(2\theta)}$.)

Solution: Let us first normalize the wave function

$$1 = \langle\psi|\psi\rangle = 2\alpha^2 + \beta^2 \implies \beta^2 = 1 - 2\alpha^2$$

Using the parameterization suggested in the hint $\alpha = \frac{1}{\sqrt{2}} \cos \theta$ we see that $\beta^2 = 1 - \cos^2 \theta = \sin^2 \theta$ or $\beta = \sin \theta$. Thus the trial state is normalized when choosing $\beta = \sin \theta$. Then the trial energy is

$$\begin{aligned} E_{tr} &= \langle\psi|\hat{H}|\psi\rangle \\ &= \langle\psi|\left(\hat{H}|1, -1\rangle\alpha + \hat{H}|0, 0\rangle\beta + \hat{H}|-1, 1\rangle\alpha\right) \\ &= \langle\psi|\left(\alpha J(|0, 0\rangle - |1, -1\rangle) + \alpha J(|0, 0\rangle - |-1, 1\rangle) + \beta J(|1, -1\rangle + |-1, 1\rangle)\right) \\ &= J\langle\psi|\left(2\alpha|0, 0\rangle + (\beta - \alpha)|1, -1\rangle + (\beta - \alpha)|-1, 1\rangle\right) \\ &= 2J(\alpha\beta + (\beta - \alpha)\alpha) \\ &= 2J(2\alpha\beta - \alpha^2) \\ &= 2J\left(\sqrt{2}\cos\theta\sin\theta - \frac{1}{2}\cos^2\theta\right) \\ &= 2J\left(\frac{1}{\sqrt{2}}\sin 2\theta - \frac{1}{4}(1 + \cos 2\theta)\right) \end{aligned}$$

Differentiating w.r.t θ and equating to zero gives

$$\frac{dE_{tr}}{d\theta} = 2J\left(\sqrt{2}\cos 2\theta + \frac{1}{2}\sin 2\theta\right) = 0 \implies \tan 2\theta = -2\sqrt{2}$$

Then using $\tan 2\theta \equiv \frac{\sin 2\theta}{\cos 2\theta} = -2\sqrt{2} \implies \sin 2\theta = -2\sqrt{2}\cos 2\theta$, the minimal trial energy is

$$E_{tr,min} = 2J\left(\left(-2 - \frac{1}{4}\right)\cos 2\theta - \frac{1}{4}\right) = \frac{J}{2}(-9\cos 2\theta - 1)$$

Then finally using the identity

$$\cos^2(2\theta) = \frac{1}{1 + \tan^2(2\theta)} = \frac{1}{1 + (-2\sqrt{2})^2} = \frac{1}{9} \implies \cos 2\theta = \frac{1}{3}$$

we get

$$E_{tr,min} = \frac{J}{2} \left(-9\frac{1}{3} - 1 \right) = \underline{\underline{-2J}}$$

which is the exact ground state energy.

In fact the best trial state is the ground state. This can be seen by working out the constants α and β . First $\cos^2 \theta = (1 + \cos 2\theta)/2$ which gives $\cos^2 \theta = \frac{2}{3}$ and implies $\cos \theta = \sqrt{\frac{2}{3}}$. Then $\sin 2\theta = \tan 2\theta \cos 2\theta = \frac{-2\sqrt{2}}{3} \implies 2 \sin \theta \cos \theta = \frac{-2\sqrt{2}}{3}$. Inserting $\cos \theta = \sqrt{\frac{2}{3}}$ we get $\sin \theta = -\frac{1}{\sqrt{3}}$. Thus $\alpha = \frac{1}{\sqrt{3}}$ and $\beta = -\frac{1}{\sqrt{3}}$ and the best trial state is

$$\frac{1}{\sqrt{3}} (|1, -1\rangle - |0, 0\rangle + |-1, 1\rangle)$$

which is the exact ground state.

Up to four points are given here for the correct expression for the variational energy before minimization. Additionally up to two points are awarded for correctly minimizing the expression and obtaining the correct answer.

An extra term

$$\hat{H}_D = \frac{D}{\hbar^2} (S_1^x S_2^y - S_1^y S_2^x)$$

is added to the Hamiltonian. D is a positive real constant with units of energy.

2.5(6 points) Treat the $\hat{H}_D$ as a perturbation and use time-independent perturbation theory to calculate the first and the second order corrections in D to the ground state energy of $\hat{H}$.

Solution: Using the ladder operators, the perturbation can be written as

$$\begin{aligned} \frac{D}{\hbar^2} (S_1^x S_2^y - S_1^y S_2^x) &= \frac{D}{\hbar^2} \left(\frac{1}{4i} (S_1^+ + S_1^-) (S_2^+ - S_2^-) - \frac{1}{4i} (S_1^+ - S_1^-) (S_2^+ + S_2^-) \right) \\ &= \frac{iD}{2\hbar^2} (S_1^+ S_2^- - S_1^- S_2^+) \end{aligned}$$

The ground state of $\hat{H}$ is non-degenerate and its ground state is the state with total spin-0 as was stated in the text before problem **2.3**. Looking up the Clebsch-Gordan table we see

that the ground state of H_0 is

$$|s_{tot} = 0, m_{tot} = 0\rangle = \frac{1}{\sqrt{3}} (|1, -1\rangle - |0, 0\rangle + |-1, 1\rangle)$$

Then applying the perturbation to this state, we get

$$\begin{aligned} \frac{iD}{2\hbar^2} (S_1^+ S_2^- - S_1^- S_2^+) |s_{tot} = 0, m_{tot} = 0\rangle &= \frac{iD}{2\hbar^2} (S_1^+ S_2^- - S_1^- S_2^+) \frac{1}{\sqrt{3}} (|1, -1\rangle - |0, 0\rangle + |-1, 1\rangle) \\ &= \frac{iD}{2\sqrt{3}} \left(-\sqrt{2}|1, -1\rangle + \sqrt{2}|0, 0\rangle - \sqrt{2}|0, 0\rangle + \sqrt{2}|-1, 1\rangle \right) \\ &= -\frac{iD}{\sqrt{6}} (|1, -1\rangle - |-1, 1\rangle) \end{aligned}$$

This is orthogonal to $|s_{tot} = 0, m_{tot} = 0\rangle$, thus the first order energy correction to the ground state is 0.

To calculate the second order correction to the ground state energy, we must seek which states the perturbation couples to. From the previous calculation, it is clear that one should look for the state $|1, -1\rangle - |-1, 1\rangle$. Inspecting the Clebsch-Gordan table one sees that the only state which involves an antisymmetric combination of these two is

$$|s_{tot} = 1, m_{tot} = 0\rangle = \frac{1}{\sqrt{2}} (|1, -1\rangle - |-1, 1\rangle)$$

which lies in the energy level with energy $E = -J$. Thus the only contributing matrix element is

$$\langle s_{tot} = 1, m_{tot} = 0 | D | s_{tot} = 0, m_{tot} = 0 \rangle = -\frac{iD}{\sqrt{3}}$$

and the second order energy correction to the ground state is

$$E_0^2 = \frac{|\langle s_{tot} = 1, m_{tot} = 0 | D | s_{tot} = 0, m_{tot} = 0 \rangle|^2}{-2J - (-J)} = -\frac{D^2}{3J}$$

No credit is given for general formulae. To get points one has to *apply* the perturbation formulae to this problem. Partial credit will be given for using the Clebsch-Gordan table to find the unperturbed states, and for carrying out calculation of matrix elements. For full score both results must be correct.

Problem 3: Two operators $\hat{T}$ and $\hat{T}^\dagger$ obey the following relations:

$$\hat{T}\hat{T} = 0, \quad \hat{T}^\dagger\hat{T}^\dagger = 0, \quad \hat{T}\hat{T}^\dagger + \hat{T}^\dagger\hat{T} = 1$$

Assume that there is at least one non-zero state in the Hilbert space $\mathcal{H}$.

3.1(2 points) Show that there exists a state $|0\rangle$ such that $\hat{T}|0\rangle = |null\rangle$, where $|null\rangle$ is the null ket with zero norm.

Solution: Let us denote the non-zero state for $|\psi\rangle$. Then either $\hat{T}|\psi\rangle = |null\rangle$ or $\hat{T}|\psi\rangle \neq |null\rangle$. In the first case we can take $|\psi\rangle = |0\rangle$ and we have shown what was required. In the second case we can apply $\hat{T}$ once more: $\hat{T}\hat{T}|\psi\rangle$. Now since $\hat{T}\hat{T} = 0$ this must be the null state: $\hat{T}\hat{T}|\psi\rangle = |null\rangle$. Thus by denoting $\hat{T}|\psi\rangle = |0\rangle$ we see that also in this case there is a state $|0\rangle$ for which $\hat{T}|0\rangle = |null\rangle$.

For full credit a convincing and logical proof must be presented.

3.2(2 points) Show that $\hat{T}^\dagger|0\rangle \neq |null\rangle$ and denote $\hat{T}^\dagger|0\rangle \equiv |1\rangle$. What is $\hat{T}|1\rangle$ and $\hat{T}^\dagger|1\rangle$? Use these results to show that $\mathcal{H}$ is two-dimensional.

Solution: Apply $\hat{T}$ to $\hat{T}^\dagger|0\rangle$. We then get

$$\hat{T}\hat{T}^\dagger|0\rangle = (1 - \hat{T}^\dagger\hat{T})|0\rangle = |0\rangle \implies \hat{T}^\dagger|0\rangle \neq |null\rangle$$

as otherwise if $\hat{T}^\dagger|0\rangle = |null\rangle$ then $\hat{T}|null\rangle = |null\rangle$.

Denote $|1\rangle \equiv \hat{T}^\dagger|0\rangle$. Then

$$\begin{aligned}\hat{T}|1\rangle &= \hat{T}\hat{T}^\dagger|0\rangle = (1 - \hat{T}^\dagger\hat{T})|0\rangle = |0\rangle \\ \hat{T}^\dagger|1\rangle &= \hat{T}^\dagger\hat{T}^\dagger|0\rangle = |null\rangle\end{aligned}$$

Summarizing

$$\begin{aligned}\hat{T}|0\rangle &= |null\rangle, & \hat{T}^\dagger|0\rangle &= |1\rangle \\ \hat{T}|1\rangle &= |0\rangle, & \hat{T}^\dagger|1\rangle &= |null\rangle\end{aligned}$$

Thus we see that no other states than $|0\rangle$ and $|1\rangle$ are generated from applying products of operators $\hat{T}$ and $\hat{T}^\dagger$ on $\mathcal{H}$. The Hilbert space is therefore two dimensional as any state can be written as a linear combination of the *two* states $|0\rangle$ and $|1\rangle$.

For full credit all four questions must be answered in a convincing way.

3.3(2 points) Find the eigenvalues and eigenstates of the Hamiltonian $\hat{H} = g \left(\hat{T}^\dagger \hat{T} - \hat{T} \hat{T}^\dagger \right)$, where g has units of energy.

Solution: Using the relation $\hat{T} \hat{T}^\dagger + \hat{T}^\dagger \hat{T} = 1$ we can rewrite the Hamiltonian

$$\hat{H} = g \left(\hat{T}^\dagger \hat{T} - \hat{T} \hat{T}^\dagger \right) = 2g \hat{T}^\dagger \hat{T} - g.$$

Thus we only need to figure out the eigenvalues and eigenvectors of $\hat{T}^\dagger \hat{T}$. Let us write down the eigenvalue equation with a general eigenvector described by constants α and β and an eigenvalue λ :

$$\hat{T}^\dagger \hat{T} (\alpha|0\rangle + \beta|1\rangle) = \lambda (\alpha|0\rangle + \beta|1\rangle)$$

Evaluating the left hand side we find

$$\beta|1\rangle = \lambda (\alpha|0\rangle + \beta|1\rangle) \implies \beta (1 - \lambda) |1\rangle = \lambda \alpha |0\rangle$$

This equation has solutions: $\lambda = 0, \alpha = 1, \beta = 0$, and $\lambda = 1, \alpha = 0, \beta = 1$. Thus the eigenvalues and eigenvectors of $\hat{T}^\dagger \hat{T}$ are

$$|0\rangle, \quad \text{with eigenvalue} = 0 \quad \& \quad |1\rangle, \quad \text{with eigenvalue} = 1.$$

Finally this gives the following eigenvectors and eigenvalues of $\hat{H}$

$$\underline{|0\rangle, \quad \text{with eigenvalue} = -g,} \quad \& \quad \underline{|1\rangle, \quad \text{with eigenvalue} = 2g - g = g}$$

Since $|0\rangle$ and $|1\rangle$ are in fact eigenfunctions of $\hat{H}$, one will also obtain full score on this subproblem by just applying $\hat{H}$ first to $|0\rangle$ and then to $|1\rangle$ and read off the corresponding eigenvalues.

Problem 4:

A particle with charge q and mass m is in a three dimensional box with length L , depth L , and height L_z . The length and depth are much larger than the height, $L \gg L_z$. You can treat the potential outside the box as being infinite.

The wavefunctions of this system are labelled by the quantum numbers n_x, n_y and

n_z , and are

$$\psi_{n_x, n_y, n_z}(x, y, z) = \sqrt{\frac{8}{L^2 L_z}} \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right) \sin\left(\frac{n_z \pi}{L_z} z\right).$$

4.1(6 points)

Find the energy eigenvalues for this particle-in-a-box system and state the allowed values of n_x , n_y and n_z .

Solution: Since the eigenstates are given, the task is to write down the correct Hamiltonian and let it act on the eigenstates to produce the eigenvalues. The Hamiltonian of this particle-in-a-box system is

$$H = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(x, y, z)$$

where V is 0 inside the box and infinity outside. Performing the derivatives, we find that the eigenvalues are

$$E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{L^2} + \frac{n_y^2}{L^2} + \frac{n_z^2}{L_z^2} \right), \quad n_x, n_y, n_z \in \{1, 2, \dots\}$$

The n 's are positive integers. None of them can be 0 as then the state is the zero state. Neither can any one of them be negative, because that eigenstate is just a phase factor (minus sign) different from the same state with positive n , and is therefore the same state.

No deep reasoning is required in this problem. Full score is given for the correct energy eigenvalues and range of ns . Partial credit is given for partially correct answers.

A time-dependent electric field with a tunable frequency ω is imposed on the box. The electric field is linearly polarized and has an amplitude E_0 and an adjustable polarization direction $\vec{d}$ (of unit length) that lies in the xy -plane.

Define the reflection operator R as

$$Rf(x, y, z) = f(L - x, L - y, L_z - z)$$

4.2(6 points) Show that electric dipole transitions between energy eigenstates with equal eigenvalues of R are forbidden. Find the frequencies of these forbidden transitions in the

interval $[0, \frac{\hbar^2 \pi^2}{2mL_z^2 \hbar}]$.

Solution: The electric dipole transition element is $-qE\vec{d} \cdot \langle f|\vec{r}|i\rangle$. Let us also assume that the energy eigenfunctions are eigenstates of R (they are!), and write

$$R\psi_f(x, y, z) = \psi_f(L - x, L - y, L_z - z) = \lambda_f \psi_f(x, y, z)$$

R is hermitian and $R^2 = 1$ which also implies $R^{-1} = R$, thus the eigenvalues λ of R are ± 1 .

To prove that R is hermitian consider the following

$$\begin{aligned} \langle a|R^\dagger|b\rangle &= \langle b|R|a\rangle^* = \left[\int dxdydz b^*(x, y, z) Ra(x, y, z) \right]^* \\ &= \int dxdydz a^*(L - x, L - y, L_z - z) b(x, y, z) = \int dxdydz a^*(x, y, z) b(L_x - x, L - y, L - z) \\ &= \langle a|R|b\rangle \implies R^\dagger = R \end{aligned}$$

Consider the matrix elements of the cartesian coordinates

$$\langle f|RxR|i\rangle = \langle f|(L - x)|i\rangle = L\langle f|i\rangle - \langle f|x|i\rangle = -\langle f|x|i\rangle$$

where we used $RxR = L - x$ which is a consequence of $Rx = (L - x)R$. On the other hand the same matrix element is

$$\langle f|RxR|i\rangle = \lambda_f \lambda_i \langle f|x|i\rangle$$

Setting them equal leads to

$$\underline{(\lambda_f \lambda_i + 1) \langle f|x|i\rangle = 0}$$

where λ_f, λ_i are the R eigenvalues of $|f\rangle$ and $|i\rangle$ respectively. Thus the matrix element $\langle f|x|i\rangle$ will be zero if $\lambda_f = \lambda_i$. The same holds for the matrix elements $\langle f|y|i\rangle$ and $\langle f|z|i\rangle$. Here the polarization vector lies in the xy -plane, so only the matrix element that involves x and y enter the transition probabilities. This concludes the proof.

The action of the operator R on ψ_{n_x, n_y, n_z} is

$$\begin{aligned} R\psi_{n_x, n_y, n_z}(x, y, z) &= \sqrt{\frac{8}{L_x L^2}} \sin\left(n_x \pi - \frac{n_x \pi}{L} x\right) \sin\left(n_y \pi - \frac{n_y \pi}{L} y\right) \sin\left(n_z \pi - \frac{n_z \pi}{L_z} z\right) \\ &= -\cos(n_x \pi) \cos(n_y \pi) \cos(n_z \pi) \sqrt{\frac{8}{L_z L^2}} \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right) \sin\left(\frac{n_z \pi}{L_z} z\right) \\ &= -\cos(n_x \pi) \cos(n_y \pi) \cos(n_z \pi) \psi_{n_x, n_y, n_z}(x, y, z) \end{aligned}$$

Thus the eigenvalue

$$\lambda_{n_x, n_y, n_z} = -\cos(n_x \pi) \cos(n_y \pi) \cos(n_z \pi)$$

The ground state energy is

$$E_{1,1,1} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{1}{L_z^2} + \frac{2}{L^2} \right)$$

increasing n_z will lead to energy increases in multiples of $\frac{\hbar^2 \pi^2}{2m L_z^2}$. Thus to keep the excitation energies lower than $\frac{\hbar^2 \pi^2}{2m L_z^2}$ above the ground state, the quantum number n_z must be one.

Thus the states in the low-energy interval $[0, \frac{\hbar^2 \pi^2}{2m L_z^2 \hbar})$ above the ground state are

$$\begin{aligned} \psi_{n_x, n_y, 1}(x, y, z) &= \sqrt{\frac{8}{L_x L^2}} \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right) \sin\left(\frac{\pi}{L_z} z\right) \\ E_{n_x, n_y, 1} &= \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2 + n_y^2}{L^2} + \frac{1}{L_z^2} \right), \quad n_x, n_y \in \{1, 2, \dots\} \\ \lambda_{n_x, n_y, 1} &= \cos n_x \pi \cos n_y \pi \end{aligned}$$

The ground state is an eigenstate of R with eigenvalue $\lambda_i = \lambda_{1,1,1} = -\cos^3(\pi) = +1$. As shown above electric dipole transitions are forbidden if the excited state also has $\lambda_f = +1$. In the energy interval $[0, \frac{\hbar^2 \pi^2}{2m L_z^2})$ this corresponds to states with n_x, n_y both odd, or both even. The forbidden electric dipole transitions in the sought low-energy interval have therefore frequencies

$$\hbar \omega_{n_x, n_y, 1} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2 + n_y^2 - 2}{L^2} \right), \quad n_x, n_y \text{ both even or both odd.}$$

Up to four points are given for the proof. Up to two points are given for obtaining the correct forbidden frequencies in a convincing way.

—— THE END ——