

Quantum Mechanics I

Week 12 (Solutions)

Spring Semester 2025

1 The Action of the Angular Momentum Operator in Position Representation

Find the action of the z -component of the angular momentum on a ket state $|\alpha\rangle$ in the position representation, i.e.

$$\langle \mathbf{x}' | L_z | \alpha \rangle = -i\hbar \frac{\partial}{\partial \phi} \langle \mathbf{x}' | \alpha \rangle. \quad (1.1)$$

Hint: Use the standard spherical-coordinate transformation

$$x' = r \cos \phi \sin \theta, \quad y' = r \sin \phi \sin \theta, \quad z' = r \cos \theta.$$

We are interested in computing the matrix element $\langle \mathbf{x}' | L_z | \alpha \rangle$. The angular momentum is defined as $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ and its components are given by $L_i = \epsilon_{ijk} r_j p_k$. The z -component is given by $L_z = x p_y - y p_x$. Thus, we have:

$$\begin{aligned} \langle \mathbf{x}' | \hat{L}_z | \alpha \rangle &= \langle \mathbf{x}' | (x p_y - y p_x) | \alpha \rangle \\ &= x' \left[-i\hbar \frac{\partial}{\partial y'} \langle \mathbf{x}' | \alpha \rangle \right] - y' \left[-i\hbar \frac{\partial}{\partial x'} \langle \mathbf{x}' | \alpha \rangle \right]. \end{aligned}$$

To proceed, we first express the derivatives in spherical coordinates using the chain rule:

$$\frac{\partial}{\partial x'} = \frac{\partial r}{\partial x'} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x'} \frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial x'} \frac{\partial}{\partial \phi}, \quad \frac{\partial}{\partial y'} = \frac{\partial r}{\partial y'} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial y'} \frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial y'} \frac{\partial}{\partial \phi}. \quad (1.2)$$

Using the hint provided in the instruction, we can determine the derivatives of the spherical coordinates with respect to the cartesian ones. We thus find:

$$\begin{aligned} \langle \mathbf{x}' | \hat{L}_z | \alpha \rangle &= -i\hbar \left[r \cos \phi \sin \theta \left(\sin \phi \sin \theta \frac{\partial}{\partial r} \right) - r \sin \phi \sin \theta \left(\cos \phi \sin \theta \frac{\partial}{\partial r} \right) \right] \langle \mathbf{x}' | \alpha \rangle \\ &\quad - i\hbar \left[r \cos \phi \sin \theta \left(-\frac{\sin \phi \cos \theta}{r} \frac{\partial}{\partial \theta} \right) - r \sin \phi \sin \theta \left(-\frac{\cos \phi \cos \theta}{r} \frac{\partial}{\partial \theta} \right) \right] \langle \mathbf{x}' | \alpha \rangle \\ &\quad - i\hbar \left[r \cos \phi \sin \theta \left(\frac{\cos \phi \csc \theta}{r} \frac{\partial}{\partial \phi} \right) - r \sin \phi \sin \theta \left(-\frac{\sin \phi \csc \theta}{r} \frac{\partial}{\partial \phi} \right) \right] \langle \mathbf{x}' | \alpha \rangle \\ &= -i\hbar \sin \theta \csc \theta \frac{\partial}{\partial \phi} \langle \mathbf{x}' | \alpha \rangle \\ &= -i\hbar \frac{\partial}{\partial \phi} \langle \mathbf{x}' | \alpha \rangle, \end{aligned}$$

and thus yield the final result.

2 Rotations about the z -axis

Let $\hat{\mathbf{L}} = (\hat{L}_x, \hat{L}_y, \hat{L}_z)$ be the angular-momentum operator of a particle. In the position representation, written in spherical coordinates (r, θ, ϕ) , we have

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}. \quad (2.1)$$

Let

$$\hat{D}_z(\alpha) = e^{-i\alpha \hat{L}_z / \hbar} \quad (2.2)$$

be the rotation operator for an angle α about the z -axis, acting in the Hilbert space of the particle.

(a) Let $\psi'(r, \theta, \phi) = \hat{D}_z(\alpha)\psi(r, \theta, \phi)$ be the wave-function obtained by applying $\hat{D}_z(\alpha)$ to an arbitrary state $\psi(r, \theta, \phi)$. Show that

$$\psi'(r, \theta, \phi) = \psi(r, \theta, \phi - \alpha). \quad (2.3)$$

where the prime corresponds to the rotated state.

We expand the exponential of the rotation operator in its Taylor series,

$$\begin{aligned} \psi'(r, \theta, \phi) &= D_z(\alpha)\psi(r, \theta, \phi) \\ &= e^{-i\alpha \hat{L}_z / \hbar} \psi(r, \theta, \phi) \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i\alpha}{\hbar} \right)^n \hat{L}_z^n \psi(r, \theta, \phi) \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} (-\alpha)^n \partial_{\phi}^n \psi(r, \theta, \phi) \\ &= \psi(r, \theta, \phi - \alpha), \end{aligned}$$

where in the last step we used the Taylor expansion of $\psi(r, \theta, \phi - \alpha)$ with respect to $\alpha = 0$.

(b) Express $\psi'(x, y, z)$ as a function of $\psi(x, y, z)$ and α .

We explicitly write the dependence of (r, θ, ϕ) as a function of (x, y, z) :

$$\begin{aligned} \tilde{\psi}(x(r, \theta, \phi), y(r, \theta, \phi), z(r, \theta, \phi)) &= \psi(x(r, \theta, \phi - \alpha), y(r, \theta, \phi - \alpha), z(r, \theta, \phi - \alpha)) \\ &= \psi(r \sin \theta \cos(\phi - \alpha), r \sin \theta \sin(\phi - \alpha), r \cos \theta) \\ &= \psi(r \sin \theta \cos \phi \cos \alpha + r \sin \theta \sin \phi \sin \alpha, r \sin \theta \sin \phi \cos \alpha - r \sin \theta \cos \phi \sin \alpha, r \cos \theta) \\ &= \psi(x \cos \alpha + y \sin \alpha, y \cos \alpha - x \sin \alpha, z). \end{aligned}$$

We have used the trigonometric identity $\cos(\alpha - \beta) = \cos \alpha \cos \beta + \sin \alpha \sin \beta$ and $\sin(\alpha - \beta) = \sin \alpha \cos \beta - \cos \alpha \sin \beta$. We remark that the result corresponds to the function ψ at coordinates rotated by an angle $-\alpha$ around the z -axis.

(c) Consider the three states described by the wave functions

$$\psi_x(\mathbf{r}) = x f(r), \psi_y(\mathbf{r}) = y f(r), \psi_z(\mathbf{r}) = z f(r), \quad (2.4)$$

where $f(r)$ vanishes for $r \rightarrow +\infty$ so that the states are normalisable. These three states are mutually orthogonal and thus form a basis of a subspace \mathcal{H}_1 of dimension 3 of the Hilbert space \mathcal{H} . Show that each $\psi_j(\mathbf{r})$ is an eigenstate of \hat{L}_j ($j = x, y, z$) and calculate the corresponding eigenvalues. *Hint: You may use $[\hat{L}_j, \hat{r}_k] = i\hbar \epsilon_{jkl} \hat{r}_l$.*

We will use the commutation relation for angular momentum and position as provided in the instruction. For the x components of angular momentum and position, the commutator is zero, i.e. $[\hat{L}_x, \hat{x}] = 0$. We can use this, together with the property of the position operator in the position representation, in the following way:

$$\begin{aligned} \hat{L}_x \psi_l(r) &= L_x x f(r) \\ &= \hat{L}_x \hat{x} f(r) \\ &= \hat{x} \hat{L}_x f(r) \\ &= x \hat{L}_x f(r) \\ &= x(\hat{y} \hat{p}_z - \hat{z} \hat{p}_y) f(r) \\ &= -i\hbar x(y \partial_z - z \partial_y) f(r) \\ &= -i\hbar x \left(y \frac{\partial r}{\partial z} - z \frac{\partial r}{\partial y} \right) \frac{\partial f(r)}{\partial r} \\ &= -i\hbar x \left(\frac{yz}{r} - \frac{zy}{r} \right) \frac{\partial f(r)}{\partial r} = 0. \end{aligned}$$

and we have used the fact that $r = \sqrt{x^2 + y^2 + z^2}$. The function $\psi_x(\mathbf{r})$ is therefore an eigenfunction of the operator L^x with eigenvalue zero. Analogously, we calculate $\hat{L}_y \psi_y(\mathbf{r})$ and $\hat{L}_z \psi_z(\mathbf{r})$ and find again zero-eigenvalues, respectively.

(d) Using the result of part (b), show that \mathcal{H}_1 is invariant under the action of $\hat{D}_z(\alpha)$. Express the matrix associated with $\hat{D}_z(\alpha)$ in the basis $\{\psi_x, \psi_y, \psi_z\}$.

We can use the general result obtained from part (a). For $\psi_x(\mathbf{r})$, we obtain:

$$\begin{aligned} \hat{D}_z(\alpha) \psi_x(\mathbf{r}) &= \hat{D}_z(\alpha) x f(r) \\ &= (x \cos \alpha + y \sin \alpha) f(r) \\ &= \psi_x(r) \cos \alpha + \psi_y(r) \sin \alpha. \end{aligned}$$

Likewise, for $\psi_y(\mathbf{r})$

$$\begin{aligned} \hat{D}_z(\alpha) \psi_y(\mathbf{r}) &= \hat{D}_z(\alpha) y f(r) \\ &= (y \cos \alpha - x \sin \alpha) f(r) \\ &= \psi_y(r) \cos \alpha - \psi_x(r) \sin \alpha, \end{aligned}$$

and $\psi_z(\mathbf{r})$:

$$\hat{D}_z(\alpha) \psi_z(\mathbf{r}) = \hat{D}_z(\alpha) z f(r) = \psi_z(r). \quad (2.5)$$

We see that the application of $\hat{D}_z(\alpha)$ to the three functions always gives linear combinations of the same three functions, which shows that the subspace \mathcal{H}_1 is indeed invariant under the action of $\hat{D}_z(\alpha)$. The expressions we have just obtained also define the matrix form of $\hat{D}_z(\alpha)$:

$$\hat{D}_z(\alpha) = \begin{pmatrix} \cos \alpha & \sin \alpha & 0 \\ -\sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (2.6)$$

3 Angular Momenta and Uncertainty

The commutator relations for the angular momenta

$$[L_i, L_j] = i\hbar\varepsilon_{ijk}L_k \quad (3.1)$$

imply an important set of uncertainty relations among the angular momenta, namely:

$$\Delta L_x \Delta L_y \geq \frac{\hbar}{2} |\langle \hat{L}_z \rangle|, \quad \Delta L_y \Delta L_z \geq \frac{\hbar}{2} |\langle \hat{L}_x \rangle|, \quad \Delta L_z \Delta L_x \geq \frac{\hbar}{2} |\langle \hat{L}_y \rangle|. \quad (3.2)$$

Now consider a particle in a normalized eigenstate of \hat{L}^2 and \hat{L}_z .

(a) Show that in this case the expectation values of the x and y components of the angular momentum are zero, i.e. $\langle L_x \rangle = \langle L_y \rangle = 0$.

We use the ladder operators L_{\pm} to show this. The x and y components can be expressed in terms of ladder operators:

$$L_x = \frac{1}{2} [L_+ + L_-], \quad L_y = \frac{1}{2i} [L_+ - L_-]. \quad (3.3)$$

First, for the x component, we have:

$$\begin{aligned} \langle L_x \rangle &= \frac{1}{2} [\langle l, m | L_+ | l, m \rangle + \langle l, m | L_- | l, m \rangle] \\ &\sim \langle l, m | l, m + 1 \rangle + \langle l, m | l, m - 1 \rangle \\ &= 0. \end{aligned}$$

due to the orthogonality condition of the eigenstates $|l, m\rangle$. Similarly, for the y component, we have:

$$\begin{aligned} \langle L_y \rangle &= \frac{1}{2i} [\langle l, m | L_+ | l, m \rangle - \langle l, m | L_- | l, m \rangle] \\ &\sim \langle l, m | l, m + 1 \rangle - \langle l, m | l, m - 1 \rangle \\ &= 0, \end{aligned}$$

and we used again the orthogonality condition of $|l, m\rangle$.

(b) Show that

$$\langle L_y^2 \rangle = \langle L_x^2 \rangle = \frac{\hbar^2}{2} [l(l+1) - m^2]. \quad (3.4)$$

We express the operator \hat{L}_x^2 as

$$\hat{L}_x^2 = \frac{1}{2}(\hat{L}_+ + \hat{L}_-)(\hat{L}_+ + \hat{L}_-) = \frac{1}{4}(\hat{L}_+^2 + \hat{L}_- \hat{L}_+ + \hat{L}_+ \hat{L}_- + \hat{L}_-^2). \quad (3.5)$$

The first and last terms are of no consequence because when we “sandwich” them between $|l, m\rangle$ to find the expectation value we get zero due to the orthonormality of $|l, m\rangle$. Thus, we are left with

$$\langle l, m | L_x^2 | l, m \rangle = \frac{1}{4} [\langle l, m | L_- L_+ | l, m \rangle + \langle l, m | L_+ L_- | l, m \rangle]. \quad (3.6)$$

We can deal with what is left by doing a little commutator algebra:

$$\begin{aligned} \hat{L}_\pm \hat{L}_\mp &= (\hat{L}_x \pm i\hat{L}_y)(\hat{L}_x \mp i\hat{L}_y) \\ &= \hat{L}_x^2 + \hat{L}_y^2 \pm i\hat{L}_y \hat{L}_x \mp i\hat{L}_x \hat{L}_y \\ &= \hat{L}^2 - \hat{L}_z^2 \pm i[\hat{L}_x, \hat{L}_y] \\ &= \hat{L}^2 - \hat{L}_z^2 \pm \hbar \hat{L}_z, \end{aligned}$$

where in the last equality we used the fact that $[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$. Thus, we have:

$$\langle l, m | L_\pm L_\mp | l, m \rangle = \hbar^2 l(l+1) - \hbar^2 m^2 \pm \hbar^2 m. \quad (3.7)$$

Putting everything together, we get

$$\langle \hat{L}_x^2 \rangle = \frac{\hbar^2}{2} [l(l+1) - m^2]. \quad (3.8)$$

By a very similar treatment, we can also compute $\langle \hat{L}_y^2 \rangle$ and verify that $\langle \hat{L}_x^2 \rangle = \langle \hat{L}_y^2 \rangle$.

(c) Using your results, verify the first uncertainty relation above. Can the uncertainty in any two components of \vec{L} ever vanish simultaneously?

Since $\langle \hat{L}_x \rangle = 0$, we have

$$\Delta L_x = \sqrt{\langle \hat{L}_x^2 \rangle - \langle \hat{L}_x \rangle^2} = \sqrt{\langle \hat{L}_x^2 \rangle} = \frac{\hbar}{\sqrt{2}} \sqrt{l(l+1) - m^2}. \quad (3.9)$$

and similarly for ΔL_y . The left-hand side of the proposed uncertainty relation thus reads

$$\Delta L_x \Delta L_y = \frac{\hbar^2}{2} [l(l+1) - m^2]. \quad (3.10)$$

For a fixed l , this quantity is minimized when m is as large as possible, i.e. when $m = l$. In such a situation we obtain $\Delta L_x \Delta L_y = l\hbar^2/2$. As for the right-hand side, we have

$$\frac{\hbar}{2} \langle \hat{L}_z \rangle = \frac{m\hbar^2}{2}. \quad (3.11)$$

This side is maximized precisely when the other side is minimized ($m = l$), giving $\frac{\hbar}{2}\langle\hat{L}_z\rangle = l\hbar^2/2$. In that case the two sides are equal; for all other cases ($m < l$) the left-hand side is greater. We can therefore conclude

$$\Delta L_x \Delta L_y \geq \frac{\hbar}{2} \langle\hat{L}_z\rangle. \quad (3.12)$$

It is possible for all components of angular momentum to vanish simultaneously. If a particle is in an eigenstate with $l = m = 0$, then from the relationships proved above we have $\langle\hat{L}_x^2\rangle = \langle\hat{L}_y^2\rangle = \langle\hat{L}_z^2\rangle = 0$ as well as $\langle\hat{L}_x\rangle = \langle\hat{L}_y\rangle = \langle\hat{L}_z\rangle = 0$; consequently $\Delta L_x = \Delta L_y = \Delta L_z = 0$.

4 The Quantum Rigid Rotator

A. Consider a spherically symmetric rigid rotor with moment of inertia $I_x = I_y = I_z = I$. For example, it might help to imagine a person curled up into a compact and uniform sphere and set spinning. Classically, its energy is given by,

$$E = \frac{L^2}{2I}. \quad (4.1)$$

(a) What are the energy eigenstates and eigenvalues for the quantum analog?

The Hamiltonian of the system is simply

$$\hat{H} = \frac{\hat{L}^2}{2I}, \quad (4.2)$$

and clearly commutes with both L^2 and L_z , and thus its eigenstates are the spherical harmonics Y_{lm} , since

$$\hat{L}^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm}. \quad (4.3)$$

The energy eigenvalues of the quantum rigid rotator are obtained by applying the Hamiltonian on the eigenstates:

$$\hat{H} Y_{lm} = \frac{\hat{L}^2}{2I} Y_{lm} = \frac{\hbar^2 l(l+1)}{2I} Y_{lm} \quad (4.4)$$

and we identify:

$$E_l = \frac{\hbar^2 l(l+1)}{2I}. \quad (4.5)$$

(b) What is the degeneracy of the n th energy eigenvalue? (Degeneracy in quantum mechanics refers to different quantum states having the same energy eigenvalue).

The energy eigenvalues above are labeled only by the total angular momentum quantum number l , and not on the quantum number corresponding to the z -component of the angular momentum. This is the case for all spherically symmetric systems. Now, we recall from the lecture that for a given l the quantum number m runs from $+l$ to $-l$, so every energy eigenvalue is $2l + 1$ degenerate.

B. Let us now imagine that the rotator is stretched a bit such that its moment of inertia in the z -direction becomes $I_z = (1 + \epsilon)I$, with the other two moments remaining unchanged.

(a) What are the new energy eigenstates and eigenvalues?

In this case, the Hamiltonian becomes

$$\hat{H} = \frac{\hat{L}_x^2 + \hat{L}_y^2}{2I} + \frac{\hat{L}_z^2}{2I(1 + \epsilon)}. \quad (4.6)$$

Using the fact that $L_x^2 + L_y^2 = L^2 - L_z^2$, we find:

$$\hat{H} = \frac{\hat{L}^2 - \hat{L}_z^2}{2I} + \frac{\hat{L}_z^2}{2I(1 + \epsilon)} = \frac{\hat{L}^2}{2I} - \frac{\epsilon}{1 + \epsilon} \frac{\hat{L}_z^2}{2I}. \quad (4.7)$$

The spherical harmonics Y_{lm} are simultaneous eigenfunctions of both \hat{L}^2 and L_z , so the energy eigenfunctions of the above Hamiltonian are again the Y_{lm} . Following a similar procedure as in part (a), we find the energies of this rotator as:

$$E_{lm} = \frac{\hbar^2 l(l+1)}{2I} - \frac{\epsilon}{1 + \epsilon} \frac{\hbar^2 m^2}{2I}. \quad (4.8)$$

(b) Sketch the spectrum of energy eigenvalues as a function of ϵ . For what sign of ϵ do the energy eigenvalues get closer together? Intuitively, why?

In Figure 1, we plot the energies in a dimensionless form,

$$\tilde{E}_{l,m}(\epsilon) = l(l+1) - \frac{\epsilon}{1 + \epsilon} m^2, \quad (4.9)$$

for $l = 0, 1, 2$.

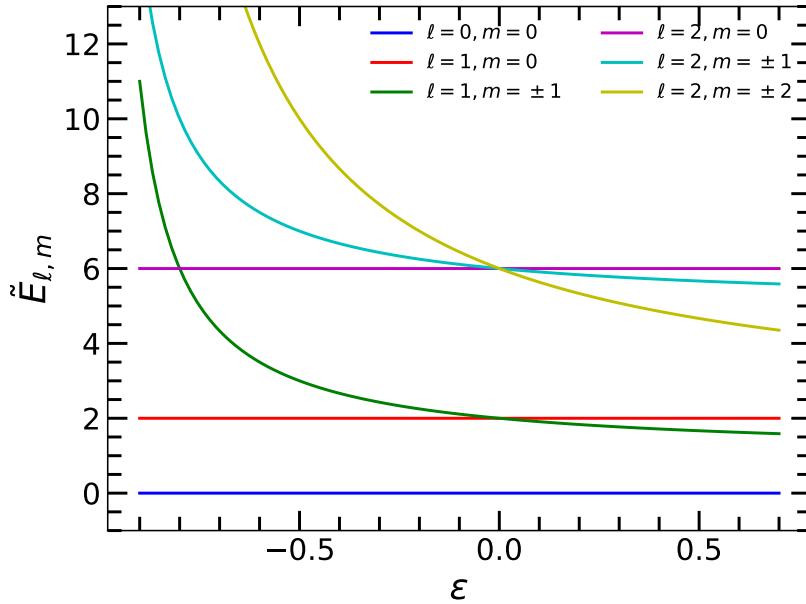


Figure 1: The (dimensionless) energies of the rotator as a function of the parameter ϵ for $l = 0, 1, 2$.

For $m = 0$, there is no dependence on ϵ since the second term in the RHS of the above equation is zero. Let us analyze the spacings between the energy eigenvalues. The difference between two energy eigenstates E_{lm} and $E_{l'm'}$ is

$$E_{lm} - E_{l'm'} = \frac{\hbar^2 [l'(l'+1) - l(l+1)]}{2I} + \frac{\epsilon}{1+\epsilon} \frac{\hbar^2 (m^2 - m'^2)}{2I}. \quad (4.10)$$

The first fraction on the right-hand side is a constant and therefore does not affect the trend of the energy differences; the absolute value of the second fraction shows how close two energies can get, since it depends on ϵ . We always assume that $m^2 > m'^2$ (if not, simply exchange $E_{lm} \leftrightarrow E_{l'm'}$), so the important term remaining is $\frac{\epsilon}{1+\epsilon}$. If $\epsilon \geq 0$ then $\left| \frac{\epsilon}{1+\epsilon} \right| \leq \frac{1}{2}$, but if $\epsilon \rightarrow -1^+$ then $\left| \frac{\epsilon}{1+\epsilon} \right| \rightarrow \infty$; thus, in the former case $\epsilon \geq 0$ the two energies are closer.

Classically this means that for a given L_z the moment of inertia in the z -direction $I_z = (1 + \epsilon)I$ increases, the associated rotational energy decreases.

(c) What is the degeneracy of the n^{th} energy eigenvalue? Is the degeneracy partially or fully lifted?

From Eq. (4.8), we see that, for a given l , the $\pm m$ eigenfunctions share the same eigenvalue, so the degeneracy is only partially lifted. This is because the system energy is still invariant under $L_z \rightarrow -L_z$, i.e. the rigid rotator starts to spin in the opposite direction but with the same angular-momentum magnitude. The two opposite rotation directions correspond to $+m$ and $-m$.

(d) Now add a magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$. Does this term lift the degeneracy?

We add an additional term to the Hamiltonian of the form $\hat{H} = -\mathbf{B} \cdot \hat{\mathbf{\mu}}$ where $\hat{\mathbf{\mu}} = \frac{q}{2m}\hat{\mathbf{L}}$. Thus, the overall Hamiltonian is:

$$\hat{H} = \frac{\hat{L}^2}{2I} - \frac{\epsilon}{1+\epsilon} \frac{\hat{L}_z^2}{2I} + \frac{q}{2m} \mathbf{B} \cdot \hat{\mathbf{L}}. \quad (4.11)$$

The magnetic field is oriented along the z -axis and thus the Hamiltonian reduces to:

$$\hat{H} = \frac{\hat{L}^2}{2I} - \frac{\epsilon}{1+\epsilon} \frac{\hat{L}_z^2}{2I} + \frac{q}{2m} B_z \hat{L}_z. \quad (4.12)$$

This Hamiltonian commutes with both L^2 and L_z , and thus its eigenstates are the usual $|l, m\rangle$ (or the spherical harmonics in position representation). The energies are thus readily obtained:

$$E_{l,m}(\epsilon) = \frac{\hbar^2 l(l+1)}{2I} - \frac{\epsilon}{1+\epsilon} \frac{\hbar^2 m^2}{2I} + \frac{q}{2m} B_z \hbar m, \quad (4.13)$$

which can be re-written in the following dimensionless form:

$$\tilde{E}_{l,m}(\epsilon) = l(l+1) - \frac{\epsilon}{1+\epsilon} m^2 + A m, \quad A = \frac{q B_z 2I}{2m \hbar} \quad (4.14)$$

where A is a dimensionless constant and is directly proportional to the magnitude of the magnetic field. This term clearly breaks the symmetry $L_z \rightarrow -L_z$, and thus degeneracy is lifted. In Figure 2, we demonstrate the breaking of the degeneracy for $\pm m$ when $B \neq 0$.

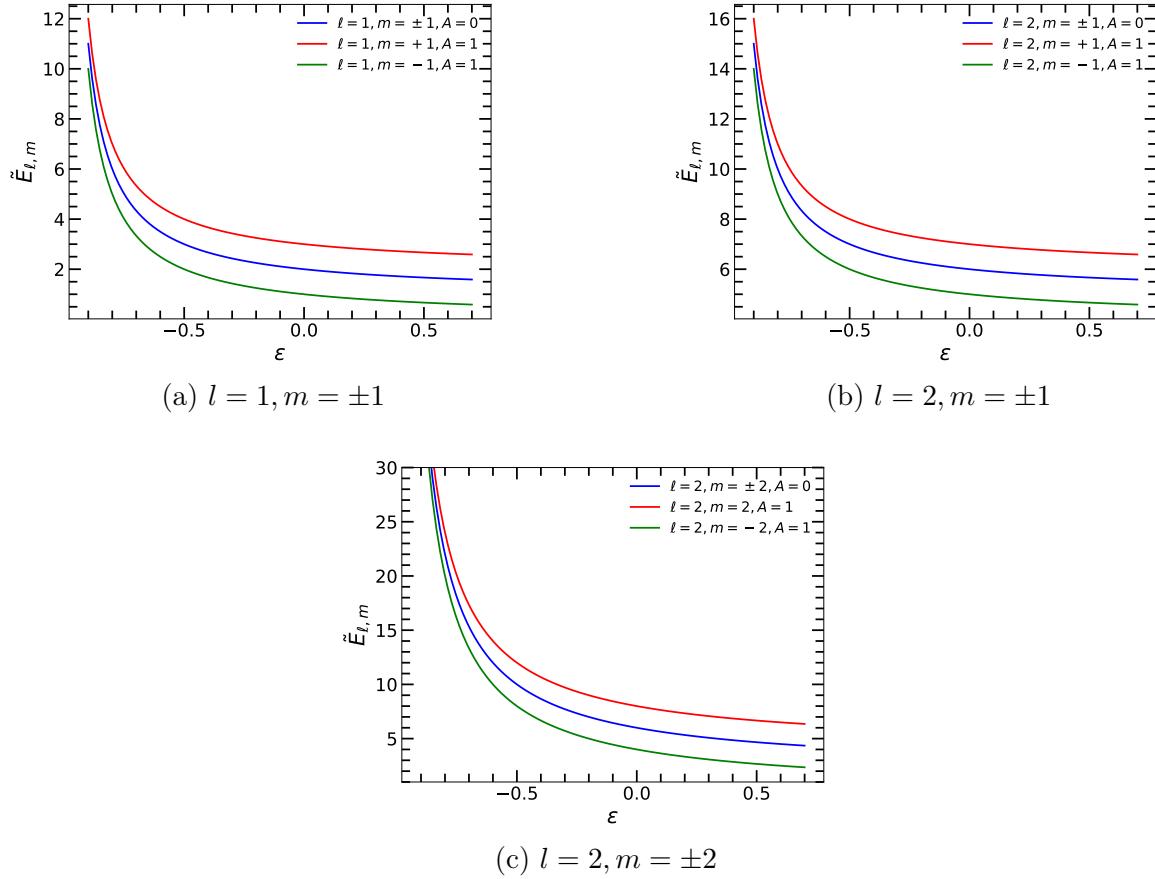


Figure 2: The energies of the rotator as a function of the parameter ϵ for a non-zero magnetic field.