Quantum Mechanics I

Week 5 (Solutions)

Spring Semester 2025

1 The Hellmann–Feynman theorem

A. Theorem Proof

Suppose a Hamiltonian $\hat{H}$ for a particular quantum system is a function of some parameter λ. As a consequence, its eigenvalues $E_n(\lambda)$ and eigenstates $|\psi_n(\lambda)\rangle$ are also functions of this parameter. The Hellman-Feynman Theorem states that

$$\frac{dE_\lambda}{d\lambda} = \left\langle \psi_\lambda \middle| \frac{d\hat{H}_\lambda}{d\lambda} \middle| \psi_\lambda \right\rangle. \tag{1.1}$$

Prove this statement.

This proof employs the following two conditions:

$$\hat{H}_\lambda|\psi_\lambda\rangle = E_\lambda|\psi_\lambda\rangle, \tag{1.2}$$

$$\langle\psi_\lambda|\psi_\lambda\rangle = 1 \Rightarrow \frac{d}{d\lambda}\langle\psi_\lambda|\psi_\lambda\rangle = 0. \tag{1.3}$$

The proof then follows through an application of the derivative product rule to the expectation value of the Hamiltonian viewed as a function of λ:

$$\begin{aligned}
\frac{dE_\lambda}{d\lambda} &= \frac{d}{d\lambda}\langle\psi_\lambda|\hat{H}_\lambda|\psi_\lambda\rangle \\
&= \left\langle \frac{d\psi_\lambda}{d\lambda} \middle| \hat{H}_\lambda \middle| \psi_\lambda \right\rangle + \left\langle \psi_\lambda \middle| \hat{H}_\lambda \middle| \frac{d\psi_\lambda}{d\lambda} \right\rangle + \left\langle \psi_\lambda \middle| \frac{d\hat{H}_\lambda}{d\lambda} \middle| \psi_\lambda \right\rangle \\
&= E_\lambda \left\langle \frac{d\psi_\lambda}{d\lambda} \middle| \psi_\lambda \right\rangle + E_\lambda \left\langle \psi_\lambda \middle| \frac{d\psi_\lambda}{d\lambda} \right\rangle + \left\langle \psi_\lambda \middle| \frac{d\hat{H}_\lambda}{d\lambda} \middle| \psi_\lambda \right\rangle \\
&= E_\lambda \frac{d}{d\lambda}\langle\psi_\lambda|\psi_\lambda\rangle + \left\langle \psi_\lambda \middle| \frac{d\hat{H}_\lambda}{d\lambda} \middle| \psi_\lambda \right\rangle \\
&= \left\langle \psi_\lambda \middle| \frac{d\hat{H}_\lambda}{d\lambda} \middle| \psi_\lambda \right\rangle.
\end{aligned}$$

B. Application to a Two-Level System

Consider a two-state system with the following total Hamiltonian:

$$\hat{H} = \begin{pmatrix} g & \omega_0 + g \\ \omega_0 + g & -g \end{pmatrix} \equiv \hat{H}_0 + g\hat{V}, \quad \hat{V} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{1.4}$$

(a) Compute the eigenvalues and eigenvectors of $\hat{H}_0$.

The eigenvalues and their respective eigenvectors are

$$E_1 = \omega_0; \quad E_2 = -\omega_0; \quad v_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}; \quad v_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

(b) We would like now to compute the first-order correction in energy δE_i when the perturbation $\hat{V}$ is introduced, i.e.

$$E_i = E_i^{(0)} + \delta E_i + \mathcal{O}(g^2), \tag{1.5}$$

where $E_i^{(0)}$ are the energies of the Hamiltonian $\hat{H}_0$. Compute the first-order variation of the energies using the Hellmann-Feynman theorem.

The variation $\delta E_i = g\, dE_1/dg|_{g=0}$ represents the first term in the Taylor expansion of the energies aroung $g = 0$. By the H.-F. theorem, we have:

$$\delta E_1 = g v_1 \cdot V v_1 = \frac{1}{2} g \begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = g,$$

$$\delta E_2 = g v_2 \cdot V v_2 = \frac{1}{2} g \begin{pmatrix} 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = -g.$$

Thus, the first-order corrected energies are $E_1 = E_1^{(0)} + g$ and $E_2 = E_2^{(0)} - g$.

(c) Compute the exact eigenvalues by diagonalizing $\hat{H}$ and verify the result found in the previous Question. Consider small g.

The exact eigenvalues are calculated from the characteristic equation (I is the identity matrix)

$$0 = \det(H - \lambda I) = \det \begin{pmatrix} g - \lambda & \omega_0 + g \\ \omega_0 + g & -g - \lambda \end{pmatrix} = \lambda^2 - \omega_0^2 - 2g\omega_0 - 2g^2$$

The roots are

$$\lambda_1 = \sqrt{\omega_0^2 + 2g\omega_0 + 2g^2}; \quad \lambda_2 = -\sqrt{\omega_0^2 + 2g\omega_0 + 2g^2}$$

Expanding in a power series of g to first order, we get

$$\lambda_1 \simeq \omega_0 + g; \quad \lambda_2 = -\omega_0 - g$$

in agreement with what was seen above.

C. Application to Atoms in an Electric Field

The coupling of any system to an external, uniform and static electric field $\mathbf{E}$ is obtained with an interaction term $-\mathbf{d}\cdot\mathbf{E}$ in the Hamiltonian, just as in the classical case,

$$\hat{H} = \hat{H}_0 - \mathbf{d}\cdot\mathbf{E}, \quad \mathbf{d} = \sum_a e_a \mathbf{r}_a\,, \tag{1.6}$$

where the index a corresponds to the number of charges. The quantity $\mathbf{d}$ is your usual dipole moment.

(a) Show that the average dipole moment of the system in the steady state $|\psi_n\rangle$ can be expressed through the variation of the energy E_n with respect to the external electric field. Here, the state $|\psi_n\rangle$ and the corresponding energy E_n are an eigenstate and energy of the Hamiltonian $\hat{H}$ respectively. Hint: Use the Hellmann-Feynman theorem.

The desired quantity is

$$\mathbf{D} = \langle\psi_n \mid \mathbf{d} \mid \psi_n\rangle \tag{1.7}$$

where $|\psi_n\rangle$ is the eigenstate of H with energy E_n. If we consider $\mathbf{E}$ as a parameter, the Hellmann-Feynman theorem tells us that

$$\frac{\partial E_n}{\partial \mathbf{E}} = \langle\psi_n \mid \frac{\partial H}{\partial \mathbf{E}} \mid \psi_n\rangle \quad \equiv \quad -\langle\psi_n \mid \mathbf{d} \mid \psi_n\rangle \tag{1.8}$$

therefore

$$\mathbf{D} = -\frac{\partial E_n}{\partial \mathbf{E}}. \tag{1.9}$$

(b) By using second-order perturbation theory (beyond of the scope of this course) we find that the energies of a closed-shell atom in a weak electric field are of the form:

$$E_n = E_0 + \frac{\alpha}{2}\vec{\mathcal{E}}^2\,, \tag{1.10}$$

where α is a constant with the appropriate units. What is the average dipole moment in this case?

In this case, the average value of the dipole is

$$\mathbf{D} = \alpha\,\mathbf{E} \tag{1.11}$$

in which we can recognize the definition of polarizability.

2 Operators and Measurements

A two-level system is described by the Hamiltonian:

$$H = E_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

In this system, we consider the measurement of two observables described by the operators A and B:

$$A = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad B = \begin{pmatrix} 2 & -\sqrt{2}i \\ \sqrt{2}i & 1 \end{pmatrix}.$$

(a) Verify that the eigenvalues of A are ± 1 and find the corresponding eigenvectors.

The eigenvalue equation $\det(\mathbb{1}\lambda - A) = 0$ is written as $\lambda^2 - 1 = 0$, and it has solutions $\lambda = \pm 1$. The corresponding (normalized) eigenvectors are

$$|A;+1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, \quad |A;-1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}. \tag{2.1}$$

(The phase was chosen arbitrarily.)

(b) Find the eigenvalues and eigenvectors of B.

The characteristic equation for B has eigenvalues $b_1 = 3$ and $b_2 = 0$ with normalized eigenvectors

$$|B;3\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} \sqrt{2} \\ i \end{pmatrix}, \quad |B;0\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} i \\ \sqrt{2} \end{pmatrix}. \tag{2.2}$$

(c) Are the observables A and B compatible? Are they conserved?

The observables do not commute with each other, i.e. $[A, B] \neq 0$, and are therefore not compatible. The simplest way to verify this is to write the observables in terms of the Pauli matrices:

$$A = \sigma_y, \quad B = \frac{3}{2}\mathbf{I} + \frac{1}{2}\sigma_z + \sqrt{2}\,\sigma_y.$$

Hence

$$[A, B] = \tfrac{1}{2}[\sigma_y, \sigma_z] = i\,\sigma_x.$$

Similarly,

$$H = E_0\,\sigma_z,$$

so these observables also do not commute with H and are not conserved.

(d) Suppose a measurement of A is performed, yielding the result measure$(A) = 1$. What would be the results and their respective probabilities if B were measured immediately after measuring A?

After measuring A, the system is in the state $|A;+1\rangle$, so the probability of observing the two possible values of B (namely 3 and 0) are:

$$P(A;1 \mid B;3) = \big|\langle B;3 \mid A;1\rangle\big|^2 = \frac{3+2\sqrt{2}}{6} \approx 0.97, \tag{2.3}$$

$$P(A;1 \mid B;0) = \big|\langle B;0 \mid A;1\rangle\big|^2 = \frac{3-2\sqrt{2}}{6} \approx 0.03 \tag{2.4}$$

(e) The system is subjected to a second measurement of the observable A. What would be the probability of finding the value $A = 1$ in the following cases?

i) Not measuring B and the measurement of A is performed immediately after the first measurement.

ii) Not measuring B and the measurement of A is performed after a time t.

iii) A is measured after performing a measurement of B, obtaining the result b_1 (the maximum eigenvalue of B)

i) The measurement of A immediately after gives the result 1.

ii) The state $|A,1\rangle$ is not an eigenstate of H. The eigenstates of H are the vectors:

$$|e1\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad |e2\rangle = \begin{pmatrix}0\\1\end{pmatrix}.$$

From the expression of $|A,1\rangle$, we have

$$|A,1\rangle = \frac{1}{\sqrt{2}}\big(|e1\rangle + i\,|e2\rangle\big) = |A1\rangle.$$

Thus, at time t

$$|A1,t\rangle = \frac{1}{\sqrt{2}}\Big(|e1\rangle\, e^{-iE_0t/\hbar} + i\,|e2\rangle\, e^{+iE_0t/\hbar}\Big).$$

The probability amplitude for the process is

$$\langle A1 \mid A1,t\rangle = \frac{1}{2}\Big(e^{-iE_0t/\hbar} + e^{+iE_0t/\hbar}\Big) = \cos\Big(\frac{E_0t}{\hbar}\Big).$$

The corresponding probability is

$$P\big(A1(t) \mid A1\big) = \Big[\cos\Big(\frac{E_0t}{\hbar}\Big)\Big]^2.$$

iii) If the result of the measurement of B gives $b_1 = 3$, then the system is in the state $|B,3\rangle$, independent of its previous state. Therefore, the (relative) probability of obtaining the value $A = 1$ in an immediately subsequent measurement is

$$P(A1 \mid A1,B3) = |\langle A,1 \mid B,3\rangle|^2 = P(A1 \mid B3) = \frac{1}{6}\big(3+2\sqrt{2}\big).$$

The term "relative" refers to the assumption that in the first measurement, the result was $b_1 = 3$. Logically, the probability of the entire sequence is obtained by multiplying the probabilities in sequence (we write the probability conditions explicitly to clarify the process):

$$P(A1 \mid B3) \cdot P(B3 \mid A1) = \frac{17}{36} + \frac{\sqrt{2}}{3}.$$

3 Two-Level Systems

A. The Bloch-sphere Representation

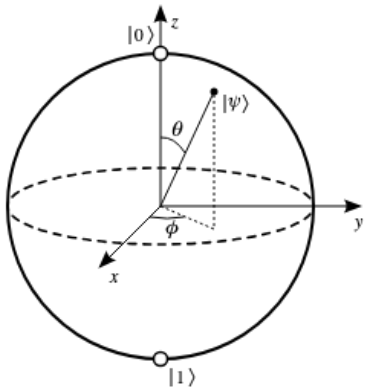

Figure 1: The Bloch sphere representation.

Show that all pure states $|\psi\rangle$ of a two-level system $|0\rangle, |1\rangle$ can be written as

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}e^{i\phi}|1\rangle \ , \tag{3.1}$$

where $\theta \in [0, \pi]$, $\phi \in [0, 2\pi[$. This result shows that the three dimensional unit sphere allows to represent any pure state of a two-level system (like a qubit, spin-1/2, photon etc). The above representation of pure states in the unit sphere is called the Bloch sphere. Recall that in Week 3, we defined the operator $\hat{S}_{\vec{n}}$ as the projection of the spin operator $\vec{S}$ along a unit vector $\vec{n} = \sin\theta\cos\phi\hat{x} + \sin\theta\sin\phi\hat{y} + \cos\theta\hat{z}$. One of the eigenvectors was precisely the state $|\psi\rangle$.

Without loss of generality, we can write any state at two levels (considered alone) in the form

$$|\psi\rangle = a|0\rangle + be^{i\phi}|1\rangle, \tag{3.2}$$

with a and b positive reals such that $a^2 + b^2 = 1$ and $\phi \in [0, 2\pi[$, since the global phase doesn't matter physically. We can therefore introduce a parameter $\theta \in [0, \pi]$ such that $a = \cos\frac{\theta}{2}$ and $b = \sin\frac{\theta}{2}$, hence the results. The angles θ and ϕ can be interpreted as the polar and azimuth angles of the spherical coordinates, which provide a parametrization of the unit sphere in three dimensions.

We are therefore immediately convinced that a point in this unit sphere (Bloch sphere) corresponds to one and only one state of the two-level system. In particular, the north pole of the Bloch sphere corresponds to the state $|0\rangle$, and the south pole to $|1\rangle$.

B. A spin-1/2 in a Magnetic Field

We consider a spin-1/2 with a magnetic moment $\boldsymbol{\mu} = -\gamma \mathbf{S}$, where $\gamma = \frac{|e|}{m}$, where $|e|$ and m are the charge and mass of an electron, respectively and $\mathbf{S}$ is the spin of the electron. This particle is in a constant magnetic field

$$\mathbf{B}_0 = \frac{\omega_x}{\gamma}\hat{x} + \frac{\omega_y}{\gamma}\hat{y} + \frac{\omega_z}{\gamma}\hat{z}\,. \tag{3.3}$$

(a) Show that the time evolution operator for this spin is given by :

$$U(t,0) = e^{-iMt}, \quad M = \frac{1}{\hbar}(\omega_x S_x + \omega_y S_y + \omega_z S_z)\,. \tag{3.4}$$

Give the matrix representation of M in the S_z eigenbasis $\{|S_z;\pm\rangle\}$.

The Hamiltonian of the system reads:

$$H = -\mu \cdot \mathbf{B}_0 = -\gamma \mathbf{S} \cdot \mathbf{B}_0, \tag{3.5}$$

The time evolution is dictated by the operator $U(t) \equiv U(t,0) = e^{-\frac{i}{\hbar}Ht} = e^{-iMt}$, where

$$M = \frac{H}{\hbar} = -\frac{1}{\hbar}(\gamma \mathbf{S}\cdot\mathbf{B}_0) = \frac{1}{\hbar}(S_x\omega_x + S_y\omega_y + S_z\omega_z) = \frac{1}{2}(\sigma_x\omega_x + \sigma_y\omega_y + \sigma_z\omega_z). \tag{3.6}$$

In the eigenbasis of S_z ($|0\rangle, |1\rangle$), we have that

$$M = \frac{1}{2}\begin{pmatrix} \omega_z & \omega_x - i\omega_y \\ \omega_x + i\omega_y & -\omega_z \end{pmatrix}. \tag{3.7}$$

The matrix representation of M, in the eigenbasis of S_z, is

$$M = \frac{1}{2}\begin{pmatrix} \omega_z & \omega_x - i\omega_y \\ \omega_x + i\omega_y & -\omega_z \end{pmatrix}. \tag{3.8}$$

(b) Show that:

$$M^2 = \frac{1}{4}\left(\omega_x^2 + \omega_y^2 + \omega_z^2\right)\mathbb{1} = \left(\frac{\omega_0}{2}\right)^2 \mathbb{1}\,, \tag{3.9}$$

where $\omega_0 = \gamma|B|$.

To obtain the above expression for M we have used that $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \mathbb{1}_2$ and $\{\sigma_i, \sigma_j\} = 2\delta_{ij}\mathbb{1}_2$,

$$M^2 = \frac{1}{4}(\sigma_x\omega_x + \sigma_y\omega_y + \sigma_z\omega_z)^2 = \frac{1}{4}(\omega_x^2 + \omega_y^2 + \omega_z^2)\mathbb{1}_2 = \frac{\omega_0^2}{4}. \tag{3.10}$$

(c) Using your previous results, show that the time evolution operator can be written as:

$$U(t,0) = \cos\left(\frac{\omega_0 t}{2}\right)\mathbb{1} - \frac{2i}{\omega_0}\sin\left(\frac{\omega_0 t}{2}\right)M\,. \tag{3.11}$$

The exponential of an operator is given by

$$e^{-iMt} = \sum_{k=0}^{\infty}\frac{(-iMt)^k}{k!} = \sum_{k=0}^{\infty}\frac{(-iMt)^{2k}}{(2k)!} + \sum_{k=0}^{\infty}\frac{(-iMt)^{2k+1}}{(2k+1)!}. \tag{3.12}$$

We have that

$$M^{2k} = (M^2)^k = \left(\frac{\omega_0}{2}\right)^{2k}\mathbb{1}_2, \quad M^{2k+1} = \left(\frac{\omega_0}{2}\right)^{2k}M. \tag{3.13}$$

and thus,

$$e^{-iMt} = \mathbb{1}_2\sum_{k=0}^{\infty}\frac{(-i\frac{\omega_0}{2}t)^{2k}}{(2k)!} + M\frac{2}{\omega_0}\sum_{k=0}^{\infty}\frac{(-i\frac{\omega_0}{2}t)^{2k+1}}{(2k+1)!} \tag{3.14}$$

$$= \mathbb{1}_2\cos\left(\frac{\omega_0}{2}t\right) - i\frac{2}{\omega_0}M\sin\left(\frac{\omega_0}{2}t\right). \tag{3.15}$$

(d) We consider a spin in the initial state $|\psi(0)\rangle = |S_z;+\rangle$. Find the time-evolved state $|\psi(t)\rangle$.

We apply the time-evolution operator on the initial state as follows:

$$|\psi(t)\rangle = U(t,0)\,|\psi(0)\rangle = \left[\cos\left(\frac{\omega_0 t}{2}\right)\mathbb{1} - \frac{2i}{\omega_0}\sin\left(\frac{\omega_0 t}{2}\right)M\right]|S_z;+\rangle\,. \tag{3.16}$$

The action of M on the eigenvector of S_z with positive eigenvalue gives:

$$M\,|S_z;+\rangle = \frac{\omega_z}{2}\,|S_z;+\rangle + \frac{\omega_x + i\omega_y}{2}\,|S_z;-\rangle\,. \tag{3.17}$$

Thus, the time-evolved state becomes:

$$|\psi(t)\rangle = \left[\cos\left(\frac{\omega_0 t}{2}\right) - i\frac{\omega_z}{\omega_0}\sin\left(\frac{\omega_0 t}{2}\right)\right]|S_z;+\rangle - i\frac{(\omega_x + i\omega_y)}{\omega_0}\sin\left(\frac{\omega_0 t}{2}\right)|S_z;-\rangle\,. \tag{3.18}$$

(e) Find the probabilities to find the system in either states $|S_z;+\rangle$ for $t > 0$.

The probability to find the system in the state $|S_z;+\rangle$ is:

$$P_+(t) = |\langle S_z;+|\psi(t)\rangle|^2 = \cos^2\left(\frac{\omega_0}{2}t\right) + \left(\frac{\omega_z}{\omega_0}\right)^2 \sin^2\left(\frac{\omega_0}{2}t\right). \tag{3.19}$$

and may further be simplified in:

$$\begin{aligned} P_+(t) &= \cos^2\left(\frac{\omega_0}{2}t\right) + \left(\frac{\omega_z}{\omega_0}\right)^2 \sin^2\left(\frac{\omega_0}{2}t\right) \\ &= 1 + \sin^2\left(\frac{\omega_0}{2}t\right)\left(\frac{\omega_z^2}{\omega_0^2} - 1\right) \\ &= 1 - \sin^2\left(\frac{\omega_0}{2}t\right)\left(\frac{\omega_x^2 + \omega_y^2}{\omega_0^2}\right). \end{aligned}$$

Note that the presence of the magnetic field determines the precession of the spin around the direction of $\mathbf{B}_0$. Thus, it is clear that if $\mathbf{S}$ and $\mathbf{B}_0$ have the same direction, there is no precession and $P_+(t)$ becomes 1.

For example, in the case where $\mathbf{B}_0$ is parallel to the z direction, we have $H = \frac{1}{2}\sigma_z\omega_z$. Therefore, $P_+ = 1$ since $\omega_x = \omega_y = 0$.

4 Advanced Operator Algebra

A. Unitary Operators

A unitary operator U is an operator whose Adjoint is its inverse, i.e.

$$U^\dagger U = \hat{\mathbb{1}} = UU^\dagger$$

(a) Show that all eigenvalues λ_i of a Unitary operator are pure phases, $\lambda_j = e^{i\phi_j}$.

Suppose $|\phi_u\rangle$ is an eigenfunction of U with eigenvalue u, i.e.

$$U|\phi_u\rangle = u|\phi_u\rangle. \tag{4.1}$$

We thus have that

$$\langle U\phi_u|U\phi_u\rangle = \langle u\phi_u|u\phi_u\rangle = |u|^2\langle\phi_u|\phi_u\rangle \tag{4.2}$$

On the other hand, since U is unitary, $U^\dagger U = 1$, we have

$$\langle U\phi_u|U\phi_u\rangle = \langle\phi_u|U^\dagger U|\phi_u\rangle = \langle\phi_u|1|\phi_u\rangle = \langle\phi_u|\phi_u\rangle. \tag{4.3}$$

From our two last arguments, we find:

$$|u|^2 \langle \phi_u | \phi_u \rangle = \langle \phi_u | \phi_u \rangle \,. \tag{4.4}$$

Thus, unless $\langle \phi_u | \phi_u \rangle = 0$, we must have that

$$|u|^2 = 1 \tag{4.5}$$

i.e., all eigenvalues u of a Unitary operator must be pure phases, $u = e^{i\theta}$.

(b) Can an operator be both Hermitian and unitary?

The condition for U to be Hermitian is that $U^\dagger = U$. The condition for U to be Unitary is that $U^\dagger U = 1$. Thus the condition for an operator to be both Unitary and Hermitian is that $U^2 = 1$, i.e. the only Unitary operators, which are also Hermitian, are those which square to one.

Note that can be easily seen from the eigenvalues: Hermitian implies the eigenvalues are all real; Unitary implies the eigenvalues are all pure phases; the only numbers which are both real and pure phases are ± 1; thus the eigenvalues of a Unitary Hermitian operator are all ± 1 and square to one.

Therefore, a Unitary operator can be Hermitian, only if it squares to one.

(c) Suppose M is a Hermitian operator. Show that e^{iM} is a Unitary operator.

Suppose M is Hermitian, $M^\dagger = M$. We would like to see that $U = e^{iM}$ is Unitary, i.e. that $U^\dagger U = \mathbb{1}$. By definition of the exponential of an operator,

$$U = e^{iM} = \sum_{n=0}^{\infty} \frac{(iM)^n}{n!} \tag{4.6}$$

Since M is Hermitian, iM is anti-Hermitian, i.e. $(iM)^\dagger = -iM$, so

$$U^\dagger = \sum_{n=0}^{\infty} \frac{(-iM)^n}{n!} = e^{-iM} \tag{4.7}$$

Thus,

$$U^\dagger U = e^{-iM} e^{iM} = 1. \tag{4.8}$$

(d) Show that the product of two unitary operators is also Unitary.

Suppose A and B are Unitary, $A^\dagger A = \mathbb{1}$ and $B^\dagger B = \mathbb{1}$, and let $W = AB$. Then

$$W^\dagger = (AB)^\dagger = B^\dagger A^\dagger \quad \Rightarrow \quad W^\dagger W = (B^\dagger A^\dagger) AB = B^\dagger (A^\dagger A) B = B^\dagger B = \mathbb{1}. \tag{4.9}$$

So $W = AB$ is Unitary.

(e) Suppose U is a unitary operator, and v a state. Show that acting on v with U preserves the norm of v.

The length of a vector v is defined as $|v| = \sqrt{\langle v|v\rangle}$. Let us make the notation $|u\rangle = U|v\rangle$. The length of u is:

$$|u| = \sqrt{\langle u|u\rangle} = \sqrt{\langle v|U^\dagger U|u\rangle} = \sqrt{\langle v|v\rangle} = |v|. \tag{4.10}$$

So unitary operators preserve the length of vectors.

(f) A space translation by L is represented by the following operator

$$\hat{T}_L = e^{-\frac{i}{\hbar}L\hat{p}}, \quad \hat{T}_L f(x) = f(x-L)\,,$$

where $\hat{p}$ is a Hermitian operator (in fact, this is the momentum operator). The operator $\hat{T}_L$ shifts the expectation value of the position by L. Verify that $\hat{T}_L$ is a unitary operator and demonstrate that

$$\hat{T}_L^\dagger = \hat{T}_{-L}\,.$$

Since $\hat{p}$ is a Hermitian operator, the operator $-\frac{L}{\hbar}\hat{p}$, being the multiplication of $\hat{p}$ by a real number, is Hermitian. Thus, from Question (c), we know that the operator

$$\hat{T}_L = e^{i\left(-\frac{L}{\hbar}\hat{p}\right)} \tag{4.11}$$

is unitary. Acting with $\hat{T}_L$ on any function $f(x)$, we find:

$$\hat{T}_{-L} f(x) = f(x+L) = e^{i\frac{L}{\hbar}p} f(x) = \left(e^{-i\left(\frac{L}{\hbar}p\right)}\right)^\dagger f(x) = \hat{T}_L^\dagger f(x). \tag{4.12}$$

Since the above equation holds for any function $f(x)$, we conclude that the first and the last members are equal at the operator level, and thus

$$\hat{T}_{-L} = \hat{T}_L^\dagger. \tag{4.13}$$

B. Anti-unitary Operators

Recall that an operator is Hermitian if it is equal to its own adjoint, $\hat{A}^\dagger = \hat{A}$. Henceforth, let $\hat{A}$ and $\hat{B}$ be Hermitian operators, and define $\hat{C} = [\hat{A}, \hat{B}]$.

(a) Show that $\hat{C}^\dagger = -\hat{C}$. Such an operator is called *anti-Hermitian*.

We show this by considering the Hermitian of the commutator:

$$C^\dagger = \Big([A,B]\Big)^\dagger = \Big(AB - BA\Big)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger = -\Big(AB - BA\Big) = -[A,B] = -C.$$

We have used the fact that both A, B are Hermitian operators.

(b) Show that the eigenvalues of the anti-Hermitian operator $\hat{C}$ are all imaginary.

Consider the operator $(i\hat{C})$:

$$(i\hat{C})^\dagger = -i\hat{C}^\dagger = i\hat{C}, \tag{4.14}$$

which means that $i\hat{C}$ is Hermitian. As a result, eigenvalues of $i\hat{C}$ are real, so eigenvalues of $\hat{C}$ must be purely imaginary.

(c) Suppose $[\hat{K}, \hat{J}] = -s\hat{J}$, where s is a real quantity and $\hat{K}$ is Hermitian. Is $\hat{J}$ Hermitian?

The operator $\hat{J}$ is not Hermitian, which is something that is mostly easily proven by contradiction. Suppose we were to assume that $\hat{J}$ were Hermitian, so that $\hat{J}^\dagger = \hat{J}$. Let us rewrite $\hat{J}$ as $-\frac{1}{s}[\hat{K}, \hat{J}]$ and consider $\hat{J}^\dagger$:

$$\hat{J}^\dagger = -\left(\frac{1}{s}[\hat{K}, \hat{J}]\right)^\dagger = -\frac{1}{s}\left(\hat{K}\hat{J} - \hat{J}\hat{K}\right)^\dagger = -\frac{1}{s}(\hat{J}^\dagger\hat{K}^\dagger - \hat{K}^\dagger\hat{J}^\dagger) = \frac{1}{s}(\hat{K}\hat{J} - \hat{J}\hat{K}),$$

where in the last equality we used the fact that $\hat{K}$ is Hermitian and our assumption that $\hat{J}$ is also Hermitian. The final expression is equal to $+\frac{1}{s}[\hat{K}, \hat{J}] = -\hat{J}$. Thus, our algebra implies that $\hat{J}^\dagger = -\hat{J}$, which contradicts our assumption of $\hat{J}^\dagger = \hat{J}$ (i.e., our assumption that $\hat{J}$ is Hermitian). Since we have a contradiction, we are forced to conclude that $\hat{J}$ is not Hermitian.

(d) Show that $[\hat{K}, \hat{J}^\dagger] = +s\hat{J}^\dagger$.

Starting with $[\hat{K}, \hat{J}]$, we have

$$\begin{aligned}[\hat{K}, \hat{J}^\dagger] = [\hat{K}^\dagger, \hat{J}^\dagger] = \hat{K}^\dagger\hat{J}^\dagger - \hat{J}^\dagger\hat{K}^\dagger = (\hat{J}\hat{K})^\dagger - (\hat{K}\hat{J})^\dagger \\ = -(\hat{K}\hat{J} - \hat{J}\hat{K})^\dagger = -[\hat{K}, \hat{J}]^\dagger = -(-s\hat{J})^\dagger = s\hat{J}^\dagger,\end{aligned}$$

where in the first equality, we used the Hermiticity of $\hat{K}$ to replace $\hat{K}$ with $\hat{K}^\dagger$. In the penultimate equality, we used our definition of $\hat{J}$, i.e., $[\hat{K}, \hat{J}] = -s\hat{J}$.

What we have, then, are two results (which really imply each other):

$$[\hat{K}, \hat{J}] = -s\hat{J} \quad \text{and} \quad [\hat{K}, \hat{J}^\dagger] = +s\hat{J}^\dagger. \tag{4.15}$$

(e) Suppose $\hat{K}\varphi_k = k\varphi_k$. Show that $(\hat{J}\varphi_k)$ is an eigenfunction of $\hat{K}$ with eigenvalue $(k - s)$.

If $\hat{K}\varphi_k = k\varphi_k$ (i.e., φ_k is an eigenstate of $\hat{K}$ with eigenvalue k), then the state $(\hat{J}\varphi_k)$ is also an eigenfunction of $\hat{K}$ with eigenvalue $(k - s)$, as we now show:

$$\hat{K}(\hat{J}\varphi_k) = \hat{K}\hat{J}\varphi_k = ([\hat{K}, \hat{J}] + \hat{J}\hat{K})\varphi_k = -s\hat{J}\varphi_k + k\hat{J}\varphi_k = (k - s)(\hat{J}\varphi_k). \tag{4.16}$$

(f) Show that $(\hat{J}^\dagger \varphi_k)$ is an eigenfunction of $\hat{K}$ with eigenvalue $(k+s)$.

Similarly, we have:

$$\hat{K}(\hat{J}^\dagger \varphi_k) = \hat{K}\hat{J}^\dagger \varphi_k = ([\hat{K}, \hat{J}^\dagger] + \hat{J}^\dagger \hat{K})\varphi_k = +s\hat{J}^\dagger \varphi_k + k\hat{J}^\dagger \varphi_k = (k+s)(\hat{J}^\dagger \varphi_k). \quad (68)$$

Remark: The algebraic structure explored in this problem is precisely analogous to the one in the quantum harmonic oscillator, which we will encounter later in the course. The $\hat{J}$ is the lowering operator that acts on an eigenstate of $\hat{K}$ and gives a result that is directly proportional to an eigenstate of $\hat{K}$ with an eigenvalue that is lower than the eigenvalue of the original eigenstate. The operator $\hat{J}^\dagger$ "raises" in an analogous way.

C. Baker-Campbell-Hausdorff formula

The Baker-Campbell-Hausdorff formula is a particularly useful formula which is commonly used to conduct unitary transforms in quantum mechanics.

(a) Prove the Baker-Campbell-Hausdorff formula for a linear operator on Hilbert space,

$$e^A B e^{-A} = \sum_{k=0}^{\infty} \frac{1}{k!}[A, B]_k,$$

where $[A, B]_0 = B$ and $[A, B]_k = [A, [A, B]]_{k-1}$.

To prove this formula, we use the Taylor expansion of the exponential, as to find:

$$G = e^A B e^{-A} = \left(\sum_n \frac{A^n}{n!}\right) B \left(\sum_m \frac{(-1)^m A^m}{m!}\right) = \sum_{n,m} \frac{(-1)^m A^n B A^m}{n! m!}. \quad (4.17)$$

We analyze G into its components based on the sum $(n+m)$:

$$G = G_0 + G_1 + G_2 + \cdots. \quad (4.18)$$

We may show the first few terms as follows (we use the notation (n, m)):

- $(0,0) : G_0 = B$
- $(1,0), (0,1) : G_1 = [A, B]$
- $(2,0), (1,1), (0,2) : G_2 = \frac{1}{2!}[A, [A, B]]$

and so forth.

Thus, we can show:

$$e^A B e^{-A} = \sum_{k=0}^{\infty} \frac{1}{k!}[A, B]_k, \quad (4.19)$$

where $[A, B]_0 = B$ and $[A, B]_k = [A, [A, B]]_{k-1}$.

(b) For the case that $[A,[A,B]] = [B,[A,B]] = 0$ (the Heisenberg algebra or the creation and annihilation operators of the harmonic oscillator – which we will encounter soon – are examples), show, using the result from Question (a), that

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]}.$$

Hint: Consider the operator $g(s) = e^{sA}e^{sB}$ and take the derivative with respect to s. Obtain a differential equation for $g(s)$ and solve it. Set $s = 1$ to your final result.

For $g(s) = e^{sA}e^{sB}$, it follows that

$$\frac{dg}{ds} = \left(A + e^{sA}Be^{-sA}\right) g(s) = (A + B + s[A,B])\, g(s), \tag{4.20}$$

whose solution is

$$g(s) = e^{s(A+B)+\frac{s^2}{2}[A,B]}. \tag{4.21}$$

Taking $s = 1$ gives one of the special cases of the Baker–Campbell–Hausdorff formula described above:

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]}. \tag{4.22}$$

5 Which-Slit Information Destroys Interference

We would like to investigate through which slits the electrons pass. We decide to set up a double-slit experiment and place test particles in front of slit A to detect the electrons passing through this slit. The electron collides with these test particles, and this process causes an uncertainty in the momentum Δp_y.

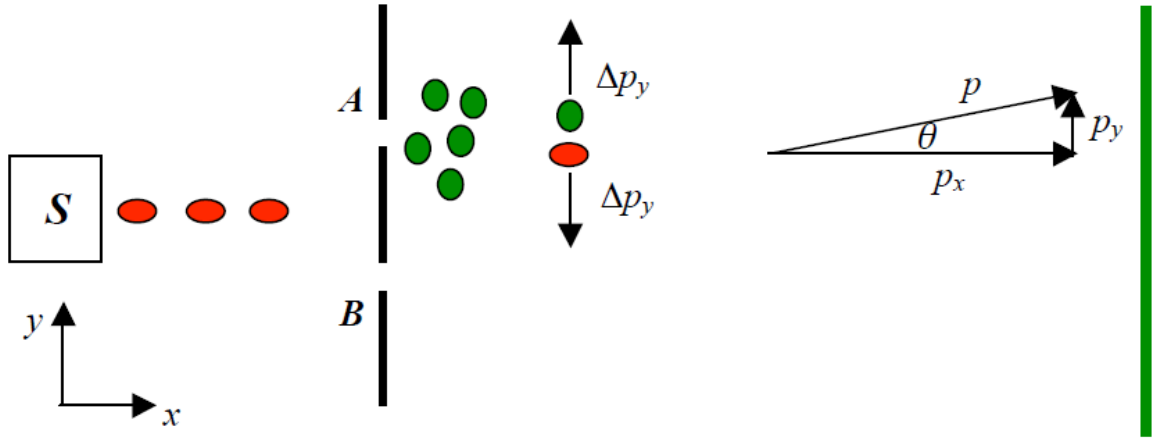

Figure 2: Modified apparatus, with test particles behind slit A. If an electron passes through slit A, it will scatter with one of the test particles, after which both particles will have some uncertainty in their momentum along the y direction, Δp_y. Also shown is the momentum for an unscattered electron. In the problem it has to be assumed that the screen is located very far away from the double-slit aperture, so that the distance between the two slits, d, is much smaller than the distance L between the plane of the two slits and the detector screen.

(a) Let us consider first the case in which the electron is not scattered by the test particles. In this case, find the angle corresponding to the first minimum of the interference pattern.

The difference in path lengths, ΔL, from each slit to point P is given by $\Delta L = d \sin\theta$. The first minimum in the interference pattern, nearest the central peak, therefore occurs for $\Delta L = (1/2)\lambda$, where λ is the wavelength of the waves passing through the slits, or

$$d \sin\theta = \frac{1}{2}\lambda \,, \tag{5.1}$$

corresponding to an angle from the initial direction of propagation given by

$$\sin\theta = \frac{\lambda}{2d} \,. \tag{5.2}$$

An electron's associated wavelength is given by the de Broglie relation,

$$\lambda = \frac{h}{p} \,, \tag{5.3}$$

where h is Planck's constant and p is the electron's momentum. Thus the minima in the interference pattern will occur at

$$\sin\theta = \frac{h}{2pd} \,. \tag{5.4}$$

(b) Using your result from Question (a) and the de Broglie relation, show that at the first minimum of the interference pattern, the y-component of the momentum of the unscattered electron is:

$$p_y = \frac{h}{2d}\,, \tag{5.5}$$

where h is the Planck's constant.

An unscattered electron that was heading toward that position on the screen, meanwhile, would have a y-component of its momentum given by $p_y = p\sin\theta$, or $\sin\theta = \frac{p_y}{p}$. Combining these expressions, we have

$$\sin\theta = \frac{p_y}{p} = \frac{h}{2pd} \quad \Rightarrow \quad p_y = \frac{h}{2d}. \tag{5.6}$$

(c) What should be the condition of the momentum and its uncertainty that guarantees the preservation of the interference pattern?

The preservation of the interference pattern requires that the uncertainty in the momentum after scattering, Δp_y, remains much smaller than the $p_y = h/(2d)$. In fact, if Δp_y was larger than $h/(2d)$, the momentum uncertainty due to the collision with the test particles would be enough to shift the momentum by an amount comparable to the distance between the interference fringes. This would destroy the interference pattern.

Thus, in order to preserve interference we have to require that:

$$\Delta p_y \ll p_y = \frac{h}{2d}\,. \tag{5.7}$$

(d) What should be the condition of the position and its uncertainty that guarantees definite measurement of which-slit information?

Any definite measurement of which slit the electron passed through also required $\Delta y \ll d$.

(e) Using your results from Questions (c) and (d), show that

$$\Delta y \Delta p_y \ll \frac{h}{2}\,, \tag{5.8}$$

which is a clear violation of the uncertainty principle! As a result, the inclusion of test particles significantly affects the electron's momentum, causing the minima of the interference pattern to smear out and ultimately leading to the loss of interference.

In order to measure the which-slit information AND not disrupt the characteristic interference pattern, we would require (considering the conditions from the previous two questions):

$$\Delta y \Delta p_y \ll d\left(\frac{h}{2d}\right) = \frac{h}{2}\,. \tag{5.9}$$

This is a clear violation of the Heisenberg's uncertainty principle!

The act of measuring through which slit the electron passed destroys the interference pattern. An electron that encounters one of the test particles would necessarily receive such a large "kick", Δp_y, that the minima of the interference pattern would get smeared out, destroying the characteristic pattern of peaks and valleys. In fact, if every electron were definitely measured to pass through either slit A or slit B, the resulting detection pattern when both slits were open would revert to the sum of the two single-slit distributions – all wavelike behavior would vanish.