Quantum Mechanics I

Week 4 (Solutions)

Spring Semester 2025

1 Finite Hamiltonian

We consider a 3-state system, described by the following Hamiltonian:

$$H = H_0 + H_1 = \begin{pmatrix} E_0 & 0 & 0 \\ 0 & E_0 & 0 \\ 0 & 0 & E_0 \end{pmatrix} - \frac{\epsilon}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{1.1}$$

(a) Calculate the eigenvalues of H and the eigenstates $|a\rangle$, $|b\rangle$, $|c\rangle$, corresponding to the ground state, the first, and the second excited states. Express the result in terms of the basis vectors:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{1.2}$$

Solving the characteristic equation, we find the eigenvalues $E_0 - \epsilon$; $\quad E_0$; $\quad E_0 + \epsilon$, with corresponding normalized eigenvectors:

$$|a\rangle = \begin{pmatrix} 1/2 \\ 1/\sqrt{2} \\ 1/2 \end{pmatrix} = \frac{|1\rangle + \sqrt{2}|2\rangle + |3\rangle}{2},$$

$$|b\rangle = \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ -1/\sqrt{2} \end{pmatrix} = \frac{|1\rangle - |3\rangle}{\sqrt{2}},$$

$$|c\rangle = \begin{pmatrix} 1/2 \\ -1/\sqrt{2} \\ 1/2 \end{pmatrix} = \frac{|1\rangle - \sqrt{2}|2\rangle + |3\rangle}{2}.$$

(b) Verify that the Hamiltonian H commutes with the operator:

$$\Pi = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \Pi^2 = 1. \tag{1.3}$$

Discuss the relevance of this fact in relation to Question (a).

By computing the commutator, we verify that $[H, \Pi] = 0$. The eigenvalues of Π are ± 1. Since the eigenvalues of H are non-degenerate, they are automatically eigenstates of Π. It is immediately verified that $|a\rangle$ and $|c\rangle$ are "even" eigenstates with eigenvalue $+1$, while $|b\rangle$ is an "odd" eigenstate with eigenvalue -1.

(c) Express the states $|1\rangle$, $|2\rangle$, $|3\rangle$ in terms of the eigenstates of H.

By inverting the relations given above, we obtain:

$$|1\rangle = \frac{|a\rangle + \sqrt{2}|b\rangle + |c\rangle}{2}, \quad |2\rangle = \frac{|a\rangle - |c\rangle}{\sqrt{2}}, \quad |3\rangle = \frac{|a\rangle - \sqrt{2}|b\rangle + |c\rangle}{2}.$$

(d) The system is initially at time $t = 0$ in state $|1\rangle$, i.e., $|\psi(0)\rangle = |1\rangle$. Determine the state at time t, $|\psi(t)\rangle$, in terms of the states $|1\rangle$, $|2\rangle$, $|3\rangle$. Compute the probability $P_2(t)$ of being in state 2 at time t and plot its evolution as a function of time.

Using the time evolution operator $U = \exp\{-iHt/\hbar\}$ and the initial state in the energy eigenbasis (see previous Question),

$$|\psi(t)\rangle = U(t)\,|1\rangle = e^{-iHt/\hbar}\left(\frac{|a\rangle + \sqrt{2}|b\rangle + |c\rangle}{2}\right), \tag{1.4}$$

we find:

$$\begin{aligned} |\psi(t)\rangle &= e^{-iE_0 t/\hbar}\left[\frac{|a\rangle e^{i\epsilon t/\hbar} + \sqrt{2}|b\rangle + |c\rangle e^{-i\epsilon t/\hbar}}{2}\right] = \\ &= e^{-iE_0 t/\hbar}\left[\frac{1}{2}(1 + \cos(\epsilon t/\hbar))|1\rangle + \frac{i}{\sqrt{2}}\sin(\epsilon t/\hbar)|2\rangle + \frac{1}{2}(-1 + \cos(\epsilon t/\hbar))|3\rangle\right] \end{aligned} \tag{1.5}$$

The probability of being in state $|2\rangle$ at time t is:

$$P_2(t) = |\langle 2|\psi(t)\rangle|^2 = \frac{1}{2}\sin^2\left(\frac{\epsilon t}{\hbar}\right).$$

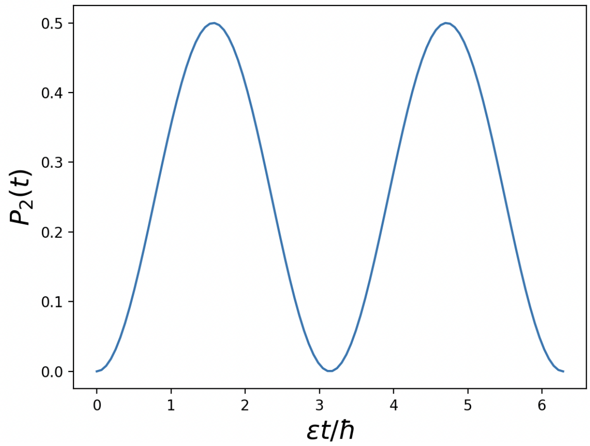

Figure 1: The probability of being in state $|2\rangle$ as a function of time.

Remark: The model represents in a very simplified way the motion of an electron on a triatomic cyclic molecule. ϵ is the transition amplitude between localized levels. If $\epsilon = 0$, the electron has three equivalent equilibrium positions, with energy E_0.

2 Two-Level Quantum System

The Hamiltonian of a two-level quantum system is described by the following operator (in the appropriate units of measurement):

$$H|1\rangle = |1\rangle + \frac{1+i}{\sqrt{2}}|2\rangle, \tag{2.1}$$

$$H|2\rangle = \frac{1-i}{\sqrt{2}}|1\rangle + |2\rangle \tag{2.2}$$

where $|1\rangle$ and $|2\rangle$ are the normalized eigenvectors of another Hermitian operator A:

$$A|1\rangle = \sqrt{2}|1\rangle, \tag{2.3}$$

$$A|2\rangle = -\sqrt{2}|2\rangle. \tag{2.4}$$

(a) Find the matrix representation of the Hamiltonian on the basis of the eigen-kets (eigenvectors) of the operator A, i.e., the matrix elements

$$H_{ij} = \langle i|H|j\rangle, \quad \text{with } i, j = 1, 2. \tag{2.5}$$

Considering the matrix elements H_{ij} obtained by the inner products $\langle i|H|j\rangle$, the Hamiltonian matrix H is:

$$H = \begin{pmatrix} 1 & \frac{1-i}{\sqrt{2}} \\ \frac{1+i}{\sqrt{2}} & 1 \end{pmatrix}, \tag{2.6}$$

In our calculations, we have used the orthonormality condition for the eigenvectors of the operator $\hat{A}$.

(b) Find the eigenvalues and eigenvectors of the Hamiltonian.

The eigenvalues are found by solving the characteristic equation obtained from:

$$P(E) = \det \begin{pmatrix} 1-E & \frac{1-i}{\sqrt{2}} \\ \frac{1+i}{\sqrt{2}} & 1-E \end{pmatrix} = 0\,. \tag{2.7}$$

We find $P(E) = (1-E)^2 - 1 = 0$, so the two eigenvalues are $E_1 = 0$ and $E_2 = 2$.

The corresponding eigenvectors are:

$$|E_1\rangle = \frac{1}{\sqrt{2}}|1\rangle - \frac{1+i}{2}|2\rangle, \quad |E_2\rangle = \frac{1}{\sqrt{2}}|1\rangle + \frac{1+i}{2}|2\rangle\,. \tag{2.8}$$

At time $t = 0$, a measurement of the observable associated with the operator A is performed. The result of this measurement is $-\sqrt{2}$.

(c) Immediately afterward, a measurement of the energy is performed. What is the probability that this energy measurement yields a value $E = 0$?

We express the eigenvectors of the operator $\hat{A}$ in the eigenbasis of the Hamiltonian, i.e.

$$|1\rangle = \frac{1}{\sqrt{2}}(|E_2\rangle + |E_1\rangle), \quad |2\rangle = \frac{1-i}{2}(|E_2\rangle - |E_1\rangle)\,. \tag{2.9}$$

Right after the measurement at time $t = 0$, we find $|\Psi\rangle = |2\rangle$. The probability of measuring $E_1 = 0$ is determined by the Born rule. Using, the expansion of the state $|2\rangle$ in the basis $\{|E_1\rangle\,, |E_2\rangle\}$, we find

$$P(E_1) = \left|\frac{1-i}{2}\right|^2 = \frac{1}{2}\,. \tag{2.10}$$

(d) How does this probability change if, instead of measuring the energy at time $t = 0$, we measure it at a time $T > 0$?

We first evolve the system in time by acting with the time evolution operator on the initial state:

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|2\rangle = \frac{1-i}{2}\left(e^{-2it/\hbar}|E_2\rangle - |E_1\rangle\right) \tag{2.11}$$

Thus,

$$P(E_1) = \left|\frac{1-i}{2}\right|^2 = \frac{1}{2}, \tag{2.12}$$

and it does not depend on time.

(e) Now imagine that no energy measurement is performed. At what time $t \geq 0$ will the system be in the physical state described by $|2\rangle$?

In Question (d), we found that

$$|\psi(t)\rangle = \frac{1-i}{2}\left(e^{-2it/\hbar}|E_2\rangle - |E_1\rangle\right), \tag{2.13}$$

so $|\psi(t)\rangle = e^{i\phi}|2\rangle$, where ϕ is an arbitrary global phase. This condition is satisfied if

$$e^{-2it/\hbar} = 1, \tag{2.14}$$

thus for $t = n\pi\hbar$ for $n = 1, 2, \cdots$.

3 Perturbing a Two-Level System

In this exercise we consider the simplest possible (non-trivial) system, namely a two-level system. This is a system that is described by wave functions belonging to $\mathbb{C}_2$. The operators are therefore, according to the idea of Heisenberg's matrix mechanics, described by 2×2 matrices. In particular, one can always choose a basis such that the Hamiltonian is given by:

$$\hat{H}_0 = \hbar \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix}. \tag{3.1}$$

Then, we introduce a perturbation:

$$\hat{W} = \begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{pmatrix}$$

The new Hamiltonian is then given by $\hat{H} = \hat{H}_0 + \hat{W}$.

(a) Write down the eigenenergies $E_1^{(0)}, E_2^{(0)}$ and orthonormal eigenstates $\{|\phi_1^{(0)}\rangle, |\phi_2^{(0)}\rangle\}$ of the unperturbed Hamiltonian $\hat{H}_0$.

The Hamiltonian $\hat{H}_0$ is diagonal and thus $E_1^{(0)} = \hbar\omega_1$ and $E_2^{(0)} = \hbar\omega_2$. It is expressed in the basis of its eigenvectors. These are:

$$|\phi_1^{(0)}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\phi_2^{(0)}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

(b) What conditions must be met by the quantities W_{ij} for $\hat{H}$ to describe a Hamiltonian?

The matrix $\hat{W}$ represents a physical Hamiltonian if it satisfies the condition $\hat{H}^\dagger = \hat{H}$ and consequently $\hat{W}^\dagger = \hat{W}$. On the level of matrix elements this equation reads $W_{ij} = W_{ji}^*$. This implies the following constraint on the matrix $\hat{W}$:

$$\hat{W} = \begin{pmatrix} W_{11} & W_{12}e^{i\chi} \\ W_{12}e^{-i\chi} & W_{22} \end{pmatrix} \tag{20}$$

where W_{11}, W_{12}, W_{22} and $\chi \in \mathbb{R}$.

(c) Find the eigenvalues $E_{1,2}$ of $\hat{H}$.

The eigenvalues of $\hat{H}$ are given by

$$E_{1,2} = \frac{1}{2}(\hbar\omega_1 + W_{11} + \hbar\omega_2 + W_{22}) \pm \frac{1}{2}\sqrt{(\hbar\omega_1 + W_{11} - \hbar\omega_2 - W_{22})^2 + 4|W_{12}|^2}.$$

We now focus on a specific case

$$\hat{W}_I = w\sigma_x = \begin{pmatrix} 0 & w/2 \\ w/2 & 0 \end{pmatrix}. \tag{3.2}$$

where $w \in \mathbb{R}$. This corresponds to a perturbation which "mixes" or couples the eigenstates of the Hamiltonian.

To simplify the notation, we further introduce the detuning parameter $\delta = \hbar(\omega_2 - \omega_1)$ such that the unperturbed Hamiltonian takes the form:

$$H_0 = \begin{pmatrix} -\frac{\delta}{2} & 0 \\ 0 & \frac{\delta}{2} \end{pmatrix}, \tag{3.3}$$

by making a suitable choice for $\hbar\omega_1$.

(d) Find the eigenvalues of the total Hamiltonian $\hat{H}$.

The eigenvalues are obtained by setting $W_{11} = W_{22} = 0$ and $W_{12} = W_{21} = w/2$ in the eigenvalues we obtained above. We find:

$$E_{1,2} = \pm\frac{1}{2}\sqrt{\delta^2 + w^2}\,. \tag{3.4}$$

We can verify that when $w = 0$, we obtain the unperturbed energies $E_{1,2} = \pm\frac{1}{2}\delta$.

(e) Find the eigenstates of the new Hamiltonian.

Diagonalizing the total matrix we find:

$$|\phi_1\rangle = \begin{pmatrix} \cos\Theta \\ \sin\Theta \end{pmatrix}, \quad |\phi_2\rangle = \begin{pmatrix} -\sin\Theta \\ \cos\Theta \end{pmatrix}, \quad \tan 2\Theta = -\frac{w}{\delta}\,. \tag{3.5}$$

The coefficients are given by

$$\cos\Theta = \frac{1}{\sqrt{1+\alpha^2}}, \quad \sin\Theta = \frac{\alpha}{\sqrt{1+\alpha^2}}$$

where $\alpha = (\sqrt{\delta^2 + w^2} + \delta)/w$. For the derivation of $\tan 2\Theta = -\frac{w}{\delta}$, the following trigonometric identity was used:

$$\tan 2\Theta = \frac{2\tan\Theta}{1 - \tan^2\Theta}.$$

These states are expressed in the energy basis of the unperturbed Hamiltonian, thus the new eigenstates are a linear combination of the original states.

(f) Plot the energies $E_{\pm}$ as a function of the detuning δ. Plot also the unperturbed energies $E_{1,2}^{(0)} = \pm\delta/2$. What happens to the eigenstates for low and high detuning?

The finite, non-zero value of the perturbation strength w introduces a gap in the energy spectrum at zero detuning. Notice that for large detunings (either positive or negative), the new energies tend to the original ones.

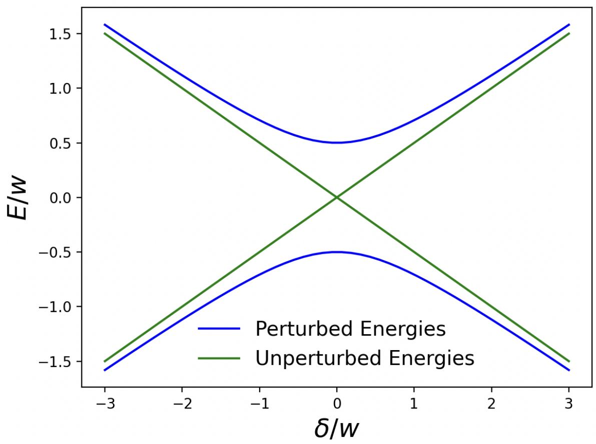

Figure 2: The energy spectrum for perturbed and unperturbed energies.

Remark: This system appears in many physical scenarios, for instance in light-matter interaction, in cavity electrodynamics and in mesoscopic physics.

4 A Particle in a Box

A box containing a particle is divided into a right and a left compartment by a thin partition. If the particle is known to be on the right (left) side with certainty, the state is represented by the position eigenket $|R\rangle$ ($|L\rangle$), where we have neglected spatial variations within each half of the box. The most general state vector can then be written as

$$|\alpha\rangle = |R\rangle\langle R|\alpha\rangle + |L\rangle\langle L|\alpha\rangle,$$

where $\langle R|\alpha\rangle$ and $\langle L|\alpha\rangle$ can be regarded as "wave functions." The particle can tunnel through the partition; this tunneling effect is characterized by the Hamiltonian

$$H = \Delta(|L\rangle\langle R| + |R\rangle\langle L|),$$

where Δ is a real number with the dimension of energy.

(a) Find the normalized energy eigenkets. What are the corresponding energy eigenvalues?

The energy eigenvalues are $E_{\pm} = \pm\Delta$ with normalized eigenstates

$$|E_{\pm}\rangle = \frac{1}{\sqrt{2}}(|R\rangle \pm |L\rangle). \tag{4.1}$$

(b) In the Schrödinger picture the base kets $|R\rangle$ and $|L\rangle$ are fixed, and the state vector moves with time. Suppose the system is represented by $|\alpha\rangle$ as given above at $t=0$. Find the state vector $|\alpha, t_0 = 0; t\rangle$ for $t > 0$ by applying the appropriate time-evolution operator to $|\alpha\rangle$.

We first express the original kets $\{|R\rangle, |L\rangle\}$ in the energy eigenbasis, $|R\rangle = (|E_+\rangle + |E_-\rangle)/\sqrt{2}$ and $|L\rangle = (|E_+\rangle - |E_-\rangle)/\sqrt{2}$. Then, we apply the time-evolution operator on the state $|\alpha\rangle$ and find (with $\omega = \Delta/\hbar$):

$$\begin{aligned} |\alpha, t\rangle &= e^{-iHt/\hbar}|\alpha, t=0\rangle \\ &= e^{-iHt/\hbar}|R\rangle\langle R|\alpha\rangle + e^{-iHt/\hbar}|L\rangle\langle L|\alpha\rangle \\ &= \frac{1}{\sqrt{2}}\left[e^{-i\omega t}|E_+\rangle + e^{i\omega t}|E_-\rangle\right]\langle R|\alpha\rangle + \frac{1}{\sqrt{2}}\left[e^{-i\omega t}|E_+\rangle - e^{i\omega t}|E_-\rangle\right]\langle L|\alpha\rangle. \end{aligned} \tag{4.2}$$

Then, we may express this state in the original basis $\{|L\rangle, |R\rangle\}$:

$$|\alpha, t\rangle = \Big[\cos\omega t\,\langle R|\alpha\rangle - i\sin\omega t\,\langle L|\alpha\rangle\Big]|R\rangle + \Big[\cos\omega t\,\langle L|\alpha\rangle - i\sin\omega t\,\langle R|\alpha\rangle\Big]|L\rangle\ . \tag{4.3}$$

(c) Suppose at $t = 0$ the particle is on the right side with certainty. What is the probability for observing the particle on the left side as a function of time?

The initial condition means that $\langle R|\alpha\rangle = 1$ and $\langle L|\alpha\rangle = 0$, so we calculate

$$|\langle L|\alpha, t\rangle|^2 = \sin^2\omega t. \tag{4.4}$$

(d) Write down the coupled Schrödinger equations for the wave functions $\langle R|\alpha, t_0 = 0; t\rangle$ and $\langle L|\alpha, t_0 = 0; t\rangle$. Show that the solutions to the coupled Schrödinger equations are just what you expect from Question (b).

We use the simplified notation $|\alpha, t\rangle \equiv |\alpha, t_0 = 0; t\rangle$, and express our state as:

$$|\alpha, t\rangle = \langle R|\alpha, t\rangle\,|R\rangle + \langle L|\alpha, t\rangle\,|L\rangle\ . \tag{4.5}$$

We may use for simplicity the notation $c_R(t) \equiv \langle R|\alpha, t\rangle$ and $c_L(t) \equiv \langle L|\alpha, t\rangle$.

We use the Schrödinger equation,

$$i\hbar d_t\,|\alpha, t\rangle = \hat{H}\,|\alpha, t\rangle\,, \quad H = \Delta(|L\rangle\langle R| + |R\rangle\langle L|). \tag{4.6}$$

Using the general time-evolved state in the Schrödinger equation, and equating the coefficients of the state kets $|L\rangle, |R\rangle$, we find:

$$i\hbar d_t c_R = \Delta c_L, \quad i\hbar d_t c_L = \Delta c_R\ ,.$$

Solving the system of coupled ordinary differential equations, we find the following solution:

$$c_R = -i\beta_1 \sin\omega t + +i\beta \cos\omega t, \quad c_L = \beta_1 \cos\omega t + \beta_2 \sin\omega t\,, \tag{4.7}$$

where the constants β_1, β_2 are determined from the initial conditions. Comparing this result to that of Question (b), we find agreement when $\beta_1 = \langle L|\alpha\rangle$ and $\beta_2 = -i\,\langle R|\alpha\rangle$.

(e) Suppose the printer made an error and wrote H as

$$H = \Delta|L\rangle\langle R|.$$

Show that the probability conservation as a function of time is violated. Suppose that the initial state is $|R\rangle$.

We will evolve this state using the time evolution operator

$$|\Psi(t)\rangle = U\,|\Psi(0)\rangle = \exp\left(-i\frac{H}{\hbar}t\right)|\Psi(0)\rangle\,, \tag{4.8}$$

Notice that for this Hamiltonian, we have $H^2 = 0$. Thus, we can expand

$$|\Psi(t)\rangle = \left[\mathbb{1} - i\frac{\hat{H}}{\hbar}t\right]|\Psi(0)\rangle\,. \tag{4.9}$$

The initial state is taken to be that of $|R\rangle$, hence we find:

$$|\Psi(t)\rangle = |R\rangle - i\frac{\Delta}{\hbar}t\,|L\rangle\,. \tag{4.10}$$

We consider the probability density as a function of time,

$$\langle\Psi(t)|\Psi(t)\rangle = 1 + \frac{\Delta^2}{\hbar^2}t^2\,. \tag{4.11}$$

Probability is no longer conserved in time. At time $t = 0$, the probability is indeed unity, but then for $t > 0$, it grows with time.