Physics Through Problem Solving - XXII
Quantum Mechanics Problems with Time-Evolution Operator

Ahmed Sayeed
Department of Physics
University of Pune
Pune - 411007
email: sayeed@physics.unipune.ac.in
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In this article we solve some quantum mechanics problems using the time-evolution operator $U(t) = e^{-iHt/\hbar}$ for a time independent Hamiltonian H. We consider here the time evolution of a particularly simple system - a two-state system.

We learn in an introductory course in quantum mechanics that any physical system (an electron, an atom, a molecule etc.) has to be described by a state-vector $|\psi\rangle(t)$. The most familiar example of a state-vector is a wave-function, such as that of an electron in a hydrogen atom. We are also familiar with the state-vector that describes the spin state of a particle. The simplest example is the spin-state of a free electron (or any spin-1/2 particle). The state-vector $|\psi\rangle$ in this case is a column vector of size 2. If this state-vector is known we can calculate the probability of obtaining a result in any measurement on the system, such as, the measurement of energy or the spin component in a given direction. One of the basic tasks in quantum mechanics is to determine the state-vector of the system $|\psi(t)\rangle$ at a given instant of time t, given the the state-vector of the system $|\psi(0)\rangle$ at a given instant of time $t = 0$. One way of doing it is by solving the Schrödinger equation $i\hbar\frac{d|\psi(t)\rangle}{dt} = H|\psi(t)\rangle$. Another equivalent way of doing this is by using the time-evolution operator $U(t) = e^{-iHt/\hbar}$. This is physically more intuitive because you can think of the change in state-vector as caused by the action of an operator - you take $|\psi(0)\rangle$ and operate $U(t)$ on it, and you get $|\psi\rangle(t)$, that is, $U(t)|\psi(0)\rangle = |\psi(t)\rangle$. In the following problems we shall demonstrate this procedure.

The Hamiltonian for a two state system is given by (in the standard basis $\{|1\rangle, |2\rangle\}$)

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

E_0 and η are not time-dependent.

Problem 1

Can E_0 and η be complex numbers?

Solution

The Hamiltonian is the operator for the observable energy. The operators representing observables have to Hermitian, that is to say, $H^\dagger = H$. Which is possible only if all the main-diagonal elements are real, and opposing off-diagonal elements are complex-conjugates of one another. In this case that means E_0 is real, and $(-\eta)^* = (-\eta) \implies \eta^* = \eta$, i.e. η is also real.

Problem 2

Find the eigenvalues and eigenvectors of H given in the previous problem.

Solution

The characteristic equation and the solutions are (λ is the eigenvalue)

$$|H - \lambda I| = 0 \implies (E_0 - \lambda)^2 - \eta^2 = 0 \implies \lambda = E_0 \pm \eta$$

where I is the 2×2 identity matrix. Let us call eigenvectors for the eigenvalues $E_1 = E_0 - \eta$ and $E_2 = E_0 + \eta$ respectively $|V_1\rangle$ and $|V_2\rangle$. We obtain the two eigenvectors by solving two eigenvalue equations $H|V_1\rangle = E_1|V_1\rangle$ and $H|V_2\rangle = E_2|V_2\rangle$. The first one is worked out as follows. Let $|V_1\rangle = \binom{x_1}{x_2}$ and we have to determine x_1 and x_2.

$$\begin{pmatrix} E_0 & -\eta \\ -\eta & E_0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = (E_0 - \eta) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

which gives us two equations $E_0 x_1 - \eta x_2 = (E_0 - \eta)x_1$ and $-\eta x_1 + E_0 x_2 = (E_0 - \eta)x_2$. But these two equations are not independent - one can be obtained from the other. So we have one linear equation to determine two unknowns, which is impossible. But we can use this equation to determine the *ratio* of x_1 and x_2, and then apply normalization requirement to fix the values of x_1 and x_2.

Simplifying any one of the 'two' equations above we get $x_2 = x_1 = c$ say. Thus we have $|V_1\rangle = \binom{c}{c}$. And c remains to be determined. But $|V_1\rangle$ is a quantum state of the system, and so must be normalized. Normalization gives us $c = 1/\sqrt{2}$. Thus we finally have $|V_1\rangle = \frac{1}{\sqrt{2}}\binom{1}{1}$. Note that we can multiply this vector by a factor $e^{i\phi}$, where ϕ any real number, and it still remains normalized. Thus the quantum states we obtain are always uncertain within this *overall phase factor*. But it does not matter, because no measurable property of a system depends on the overall phase-factor of the state-vector. So for simplicity we usually set $\phi = 0$ so that the phase-factor is unity.

Working in the same way, the reader can easily find the second eigenvector as $|V_2\rangle = \frac{1}{\sqrt{2}}\binom{1}{-1}$. At this point it is important to do a check - we know that the eigenvectors of a Hermitian matrix, for distinct eigenvalues, are always mutually orthogonal. We can readily verify that the inner-products $\langle V_1|V_2\rangle$ and $\langle V_2|V_1\rangle$ are both zero and so everything is in order. One common practice in quantum mechanics is to label the eigenvectors of a matrix by the respective eigenvalue. That is, we call $|V_1\rangle$ and $|V_2\rangle$ above $|E_1\rangle$ and $|E_2\rangle$. Thus the eigenvalue equations become simply $H|E_1\rangle = E_1|E_1\rangle$ and $H|E_1\rangle = E_1|E_1\rangle$. This can be slightly confusing for a beginner, but once you get used to it, it is very convenient when doing quantum mechanics linear algebra. We shall use this notation in the rest this article.

Problem 3

Consider a system described by the Hamiltonian H given in problem 1. At $t = 0$ the system is in the state

$$|\psi(0)\rangle = \frac{|1\rangle + i|2\rangle}{\sqrt{2}}$$

What are the probabilities that at time $t = 0$ the system is found in the states $|1\rangle$ and $|2\rangle$? What are the probabilities that the system is found in each of the two energy eigenstates?

Solution

Here $|1\rangle = \left(\begin{smallmatrix}1\\0\end{smallmatrix}\right)$ and $|2\rangle = \left(\begin{smallmatrix}0\\1\end{smallmatrix}\right)$ (i.e.,*standard basis vectors*). We know from one of the basic postulates of quantum mechanics that if at a given moment of time the system is in the state $|\psi\rangle$, the probability that an observation will find it in a state $|\phi\rangle$ is (assuming both the state vectors are normalized) $|\langle\phi|\psi\rangle|^2$. Thus the probability that at $t = 0$ the system is found in the state $|1\rangle$ is

$$\begin{aligned}|\langle 1|\psi(0)\rangle|^2 &= \left|\langle 1|\left[\frac{1}{\sqrt{2}}|1\rangle + \frac{i}{\sqrt{2}}|2\rangle\right]\right|^2\\ &= \left|\frac{1}{\sqrt{2}}\left[\langle 1|1\rangle + i\langle 1|2\rangle\right]\right|^2\\ &= \left|\frac{1}{\sqrt{2}}\left[1+0\right]\right|^2\\ &= \frac{1}{2}\end{aligned}$$

We have used above the orthonormality of the basis vectors, i.e. $\langle 1|1\rangle = 1$ and $\langle 1|2\rangle = 0$. Similarly we get the probability that at $t = 0$ the system is found in the state $|2\rangle$ also $\frac{1}{2}$.

The probabilities for finding the system in energy eigenstates $|E_1\rangle$ and $|E_1\rangle$ are respectively $|\langle E_1|\psi(0)\rangle|^2$ and $|\langle E_2|\psi(0)\rangle|^2$. Let us first evaluate the components $\langle E_1|\psi(0)\rangle$ and $\langle E_2|\psi(0)\rangle$. We have

$$|E_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle \tag{1}$$

And

$$|E_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}|1\rangle - \frac{1}{\sqrt{2}}|2\rangle \tag{2}$$

And we are given

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}|1\rangle + \frac{i}{\sqrt{2}}|1\rangle \tag{3}$$

From Eqs. (1) and (3) we get

$$\begin{aligned}\langle E_1|\psi(0)\rangle =&\langle E_1|\left[\frac{|1\rangle + i|2\rangle}{\sqrt{2}}\right]\\ =&\left[\langle 1|\frac{1}{\sqrt{2}} + \langle 2|\frac{1}{\sqrt{2}}\right]\left[\frac{|1\rangle + i|2\rangle}{\sqrt{2}}\right]\\ =&\frac{1}{2}\left[\langle 1|1\rangle + \langle 2|1\rangle + i\langle 1|2\rangle + i\langle 2|2\rangle\right]\\ =&\frac{1}{2}\left[1+i\right]\end{aligned} \tag{4}$$

And from Eqs. (2) and (3) we get

$$\begin{aligned}\langle E_2|\psi(0)\rangle =&\langle E_1|\left[\frac{|1\rangle + i|2\rangle}{\sqrt{2}}\right]\\ =&\frac{1}{2}\left[1-i\right]\end{aligned} \tag{5}$$

And from Eqs. (4) and (5) we immediately get $|\langle E_1|\psi(0)\rangle|^2 = \frac{1}{2}$ and $|\langle E_2|\psi(0)\rangle|^2 = \frac{1}{2}$.

Problem 4

Answer the questions in the previous problem for $t > 0$, using the time-evolution operator.

Solution

We begin by expanding the state vector $|\psi(0)\rangle$ in the $\{|E_1\rangle, |E_2\rangle\}$ basis:

$$|\psi(0)\rangle = |E_1\rangle\langle E_1|\psi(0)\rangle + |E_2\rangle\langle E_2|\psi(0)\rangle \tag{6}$$

Using Eqs (4) and (5) in Eq. (6) we get

$$|\psi(0)\rangle = \frac{1}{2}(1+i)|E_1\rangle + \frac{1}{2}(1-i)|E_2\rangle \tag{7}$$

In Eq. (7) we have expressed the state vector $|\psi(0)\rangle$ in the energy eigenbasis. Now we can operate the time-evolution operator for the time independent Hamiltonian, $U(t) = e^{-iHt/\hbar}$, on this state vector and obtain the state vector at time t, that is $|\psi(t)\rangle$:

$$\begin{aligned}|\psi(t)\rangle &= U(t)|\psi(0)\rangle\\ &= e^{-iHt/\hbar}|\psi(0)\rangle\\ &= e^{-iHt/\hbar}\left[\frac{1}{2}(1+i)|E_1\rangle + \frac{1}{2}(1-i)|E_2\rangle\right]\\ &= \left[\frac{1}{2}(1+i)e^{-iHt/\hbar}|E_1\rangle + \frac{1}{2}(1-i)e^{-iHt/\hbar}|E_2\rangle\right]\\ &= \left[\frac{1}{2}(1+i)e^{-iE_1t/\hbar}|E_1\rangle + \frac{1}{2}(1-i)e^{-iE_2t/\hbar}|E_2\rangle\right]\end{aligned} \tag{8}$$

In the last step we have used the fact that when the time-evolution operator $e^{-iHt/\hbar}$ (H being time-independent) acts on an energy eigenstate $|E\rangle$, the eigenstate gets multiplied by the factor $e^{-iEt/\hbar}$, E being the energy eigenvalue for the state. Note that $e^{-iEt/\hbar}$ is a number (or scalar).

We are now ready to calculate the probabilities that at time t, the system is in the states represented by vectors $|1\rangle$ and $|2\rangle$. The probability that at time t the system is found in the state $|1\rangle$ is :

$$\begin{aligned} P_1(t) &= |\langle 1|\psi(t)\rangle|^2 \\ &= \left|\langle 1| \left[\frac{1}{2}(1+i)e^{-iE_1t/\hbar}|E_1\rangle + \frac{1}{2}(1-i)e^{-iE_2t/\hbar}|E_2\rangle\right]\right|^2 \\ &= \left|\left[\frac{1}{2}(1+i)e^{-iE_1t/\hbar}\langle 1|E_1\rangle + \frac{1}{2}(1-i)e^{-iE_2t/\hbar}\langle 1|E_2\rangle\right]\right|^2 \end{aligned}$$

From Eqs. (1) and (2) we have $\langle 1|E_1\rangle = \frac{1}{\sqrt{2}}$ and $\langle 1|E_2\rangle = \frac{1}{\sqrt{2}}$. Using this the last equation above we have

$$\begin{aligned} P_1(t) &= \left|\left[\frac{1}{2}(1+i)e^{-iE_1t/\hbar}\frac{1}{\sqrt{2}} + \frac{1}{2}(1-i)e^{-iE_2t/\hbar}\frac{1}{\sqrt{2}}\right]\right|^2 \\ &= \left(\frac{1}{2\sqrt{2}}\right)^2 \left|\left[(1+i)e^{-iE_1t/\hbar} + (1-i)e^{-iE_2t/\hbar}\right]\right|^2 \\ &= \frac{1}{8}\left|\left[(1+i)e^{-iE_1t/\hbar} + (1-i)e^{-iE_2t/\hbar}\right]\right|^2 \end{aligned}$$

We can simplify the modulus-squared term in the last expression above by noting that for a complex number z, $|z|^2 = zz^*$, and also $e^{i\theta} - e^{-i\theta} = 2i\sin\theta$. After a few lines of simplification, we get

$$\begin{aligned} P_1(t) &= \frac{1}{2}\left[1 - \sin\left(\frac{E_2 - E_1}{\hbar}t\right)\right] \\ &= \frac{1}{2}\left[1 - \sin\left(\frac{2\eta}{\hbar}t\right)\right] \end{aligned}$$

In the last line we have used $E_2 - E_1 = 2\eta$. An almost identical calculation gives the probability that at time t the system is found in the state $|2\rangle$:

$$\begin{aligned} P_2(t) &= |\langle 2|\psi(t)\rangle|^2 \\ &= \frac{1}{2}\left[1 + \sin\left(\frac{2\eta}{\hbar}t\right)\right] \end{aligned}$$

Note that the two probabilities add to 1. This is because this is a two-state system, and the states $|1\rangle$ and $|2\rangle$ are mutually orthogonal. Thus is the system in not one state, it must be in the other.

Similarly, the probability that at time t the system is found in the energy eigenstate E_1 is given by $|\langle E_1|\psi(t)|^2$. This we can calculate by using Eq. (1) in (8):

$$\begin{aligned} P(t, E = E_1) &= |\langle E_1|\psi(t)\rangle|^2 \\ &= \left|\langle E_1| \left[\frac{1}{2}(1+i)e^{-iE_1t/\hbar}|E_1\rangle + \frac{1}{2}(1-i)e^{-iE_2t/\hbar}|E_2\rangle\right]\right|^2 \\ &= \left|\left[\frac{1}{2}(1+i)e^{-iE_1t/\hbar}\langle E_1|E_1\rangle + \frac{1}{2}(1-i)e^{-iE_2t/\hbar}\langle E_1|E_2\rangle\right]\right|^2 \\ &= \left|\left[\frac{1}{2}(1+i)e^{-iE_1t/\hbar} + 0\right]\right|^2 \\ &= \frac{1}{2} \end{aligned}$$

In the above we have used the orthonormality of $|E_1\rangle$ and $|E_2\rangle$ (i.e. $\langle E_1|E_1\rangle = 1$, $\langle E_1|E_2\rangle = 0$) and $|e^{-iE_1t/\hbar}|^2 = 1$.

In the same manner we get

$$\begin{aligned}
P(t, E = E_2) &= |\langle E_2|\psi(t)\rangle|^2 \\
&= \left|\langle E_2| \left[\frac{1}{2}(1+i)e^{-iE_1t/\hbar}|E_1\rangle + \frac{1}{2}(1-i)e^{-iE_2t/\hbar}|E_2\rangle\right]\right|^2 \\
&= \left|\left[\frac{1}{2}(1+i)e^{-iE_1t/\hbar}\langle E_2|E_1\rangle + \frac{1}{2}(1-i)e^{-iE_2t/\hbar}\langle E_2|E_2\rangle\right]\right|^2 \\
&= \left|\left[0 + \frac{1}{2}(1+i)e^{-iE_2t/\hbar}\right]\right|^2 \\
&= \frac{1}{2}
\end{aligned}$$

Once again the two probabilities add up to 1, for the same reason - the states $|E_1\rangle$ and $|E_2\rangle$ are mutually orthogonal for a two-state system. Note that the probabilities of finding the system in an energy eigenstates is *independent of time*, that is, they are same as at time $t = 0$, as we have seen in the previous problem. This is true in general when the Hamiltonian is time independent. But we have also seen that the probabilities of finding the system in some arbitrary state, such as $|1\rangle$ and $|2\rangle$ considered above, in general vary with time.