PHYS-C0252 - Quantum Mechanics

Exercise set 3 - model solutions

Due date: May 15, 2024 by 23:59 on MyCourses
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1. Consider the temporal evolution of quantum states $\{|\psi\rangle\}$ determined by a Hamiltonian $\hat{H}(t)$. We define the evolution operator $\hat{U}(t, t_0)$ as

$$\hat{U}(t, t_0)|\psi(t_0)\rangle = |\psi(t)\rangle, \text{ for all } t \geq t_0 \in \mathbb{R} \text{ and } |\psi(t_0)\rangle \in \mathcal{H}$$

(a) Prove the following identities:

i. $\hat{U}(t_0, t_0) = \hat{I}$, for all $t_0 \in \mathbb{R}$.

ii. $\hat{U}^\dagger(t, t_0)\hat{U}(t, t_0) = \hat{I}$, for all $t > t_0 \in \mathbb{R}$. Hint: Calculate $\partial_t[\hat{U}^\dagger(t, t_0)\hat{U}(t, t_0)]$, use the Schrödinger equation equivalent for $\hat{U}(t, t_0)$, and use the result of i. as an initial condition. Note that we do not assume the Hamiltonian to be independent of time.

iii. $\hat{U}(t_2, t_0) = \hat{U}(t_2, t_1)\hat{U}(t_1, t_0)$, for all $t_0 < t_1 < t_2 \in \mathbb{R}$.

(b) Construct the evolution operator $\hat{U}(t, t_0)$ for a time-dependent Hamiltonian $\hat{H}(t)$ using the following steps:

1. Using the Schrödinger equation for U, show that U is formally given by

$$U(t, t_0) = \hat{I} + \sum_{n=1}^{\infty} \left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \cdots \int_{t_0}^{t_{n-1}} \mathrm{d}t_n \, \hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n).$$

2. Find $U(t, t_0)$ when $\hat{H}$ is time-independent using the fact that

$$\int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \cdots \int_{t_0}^{t_{n-1}} \mathrm{d}t_n \, C = \frac{1}{n!} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t} \mathrm{d}t_2 \cdots \int_{t_0}^{t} \mathrm{d}t_n \, C$$

for a constant C.

3. Find an expression for $U(t, t_0)$ when $\hat{H}$ is piecewise constant in time. Use the above result, divide the interval $[t_0, t]$ into n intervals $[t_0, t_1]$, $(t_1, t_2]$, $\ldots$, $(t_{n-1}, t_n]$, where $t_k = t_0 + k\delta t$, $t_n = t$, and assume that $\hat{H}$ is constant in each interval and that $\hat{H}(t_k)$ commute.

4. Take the limit $\delta t \to 0$ to convert the sum in the above result to an integral in order to obtain the final result for $U(t, t_0)$.

Solution:

(a) i. By definition,

$$\hat{U}(t_0, t_0)|\psi(t_0)\rangle = |\psi(t_0)\rangle,$$

thus $\hat{U}(t_0, t_0) = \hat{I}$.

ii. Consider the time-dependent Schrödinger's equation:

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \hat{H}|\psi(t)\rangle.$$

Substitute $|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle$

$$i\hbar\frac{\partial\hat{U}(t,t_0)}{\partial t}|\psi(t_0)\rangle = \hat{H}\hat{U}(t,t_0)|\psi(t_0)\rangle.$$

For this to hold for any $|\psi(t_0)\rangle$, the operators on the LHS and RHS should be equal:

$$i\hbar\frac{\partial\hat{U}(t,t_0)}{\partial t} = \hat{H}\hat{U}(t,t_0).$$
$$\Rightarrow \frac{\partial\hat{U}(t,t_0)}{\partial t} = \frac{-i}{\hbar}\hat{H}\hat{U}(t,t_0).$$

This is the Schrödinger equation equivalent for $\hat{U}(t,t_0)$. Using the chain rule and $\frac{\partial}{\partial t}(\hat{A}(t)^\dagger) = \left(\frac{\partial}{\partial t}\hat{A}(t)\right)^\dagger$, we have

$$\begin{aligned}\frac{\partial}{\partial t}\left(\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0)\right) &= \hat{U}^\dagger(t,t_0)\frac{\partial\hat{U}(t,t_0)}{\partial t} + \frac{\partial\hat{U}^\dagger(t,t_0)}{\partial t}\hat{U}(t,t_0)\\ &= \frac{-i}{\hbar}\hat{U}^\dagger(t,t_0)(\hat{H}\hat{U}(t,t_0)) + \frac{i}{\hbar}(\hat{U}^\dagger(t,t_0)\hat{H})\hat{U}(t,t_0)\\ &= 0.\end{aligned}$$

Thus, the time derivative of $\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0)$ is zero, i.e., it is a constant, independent of t. We can thus choose $t = t_0$, and using the result of (i), we then have

$$\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0) = \hat{U}^\dagger(t_0,t_0)\hat{U}(t_0,t_0) = \hat{I}^\dagger\hat{I} = \hat{I}.$$

iii. Using the definition of $\hat{U}$, we have

$$|\psi(t_1)\rangle = \hat{U}(t_1,t_0)|\psi(t_0)\rangle$$

$$|\psi(t_2)\rangle = \hat{U}(t_2,t_1)|\psi(t_1)\rangle = \hat{U}(t_2,t_1)\hat{U}(t_1,t_0)|\psi(t_0)\rangle.$$

thus

$$\hat{U}(t_2,t_0) = \hat{U}(t_2,t_1)\hat{U}(t_1,t_0).$$

(b) 1. Consider the Schrödinger equation equivalent for $\hat{U}(t,t_0)$.

$$\mathrm{i}\hbar\frac{\partial\hat{U}(t,t_0)}{\partial t} = \hat{H}(t)\hat{U}(t,t_0).$$

We must solve this operator differential equation subject to the initial condition $\hat{U}(t_0,t_0) = \hat{I}$. Integrating both sides of the differential equation and using the initial condition, we get the following integral equation:

$$\hat{U}(t,t_0) = \hat{I} - \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\hat{H}(t_1)\hat{U}(t_1,t_0)dt_1.$$

By recursively inserting the RHS of this equation in place of U on the RHS, we get a series of equations

$$\begin{aligned} U(t,t_0) &= \hat{I} - \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t} \hat{H}(t_1)\left(\hat{I} - \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t_1} \hat{H}(t_2)\hat{U}(t_2,t_0)dt_2\right)dt_1 \\ &= \hat{I} - \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t} \hat{H}(t_1)dt_1 - \frac{1}{\hbar^2}\int_{t_0}^{t}\int_{t_0}^{t_1} \hat{H}(t_1)\hat{H}(t_2)\hat{U}(t_2,t_0)dt_1 dt_2, \end{aligned}$$

and so on. Repeating this n times, this produces a sum on the RHS, where the nth term is

$$\left(\frac{-\mathrm{i}}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n\ \hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n)\hat{U}(t_n,t_0),$$

and the other terms up to $(n-1)$ will only contain $\hat{H}$, not $\hat{U}$. When we take the limit $n \longrightarrow \infty$, the contribution of $U(t_n,t_0)$ in the $\int_{t_0}^{t_{n-1}} dt_n$ term vanishes, so we obtain the infinite series expansion

$$\hat{U}(t,t_0) = \hat{I} + \sum_{n=1}^{\infty}\left(\frac{-\mathrm{i}}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n\ \hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n).$$

This expansion is called the Dyson series.

2. Since the Hamiltonian is time independent, we can factor it out in the front to obtain

$$\begin{aligned} \hat{U}(t,t_0) &= \hat{I} + \sum_{n=1}^{\infty}\left(\frac{-\mathrm{i}}{\hbar}\right)^n \hat{H}^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \\ &= \hat{I} + \sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{-\mathrm{i}}{\hbar}\right)^n \hat{H}^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \qquad \text{(Using the given relation)} \\ &= \hat{I} + \sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{-\mathrm{i}}{\hbar}\right)^n \hat{H}^n \cdot (t-t_0)^n \\ &= \hat{I} + \sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{-\mathrm{i}}{\hbar}(t-t_0)\hat{H}\right)^n = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{-\mathrm{i}}{\hbar}(t-t_0)\hat{H}\right)^n \\ &= \exp\left(\frac{-\mathrm{i}}{\hbar}(t-t_0)\hat{H}\right). \end{aligned}$$

3. The Hamiltonian $\hat{H}$ depends on time but the operators $\hat{H}(t_k)$ corresponding to different moments of time commute. Dividing the interval $[t_0,t]$ into intervals $[t_0,t_1)$, $[t_1,t_2)$, $\ldots$, $(t_{n-1},t_n]$, based on the above result, the time evolution operator $U(t_{k+1},t_k)$ for each interval is given by

$$U(t_{k+1},t_k) = \exp\left(\frac{-\mathrm{i}}{\hbar}(t_{k+1}-t_k)\hat{H}(t_k)\right)$$

and based on the result of part (a) (iii), we have

$$\begin{aligned} U(t,t_0) &= \hat{U}(t,t_{n-1})\hat{U}(t_{n-1},t_{n-2})\cdots\hat{U}(t_1,t_0) \\ &= e^{-\mathrm{i}\hat{H}(t_n)\delta t/\hbar}\, e^{-\mathrm{i}\hat{H}(t_{n-1})\delta t/\hbar}\cdots e^{-\mathrm{i}\hat{H}(t_0)\delta t/\hbar}, \end{aligned}$$

where $\delta t = t_{k+1} - t_k$. When $\hat{A}$ and $\hat{B}$ commute, we can use the relation $e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}}$, so that we obtain

$$U(t, t_0) = \exp\left(\frac{-\mathrm{i}}{\hbar}\sum_{m=0}^{n} H(t_m)\delta t\right)$$

4. Taking the limit converts the sum to an integral: $\lim_{\delta t\to 0}\sum_{m=0}^{n} H(t_m)\delta t = \int_{t_0}^{t}\hat{H}(t')dt'$, so that we obtain

$$U(t, t_0) = \exp\left(\frac{-\mathrm{i}}{\hbar}\int_{t_0}^{t}\hat{H}(t')dt'\right).$$

2. Let $\vec{a}$ be any real-valued three-dimensional unit vector and $\theta \in \mathbb{R}$.

   (a) Prove that
   $$\mathrm{e}^{\mathrm{i}\theta(\vec{a}\cdot\hat{\vec{\sigma}})} = \hat{I}\cos(\theta) + \mathrm{i}(\vec{a}\cdot\hat{\vec{\sigma}})\sin(\theta),$$
   where $\vec{a}\cdot\hat{\vec{\sigma}} = a_x\hat{\sigma}_x + a_y\hat{\sigma}_y + a_z\hat{\sigma}_z$, $\{a_k\}$ are the Cartesian components of $\vec{a}$, and $\{\hat{\sigma}_k\}$ are the Pauli matrices. Hint: Use the Taylor series definition of the operator exponential. Then, try to find a simplified expression for $(\theta\vec{a}\cdot\hat{\vec{\sigma}})^k$, depending on whether k is even or odd.

   (b) Consider the operator $\mathrm{e}^{-\mathrm{i}\frac{\pi}{2}(\vec{a}\cdot\hat{\vec{\sigma}})}$. Show that the case
   $$\vec{a} = \vec{z} = \begin{bmatrix}0\\0\\1\end{bmatrix}$$
   corresponds to a rotation by the angle π about the z axis of the Bloch sphere. Hint: operate on lea general state $|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$ and compare the Bloch vectors of the original and resultant states. Also note that you can always ignore the global phase, that is,
   $$e^{\mathrm{i}\phi_1}|0\rangle + e^{\mathrm{i}\phi_2}|1\rangle = \underbrace{e^{\mathrm{i}\phi_1}}_{\text{global phase}}\left(|0\rangle + e^{\mathrm{i}(\phi_2-\phi_1)}|1\rangle\right)$$
   has the same Bloch sphere representation as
   $$|0\rangle + e^{\mathrm{i}(\phi_2-\phi_1)}|1\rangle.$$
   If you want, you can also show that $\vec{a} = \vec{x}$ and $\vec{a} = \vec{y}$ correspond to rotations about the x and y axis, respectively (but points are awarded only for the case $\vec{a} = \vec{z}$).

Solution:

Consider the series expansion of $\mathrm{e}^{\mathrm{i}\theta(\vec{a}\cdot\hat{\vec{\sigma}})}$

$$\begin{aligned}\mathrm{e}^{\mathrm{i}\theta(\vec{a}\cdot\hat{\vec{\sigma}})} &= \sum_{k=0}^{\infty}\frac{1}{k!}(\mathrm{i}\theta\vec{a}\cdot\hat{\vec{\sigma}})^k \\ &= \sum_{k'=0}^{\infty}\frac{(-1)^{k'}}{(2k')!}\left(\theta\vec{a}\cdot\hat{\vec{\sigma}}\right)^{2k'} + \sum_{k'=0}^{\infty}\frac{\mathrm{i}(-1)^{k'}}{(2k'+1)!}\left(\theta\vec{a}\cdot\hat{\vec{\sigma}}\right)^{2k'+1},\end{aligned}$$

where the first sum is over the even and the second over the odd values of k, and we have used the fact that $\mathrm{i}^{2k} = (\mathrm{i}^2)^k = (-1)^k$ and $\mathrm{i}^{2k+1} = \mathrm{i} \cdot \mathrm{i}^{2k} = \mathrm{i}(-1)^{2k}$. Note that

$$\left(\vec{a} \cdot \hat{\vec{\sigma}}\right)^2 = \sum_{i,j} a_i a_j \hat{\sigma}_i \hat{\sigma}_j$$

where i, j are x, y, z,

$$\hat{\sigma}_i \hat{\sigma}_j + \hat{\sigma}_j \hat{\sigma}_i = 0$$

and

$$\hat{\sigma}_i^2 = \hat{I}.$$

Thus

$$(\vec{a} \cdot \hat{\vec{\sigma}})^2 = \sum_i a_i^2 \hat{I} = \hat{I},$$

since $\vec{a}$ is a unit vector. From this, we obtain

$$\left(\theta \vec{a} \cdot \hat{\vec{\sigma}}\right)^{2k'} = \theta^{2k'} \hat{I}$$
$$\left(\theta \vec{a} \cdot \hat{\vec{\sigma}}\right)^{2k'+1} = \theta^{2k'+1} \, \vec{a} \cdot \hat{\vec{\sigma}},$$

and therefore

$$\begin{aligned}
\mathrm{e}^{\mathrm{i}\theta(\vec{a}\cdot\vec{\sigma})} &= \sum_{k'}^{\infty} \frac{(-1)^{k'}}{(2k')!} (\theta \vec{a} \cdot \hat{\vec{\sigma}})^{2k'} + \sum_{k'}^{\infty} \frac{\mathrm{i}(-1)^{k'}}{(2k'+1)!} (\theta \vec{a} \cdot \hat{\vec{\sigma}})^{2k'+1} \\
&= \sum_{k'}^{\infty} \frac{(-1)^{k'}}{(2k')!} \theta^{2k'} \hat{I} + \sum_{k'}^{\infty} \frac{\mathrm{i}(-1)^{k'}}{(2k'+1)!} \theta^{2k'+1} \vec{a} \cdot \hat{\vec{\sigma}} \\
&= \hat{I} \cos(\theta) + \mathrm{i}(\vec{a} \cdot \hat{\vec{\sigma}}) \sin(\theta).
\end{aligned}$$

(b) Take a general state

$$|\psi\rangle = \cos(\theta/2)\,|0\rangle + e^{i\phi} \sin(\theta/2)\,|1\rangle \;\hat{=}\; \begin{bmatrix} \cos(\theta/2) \\ e^{i\phi} \sin(\theta/2) \end{bmatrix}$$

with the Bloch representation

$$\vec{\psi} = \begin{bmatrix} \cos\phi \sin\theta \\ \sin\phi \sin\theta \\ \cos\theta \end{bmatrix}$$

And check the action of $e^{-i\frac{\pi}{2}(\vec{a}\cdot\vec{\sigma})}$

From part (a), we know

$$e^{-i\frac{\pi}{2}(\vec{a}\cdot\vec{\sigma})} = \hat{I} \cos\left(\frac{\pi}{2}\right) + i(\vec{a} \cdot \vec{\sigma}) \sin\left(\frac{\pi}{2}\right) = i(\vec{a} \cdot \vec{\sigma})$$

.

Take

$$\vec{a} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \Rightarrow \vec{a} \cdot \vec{\sigma} = \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

to find

$$e^{-i\frac{\pi}{2}(\vec{a}\cdot\vec{\sigma})} |\psi\rangle = i \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \cos(\theta/2) \\ e^{i\phi}\sin(\theta/2) \end{bmatrix} = i \begin{bmatrix} \cos(\theta/2) \\ -e^{i\phi}\sin(\theta/2) \end{bmatrix} = i \begin{bmatrix} \cos(\theta/2) \\ e^{i\pi}e^{i\phi}\sin(\theta/2) \end{bmatrix}$$

$$= i \begin{bmatrix} \cos(\theta/2) \\ e^{i(\phi+\pi)}\sin(\theta/2) \end{bmatrix},$$

where we made use of the Euler's formula $e^{i\pi} = -1$. We can ignore the global phase i to get

$$\begin{bmatrix} \cos(\theta/2) \\ e^{i(\phi+\pi)}\sin(\theta/2) \end{bmatrix},$$

which has the Bloch sphere representation

$$\begin{bmatrix} \cos(\phi+\pi)\sin(\theta) \\ \sin(\phi+\pi)\sin(\theta) \\ \cos(\theta) \end{bmatrix},$$

meaning our Bloch angle ϕ has changed to $\phi + \pi$. Using the identities

$$\sin(\phi+\pi) = -\sin\phi,$$
$$\cos(\phi+\pi) = -\cos\phi,$$

this is

$$\begin{bmatrix} -\cos\phi\sin\theta \\ -\sin\phi\sin\theta \\ \cos\theta \end{bmatrix},$$

which is the same as the original Bloch vector, but with the x and y components having the opposite sign, meaning that it's a rotation about the z axis. Another option is to confirm this by drawing.

X and Y rotations (optional)

Similarly for

$$\vec{a} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \Rightarrow \vec{a} \cdot \vec{\sigma} = \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

to find

$$e^{-i\frac{\pi}{2}(\vec{a}\cdot\vec{\sigma})} |\psi\rangle = i \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \cos(\theta/2) \\ e^{i\phi}\sin(\theta/2) \end{bmatrix} = i \begin{bmatrix} e^{i\phi}\sin(\theta/2) \\ \cos(\theta/2) \end{bmatrix} = ie^{i\phi} \begin{bmatrix} \sin(\theta/2) \\ e^{-i\phi}\cos(\theta/2) \end{bmatrix}$$

$$= ie^{i\phi} \begin{bmatrix} -\cos\left(\frac{\theta+\pi}{2}\right) \\ e^{-i\phi}\sin\left(\frac{\theta+\pi}{2}\right) \end{bmatrix} = -ie^{i\phi} \begin{bmatrix} \cos\left(\frac{\theta+\pi}{2}\right) \\ e^{-i(\phi+\pi)}\sin\left(\frac{\theta+\pi}{2}\right) \end{bmatrix},$$

where in the last step, we have used $e^{-i(\phi+\pi)} = e^{-i\phi}e^{-i\pi} = -e^{-i\phi}$. We can ignore the global phase $-ie^{i\phi}$ to get

$$\begin{bmatrix} \cos\left(\frac{\theta+\pi}{2}\right) \\ e^{-i(\phi+\pi)} \sin\left(\frac{\theta+\pi}{2}\right) \end{bmatrix},$$

which has the Bloch sphere representation

$$\begin{bmatrix} \cos(-\phi-\pi)\sin(\theta+\pi) \\ \sin(-\phi-\pi)\sin(\theta+\pi) \\ \cos(\theta+\pi) \end{bmatrix},$$

meaning our Bloch angles have changed to $\theta \to \theta+\pi$, $\phi \to -\phi-\pi$. We can simplify this vector to

$$\begin{bmatrix} \cos\phi\sin\theta \\ -\sin\phi\sin\theta \\ -\cos\theta \end{bmatrix},$$

which is the same as the original Bloch vector, but with the y and z components having the opposite sign, meaning that it's a rotation about the x axis.

Finally, consider

$$\vec{a} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \Rightarrow \vec{a}\cdot\vec{\sigma} = \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}.$$

We get

$$e^{-i\pi(\vec{a}\cdot\vec{\sigma})/2}|\psi\rangle = i\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} \cos(\theta/2) \\ e^{i\phi}\sin(\theta/2) \end{bmatrix} = \begin{bmatrix} e^{i\phi}\sin(\theta/2) \\ -\cos(\theta/2) \end{bmatrix}$$

$$= -e^{i\phi}\begin{bmatrix} -\sin(\theta/2) \\ e^{-i\phi}\cos(\theta/2) \end{bmatrix} = -e^{i\phi}\begin{bmatrix} \cos\left(\frac{\theta+\pi}{2}\right) \\ e^{-i\phi}\sin\left(\frac{\theta+\pi}{2}\right) \end{bmatrix}$$

again, we ignore the global phase to get

$$\begin{bmatrix} \cos\left(\frac{\theta+\pi}{2}\right) \\ e^{-i\phi}\sin\left(\frac{\theta+\pi}{2}\right) \end{bmatrix},$$

which has the Bloch representation

$$\begin{bmatrix} \cos(-\phi)\sin(\theta+\pi) \\ \sin(-\phi)\sin(\theta+\pi) \\ \cos(\theta+\pi) \end{bmatrix},$$

meaning our Bloch angles have changed as $\phi \to -\phi$, $\theta \to \theta+\pi$, which is a rotation about the y axis.

3. Consider a system described by the Hamiltonian $\hat{H} = \epsilon(-\mathrm{i}|0\rangle\langle 1| + \mathrm{i}|1\rangle\langle 0|)$, where $\{|0\rangle, |1\rangle\}$ form an orthonormal basis of the considered Hilbert space and ϵ is a real-valued constant with the dimension of energy. The eigenergies of $\hat{H}$ are $\pm\epsilon$ and the corresponding eigenstates are

$$|\epsilon\rangle = \frac{|0\rangle + \mathrm{i}\,|1\rangle}{\sqrt{2}}, \qquad |-\epsilon\rangle = \frac{|0\rangle - \mathrm{i}\,|1\rangle}{\sqrt{2}}.$$

.

   (a) (2 points) What are the probabilities to measure ϵ and $-\epsilon$ if the system is in the state $|1\rangle$? What is the value of $\langle H\rangle$?

   (b) (4 points) Find the state $|\psi(t)\rangle$ at an arbitrary time t, when the system is initially in the state $|\psi(t=0)\rangle = |0\rangle$. What is the probability to find the system in the state $|0\rangle$ as a function of time? How does $\langle H\rangle$ change with time? Hint: you need to solve the Schrödinger equation.

Solution:

(a)

$$|1\rangle = \frac{-\mathrm{i}}{\sqrt{2}}\left(|\epsilon\rangle - |-\epsilon\rangle\right) \Rightarrow \begin{cases} P(\epsilon) = |\langle \epsilon|1\rangle|^2 = \left|\frac{-\mathrm{i}}{\sqrt{2}}\right|^2 = \frac{1}{2} \\ P(-\epsilon) = |\langle -\epsilon|1\rangle|^2 = \left|\frac{\mathrm{i}}{\sqrt{2}}\right|^2 = \frac{1}{2} \end{cases}$$

$$\langle H\rangle = \frac{1}{2}\cdot\epsilon + \frac{1}{2}\cdot(-\epsilon) = 0$$

(b) In the case of a time-independent Hamiltonian, the Schrödinger equation is solved by (See chapter 5.2 in the lecture notes)

$$|\psi(t)\rangle = \sum_m c_m(t)\,|\psi_m\rangle = \sum_m c_m(0)e^{-\mathrm{i}E_m t/\hbar}\,|\psi_m\rangle\,,$$

where $\{|\psi_m\rangle\}$ is an eigenbasis of the Hamiltonian and $\{E_m\}$ are the corresponding eigenvalues. Since $\{|\epsilon\rangle, |-\epsilon\rangle\}$ is an eigenbasis of the Hamiltonian, we identify $E_1 = \epsilon,\ E_2 = -\epsilon,\ c_1(0) = c_2(0) = \frac{1}{\sqrt{2}}$, and write

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}e^{-\mathrm{i}\epsilon t/\hbar}\,|\epsilon\rangle + \frac{1}{\sqrt{2}}e^{\mathrm{i}\epsilon t/\hbar}\,|-\epsilon\rangle\,,$$

from which we also find

$$\langle H\rangle(t) = \langle \epsilon|\psi(t)\rangle\,\epsilon - \langle -\epsilon|\psi(t)\rangle\,\epsilon = \frac{1}{2}\epsilon - \frac{1}{2}\epsilon = 0 = \langle H\rangle(0),$$

meaning the expectation value does not change. For a system with a time-independent Hamiltonian, it is generally true that the expectation value of the Hamiltonian does not change with time, which is evident from the fact that, according to the Schrödinger equation, the eigenstates of the Hamiltonian gain a complex phase $e^{iEt/\hbar}$ with time, but the amplitude of their coefficients does not change, since $|e^{iEt/\hbar}| = 1$.

To find $P(|0\rangle, t)$, it is useful to express $|\psi(t)\rangle$ in the $\{|0\rangle, |1\rangle\}$ basis:

$$\begin{aligned}
|\psi(t)\rangle &= \frac{1}{2}e^{-\mathrm{i}\epsilon t/\hbar}\left(|0\rangle + \mathrm{i}\,|1\rangle\right) + \frac{1}{2}e^{\mathrm{i}\epsilon t/\hbar}\left(|0\rangle - \mathrm{i}\,|1\rangle\right) \\
&= \frac{1}{2}\left(e^{\mathrm{i}\epsilon t/\hbar} + e^{-\mathrm{i}\epsilon t/\hbar}\right)|0\rangle - \frac{1}{2}\left(e^{\mathrm{i}\epsilon t/\hbar} - e^{-\mathrm{i}\epsilon t/\hbar}\right)|1\rangle \\
&= \cos\left(\frac{\epsilon t}{\hbar}\right)|0\rangle - \sin\left(\frac{\epsilon t}{\hbar}\right)|1\rangle .
\end{aligned}$$

Then,

$$P(|0\rangle, t) = |\langle 0|\psi(t)\rangle|^2 = \cos^2\left(\frac{\epsilon t}{\hbar}\right) = \frac{1}{2} + \frac{1}{2}\cos\left(\frac{2\epsilon t}{\hbar}\right).$$

Similarly, you can also find

$$P(|1\rangle, t) = \frac{1}{2} - \frac{1}{2}\cos\left(\frac{2\epsilon t}{\hbar}\right).$$

Notice that these results mean that the system starts out at $P(|0\rangle, 0) = 1$ (as we wanted), after which the probability to find the system in a particular state oscillates with frequency $\frac{2\epsilon}{\hbar}$. On the Bloch sphere, this corresponds to the Bloch vector rotating on the surface of the sphere along the x-z plane.

(4) Consider a peculiar gate known as square-root of NOT with the matrix representation

$$\sqrt{\mathrm{NOT}} \mathrel{\hat{=}} \frac{1}{2}\begin{bmatrix} 1+\mathrm{i} & 1-\mathrm{i} \\ 1-\mathrm{i} & 1+\mathrm{i} \end{bmatrix}.$$

(a) Is this gate unitary? Is it Hermitian? How does it act on the $|0\rangle$ and $|1\rangle$ basis states?

(b) Show that the square-root of NOT gate is worthy of its name by verifying that $\left(\sqrt{\mathrm{NOT}}\right)^2 = \sigma_x$.

(c) Let us define the action of the following gates on a two-qubit system:

$$\mathrm{NOT}^{(2)}|x0\rangle = |x1\rangle, \quad \mathrm{NOT}^{(2)}|x1\rangle = |x0\rangle, \tag{1}$$

$$H^{(2)}|x0\rangle = \frac{1}{\sqrt{2}}\left(|x0\rangle + |x1\rangle\right), \quad H^{(2)}|x1\rangle = \frac{1}{\sqrt{2}}\left(|x0\rangle - |x1\rangle\right), \tag{2}$$

$$\mathrm{CNOT}^{(2,1)}|x0\rangle = |x0\rangle, \quad \mathrm{CNOT}^{(2,1)}|01\rangle = |11\rangle, \quad \mathrm{CNOT}^{(2,1)}|11\rangle = |01\rangle, \tag{3}$$

where $x \in \{0, 1\}$, so for instance $\mathrm{NOT}^{(2)}|00\rangle = |01\rangle$. The matrix representation of $\mathrm{NOT}^{(2)}$ is

$$\mathrm{NOT}^{(2)} \mathrel{\hat{=}} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix},$$

which you can verify by operating on the basis states and checking that they match the definition (1). Find the matrix representations for $H^{(2)}$ and $\mathrm{CNOT}^{(2,1)}$.

(d) Either by using the action of the gates defined in equations (1-3) or by using the matrices derived in the previous problem, find a series of gates to construct the Bell state $\frac{1}{\sqrt{2}}\left(|00\rangle - |11\rangle\right)$ starting from $|00\rangle$.

Solution:

(a)

$$\sqrt{\mathrm{NOT}}^\dagger = \frac{1}{2}\begin{bmatrix} 1-\mathrm{i} & 1+\mathrm{i} \\ 1+\mathrm{i} & 1-\mathrm{i}\end{bmatrix} \neq \sqrt{\mathrm{NOT}},$$

hence $\sqrt{\mathrm{NOT}}$ is *not* Hermitian. Let's check if it is unitary:

$$\begin{aligned}\sqrt{\mathrm{NOT}}^\dagger\sqrt{\mathrm{NOT}} &= \frac{1}{4}\begin{bmatrix} 1-\mathrm{i} & 1+\mathrm{i} \\ 1+\mathrm{i} & 1-\mathrm{i}\end{bmatrix}\begin{bmatrix} 1+\mathrm{i} & 1-\mathrm{i} \\ 1-\mathrm{i} & 1+\mathrm{i}\end{bmatrix} \\ &= \frac{1}{4}\begin{bmatrix} 1+1+1+1 & 1-1+1-1 \\ 1-1+1-1 & 1+1+1+1\end{bmatrix} = \frac{1}{4}\begin{bmatrix} 4 & 0 \\ 0 & 4\end{bmatrix} = I,\end{aligned}$$

$$\begin{aligned}\sqrt{\mathrm{NOT}}\sqrt{\mathrm{NOT}}^\dagger &= \frac{1}{4}\begin{bmatrix} 1+\mathrm{i} & 1-\mathrm{i} \\ 1-\mathrm{i} & 1+\mathrm{i}\end{bmatrix}\begin{bmatrix} 1-\mathrm{i} & 1+\mathrm{i} \\ 1+\mathrm{i} & 1-\mathrm{i}\end{bmatrix} \\ &= \frac{1}{4}\begin{bmatrix} 1+1+1+1 & 1-1+1-1 \\ 1-1+1-1 & 1+1+1+1\end{bmatrix} = \frac{1}{4}\begin{bmatrix} 4 & 0 \\ 0 & 4\end{bmatrix} = I,\end{aligned}$$

thus $\sqrt{\mathrm{NOT}}$ *is* unitary.

(b) By direct calculation

$$\begin{aligned}\sqrt{\mathrm{NOT}}^2 = \sqrt{\mathrm{NOT}}\sqrt{\mathrm{NOT}} &= \frac{1}{2}\begin{bmatrix} 1+\mathrm{i} & 1-\mathrm{i} \\ 1-\mathrm{i} & 1+\mathrm{i}\end{bmatrix}\frac{1}{2}\begin{bmatrix} 1+\mathrm{i} & 1-\mathrm{i} \\ 1-\mathrm{i} & 1+\mathrm{i}\end{bmatrix} \\ &= \frac{1}{4}\begin{bmatrix} 1-1+1-1 & 1+1+1+1 \\ 1+1+1+1 & 1-1+1-1\end{bmatrix} = \frac{1}{4}\begin{bmatrix} 0 & 4 \\ 4 & 0\end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0\end{bmatrix} = \sigma_x.\end{aligned}$$

As an aside, let's think about $\sqrt{\mathrm{NOT}}$ gate in terms of its operation on the Bloch sphere. From Exercise 2 you might have already surmised that $e^{\mathrm{i}\theta(\vec{a}\cdot\hat{\vec{\sigma}})}$ generates a rotation by an angle 2θ around the axis spanned by the vector $\vec{a}$. Specifically, we have seen that up to a global phase factor, the Pauli operators $\{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$ generate rotations by an angle π about the x, y, and z axes, respectively. Consequently, if one thinks about it geometrically, one might suspect that the "square-root" of $\hat{\sigma}_x$ is an operation that should take you to the half-way point of this rotation, i.e. it would generate a rotation about the x axis by an angle $\pi/2$. Let us verify this intuition. First, we can decompose $\sqrt{\mathrm{NOT}}$ in terms of the Pauli matrices and the identity matrix as follows:

$$\begin{aligned}\sqrt{\mathrm{NOT}} &= \frac{1}{2}\begin{bmatrix} 1+\mathrm{i} & 1-\mathrm{i} \\ 1-\mathrm{i} & 1+\mathrm{i}\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} \frac{1+\mathrm{i}}{\sqrt{2}} & \frac{1-\mathrm{i}}{\sqrt{2}} \\ \frac{1-\mathrm{i}}{\sqrt{2}} & \frac{1+\mathrm{i}}{\sqrt{2}}\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} e^{\mathrm{i}\frac{\pi}{4}} & e^{-\mathrm{i}\frac{\pi}{4}} \\ e^{-\mathrm{i}\frac{\pi}{4}} & e^{\mathrm{i}\frac{\pi}{4}}\end{bmatrix} \\ &= \frac{e^{\mathrm{i}\frac{\pi}{4}}}{\sqrt{2}}\begin{bmatrix} 1 & e^{-\mathrm{i}\frac{\pi}{2}} \\ e^{-\mathrm{i}\frac{\pi}{2}} & 1\end{bmatrix} = \frac{e^{\mathrm{i}\frac{\pi}{4}}}{\sqrt{2}}\begin{bmatrix} 1 & -\mathrm{i} \\ -\mathrm{i} & 1\end{bmatrix} = e^{\mathrm{i}\frac{\pi}{4}}\left(\frac{1}{\sqrt{2}}I - \frac{1}{\sqrt{2}}\mathrm{i}\sigma_x\right).\end{aligned}$$

Now, from basic trigonometry we may recognize $\frac{1}{\sqrt{2}}$ and $-\frac{1}{\sqrt{2}}$ as the cosine and sine of the angle $-\pi/4$, which, combined with the idenitity derived in Exercise 2a allows us to write

$$\sqrt{\mathrm{NOT}} = e^{\mathrm{i}\frac{\pi}{4}} \left[I \cos\left(-\frac{\pi}{4}\right) + \mathrm{i}\sigma_x \sin\left(-\frac{\pi}{4}\right)\right] = e^{\mathrm{i}\frac{\pi}{4}} e^{-\mathrm{i}\frac{\pi}{4}\sigma_x} \propto e^{\mathrm{i}\left(-\frac{\pi}{4}\right)\sigma_x}.$$

Ignoring the global phase constant, we see that $\sqrt{\mathrm{NOT}}$ corresponds to a rotation by angle $-\pi/2$ about the x axis. Although the rotation angle is negative, performing it twice we will get us to the same pole on the opposite side of the Bloch sphere, and the sign refers to the clockwise/counterclockwise direction of rotation. So indeed, our geometrical guess was not a fluke! Additionally, we can infer that there are at least two ways to define $\sqrt{\mathrm{NOT}}$ relating to the direction of rotation of the state. Moreover, in the case of single-qubit systems that do not interact with the environment, the amount of possible $\sqrt{\mathrm{NOT}}$ is infinite, since the phase factor can be chosen arbitrarily. In quantum mechanics you get to learn that even abstract objects like matrices or operators can be exponentiated and have square-roots under certain circumstances, fascinating isn't it?

(c) The matrix representations are

$$H^{(2)} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix}, \ \mathrm{CNOT}^{(2,1)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}.$$

There are several ways you can find these; the fastest option may be to use the Feynman problem-solving algorithm: i) Write down the problem, ii) think very hard, iii) write down the answer.
By identifying the basis states as column vectors, it is possible to deduce the form of the matrix that has the action of the given gate on the basis vectors.
However, it is also possible to use methods that are more certain to terminate than the Feynman algorithm. For instance, one can use the typical method of finding matrix elements using inner products:

$$\langle 00|\hat{H}^{(2)}|00\rangle = \langle 00| \frac{1}{\sqrt{2}} \left(|00\rangle + |01\rangle\right) = \frac{1}{\sqrt{2}}$$
$$\langle 10|\hat{H}^{(2)}|00\rangle = \langle 10| \frac{1}{\sqrt{2}} \left(|00\rangle + |01\rangle\right) = 0,$$

and so on (and similarly for $\mathrm{CNOT}^{(2,1)}$). Another option is to use tensor products, if you are familiar with them. $H^{(2)}$ can be represented as a tensor product of the Identity operator on qubit 1, and the Hadamard gate on qubit 2:

$$H^{(2)} = I \otimes H = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \cdot \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix} & 0 \cdot \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \\ 0 \cdot \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} & 1 \cdot \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \end{bmatrix}$$

$$= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix}$$

$\mathrm{CNOT}^{(2,1)}$ is a sum of two tensor products: a NOT on qubit 1 and the projection onto state $|1\rangle$ on qubit 2, and the identity operator on qubit 1 and the projection onto state $|0\rangle$ on qubit 1:

$$\begin{aligned}
\mathrm{CNOT}^{(2,1)} &= \mathrm{NOT} \otimes P_1 + I \otimes P_0 \\
&= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \\
&= \begin{bmatrix} 0 \cdot \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} & 1 \cdot \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \\ 1 \cdot \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} & 0 \cdot \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \end{bmatrix} + \begin{bmatrix} 1 \cdot \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} & 0 \cdot \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \\ 0 \cdot \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} & 1 \cdot \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}
\end{aligned}$$

(d) A possible series of gates is $\mathrm{NOT}^{(2)} \to H^{(2)} \to \mathrm{CNOT}^{(2,1)}$, since

$$\begin{aligned}
\mathrm{CNOT}^{(2,1)} H^{(2)} \mathrm{NOT}^{(2)} |00\rangle &= \mathrm{CNOT}^{(2,1)} H^{(2)} |01\rangle \\
&= \frac{1}{\sqrt{2}} \mathrm{CNOT}^{(2,1)} (|00\rangle - |01\rangle) \\
&= \frac{1}{\sqrt{2}} \left(\mathrm{CNOT}^{(2,1)} |00\rangle - \mathrm{CNOT}^{(2,1)} |01\rangle \right) \\
&= \frac{1}{\sqrt{2}} (|00\rangle - |11\rangle) .
\end{aligned}$$

Note that the matrix representation of the full operation is

$$\mathrm{CNOT}^{(2,1)} H^{(2)} \mathrm{NOT}^{(2)} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \tag{4}$$

$$= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 1 \\ -1 & 1 & 0 & 0 \end{bmatrix} . \tag{5}$$

The problem can also be worded in the following way:
Given a gate $\hat{G}$ with the matrix representation

$$G = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 1 \\ -1 & 1 & 0 & 0 \end{bmatrix}, \tag{6}$$

and the action $\hat{G}\left|00\right\rangle = \frac{1}{\sqrt{2}}\left(\left|00\right\rangle - \left|11\right\rangle\right)$, find the decomposition into the gateset $\{\mathrm{NOT}^{(2)}, H^{(2)}, \mathrm{CNOT}^{(2,1)}\}$. Such problems are a very integral part of quantum computing. Just like a classical computer, a quantum computer is only capable of running a few different elementary operations. All gates/algorithms more complicated than these basic operations need to be decomposed into a series of basic operations. This process is called *Quantum compiling*.