Sakurai Chapter-2
Solution

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
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((**2-1**))

1. Consider the spin-precession problem discussed in the text. It can also be solved in the Heisenberg picture. Using the Hamiltonian

$$H = -\left(\frac{eB}{mc}\right)S_z = \omega S_z,$$

write the Heisenberg equations of motion for the time-dependent operators $S_x(t)$, $S_y(t)$, and $S_z(t)$. Solve them to obtain $S_{x,y,z}$ as functions of time.

((**Solution**))

S_x, S_y, and S_z are the operators in the Schrödinger picture and $S_x(t)$, $S_y(t)$, and $S_z(t)$ are the operators in the Heisenberg picture:

$$S_i(t) = e^{\frac{i}{\hbar}Ht} S_i e^{-\frac{i}{\hbar}Ht}$$

$$\dot{S}_i(t) = \frac{1}{i\hbar}[S_i(t), H]$$

$$\frac{dS_z(t)}{dt} = \frac{1}{i\hbar}[S_z(t), \omega S_z] = \frac{1}{i\hbar}[S_z(t), \omega S_z(t)] = 0$$

$$S_z(t) = S_z \qquad \text{(no time dependent)}$$

$$\frac{dS_x(t)}{dt} = \frac{1}{i\hbar}[S_x(t), \omega S_z] = \frac{1}{i\hbar}[S_x(t), \omega S_z(t)] = -\omega S_y(t) \qquad (1)$$

where

$$[S_z(t), S_x(t)] = i\hbar S_y(t).$$

$$\frac{dS_y(t)}{dt} = \frac{1}{i\hbar}[S_y(t), \omega S_z] = \frac{1}{i\hbar}[S_y(t), \omega S_z(t)] = \omega S_x(t) \qquad (2)$$

where

$$[S_y(t), S_z(t)] = i\hbar S_x(t).$$

From Eqs. (1) and (2), we get

$$\frac{d^2 S_x(t)}{dt^2} = -\omega \frac{dS_y}{dt} = -\omega^2 S_x(t)$$

and

$$\frac{d^2 S_y(t)}{dt^2} = \omega \frac{dS_x}{dt} = -\omega^2 S_y(t).$$

The general solution of the differential equation is

$$S_x(t) = C_1 \cos(\omega t) + C_2 \sin(\omega t)$$

and

$$S_y(t) = D_1 \cos(\omega t) + D_2 \sin(\omega t).$$

At $t = 0$,

$$S_x(t) = S_x \qquad \text{(Schrödinger picture)}$$
$$S_y(t) = S_y \qquad \text{(Schrödinger picture)}$$
$$\frac{dS_x(t=0)}{dt} = -\omega S_y(t=0) = -\omega S_y$$
$$\frac{dS_y(t=0)}{dt} = \omega S_x(t=0) = \omega S_x.$$

Then we have

$$S_x(t) = S_x \cos(\omega t) - S_y \sin(\omega t)$$

$$S_y(t) = S_x \sin(\omega t) + S_y \cos(\omega t).$$

((**2-2**))

2. Look again at the Hamiltonian of Chapter 1, Problem 11. Suppose the typist made an error and wrote H as

$$H = H_{11}|1\rangle\langle 1| + H_{22}|2\rangle\langle 2| + H_{12}|1\rangle\langle 2|.$$

What principle is now violated? Illustrate your point explicitly by attempting to solve the most general time-dependent problem using an illegal Hamiltonian of this kind. (You may assume $H_{11} = H_{22} = 0$ for simplicity.)

((**Solution**))

We assume that $H_{11} = H_{22} = 0$. Hamiltonian is not a Hermitian operator.

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$$

$$\hat{U}(t) = \exp\left(-\frac{i}{\hbar}\hat{H}t\right) = 1 + \left(-\frac{i}{\hbar}\hat{H}t\right) + \frac{1}{2!}\left(-\frac{i}{\hbar}\hat{H}t\right)^2 + \cdots$$

$$\hat{H} = \begin{pmatrix} 0 & H_{12} \\ 0 & 0 \end{pmatrix} = H_{12}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$\hat{H}^2 = \begin{pmatrix} 0 & H_{12} \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & H_{12} \\ 0 & 0 \end{pmatrix} = 0$$

$$\hat{U}(t) = 1 - \frac{i}{\hbar}\hat{H}t = \begin{pmatrix} 1 & -\frac{i}{\hbar}H_{12}t \\ 0 & 1 \end{pmatrix}$$

$$\hat{U}(t)^+ = \begin{pmatrix} 1 & 0 \\ \frac{i}{\hbar}H_{12}t & 1 \end{pmatrix}$$

$$\hat{U}(t)\hat{U}(t)^+ = \begin{pmatrix} 1 & -\frac{i}{\hbar}H_{12}t \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ \frac{i}{\hbar}H_{12}t & 1 \end{pmatrix} = \begin{pmatrix} 1 + \frac{H_{12}^2 t^2}{\hbar^2} & -\frac{i}{\hbar}H_{12}t \\ \frac{i}{\hbar}H_{12}t & 1 \end{pmatrix} \neq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Therefore $\hat{U}(t)$ is not a Unitary operator. The conservation law of probability is violated.

((Mathematica 5.2))

```
H={{0,H12},{0,0}}
```
{{0,H12},{0,0}}

```
U = MatrixExp[-ⅈ/ℏ H t] // Simplify
```
$\{\{1, -\frac{i\, H12\, t}{\hbar}\}, \{0, 1\}\}$

```
UT=Transpose[U]
```
$\{\{1, 0\}, \{-\frac{i\, H12\, t}{\hbar}, 1\}\}$

```
UH = {{1, 0}, {ⅈ H12 t/ℏ, 1}}
```
$\{\{1, 0\}, \{\frac{i\, H12\, t}{\hbar}, 1\}\}$

```
A=UH.U//Simplify
```
$\{\{1, -\frac{i\, H12\, t}{\hbar}\}, \{\frac{i\, H12\, t}{\hbar}, 1 + \frac{H12^2\, t^2}{\hbar^2}\}\}$

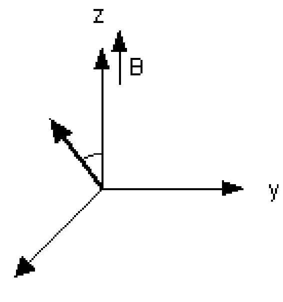
```
A//MatrixForm
```
$$\begin{pmatrix} 1 & -\frac{i\, H12\, t}{\hbar} \\ \frac{i\, H12\, t}{\hbar} & 1 + \frac{H12^2\, t^2}{\hbar^2} \end{pmatrix}$$

```
B=U.UH//Simplify
```
$\{\{1 + \frac{H12^2\, t^2}{\hbar^2}, -\frac{i\, H12\, t}{\hbar}\}, \{\frac{i\, H12\, t}{\hbar}, 1\}\}$

```
B//MatrixForm
```
$$\begin{pmatrix} 1 + \frac{H12^2\, t^2}{\hbar^2} & -\frac{i\, H12\, t}{\hbar} \\ \frac{i\, H12\, t}{\hbar} & 1 \end{pmatrix}$$

((**2-3**))

3. An electron is subject to a uniform, time-independen[t] strength B in the positive z-direction. At $t = 0$ the el[ectron] be in an eigenstate of $\mathbf{S}\cdot\hat{\mathbf{n}}$ with eigenvalue $\hbar/2$, wher[e] lying in the xz-plane, that makes an angle β with th[e]
   a. Obtain the probability for finding the electron in as a function of time.
   b. Find the expectation value of S_x as a function of
   c. For your own peace of mind show that your answers make good sense in the extreme cases (i) $\beta \to 0$ and (ii) $\beta \to \pi/2$.



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a.

Initial state is

$$|\alpha(t=0)\rangle = \cos\left(\frac{\beta}{2}\right)|+\rangle + \sin\left(\frac{\beta}{2}\right)|-\rangle$$

and final state is

$$|+\rangle_x = \frac{1}{\sqrt{2}}[|+\rangle + |-\rangle].$$

Hamiltonian is described as

$$H = -\frac{eB}{mc}S_z = \omega S_z. \quad (e<0)$$

At time t

$$\begin{aligned}|\alpha(t)\rangle &= e^{-\frac{i\omega t}{\hbar}S_z}|\alpha(t=0)\rangle \\ &= e^{-\frac{i\omega t}{\hbar}S_z}\left\{\cos\left(\frac{\beta}{2}\right)|+\rangle + \sin\left(\frac{\beta}{2}\right)|-\rangle\right\}. \\ &= \cos\left(\frac{\beta}{2}\right)e^{-\frac{i\omega t}{2}}|+\rangle + \sin\left(\frac{\beta}{2}\right)e^{\frac{i\omega t}{2}}|-\rangle\end{aligned}$$

The probability of finding the electron in the state $|+\rangle_x$:

$$P(t) = \left|{}_x\langle+|\alpha(t)\rangle\right|^2$$

$$ {}_x\langle +|\alpha(t)\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) e^{-\frac{i\omega t}{2}} \\ \sin\left(\frac{\beta}{2}\right) e^{\frac{i\omega t}{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}\left[\cos\left(\frac{\beta}{2}\right)e^{-\frac{i\omega t}{2}} + \sin\left(\frac{\beta}{2}\right)e^{\frac{i\omega t}{2}}\right] $$

$$ \begin{aligned} \left|{}_x\langle +|\alpha(t)\rangle\right|^2 &= \frac{1}{2}\left[\cos\left(\frac{\beta}{2}\right)e^{\frac{i\omega t}{2}} + \sin\left(\frac{\beta}{2}\right)e^{-\frac{i\omega t}{2}}\right]\left[\cos\left(\frac{\beta}{2}\right)e^{-\frac{i\omega t}{2}} + \sin\left(\frac{\beta}{2}\right)e^{\frac{i\omega t}{2}}\right] \\ &= \frac{1}{2}\left[\cos^2\left(\frac{\beta}{2}\right) + \sin^2\left(\frac{\beta}{2}\right) + \sin\left(\frac{\beta}{2}\right)\cos\left(\frac{\beta}{2}\right)\left(e^{i\omega t} + e^{-i\omega t}\right)\right] \\ &= \frac{1}{2}\left(1 + \sin\beta\cos\omega t\right) \end{aligned} $$

b.

$$ \begin{aligned} \langle S_x\rangle &= \langle\alpha(t)|S_x|\alpha(t)\rangle \\ &= \frac{\hbar}{2}\begin{pmatrix} \cos\frac{\beta}{2}e^{i\frac{\omega t}{2}} & \sin\frac{\beta}{2}e^{-i\frac{\omega t}{2}} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \cos\frac{\beta}{2}e^{-i\frac{\omega t}{2}} \\ \sin\frac{\beta}{2}e^{i\frac{\omega t}{2}} \end{pmatrix} \\ &= \frac{\hbar}{2}\begin{pmatrix} \cos\frac{\beta}{2}e^{i\frac{\omega t}{2}} & \sin\frac{\beta}{2}e^{-i\frac{\omega t}{2}} \end{pmatrix}\begin{pmatrix} \sin\frac{\beta}{2}e^{i\frac{\omega t}{2}} \\ \cos\frac{\beta}{2}e^{-i\frac{\omega t}{2}} \end{pmatrix} \\ &= \frac{\hbar}{2}\cos\frac{\beta}{2}\sin\frac{\beta}{2}\left(e^{i\omega t} + e^{-i\omega t}\right) \\ &= \frac{\hbar}{2}\sin\beta\cos\omega t \end{aligned} $$

c.

For $\beta = 0$

$$ |\alpha(t=0)\rangle = |+\rangle $$

$$ |\alpha(t)\rangle = e^{-i\frac{\omega t}{2}}|+\rangle $$

$$ P(t) = \left|{}_x\langle +|\alpha(t)\rangle\right|^2 = \frac{1}{2} $$

$$ \langle S_x\rangle = 0 $$

For $\beta = \pi/2$

$$|\alpha(t=0)\rangle = |+\rangle_x$$

$$|\alpha(t)\rangle = \frac{1}{\sqrt{2}}\left[e^{-i\frac{\omega t}{2}}|+\rangle + e^{i\frac{\omega t}{2}}|-\rangle\right]$$

$$P(t) = \left|{}_x\langle+|\alpha(t)\rangle\right|^2 = \frac{1}{2}(1+\cos\omega t)$$

$$\langle S_x\rangle = \frac{\hbar}{2}\cos\omega t$$

((2-4))

4. Let $x(t)$ be the coordinate operator for a free particle in one dimension in the Heisenberg picture. Evaluate

$$[x(t), x(0)].$$

$$H = \frac{1}{2m}p^2$$

$$\frac{dx(t)}{dt} = \frac{1}{i\hbar}\left[x(t), \frac{p^2}{2m}\right] = \frac{1}{i\hbar}\left[x(t), \frac{p(t)^2}{2m}\right] = \frac{1}{i\hbar}i\hbar\frac{\partial}{\partial p(t)}\frac{p(t)^2}{2m} = \frac{1}{m}p(t)$$

$$\frac{dp(t)}{dt} = \frac{1}{i\hbar}\left[p(t), \frac{p^2}{2m}\right] = \frac{1}{i\hbar}\left[p(t), \frac{p(t)^2}{2m}\right] = 0$$

Then

$$x(t) = \frac{p(0)}{m}t + x(0)$$

$$[x(t), x(0)] = \left[\frac{p(0)}{m}t + x(0), x(0)\right] = -\frac{1}{m}t[x(0), p(0)] = -\frac{i\hbar}{m}t$$

((2-5))

5. Consider a particle in one dimension whose Hamiltonian is given by

$$H = \frac{p^2}{2m} + V(x).$$

By calculating $[[H, x], x]$ prove

$$\sum_{a'} |\langle a''|x|a'\rangle|^2 (E_{a'} - E_{a''}) = \frac{\hbar^2}{2m},$$

where $|a'\rangle$ is an energy eigenket with eigenvalue $E_{a'}$.

$$[[H,x],x] = \left[\left[\frac{p^2}{2m}, x\right], x\right] + [[V(x),x],x] = \left[\left[\frac{p^2}{2m}, x\right], x\right]$$

$$= \left[-i\hbar\frac{\partial}{\partial p}\left(\frac{p^2}{2m}\right), x\right] = \left[-i\hbar\frac{p}{m}, x\right] = i\hbar\frac{1}{m}[x,p] = (i\hbar)^2\frac{1}{m} = -\frac{\hbar^2}{m}$$

Then

$$\langle a''|[[H,x],x]|a''\rangle = -\frac{\hbar^2}{m} \qquad (1)$$

On the other hand

$$\begin{aligned}
\langle a''|[[H,x],x]|a''\rangle &= \langle a''|[H,x]x|a''\rangle - \langle a''|x[H,x]|a''\rangle \\
&= \sum_{a'} \{\langle a''|[H,x]|a'\rangle\langle a'|x|a''\rangle - \langle a''|x|a'\rangle\langle a'|[H,x]|a''\rangle\} \\
&= \sum_{a'} \{(E_{a''} - E_{a'})\langle a''|x|a'\rangle\langle a'|x|a''\rangle - (E_{a'} - E_{a''})\langle a''|x|a'\rangle\langle a'|x|a''\rangle\} \\
&= -2\sum_{a'} (E_{a'} - E_{a''})|\langle a''|x|a'\rangle|^2
\end{aligned}$$

(2)

Combining Eqs. (1) and (2), we obtain

$$\sum_{a'} |\langle a''|x|a'\rangle|^2 (E_{a'} - E_{a''}) = \frac{\hbar^2}{2m} \qquad (3)$$

((2-6))

$$
\begin{aligned}
[\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}, H] &= \left[\sum_i \hat{x}_i\hat{p}_i, \frac{1}{2m}\sum_l \hat{p}_j^2 + V(\hat{\mathbf{r}})\right] \\
&= \sum_i\left(\left[\hat{x}_i\hat{p}_i, \frac{1}{2m}\sum_l \hat{p}_j^2\right] + [\hat{x}_i\hat{p}_i, V(\hat{\mathbf{r}})]\right) \\
&= \sum_i\left(\left[\hat{x}_i, \frac{1}{2m}\sum_l \hat{p}_j^2\right]\hat{p}_i + \hat{x}_i[\hat{p}_i, V(\hat{\mathbf{r}})]\right) \\
&= i\hbar\sum_i\left\{\left(\frac{\partial}{\partial\hat{p}_i}\frac{1}{2m}\hat{p}_i^2\right)\hat{p}_i - \hat{x}_i\frac{\partial V(\hat{\mathbf{r}})}{\partial\hat{x}_i}\right\} \\
&= i\hbar\sum_i\left(\frac{1}{m}\hat{p}_i^2 - \hat{x}_i\frac{\partial V(\hat{\mathbf{r}})}{\partial\hat{x}_i}\right)
\end{aligned}
$$

Then

$$\frac{d}{dt}\langle\psi(t)|\hat{A}|\psi(t)\rangle = -\frac{i}{\hbar}\langle\psi(t)|[\hat{A},\hat{H}]|\psi(t)\rangle$$

When $\hat{A} = \hat{\mathbf{r}}\cdot\hat{\mathbf{p}}$

$$\frac{d}{dt}\langle\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}\rangle = -\frac{i}{\hbar}\langle[\hat{\mathbf{r}}\cdot\hat{\mathbf{p}},\hat{H}]\rangle = \left\langle\frac{\hat{\mathbf{p}}^2}{m}\right\rangle - \langle\hat{\mathbf{r}}\cdot\nabla V(\hat{\mathbf{r}})\rangle$$

When $\frac{d}{dt}\langle\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}\rangle = 0$,

$$\left\langle\frac{\hat{\mathbf{p}}^2}{m}\right\rangle - \langle\hat{\mathbf{r}}\cdot\nabla V(\hat{\mathbf{r}})\rangle = 0\,.$$

Since $\hat{T} = \frac{1}{2m}\hat{\mathbf{p}}^2$ (kinetic energy),

$$2\langle\hat{T}\rangle - \langle\hat{\mathbf{r}}\cdot\nabla V(\hat{\mathbf{r}})\rangle = 0 \text{ (Virial theorem)}$$

We now consider the following case.

$$\langle\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}\rangle = \langle\varphi_n(t)|\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}|\varphi_n(t)\rangle = \langle\varphi_n|e^{\frac{i}{\hbar}\hat{H}t}\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}e^{-\frac{i}{\hbar}\hat{H}t}|\varphi_n\rangle = e^{\frac{i}{\hbar}\varepsilon_n t}\langle\varphi_n|\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}|\varphi_n\rangle e^{-\frac{i}{\hbar}\varepsilon_n t} = \langle\varphi_n|\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}|\varphi_n\rangle$$

which is independent of *t*. Therefore $\frac{d}{dt}\langle\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}\rangle = 0$.

((**2-8**))

8. Let $|a'\rangle$ and $|a''\rangle$ be eigenstates of a Hermitian operator A with eigenvalues a' and a'', respectively ($a' \neq a''$). The Hamiltonian operator is given by

$$H = |a'\rangle\delta\langle a''| + |a''\rangle\delta\langle a'|,$$

where δ is just a real number.

a. Clearly, $|a'\rangle$ and $|a''\rangle$ are not eigenstates of the Hamiltonian. Write down the eigenstates of the Hamiltonian. What are their energy eigenvalues?

b. Suppose the system is known to be in state $|a'\rangle$ at $t = 0$. Write down the state vector in the Schrödinger picture for $t > 0$.

c. What is the probability for finding the system in $|a''\rangle$ for $t > 0$ if the system is known to be in state $|a'\rangle$ at $t = 0$?

d. Can you think of a physical situation corresponding to this problem?

(**a**)

$$\hat{H} = \begin{pmatrix} 0 & \delta \\ \delta & 0 \end{pmatrix} = \delta\hat{\sigma}_x$$

$$|\psi\rangle = \begin{pmatrix} A \\ B \end{pmatrix}$$

Eigenvalue equation

$$H|\psi\rangle = E|\psi\rangle$$

$$\begin{vmatrix} -E & \delta \\ \delta & -E \end{vmatrix} = 0$$

$$E^2 = \delta^2$$

$$E = \pm\delta$$

For $E = \delta$

$$|+\delta\rangle = \begin{pmatrix} A_+ \\ B_+ \end{pmatrix}$$

$$\begin{pmatrix} -\delta & \delta \\ \delta & -\delta \end{pmatrix}\begin{pmatrix} A_+ \\ B_+ \end{pmatrix} = 0$$

$$A_+ = B_+$$

Normalization

$$|A_+|^2 + |B_+|^2 = 1$$

$$|A_+| = |B_+| = \frac{1}{\sqrt{2}}$$

$$|+\delta\rangle = \frac{1}{\sqrt{2}}\left(|a'\rangle + |a''\rangle\right) \qquad H|+\delta\rangle = \delta|+\delta\rangle$$

For $E = -\delta$

$$|-\delta\rangle = \frac{1}{\sqrt{2}}\left(|a'\rangle - |a''\rangle\right) \qquad H|-\delta\rangle = -\delta|-\delta\rangle$$

(Note)

$|+\delta\rangle = U|a'\rangle$ $\qquad$ U: Unitary operator

$|-\delta\rangle = U|a''\rangle$

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix}$$

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix}$$

=> $$U = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

b.

At $t = 0$ $\quad |\psi(t=0)\rangle = |a'\rangle$

$$|a'\rangle = \frac{1}{\sqrt{2}}\left[|+\delta\rangle + |-\delta\rangle\right]$$

$$\begin{aligned}
|\psi(t)\rangle &= \exp\left(-\frac{i\hat{H}}{\hbar}t\right)|\psi(t=0)\rangle \\
&= \exp\left(-\frac{i\hat{H}}{\hbar}t\right)\frac{1}{\sqrt{2}}\left[|+\delta\rangle + |-\delta\rangle\right] \\
&= \frac{1}{\sqrt{2}}\left[e^{-\frac{i\delta}{\hbar}t}|+\delta\rangle + e^{\frac{i\delta}{\hbar}t}|-\delta\rangle\right] \\
&= \frac{1}{\sqrt{2}}\left[\left\{\cos\left(\frac{\delta t}{\hbar}\right) - i\sin\left(\frac{\delta t}{\hbar}\right)\right\}|+\delta\rangle + \left\{\cos\left(\frac{\delta t}{\hbar}\right) + i\sin\left(\frac{\delta t}{\hbar}\right)\right\}|-\delta\rangle\right] \\
&= \cos\left(\frac{\delta t}{\hbar}\right)|a'\rangle - i\sin\left(\frac{\delta t}{\hbar}\right)|a''\rangle
\end{aligned}$$

More powerful solution is as follows.

$$\hat{U}^{+}\hat{H}\hat{U} = \begin{pmatrix} \delta & 0 \\ 0 & -\delta \end{pmatrix}$$

$$\hat{U}^{+}\exp\left(-\frac{i\hat{H}}{\hbar}t\right)\hat{U} = \exp\left(-\frac{i\hat{U}^{+}\hat{H}\hat{U}}{\hbar}t\right) = \begin{pmatrix} e^{-\frac{i\delta}{\hbar}t} & 0 \\ 0 & e^{\frac{i\delta}{\hbar}t} \end{pmatrix}$$

$$\exp\left(-\frac{i\hat{H}}{\hbar}t\right) = \hat{U}\begin{pmatrix} e^{-\frac{i\delta}{\hbar}t} & 0 \\ 0 & e^{\frac{i\delta}{\hbar}t} \end{pmatrix}\hat{U}^{+} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}\begin{pmatrix} e^{-\frac{i\delta}{\hbar}t} & 0 \\ 0 & e^{\frac{i\delta}{\hbar}t} \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

or

$$\exp\left(-\frac{i\hat{H}}{\hbar}t\right) = \begin{pmatrix} \cos\left(\frac{t\delta}{\hbar}\right) & -i\sin\left(\frac{t\delta}{\hbar}\right) \\ -i\sin\left(\frac{t\delta}{\hbar}\right) & \cos\left(\frac{t\delta}{\hbar}\right) \end{pmatrix}$$

$$|\psi(t)\rangle = \exp\left(-\frac{i\hat{H}}{\hbar}t\right)|\psi(t=0)\rangle = \begin{pmatrix} \cos\left(\frac{t\delta}{\hbar}\right) & -i\sin\left(\frac{t\delta}{\hbar}\right) \\ -i\sin\left(\frac{t\delta}{\hbar}\right) & \cos\left(\frac{t\delta}{\hbar}\right) \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\left(\frac{t\delta}{\hbar}\right) \\ -i\sin\left(\frac{t\delta}{\hbar}\right) \end{pmatrix}$$

((Mathematica 5.2))

```
(*Sakurai 2-8*)
U = {{1/√2, 1/√2}, {1/√2, -1/√2}}
{{1/√2, 1/√2}, {1/√2, -1/√2}}
UH=U
{{1/√2, 1/√2}, {1/√2, -1/√2}}
UH.U
{{1,0},{0,1}}
HD = {{Exp[-ⅈ t δ/ℏ], 0}, {0, Exp[ⅈ t δ/ℏ]}}
{{ⅇ^(-ⅈ t δ/ℏ), 0}, {0, ⅇ^(ⅈ t δ/ℏ)}}
HD//MatrixForm
(ⅇ^(-ⅈ t δ/ℏ)   0
 0              ⅇ^(ⅈ t δ/ℏ))
U.HD.UH//ExpToTrig//Simplify
{{Cos[t δ/ℏ], -ⅈ Sin[t δ/ℏ]}, {-ⅈ Sin[t δ/ℏ], Cos[t δ/ℏ]}}
```

(c)

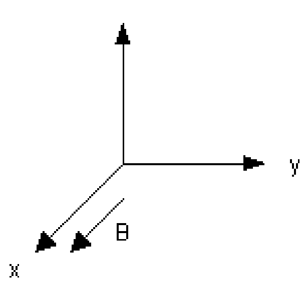
$$P = |\langle a''|\psi(t)\rangle|^2 = \left|-i\sin\left(\frac{\delta t}{\hbar}\right)\right|^2 = \sin^2\left(\frac{\delta t}{\hbar}\right)$$

(d)

We choose $\hat{S}_x$ as Hermitian operator

$$|a'\rangle = |+\rangle, \qquad |a''\rangle = |-\rangle$$

$$\hat{H} = \frac{2\delta}{\hbar}\hat{S}_x = \frac{eB}{mc}\hat{S}_x \quad (B = \frac{2mc}{|e|\hbar}\delta)$$



$|+\delta\rangle = |+\rangle_x$ and $|-\delta\rangle = |-\rangle_x$

precession motion of electron in the presence of a magnetic field *B* along the *x*-axis.

((2-9))

9. A box containing a particle is divided into a right and 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?

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 $|\alpha\rangle$.

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?

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 (b).

e. Suppose the printer made an error and wrote H as

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

By explicitly solving the most general time-evolution problem with this Hamiltonian, show that probability conservation is violated.

$$|\alpha\rangle = |R\rangle\underbrace{\langle R|\alpha\rangle}_{B} + |L\rangle\underbrace{\langle L|\alpha\rangle}_{A}$$

Hamiltonian

$$\hat{H} = \Delta\left(|L\rangle\langle R| + |R\rangle\langle L|\right)$$

a.
Eigenvalue equation

$$\hat{H}|\alpha\rangle = E|\alpha\rangle$$

$$\begin{pmatrix} 0 & \Delta \\ \Delta & 0 \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = E\begin{pmatrix} A \\ B \end{pmatrix}$$

$$\begin{vmatrix} -E & \Delta \\ \Delta & -E \end{vmatrix} = 0$$

$$E^2 - \Delta^2 = 0$$

$$E = \pm\Delta$$

For $E_1 = \Delta$ $\quad |E_1\rangle = \frac{1}{\sqrt{2}}\left(|L\rangle + |R\rangle\right)$

For $E_2 = -\Delta$ $\quad |E_2\rangle = \frac{1}{\sqrt{2}}\left(|L\rangle - |R\rangle\right)$

=> $\quad |R\rangle = \frac{1}{\sqrt{2}}\left(|E_1\rangle - |E_2\rangle\right)$

$\quad |L\rangle = \frac{1}{\sqrt{2}}\left(|E_1\rangle + |E_2\rangle\right)$

b.

$$
\begin{aligned}
|\alpha(t)\rangle &= e^{-\frac{i}{\hbar}Ht}|\alpha(0)\rangle = e^{-\frac{i}{\hbar}Ht}\left(|R\rangle\langle R|\alpha\rangle + |L\rangle\langle L|\alpha\rangle\right) \\
&= e^{-\frac{i}{\hbar}Ht}\left[\frac{1}{\sqrt{2}}\left(|E_1\rangle - |E_2\rangle\right)\langle R|\alpha\rangle + \frac{1}{\sqrt{2}}\left(|E_1\rangle + |E_2\rangle\right)\langle L|\alpha\rangle\right] \\
&= \left[e^{-\frac{i}{\hbar}\Delta t}\frac{1}{\sqrt{2}}|E_1\rangle - e^{\frac{i}{\hbar}\Delta t}\frac{1}{\sqrt{2}}|E_2\rangle\right]\langle R|\alpha\rangle + \left[e^{-\frac{i}{\hbar}\Delta t}\frac{1}{\sqrt{2}}|E_1\rangle + e^{\frac{i}{\hbar}\Delta t}\frac{1}{\sqrt{2}}|E_2\rangle\right]\langle L|\alpha\rangle \\
&= \frac{1}{\sqrt{2}}e^{-\frac{i}{\hbar}\Delta t}|E_1\rangle\left(\langle R|\alpha\rangle + \langle L|\alpha\rangle\right) + \frac{1}{\sqrt{2}}e^{\frac{i}{\hbar}\Delta t}|E_2\rangle\left(-\langle R|\alpha\rangle + \langle L|\alpha\rangle\right) \\
&= \frac{1}{2}e^{-\frac{i}{\hbar}\Delta t}\left(|L\rangle + |R\rangle\right)\left(\langle R|\alpha\rangle + \langle L|\alpha\rangle\right) + \frac{1}{2}e^{\frac{i}{\hbar}\Delta t}\left(|L\rangle - |R\rangle\right)\left(-\langle R|\alpha\rangle + \langle L|\alpha\rangle\right) \\
&= \left[\cos\left(\frac{\Delta t}{\hbar}\right)\langle L|\alpha\rangle - i\sin\left(\frac{\Delta t}{\hbar}\right)\langle R|\alpha\rangle\right]|L\rangle + \left[\cos\left(\frac{\Delta t}{\hbar}\right)\langle R|\alpha\rangle - i\sin\left(\frac{\Delta t}{\hbar}\right)\langle L|\alpha\rangle\right]|R\rangle
\end{aligned}
$$

More powerful method:

Unitary operator

$$
\hat{U} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}, \qquad \hat{U}^+ = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}
$$

$$
\hat{H} = \begin{pmatrix} 0 & \Delta \\ \Delta & 0 \end{pmatrix}
$$

$$
\hat{U}^+\hat{H}\hat{U} = \begin{pmatrix} \Delta & 0 \\ 0 & -\Delta \end{pmatrix}
$$

$$
\hat{U}^+\exp(-\frac{i}{\hbar}\hat{H}t)\hat{U} = \exp(-\frac{i}{\hbar}\hat{U}^+\hat{H}\hat{U}t) = \begin{pmatrix} e^{-\frac{i}{\hbar}\Delta t} & 0 \\ 0 & e^{\frac{i}{\hbar}\Delta t} \end{pmatrix}
$$

or

$$
\exp(-\frac{i}{\hbar}\hat{H}t) = \hat{U}\begin{pmatrix} e^{-\frac{i}{\hbar}\Delta t} & 0 \\ 0 & e^{\frac{i}{\hbar}\Delta t} \end{pmatrix}\hat{U}^+ = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}\begin{pmatrix} e^{-\frac{i}{\hbar}\Delta t} & 0 \\ 0 & e^{\frac{i}{\hbar}\Delta t} \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}
$$

$$= \begin{pmatrix} \cos(\frac{\Delta t}{\hbar}) & -i\sin(\frac{\Delta t}{\hbar}) \\ -i\sin(\frac{\Delta t}{\hbar}) & \cos(\frac{\Delta t}{\hbar}) \end{pmatrix}$$

$$|\alpha(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\alpha(0)\rangle = \begin{pmatrix} \cos(\frac{\Delta t}{\hbar}) & -i\sin(\frac{\Delta t}{\hbar}) \\ -i\sin(\frac{\Delta t}{\hbar}) & \cos(\frac{\Delta t}{\hbar}) \end{pmatrix} \begin{pmatrix} \langle R|\alpha\rangle \\ \langle L|\alpha\rangle \end{pmatrix}$$

$$= \begin{pmatrix} \cos(\frac{\Delta t}{\hbar})\langle R|\alpha\rangle - i\sin(\frac{\Delta t}{\hbar})\langle L|\alpha\rangle \\ -i\sin(\frac{\Delta t}{\hbar})\langle R|\alpha\rangle + \cos(\frac{\Delta t}{\hbar})\langle L|\alpha\rangle \end{pmatrix}$$

c.
At $t = 0$, $|\alpha(t=0)\rangle = |R\rangle$, which means $\langle L|\alpha\rangle = 0$ and $\langle R|\alpha\rangle = 1$.

$$|\alpha(t)\rangle = -i\sin\left(\frac{\Delta t}{\hbar}\right)|L\rangle + \cos\left(\frac{\Delta t}{\hbar}\right)|R\rangle$$

The probability of observing the particle on the left side is

$$P_L = |\langle L|\alpha(t)\rangle|^2 = \left|-i\sin\left(\frac{\Delta t}{\hbar}\right)\right|^2 = \sin^2\left(\frac{\Delta t}{\hbar}\right)$$

d.
Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\alpha(t)\rangle = \hat{H}|\alpha(t)\rangle \qquad \text{with} \qquad |\alpha(t_0)\rangle = |\alpha\rangle$$

Multiplying $\langle R|$ and $\langle L|$

$$i\hbar\frac{\partial}{\partial t}\langle R|\alpha(t)\rangle = \langle R|H|\alpha(t)\rangle = \Delta\langle L|\alpha(t)\rangle$$

$$i\hbar\frac{\partial}{\partial t}\langle L|\alpha(t)\rangle = \langle L|H|\alpha(t)\rangle = \Delta\langle R|\alpha(t)\rangle,$$

where

$$\langle R|H|\alpha(t)\rangle = \Delta\langle L|\alpha(t)\rangle$$
$$\langle L|H|\alpha(t)\rangle = \Delta\langle R|\alpha(t)\rangle .$$

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\langle R|\alpha(t)\rangle\\ \langle L|\alpha(t)\rangle\end{pmatrix} = \begin{pmatrix}0 & \Delta\\ \Delta & 0\end{pmatrix}\begin{pmatrix}\langle R|\alpha(t)\rangle\\ \langle L|\alpha(t)\rangle\end{pmatrix}$$

$$\begin{pmatrix}\langle R|\alpha(t)\rangle\\ \langle L|\alpha(t)\rangle\end{pmatrix} = \exp\left[-\frac{i}{\hbar}\begin{pmatrix}0 & \Delta\\ \Delta & 0\end{pmatrix}t\right]\begin{pmatrix}\langle R|\alpha\rangle\\ \langle L|\alpha\rangle\end{pmatrix}$$

Here

$$\begin{aligned}\exp\left[-\frac{i}{\hbar}\begin{pmatrix}0 & \Delta\\ \Delta & 0\end{pmatrix}t\right] &= I + \left(-\frac{i\Delta}{\hbar}t\right)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} + \frac{1}{2!}\left(-\frac{i\Delta}{\hbar}t\right)^2\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\\ &\quad + \frac{1}{3!}\left(-\frac{i\Delta}{\hbar}t\right)^3\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} + \cdots\\ &= \cos\left(\frac{\Delta t}{\hbar}\right)\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} - i\sin\left(\frac{\Delta t}{\hbar}\right)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\\ &= \begin{pmatrix}\cos\left(\frac{\Delta t}{\hbar}\right) & -i\sin\left(\frac{\Delta t}{\hbar}\right)\\ -i\sin\left(\frac{\Delta t}{\hbar}\right) & \cos\left(\frac{\Delta t}{\hbar}\right)\end{pmatrix}\end{aligned}$$

Therefore

$$\begin{pmatrix}\langle R|\alpha(t)\rangle\\ \langle L|\alpha(t)\rangle\end{pmatrix} = \begin{pmatrix}\cos\left(\frac{\Delta t}{\hbar}\right) & -i\sin\left(\frac{\Delta t}{\hbar}\right)\\ -i\sin\left(\frac{\Delta t}{\hbar}\right) & \cos\left(\frac{\Delta t}{\hbar}\right)\end{pmatrix}\begin{pmatrix}\langle R|\alpha\rangle\\ \langle L|\alpha\rangle\end{pmatrix}$$

((**2-10**))

10. Using the one-dimensional simple harmonic oscillator as an example, illustrate the difference between the Heisenberg picture and the Schrödinger picture. Discuss in particular how (a) the dynamic variables x and p and (b) the most general state vector evolve with time in each of the two pictures.

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

a. variables *x* and *p*

Schrödinger picture => no change

Heisenberg picture

$$\frac{dx(t)}{dt} = \frac{1}{i\hbar}\left[x(t), H\right] = \frac{1}{m}p(t)$$
$$\frac{dp(t)}{dt} = \frac{1}{i\hbar}\left[p(t), H\right] = -m\omega^2 x(t)$$

$$x(t) = x(0)\cos\omega t + \left(\frac{p(0)}{m\omega}\right)\sin\omega t$$
$$p(t) = -m\omega x(0)\sin\omega t + p(0)\cos\omega t$$

b. state vector

Heisenberg picture => no change

Schrödinger picture

$$\left|\psi(t)\right\rangle = \exp\left(-\frac{iH}{\hbar}t\right)\left|\psi(t=0)\right\rangle$$

with

$$\left|\psi(t=0)\right\rangle = \sum_n c_n\left|n\right\rangle,\ c_n = \left\langle n\middle|\psi(t=0)\right\rangle$$

$$\left|\psi(t)\right\rangle = \sum_n c_n e^{-\frac{i}{\hbar}E_n t}\left|n\right\rangle$$
$$= \sum_n c_n e^{-i\omega(n+\frac{1}{2})}\left|n\right\rangle$$
$$= \begin{pmatrix} c_0 e^{-i\frac{1}{2}\omega} \\ c_1 e^{-i\frac{3}{2}\omega} \\ \vdots \\ \vdots \end{pmatrix}$$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

((**2-11**))

11. Consider a particle subject to a one-dimensional simple harmonic oscillator potential. Suppose at $t = 0$ the state vector is given by

$$\exp\left(\frac{-ipa}{\hbar}\right)|0\rangle,$$

where p is the momentum operator and a is some number with dimension of length. Using the Heisenberg picture, evaluate the expectation value $\langle x\rangle$ for $t \geq 0$.

In the Heisenberg picture

$$x(t) = x\cos\omega t + \frac{p}{m\omega}\sin\omega t$$

Using

$$\exp\left(\frac{ipa}{\hbar}\right)x\exp\left(-\frac{ipa}{\hbar}\right) = x + a$$

$$\exp\left(\frac{ipa}{\hbar}\right)p\exp\left(-\frac{ipa}{\hbar}\right) = p$$

Note

$$\left[x, \exp\left(\frac{ipa}{\hbar}\right)\right] = i\hbar\frac{\partial}{\partial p}\exp\left(\frac{ipa}{\hbar}\right) = i\hbar\left(\frac{ia}{\hbar}\right)\exp\left(\frac{ipa}{\hbar}\right) = -a\exp\left(\frac{ipa}{\hbar}\right)$$

$$\exp\left(\frac{ipa}{\hbar}\right)x - x\exp\left(\frac{ipa}{\hbar}\right) = a\exp\left(\frac{ipa}{\hbar}\right)$$

$$\langle x(t)\rangle = \langle 0|\exp\left(\frac{ipa}{\hbar}\right)x(t)\exp\left(-\frac{ipa}{\hbar}\right)|0\rangle$$

$$= \cos\omega t\langle 0|\exp\left(\frac{ipa}{\hbar}\right)x\exp\left(-\frac{ipa}{\hbar}\right)|0\rangle + \frac{1}{m\omega}\sin\omega t\langle 0|\exp\left(\frac{ipa}{\hbar}\right)p\exp\left(-\frac{ipa}{\hbar}\right)|0\rangle$$

$$= \cos\omega t\langle 0|(x+a)|0\rangle + \frac{1}{m\omega}\sin\omega t\langle 0|p|0\rangle$$

$$= a\cos\omega t$$

where

$$\langle 0|x|0\rangle = 0, \quad \langle 0|p|0\rangle = 0.$$

At $t = 0$, the wave function is given by

$$\langle x|\psi(0)\rangle = \langle x|\exp\left(-\frac{ipa}{\hbar}\right)|0\rangle$$

((**2-12**))

12. a. Write down the wave function (in coordinate space) for the state specified in Problem 11 at $t = 0$. You may use

$$\langle x'|0\rangle = \pi^{-1/4}x_0^{-1/2}\exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right], \quad \left(x_0 \equiv \left(\frac{\hbar}{m\omega}\right)^{1/2}\right).$$

b. Obtain a simple expression for the probability that the state is found in the ground state at $t = 0$. Does this probability change for $t > 0$?

---

a.

$$\langle x'|\exp\left(-\frac{ipa}{\hbar}\right)|0\rangle = \langle x'|\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{ia}{\hbar}\right)^n p^n|0\rangle$$

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{ia}{\hbar}\right)^n\langle x'|p^n|0\rangle$$

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{ia}{\hbar}\right)^n\left(\frac{\hbar}{i}\right)^n\frac{\partial^n}{\partial x'^n}\langle x'|0\rangle$$

$$= \pi^{-\frac{1}{4}}x_0^{-\frac{1}{2}}\exp\left[-\frac{1}{2}\left(\frac{x'-a}{x_0}\right)^2\right]$$

$(\langle x'|p = \langle x'|\frac{\hbar}{i}\frac{\partial}{\partial x'} = \frac{\hbar}{i}\langle x'|\frac{\partial}{\partial x'})$

b.

$$\langle 0|\exp\left(-\frac{ipa}{\hbar}\right)|0\rangle = \int dx'\langle 0|x'\rangle\langle x'|\exp\left(-\frac{ipa}{\hbar}\right)$$

$$= \pi^{-\frac{1}{4}}x_0^{-\frac{1}{2}}\int dx'\exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right]\pi^{-\frac{1}{4}}x_0^{-\frac{1}{2}}\exp\left[-\frac{1}{2}\left(\frac{x'-a}{x_0}\right)^2\right]$$

$$= \pi^{-\frac{1}{2}}x_0^{-1}\exp\left(-\frac{a^2}{4x_0^2}\right)\int dx'\exp\left[-\left(\frac{x'-\frac{1}{2}a}{x_0}\right)^2\right]$$

$$= \exp\left(-\frac{a^2}{4x_0^2}\right)$$

Therefore the probability is given by

$$P(t=0) = \left|\langle 0|\exp\left(-\frac{ipa}{2x_0^2}\right)|0\rangle\right|^2 = \exp\left(-\frac{a^2}{2x_0^2}\right)$$

$$P(t) = \left|\langle 0|\exp\left(-\frac{iH}{\hbar}t\right)\exp\left(-\frac{ipa}{2x_0^2}\right)|0\rangle\right|^2$$

$$= \left|\exp\left(-\frac{i\omega t}{2}\right)\langle 0|\exp\left(-\frac{ipa}{2x_0^2}\right)|0\rangle\right|^2 = P(t=0)$$

invariant

((**2-13**))

13. Consider a one-dimensional simple harmonic oscillator.

a. Using

$$\left.\begin{matrix} a \\ a^\dagger \end{matrix}\right\} = \sqrt{\frac{m\omega}{2\hbar}}\left(x \pm \frac{ip}{m\omega}\right), \quad \left.\begin{matrix} a|n\rangle \\ a^\dagger|n\rangle \end{matrix}\right\} = \left\{\begin{matrix} \sqrt{n}\,|n-1\rangle \\ \sqrt{n+1}\,|n+1\rangle, \end{matrix}\right.$$

evaluate $\langle m|x|n\rangle$, $\langle m|p|n\rangle$, $\langle m|\{x, p\}|n\rangle$, $\langle m|x^2|n\rangle$, and $\langle m|p^2|n\rangle$.

b. Check that the virial theorem holds for the expectation values of the kinetic and the potential energy taken with respect to an energy eigenstate.

---

a.

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^+\right)$$

$$\hat{p} = -i\sqrt{\frac{m\hbar\omega}{2}}\left(\hat{a} - \hat{a}^+\right)$$

$$\begin{aligned}\langle m|\hat{x}|n\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left(\langle m|\hat{a}|n\rangle + \langle m|\hat{a}^+|n\rangle\right) \\ &= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right)\end{aligned}$$

$$\begin{aligned}\langle m|\hat{p}|n\rangle &= -i\sqrt{\frac{m\hbar\omega}{2}}\left(\langle m|\hat{a}|n\rangle - \langle m|\hat{a}^+|n\rangle\right) \\ &= -i\sqrt{\frac{m\hbar\omega}{2}}\left(\sqrt{n}\delta_{m,n-1} - \sqrt{n+1}\delta_{m,n+1}\right)\end{aligned}$$

$$\begin{aligned}\{\hat{x}, \hat{p}\} &= \sqrt{\frac{\hbar}{2m\omega}}\left(-i\sqrt{\frac{m\hbar\omega}{2}}\right)\{\hat{a} + \hat{a}^+, \hat{a} - \hat{a}^+\} \\ &= -\frac{i\hbar}{2}\{\hat{a} + \hat{a}^+, \hat{a} - \hat{a}^+\} \\ &= -\frac{i\hbar}{2}\{(\hat{a} + \hat{a}^+)(\hat{a} - \hat{a}^+) + (\hat{a} - \hat{a}^+)(\hat{a} + \hat{a}^+)\} \\ &= -\frac{i\hbar}{2}\left(\hat{a}^2 - \hat{a}\hat{a}^+ + \hat{a}^+\hat{a} - \hat{a}^{+^2} + \hat{a}^2 + \hat{a}\hat{a}^+ - \hat{a}^+\hat{a} - a^{+^2}\right) \\ &= -i\hbar\left(\hat{a}^2 - \hat{a}^{+^2}\right)\end{aligned}$$

$$\langle m|\{\hat{x},\hat{p}\}|n\rangle = -i\hbar\left(\langle m|\hat{a}^2|n\rangle - \langle m|\hat{a}^{+2}|n\rangle\right)$$
$$= -i\hbar\{\sqrt{n(n-1)}\delta_{m,n-2} - \sqrt{(n+1)(n+2)}\delta_{m,n+2}\}$$

$$\langle m|x^2|n\rangle = \frac{\hbar}{2m\omega}\langle m|\hat{a}^2 + \hat{a}\hat{a}^+ + \hat{a}^+\hat{a} + \hat{a}^{+2}|n\rangle$$
$$= \frac{\hbar}{2m\omega}\langle m|\hat{a}^2 + \hat{a}^{+2} + (2\hat{a}^+\hat{a}+1)|n\rangle$$
$$= \frac{\hbar}{2m\omega}\{\sqrt{n(n+1)}\delta_{m,n-2} + \sqrt{(n+1)(n+2)}\delta_{m,n+2} + (2n+1)\delta_{m,n}\}$$

$$\langle m|\hat{p}^2|n\rangle = -\frac{m\hbar\omega}{2}\langle m|\hat{a}^2 - \hat{a}\hat{a}^+ - \hat{a}^+\hat{a} + \hat{a}^{+2}|n\rangle$$
$$= -\frac{m\hbar\omega}{2}\{\sqrt{n(n+1)}\delta_{m,n-2} + \sqrt{(n+1)(n+2)}\delta_{m,n+2} - (2n+1)\delta_{m,n}\}$$

b.

$$\langle n|\frac{\hat{p}^2}{m}|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right)$$

Then $\langle n|\hat{x}\frac{dV}{d\hat{x}}|n\rangle = \langle n|\hat{x}\frac{d}{d\hat{x}}\left(\frac{1}{2}m\omega^2\hat{x}^2\right)|n\rangle = m\omega^2\langle n|\hat{x}^2|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right)$

$$\langle n|\frac{\hat{p}^2}{m}|n\rangle = \langle n|\hat{x}\frac{dV}{d\hat{x}}|n\rangle,$$

showing that the virial theorem holds.

<u>Note</u>

$$\left\langle\frac{\hat{p}^2}{2m}\right\rangle = \left\langle\frac{1}{2}m\omega^2\hat{x}^2\right\rangle$$

The kinetic energy = potential energy

((**2-14**))

14. a. Using

$$\langle x'|p'\rangle = (2\pi\hbar)^{-1/2} e^{ip'x'/\hbar} \qquad \text{(one dimension)}$$

prove

$$\langle p'|x|\alpha\rangle = i\hbar \frac{\partial}{\partial p'} \langle p'|\alpha\rangle.$$

b. Consider a one-dimensional simple harmonic oscillator. Starting with the Schrödinger equation for the state vector, derive the Schrödinger equation for the *momentum-space* wave function. (Make sure to distinguish the operator p from the eigenvalue p'.) Can you guess the energy eigenfunctions in momentum space?

---

a.

$$\begin{aligned}
\langle p'|x|\alpha\rangle &= \int dx' \langle p'|x|x'\rangle\langle x'|\alpha\rangle \\
&= \int dx' x' \langle p'|x'\rangle\langle x'|\alpha\rangle \\
&= \int dx' x' \left(\frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{-ipx'}{\hbar}\right)\right)\langle x'|\alpha\rangle \\
&= \int dx' i\hbar \frac{\partial}{\partial p'} \left(\frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{-ipx'}{\hbar}\right)\right)\langle x'|\alpha\rangle \\
&= i\hbar \frac{\partial}{\partial p'} \int dx' \langle p'|x'\rangle\langle x'|\alpha\rangle \\
&= i\hbar \frac{\partial}{\partial p'} \langle p'|\alpha\rangle
\end{aligned}$$

b.

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

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} \langle p'|\psi(t)\rangle &= \langle p'| \frac{1}{2m} p^2 + \frac{1}{2} m\omega^2 x^2 |\psi(t)\rangle \\
&= \frac{1}{2m} p'^2 \langle p'|\psi(t)\rangle + \frac{1}{2} m\omega^2 (i\hbar)^2 \frac{\partial^2}{\partial p'^2} \langle p'|\psi(t)\rangle
\end{aligned}$$

Therefore

$$i\hbar \frac{\partial}{\partial t} \langle p'|\psi(t)\rangle = -\frac{1}{2} m\omega^2\hbar^2 \frac{\partial^2}{\partial p'^2} \langle p'|\psi(t)\rangle + \frac{1}{2m} p'^2 \langle p'|\psi(t)\rangle$$

Suppose that

$$\left|\psi(t)\right\rangle = e^{-\frac{i}{\hbar}Ht}\left|\psi(t=0)\right\rangle = e^{-\frac{i}{\hbar}E_n t}\left|n\right\rangle,$$

we have

$$E_n\left\langle p'\middle|n\right\rangle = -\frac{1}{2}m\omega^2\hbar^2\frac{\partial^2}{\partial p'^2}\left\langle p'\middle|n\right\rangle + \frac{1}{2m}p'^2\left\langle p'\middle|n\right\rangle.$$

Here note that the Schrödinger equation in the position space is

$$E_n\left\langle x'\middle|n\right\rangle = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x'^2}\left\langle x'\middle|n\right\rangle + \frac{1}{2}m\omega^2 x'^2\left\langle x'\middle|n\right\rangle.$$

The eigenfunction in momentum space is

$$\left\langle p'\middle|n\right\rangle = \left(2^n n!\right)^{-\frac{1}{2}}\left(\frac{1}{m\omega\hbar\pi}\right)^{\frac{1}{4}}\exp\left(-\frac{1}{2}\zeta^2\right)H_n(\zeta)$$

with $\zeta = \frac{p'}{\sqrt{m\omega\hbar}}$.

((2-15))

15. Consider a function, known as the **correlation function**, defined by

$$C(t) = \langle x(t)x(0)\rangle,$$

where $x(t)$ is the position operator in the Heisenberg picture. Evaluate the correlation function explicitly for the ground state of a one-dimensional simple harmonic oscillator.

For the 1D harmonic oscillator (Heisenberg picture)

$$\hat{x}_H(t) = \hat{x}\cos\omega t + \frac{1}{m\omega}\hat{p}\sin\omega t.$$

$$C(t) = \langle 0|\hat{x}_H(t)\hat{x}_H(0)|0\rangle$$
$$= \langle 0|\hat{x}^2 \cos\omega_0 t + \frac{1}{m\omega_0}\hat{p}\hat{x}\sin\omega_0 t|0\rangle$$
$$= \cos\omega_0 t\langle 0|\hat{x}^2|0\rangle + \frac{\sin\omega t}{m\omega}\langle 0|\hat{p}\hat{x}|0\rangle$$
$$= \cos\omega_0 t\frac{\hbar}{2m\omega_0} + \frac{\sin\omega_0 t}{m\omega_0}\left(-\frac{i\hbar}{2}\right)$$
$$= \frac{\hbar}{2m\omega_0}e^{-i\omega_0 t}$$

where we use

$$\hat{p}\hat{x} = -\frac{i\hbar}{2}(\hat{a}^2 - \hat{a}^{+2} - \hat{a}^+\hat{a} + \hat{a}\hat{a}^+)$$
$$\langle 0|\hat{p}\hat{x}|0\rangle = -\frac{i\hbar}{2}$$
$$\langle 0|\hat{x}^2|0\rangle = \frac{\hbar}{2m\omega_0}$$

((**2-16**))

16. Consider again a one-dimensional simple harmonic oscillator. Do the following algebraically, that is, without using wave functions.
    a. Construct a linear combination of $|0\rangle$ and $|1\rangle$ such that $\langle x\rangle$ is as large as possible.
    b. Suppose the oscillator is in the state constructed in (a) at $t = 0$. What is the state vector for $t > 0$ in the Schrödinger picture? Evaluate the expectation value $\langle x\rangle$ as a function of time for $t > 0$ using (i) the Schrödinger picture and (ii) the Heisenberg picture.
    c. Evaluate $\langle(\Delta x)^2\rangle$ as a function of time using either picture.

---

a.
In Schrödinger picture

$$|\alpha\rangle = c_0|0\rangle + c_1|1\rangle$$

$$
\begin{aligned}
\langle \hat{x} \rangle &= \langle \alpha | \hat{x} | \alpha \rangle \\
&= |c_0|^2 \langle 0 | \hat{x} | 0 \rangle + |c_1|^2 \langle 1 | \hat{x} | 1 \rangle + c_0^* c_1 \langle 0 | \hat{x} | 1 \rangle + c_0 c_1^* \langle 1 | \hat{x} | 0 \rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}} (c_0^* c_1 + c_0 c_1^*)
\end{aligned}
$$

$c_0 \equiv r_0 e^{i\theta_0}$, $c_1 \equiv r_1 e^{i\theta_1}$

or using the matrix,

$$
\langle \alpha | \hat{x} | \alpha \rangle = \frac{1}{\sqrt{2}\beta} \begin{pmatrix} c_0^* & c_1^* \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = \sqrt{\frac{\hbar}{2m\omega}} (c_0^* c_1 + c_0 c_1^*)
$$

$|c_0|^2 + |c_1|^2 = 1$ => $r_0^2 + r_1^2 = 1$

(r_i, θ_i: real numbers) $r_0 = \cos \phi$, $r_1 = \sin \phi$,

$$
\begin{aligned}
\langle x \rangle &= \sqrt{\frac{\hbar}{2m\omega}} r_0 r_1 \left[e^{i(\theta_1 - \theta_0)} + e^{-i(\theta_1 - \theta_0)} \right] \\
&= \sqrt{\frac{\hbar}{2m\omega}} 2 r_0 r_1 \cos(\theta_0 - \theta_1) \\
&= \sqrt{\frac{\hbar}{2m\omega}} \sin(2\phi) \cos(\theta_0 - \theta_1)
\end{aligned}
$$

The maximum of $\langle x \rangle$ is given when

$\sin(2\phi) = 1$, $\cos(\theta_0 - \theta_1) = 1$

$\phi = \frac{\pi}{4}$, $r_0 = r_1 = \frac{1}{\sqrt{2}}$

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

b.

$$\left|\alpha(t)\right\rangle = \exp\left(-\frac{iH}{\hbar}t\right)\left|\alpha(t=0)\right\rangle$$
$$= \exp\left(-\frac{iH}{\hbar}t\right)\frac{1}{\sqrt{2}}(\left|0\right\rangle + \left|1\right\rangle)$$
$$= \frac{1}{\sqrt{2}}e^{-\frac{1}{2}i\omega t}\left|0\right\rangle + \frac{1}{\sqrt{2}}e^{-\frac{3}{2}i\omega t}\left|1\right\rangle$$

$$\left\langle \hat{x}\right\rangle = \left\langle \alpha(t)\right|\hat{x}\left|\alpha(t)\right\rangle$$
$$= \frac{1}{2}\left(e^{-i\omega t}\left\langle 0\right|\hat{x}\left|1\right\rangle + e^{i\omega t}\left\langle 1\right|\hat{x}\left|0\right\rangle\right)$$
$$= \sqrt{\frac{\hbar}{2m\omega}}\cos\omega t$$

In the Heisenberg picture

$$\left\langle x\right\rangle = \left\langle \alpha(0)\right|\hat{x}_H\left|\alpha(0)\right\rangle$$
$$= \left\langle \alpha\right|\left(\hat{x}\cos\omega t + \frac{\hat{p}}{m\omega}\sin\omega t\right)\left|\alpha\right\rangle$$
$$= \left(\frac{1}{\sqrt{2}}\left\langle 0\right| + \frac{1}{\sqrt{2}}\left\langle 1\right|\right)\left(\hat{x}\cos\omega t + \frac{\hat{p}}{m\omega}\sin\omega t\right)\left(\frac{1}{\sqrt{2}}\left|0\right\rangle + \frac{1}{\sqrt{2}}\left|1\right\rangle\right)$$
$$= \sqrt{\frac{\hbar}{2m\omega}}\cos\omega t$$

Note:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^+) \qquad \hat{x}^2 = \frac{\hbar}{2m\omega}(\hat{a} + \hat{a}^+)^2 = \frac{\hbar}{2m\omega}(\hat{a}^2 + \hat{a}^{+2} + 2\hat{a}^+\hat{a} + \hat{1})$$

$$\begin{cases}\left\langle 0\right|\hat{x}\left|1\right\rangle \neq 0 \\ \left\langle 1\right|\hat{x}\left|0\right\rangle \neq 0 \\ \left\langle 0\right|\hat{x}\left|0\right\rangle = 0 \\ \left\langle 1\right|\hat{x}\left|1\right\rangle = 0\end{cases} \qquad \begin{cases}\left\langle 0\right|\hat{x}^2\left|1\right\rangle = 0 \\ \left\langle 1\right|\hat{x}^2\left|0\right\rangle = 0 \\ \left\langle 0\right|\hat{x}^2\left|0\right\rangle \neq 0 \\ \left\langle 1\right|\hat{x}^2\left|1\right\rangle \neq 0\end{cases}$$

c.
In Schrödinger picture, we calculate

Then

$$\left\langle (\Delta x)^2 \right\rangle = \left\langle \hat{x}^2 \right\rangle - \left\langle \hat{x} \right\rangle^2$$
$$= \frac{\hbar}{m\omega} - \frac{\hbar}{2m\omega}\cos^2 \omega t$$
$$= \frac{\hbar}{m\omega} - \frac{\hbar}{2m\omega}(1 - \sin^2 \omega t)$$
$$= \frac{\hbar}{2m\omega}(1 + \sin^2 \omega t)$$

$$\langle \alpha(t)|\hat{x}^2|\alpha(t)\rangle = \frac{1}{2}\left(e^{\frac{1}{2}i\omega t}\langle 0| + e^{\frac{3}{2}i\omega t}\langle 1| \right)\hat{x}^2\left(e^{-\frac{1}{2}i\omega t}|0\rangle + e^{-\frac{3}{2}i\omega t}|1\rangle \right)$$
$$= \frac{1}{2}\left(\langle 0|\hat{x}^2|0\rangle + \langle 1|\hat{x}^2|1\rangle + e^{-i\omega t}\langle 0|\hat{x}^2|1\rangle + e^{i\omega t}\langle 1|\hat{x}^2|0\rangle \right)$$
$$= \frac{1}{2}\left(\langle 0|\hat{x}^2|0\rangle + \langle 1|\hat{x}^2|1\rangle \right)$$
$$= \frac{1}{2}\frac{\hbar}{2m\omega}(1+3) = \frac{\hbar}{m\omega}$$

((**2-17**))

17. Show for the one-dimensional simple harmonic oscillator

$$\langle 0|e^{ikx}|0\rangle = \exp[-k^2\langle 0|x^2|0\rangle/2],$$

where x is the position *operator*.

$$\langle 0|e^{ikx}|0\rangle = \int dx'\langle 0|x'\rangle\langle x'|e^{ikx}|0\rangle$$
$$= \int dx' e^{ikx'}\left|\langle x'|0\rangle\right|^2$$
$$= \int dx' e^{ikx'}\frac{1}{\pi^{1/2}x_0}\exp\left(-\frac{x'^2}{x_0^2}\right)$$
$$= \int dx'\frac{1}{\pi^{1/2}x_0}\exp\left[-\frac{1}{x_0^2}\left(x' - \frac{ikx_0}{2}\right)^2 - \frac{k^2}{4}x_0^2\right]$$
$$= \exp\left(-\frac{k^2}{4}x_0^2\right)$$
$$= \exp\left(-\frac{k^2\langle 0|x^2|0\rangle}{2}\right)$$

where

$$\langle 0|x^2|0\rangle = \frac{\hbar}{2m\omega} = \frac{x_0}{2}$$

$$\langle x'|0\rangle = \frac{1}{\pi^{1/4}x_0^{1/2}}\exp\left(-\frac{x'^2}{2x_0^2}\right)$$

((**2-20**))

20. Consider a particle of mass m subject to a one-dimensional potential of the following form:

$$V = \begin{cases} \frac{1}{2}kx^2 & \text{for } x > 0 \\ \infty & \text{for } x < 0. \end{cases}$$

a. What is the ground-state energy?
b. What is the expectation value $\langle x^2\rangle$ for the ground state?

(a)
The wave function for the simple harmonics has either an even parity or a odd parity.

Since the potential becomes infinity for x<0, the wave function should be zero at x – 0.

Thr odd function should be zero at x = 0, since $\psi(-x) = -\psi(x)$, or $\psi(0) = -\psi(0)$.

Then we have the eigenfunction with the odd parity.

The wave function with the odd parity is $|n\rangle$ with n = 1, 3, 5, 7, ……

The energy of the ground state is $\hbar\omega(1+\frac{1}{2}) = \frac{3}{2}\hbar\omega$

(b)

$$\langle x^2\rangle = \frac{\int_0^\infty x^2|\varphi_1|^2 dx}{\int_0^\infty {}^2|\varphi_1|^2 dx} = \frac{\int_0^\infty x^2|\varphi_1|^2 dx}{\int_0^\infty {}^2|\varphi_1|^2 dx} = \langle 1|\hat{x}^2|1\rangle = \frac{\hbar}{2m\omega}3 = \frac{3\hbar}{2m\omega}$$

((**2-21**))

21. A particle in one dimension is trapped between two rigid walls:

$$V(x) = \begin{cases} 0, & \text{for } 0 < x < L \\ \infty, & \text{for } x < 0, \quad x > L. \end{cases}$$

At $t = 0$ it is known to be exactly at $x = L/2$ with certainty. What are the *relative* probabilities for the particle to be found in various energy eigenstates? Write down the wave function for $t \geq 0$. (You need not worry about absolute normalization, convergence, and other mathematical subtleties.)

$$\left|\psi(t=0)\right\rangle = \left|x = L/2\right\rangle$$

$$\left\langle x|\varphi_n\right\rangle = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L})$$

with

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

$$\left|\psi(t)\right\rangle = \exp(-\frac{i\hat{H}t}{\hbar})\left|x = L/2\right\rangle = \sum_n \exp(-\frac{i\hat{H}t}{\hbar})\left|\varphi_n\right\rangle\left\langle\varphi_n\right|x = L/2\rangle$$

$$\left|\psi(t)\right\rangle = \sum_n \exp(-\frac{iE_n t}{\hbar})\left|\varphi_n\right\rangle\varphi_n^*(x = L/2) = \sum_n a_n(t)\left|\varphi_n\right\rangle$$

where

$$a_n(t) = \exp(-\frac{iE_n t}{\hbar})\varphi_n^*(x = L/2) = \sqrt{\frac{2}{L}}\exp(-\frac{iE_n t}{\hbar})\sin(\frac{n\pi}{2})$$

Note that $a_n = 0$, when n is even.

((**2-22**)

22. Consider a particle in one dimension bound to a fixed center by a δ-function potential of the form

$$V(x) = -v_0\delta(x), \quad (v_0 \text{ real and positive}).$$

Find the wave function and the binding energy of the ground state. Are there excited bound states?

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - v_0\delta(x)\psi(x) = E\psi(x)$$

$$\int_{-\varepsilon}^{\varepsilon}[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - v_0\delta(x)\psi(x)]dx = \int_{-\varepsilon}^{\varepsilon}E\psi(x)dx$$

or

The right-hand side is equal to zero in the limit of $\varepsilon \rightarrow 0$

$$-\frac{\hbar^2}{2m}\frac{d}{dx}\psi(x)|_{-\varepsilon}^{\varepsilon} = v_0\psi(0)$$

This is the boundary condition.

We consider the case of E<0. For x>0 and x<0, we have

$$\frac{d^2}{dx^2}\psi(x) = -\frac{2mE}{\hbar^2}\psi(x) = \frac{2m|E|}{\hbar^2}\psi(x) = \rho^2\psi(x)$$

where

$$\rho = \sqrt{\frac{2m|E|}{\hbar^2}}$$

$\psi(x)$ has the form,

$\psi(x) = Ae^{-\rho x}$ for x>0.

$\psi(x) = Be^{\rho x}$ for x<0.

The potential is symmetric with respect to $x = 0$. Thus the wave function should be even function or odd function.

(i) The wave function is even function.

$\psi(x) = Ae^{-\rho x}$ for x>0.

$\psi(x) = Ae^{\rho x}$ for x<0.

$$-\frac{\hbar^2}{2m}(-A\rho e^{-\rho\varepsilon} - A\rho e^{-\rho\varepsilon}) = v_0 A$$

or

$$A[\frac{\hbar^2}{m}\rho e^{-\rho\varepsilon} - v_0] = 0$$

or in the limit of $\varepsilon \to 0$

$$A(\frac{\hbar^2}{m}\rho - v_0) = 0$$

When $A \neq 0$,

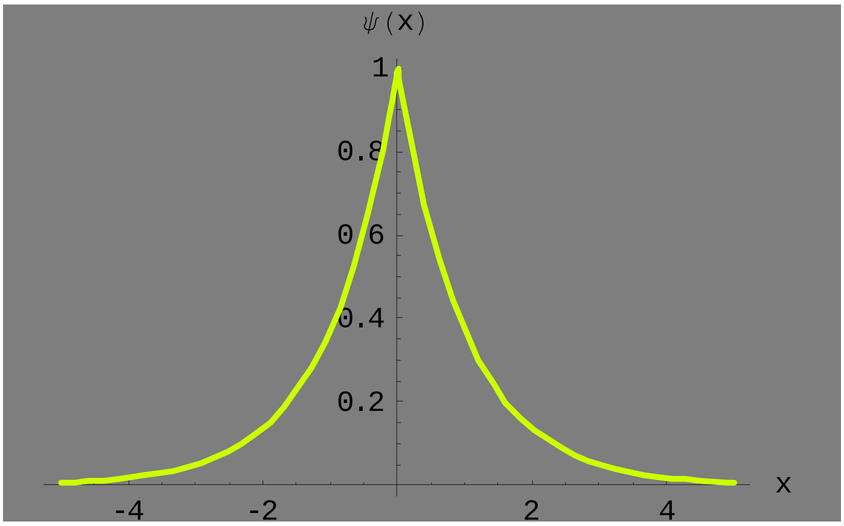
$$\rho = \sqrt{\frac{2m|E|}{\hbar^2}} = \frac{m v_0}{\hbar^2}$$

or

$$|E| = \frac{m {v_0}^2}{2\hbar^2}$$

The normalized wave function is

$$\psi(x) = \sqrt{\rho} e^{-\rho|x|}$$



There is no excited bound state.

(ii) The wave function is odd function.

$\psi(x) = Ae^{-\rho x}$ for $x>0$.

$\psi(x) = -Ae^{\rho x}$ for $x<0$.

$$-\frac{\hbar^2}{2m}(-A\rho e^{-\rho\varepsilon} + A\rho e^{-\rho\varepsilon}) = v_0 A$$

or in the limit of $\varepsilon \to 0$

$A=0$.

So there is no solution.

((**2-23**))

23. A particle of mass m in one dimension is bound to a fixed center by an attractive δ-function potential:

$$V(x) = -\lambda\delta(x), \quad (\lambda > 0).$$

At $t = 0$, the potential is suddenly switched off (that is, $V = 0$ for $t > 0$). Find the wave function for $t > 0$. (Be quantitative! But you need not attempt to evaluate an integral that may appear.)

(a)

Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - \lambda\delta(x)\psi(x) = E\psi(x)$$

$$\psi(x) = \langle x|\psi\rangle = \int \langle x|p\rangle\langle p|\psi\rangle dp = \int \frac{e^{\frac{ipx}{\hbar}}}{\sqrt{2\pi\hbar}}\langle p|\psi\rangle dp$$

Here we note that

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)=-\frac{\hbar^2}{2m}\int\left(\frac{ip}{\hbar}\right)^2\frac{e^{\frac{ipx}{\hbar}}}{\sqrt{2\pi\hbar}}\langle p|\psi\rangle dp=\int\frac{p^2}{2m}\frac{e^{\frac{ipx}{\hbar}}}{\sqrt{2\pi\hbar}}\langle p|\psi\rangle dp$$

and

$$\delta(x)\psi(x)=\psi(0)\delta(x)=\frac{\psi(0)}{\sqrt{2\pi\hbar}}\int\frac{e^{\frac{ipx}{\hbar}}}{\sqrt{2\pi\hbar}}dp$$

Thus we have

$$\frac{p^2}{2m}\langle p|\psi\rangle-\lambda\frac{\psi(0)}{\sqrt{2\pi\hbar}}=E\langle p|\psi\rangle$$

or

$$\psi(p)=\langle p|\psi\rangle=\frac{-\lambda\psi(0)}{\sqrt{2\pi\hbar}}\frac{1}{E-\frac{p^2}{2m}}$$

When E is negative, $\psi(p)$ will not diverge.

We now consider the time evolution operator.

$$\hat{U}(t)=\exp(-\frac{i}{\hbar}\hat{H}t)=\exp(-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}t)$$

$$|\psi(t)\rangle=\hat{U}(t)|\psi(t=0)\rangle=\exp(-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}t)|\psi\rangle=\int|p\rangle\langle p|\exp(-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}t)|\psi\rangle dp$$

$$=\int\exp(-\frac{i}{\hbar}\frac{p^2}{2m}t)|p\rangle\langle p|\psi\rangle dp=\frac{-\lambda\psi(0)}{\sqrt{2\pi\hbar}}\int|p\rangle dp\exp(-\frac{i}{\hbar}\frac{p^2}{2m}t)\frac{1}{E-\frac{p^2}{2m}}$$

Then we have

$$\langle x|\psi\rangle=\frac{-\lambda\psi(0)}{\sqrt{2\pi\hbar}}\int\langle x|p\rangle dp\exp(-\frac{i}{\hbar}\frac{p^2}{2m}t)\frac{1}{E-\frac{p^2}{2m}}$$

$$= \frac{-\lambda\psi(0)}{\sqrt{2\pi\hbar}} \int \frac{\exp(\frac{ipx}{\hbar} - \frac{i}{\hbar}\frac{p^2}{2m}t)}{E - \frac{p^2}{2m}} dp$$

((**2-28**))

28. Derive (2.5.16) and obtain the three-dimensional generalization of (2.5.16).

$$\langle x|\psi(t)\rangle = \langle x|\hat{U}(t,t')|\psi(t')\rangle = \int dx' \langle x|\hat{U}(t,t')|x'\rangle\langle x'|\psi(t')\rangle$$

$$K(x,t;x',t') = \langle x|\hat{U}(t,t')|x'\rangle = \langle x|\exp[-\frac{i}{\hbar}\hat{H}(t-t')]|x'\rangle$$

or

$$\langle x|\psi(t)\rangle = \int dx' K(x,t;x',t')\langle x'|\psi(t')\rangle$$

K(*x*, *t*; *x*', *t*') is referred to the propagator (kernel)

For the free particle, the propagator is given by

$$K(x,t;x',t') = \sqrt{\frac{m}{2\pi i\hbar(t-t')}} \exp[\frac{im(x-x')^2}{2\hbar(t-t')}]$$

Let's give a proof for this.

$\hat{H}$ is the Hamiltonian of the free particle.

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

$$\hat{H}|k\rangle = E_k|k\rangle$$

with

$$E_k = \frac{\hbar^2 k^2}{2m}, \qquad \omega_k = \frac{E_k}{\hbar}$$

$$K(x,t;x',t') = \langle x | \exp[-\frac{i}{\hbar}\hat{H}(t-t')) | x' \rangle$$

$$= \int dk \langle x | k \rangle \langle k | \exp[-\frac{i}{\hbar}\hat{H}(t-t')) | x' \rangle$$

$$= \int dk \langle x | k \rangle \langle k | \exp[-\frac{i\hbar k^2}{2m}(t-t')) | x' \rangle$$

$$= \int dk \frac{1}{2\pi} \exp[ik(x-x') - \frac{i\hbar k^2}{2m}(t-t')]$$

Note that

$$\exp[ik(x-x') - \frac{i\hbar k^2}{2m}(t-t')] = \exp[-\frac{i\hbar(t-t')}{2m}\{k - \frac{m(x-x')}{\hbar(t-t')}\}^2 - \frac{m(x-x')^2}{2i\hbar(t-t')}]$$

and

$$\int_{-\infty}^{\infty} dk \exp(-i\alpha k^2) = \sqrt{\frac{\pi}{i\alpha}}$$

or

$$K(x,t;x',t') = \sqrt{\frac{m}{2\pi i\hbar(t-t')}} \exp[\frac{im(x-x')^2}{2\hbar(t-t')}]$$

Probability amplitude that a particle initially at x' propagates to x in the interval t-t'.

This expression is generalized to that for the three dimension.

$$K(\mathbf{r},t;r',t') = [\frac{m}{2\pi i\hbar(t-t')}]^{3/2} \exp[\frac{im|\mathbf{r}-r'|^2}{2\hbar(t-t')}]$$

((**2-30**))

30. **The propagator in momentum space analogous to (2.5.26) is given by $\langle \mathbf{p}'', t | \mathbf{p}', t_0 \rangle$. Derive an explicit expression for $\langle \mathbf{p}'', t | \mathbf{p}', t_0 \rangle$ for the free-particle case.**

The propagator in the momentum space is defined by

$$K(\mathbf{p},t;\mathbf{p}'t') = \langle \mathbf{p} | \exp[-\frac{i}{\hbar}\hat{H}(t-t')] | \mathbf{p}' \rangle$$

with

$$\hat{H}|\mathbf{p}\rangle = \frac{\mathbf{p}^2}{2m}|\mathbf{p}\rangle$$

$$K(\mathbf{p},t;\mathbf{p}'t') = \exp[-\frac{i\mathbf{p}^2(t-t')}{2m\hbar}]\langle\mathbf{p}|\mathbf{p}'\rangle = \exp[-\frac{i\mathbf{p}^2(t-t')}{2m\hbar}]\delta(\mathbf{p}-\mathbf{p}')$$

((2-31))

$$L = \frac{m}{2}\dot{x}^2 - \frac{1}{2}m\omega_0{}^2x^2$$

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{x}}) = (\frac{\partial L}{\partial x}) = 0$$

$$\ddot{x} = -\omega_0{}^2 x$$

$$x'' = A\cos\omega_0 t'' + B\cos\omega_0 t''$$

Initial conditions

$$x = A\cos\omega_0 t + B\sin\omega_0 t$$

and

$$x' = A\cos\omega_0 t' + B\sin\omega_0 t'$$

A and *B* are determined from the above two equations.

$$x'' = \frac{x'\sin[\omega_0(t-t'')] - x\sin[\omega_0(t'-t'')]}{\sin[\omega_0(t-t')]}$$

$$\dot{x}'' = \frac{-x'\omega_0\cos[\omega_0(t-t'')] + x\omega_0\cos[\omega_0(t'-t'')]}{\sin[\omega_0(t-t')]}$$

$$L(x'',\dot{x}'',t'') = \frac{m}{2}\dot{x}''^2 - \frac{1}{2}m\omega_0{}^2x''^2$$

$$= \frac{m\omega_0{}^2}{2\sin^2[\omega_0(t-t')]}[-2xx'\cos[\omega_0(t++t'-2t'')$$

$$+ x'^2\cos[2\omega_0(t-t'')] + x^2\cos[\omega_0(t'-t'')])$$

$$S_{cl}=\int_{t'}^{t} L(t'')dt''=\frac{m\omega_0}{2\sin[\omega_0(t-t'))}[(x^2+x'^2)\cos\{\omega_0(t-t')\}-2xx']$$

$$K(x,t,x',t')=A\exp[\frac{i}{\hbar}S_{cl}]$$

$$=A\exp[\frac{im\omega_0}{2\hbar\sin[\omega_0(t-t')]}[(x^2+x'^2)\cos\{\omega_0(t-t')\}-2xx']]$$

In the limit of $t-t'\to 0$, we have

$$K(x,t,x',t')=A\exp[\frac{im\omega_0}{2\hbar\sin\{\omega_0(t-t')\}}(x-x')^2]$$

To find A, we use the fact that as $t-t'\to 0$, K must tend to $\delta(x\text{-}x')$

$$\delta(x-x')=\lim_{\Delta\to 0}\frac{1}{(\pi\Delta^2)^{1/2}}\exp[-\frac{(x-x')^2}{\Delta^2}]$$

In other words

$$A=\frac{1}{(\pi\Delta^2)^{1/2}}, \qquad \frac{1}{\Delta^2}=\frac{m\omega_0}{2i\hbar\sin\{\omega_0(t-t')\}}$$

So we get

$$\Delta=\sqrt{\frac{2i\hbar\sin\{\omega_0(t-t')\}}{m\omega_0}}$$

$$A=\frac{1}{(\pi\Delta^2)^{1/2}}=\sqrt{\frac{m\omega_0}{2\pi\hbar i\sin\{\omega_0(t-t')\}}}$$

or

$$K(x,t,x',t')$$
$$=\sqrt{\frac{m\omega_0}{2\pi\hbar i\sin\{\omega_0(t-t')\}}}\exp[\frac{im\omega_0}{2\hbar\sin[\omega_0(t-t')]}[(x^2+x'^2)\cos\{\omega_0(t-t')\}-2xx']]$$