Part IB — Quantum Mechanics Example Sheet 2

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QUESTION 1

The potential $V(x) = 0$ so our time independent SE is:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi$$

$$\iff \psi'' + k^2\psi = 0$$

setting $E = k^2\hbar^2/2m$, thus

$$\psi(x) = A\cos kx + B\sin kx$$

Using BCs, $\psi(0) = 0 \Rightarrow A = 0$

$\psi(a) = 0 \Rightarrow \sin ka = 0 \Rightarrow ka = n\pi$ for integer n, thus energy eigenvalues are $E_n = n^2\pi^2\hbar^2/2ma^2$ with corresponding energy eigenstates $B_n \sin k_n x = B_n \sin(\sqrt{2ma^2E_n/\hbar^2}x)$, and

$$\begin{aligned} 1 &= \int_0^a |\psi(x)|^2 \,\mathrm{d}x \\ &= \int_0^a B_n^2 \sin^2(k_n x)\,\mathrm{d}x \\ &= B_n^2\left[\frac{x}{2} - \frac{1}{4}\sin(2k_n x)\right]_0^a \\ &= B_n^2\frac{a}{2} \end{aligned}$$

$$\Rightarrow B_n = \sqrt{\frac{2}{a}}$$

$$\Rightarrow \text{norm. states are } \psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\sqrt{\frac{2ma^2E_n}{\hbar^2}}x\right)$$

Let ψ_n denote the expectation value of $\hat{x}$ in state ψ_n, then

$$\begin{aligned} \langle\hat{x}\rangle_n &= (\psi_n, \hat{x}\psi_n) \\ &= \int_0^a \psi_n^* x \psi_n \,\mathrm{d}x \\ &= \frac{2}{a}\int_0^a x\sin^2 k_n x\,\mathrm{d}x \end{aligned}$$

By parts,

$$
\begin{aligned}
\int_0^a x\sin^2 k_n x \,\mathrm{d}x &= \left[\frac{x^2}{2} - \frac{1}{4k_n}x\sin(2k_n x)\right]_0^a - \int_0^a \frac{x}{2} - \frac{1}{4k_n}\sin(2k_n x)\,\mathrm{d}x \\
&= \frac{a^2}{2} - \left[\frac{x^2}{4} + \frac{1}{8k_n^2}\cos(2k_n x)\right]_0^a \\
&= \frac{a^2}{2} - \left[\frac{x^2}{4} + \frac{1}{8k_n^2}\left(1-\sin^2(k_n x)\right)\right]_0^a \\
&= \frac{a^2}{2} - \frac{a^2}{4} \\
&= \frac{a^2}{4}
\end{aligned}
$$

Thus $\langle \hat{x}\rangle_n = a/2$ as required.
Next, uncertainty of measurement of $\hat{x}$ in state ψ given by

$$
\begin{aligned}
(\Delta x)_n^2 &= \langle \hat{x}^2\rangle_\psi - \langle \hat{x}\rangle_\psi^2 \\
&= \frac{2}{a}\int_0^a x^2\sin^2(k_n x)\,\mathrm{d}x - \frac{a^2}{4}
\end{aligned}
$$

By parts,

$$
\begin{aligned}
\int_0^a x^2\sin^2(k_n x)\,\mathrm{d}x &= \left[\frac{x^3}{2} - \frac{1}{4k_n}x^2\sin(2k_n x)\right]_0^a - \int_0^a x^2 - \frac{1}{2k_n}x\sin(2k_n x)\,\mathrm{d}x \\
&= \frac{a^3}{2} - \frac{a^3}{3} + \frac{1}{2k_n}\int_0^a x\sin(2k_n x)\,\mathrm{d}x \\
&= \frac{a^3}{6} + \frac{1}{2k_n}\left(\left[-\frac{1}{2k_n}x\cos(2k_n x)\right]_0^a + \frac{1}{2k_n}\int_0^a \frac{1}{2k_n}\cos(2k_n x)\,\mathrm{d}x\right) \\
&= \frac{a^3}{6} - \frac{a}{4k_n^2}\cos(2k_n a) \\
&= \frac{a^3}{6} - \frac{a}{4k_n^2}\left(1-\sin^2 k_n a\right) \\
&= \frac{a^3}{6} - \frac{a^3}{4n^2\pi^2}
\end{aligned}
$$

Hence

$$
\begin{aligned}
(\Delta x)_n^2 &= \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} - \frac{a^2}{4} \\
&= \frac{a^2}{12}\left(1 - \frac{6}{\pi^2 n^2}\right)
\end{aligned}
$$

as required.

QUESTION 2

Harmonic oscillator, mass m, frequency ω, has potential $V(x) = \frac{1}{2}m\omega^2 x^2$, hence Hamiltonian is given by

$$H\psi = -\frac{\hbar^2}{2m}\psi'' + \frac{1}{2}m\omega^2 x^2 \psi$$

Writing H in terms of momentum and position operators, we show that

$$\begin{aligned}
\langle H \rangle_\psi &= (\psi, H\psi) \\
&= (\psi, \frac{1}{2m}\hat{p}^2\psi + \frac{1}{2}m\omega^2\hat{x}^2\psi) \\
&= \frac{1}{2m}(\psi, \hat{p}^2\psi) + \frac{1}{2}m\omega^2(\psi, \hat{x}^2\psi) \\
&= \frac{1}{2m}\left((\Delta p)^2_\psi + \langle \hat{p} \rangle^2_\psi\right) + \frac{1}{2}m\omega^2\left((\Delta x)^2_\psi + \langle \hat{x} \rangle^2_\psi\right)
\end{aligned}$$

Energy eigenvalues given by

$$\begin{aligned}
\langle H \rangle_\psi &\geq \frac{1}{2m}(\Delta p)^2_\psi + + \frac{1}{2}m\omega^2(\Delta x)^2_\psi \\
&= \frac{1}{2m}\left((\Delta p)^2_\psi + + m^2\omega^2(\Delta x)^2_\psi\right) \\
&\geq \frac{1}{2m}\left(\hbar m\omega\right) = \frac{\hbar\omega}{2}
\end{aligned}$$

where the last inequality follows from the uncertainty relation.

QUESTION 3

Let $\Psi(x,t)$ be a solution of the time-dependent SE for a free particle ie. $\Psi(x,t)$ satisfies

$$i\hbar\dot{\Psi} = -\frac{\hbar^2}{2m}\Psi''$$

Define $\Phi(x,t) = \Psi(x-ut,t)e^{ikx}e^{-i\omega t}$, and setting $\Psi(\xi,\eta) = \Psi(x-ut,t)$,

$$\begin{aligned}\frac{\partial}{\partial t}\Psi(\xi,\eta) &= \frac{\partial\xi}{\partial t}\frac{\partial\Psi}{\partial\xi} + \frac{\partial\eta}{\partial t}\frac{\partial\Psi}{\partial\eta} \\ &= -u\frac{\partial\Psi}{\partial\xi} + \frac{\partial\Psi}{\partial\eta}\end{aligned}$$

and

$$\begin{aligned}\frac{\partial}{\partial x}\Psi(\xi,\eta) &= \frac{\partial\xi}{\partial x}\frac{\partial\Psi}{\partial\xi} + \frac{\partial\eta}{\partial x}\frac{\partial\Psi}{\partial\eta} \\ &= \frac{\partial\Psi}{\partial\xi}\end{aligned}$$

similarly the second derivative is

$$\frac{\partial^2\Psi}{\partial x^2} = \frac{\partial^2\Psi}{\partial\xi^2}$$

First calculate time derivatives,

$$\begin{aligned}\dot{\Phi} &= e^{ikx}\left(e^{-i\omega t}\frac{\partial}{\partial t}\Psi(\xi,\eta) - i\omega e^{-i\omega t}\Psi(\xi,\eta)\right) \\ &= e^{ikx}e^{-i\omega t}\left(-u\frac{\partial\Psi}{\partial\xi} + \frac{\partial\Psi}{\partial\eta} - i\omega\Psi\right)\end{aligned}$$

Next, spatial

$$\Phi' = e^{-i\omega t}\left(e^{ikx}\frac{\partial}{\partial x}\Psi(x-ut,t) + ike^{ikx}\Psi(x-ut,t)\right)$$

$$\begin{aligned}\Phi'' &= e^{-i\omega t}\left(e^{ikx}\frac{\partial^2}{\partial x^2}\Psi(x-ut,t) + 2ike^{ikx}\frac{\partial}{\partial x}\Psi(x-ut,t) - k^2e^{ikx}\Psi(x-ut,t)\right) \\ &= e^{-i\omega t}e^{ikx}\left(\frac{\partial^2\Psi}{\partial\xi^2} + 2ik\frac{\partial\Psi}{\partial\xi} - k^2\Psi\right)\end{aligned}$$

So time-dependent SE becomes

$$i\hbar\left(-u\frac{\partial\Psi}{\partial\xi}+\frac{\partial\Psi}{\partial\eta}-i\omega\Psi\right)=-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial\xi^2}+2ik\frac{\partial\Psi}{\partial\xi}-k^2\Psi\right)$$

Linear independence allows us to compare the coefficients of $\frac{\partial\Psi}{\partial\xi}$ and Ψ to obtain

$$-i\hbar u=-\frac{\hbar^2}{2m}2ik \qquad \hbar\omega=\frac{\hbar^2k^2}{2m}$$

$$mu=\hbar k \qquad 2m\omega=\hbar k^2$$

Thus Φ is a solution if $k=\frac{mu}{\hbar}$ and $\omega=\frac{\hbar}{2m}k^2=\frac{mu^2}{2\hbar}$
Next, comparing expectation values.
Note

$$\begin{aligned}\langle\hat{x}\rangle_\Psi&=(\Psi,\hat{x}\Psi)\\&=\int_{-\infty}^{\infty}x|\Psi|^2\,\mathrm{d}x\end{aligned}$$

Clearly

$$|\Phi|^2=|\Psi|^2$$

and so

$$\langle\hat{x}\rangle_\Phi=\langle\hat{x}\rangle_\Psi$$

But

$$\begin{aligned}\langle\hat{p}\rangle_\Phi&=\int_{-\infty}^{\infty}\Phi^*(-i\hbar\Phi')\,\mathrm{d}x\\&=\int_{-\infty}^{\infty}\Psi^*(-i\hbar\Psi')\,\mathrm{d}x+\int_{-\infty}^{\infty}\Psi^*\Psi\,\mathrm{d}x\\&=\langle\hat{p}\rangle_\Psi+\hbar k\end{aligned}$$

To show consistency with Ehrenfest's Thm, want to check

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{x}\rangle_\Phi=\frac{1}{m}\langle\hat{p}\rangle_\Psi$$

However since $\langle\hat{x}\rangle_\Phi=\langle\hat{x}\rangle_\Psi$, their derivatives must also be equal; this cannot happen as $\langle\hat{p}\rangle_\Phi\neq\langle\hat{p}\rangle_\Psi$, so the first part of Ehrenfest's does not hold.
The next part

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{p}\rangle_\Phi=-\langle V'(\hat{x})\rangle_\Psi$$

does hold, as the difference in momenta does not depend on t.

QUESTION 4

We have

$$H\psi_n(x) = E_n\psi_n(x)$$

For energy levels $E_n = (n+\frac{1}{2})\hbar\omega$ with corresponding energy eigenstates $\psi_n(x) = h_n(y)e^{-y^2/2}$ where $y = (m\omega/\hbar)^{1/2}x$ and h_n is a polynomial of degree n with $h_n(-y) = (-1)^n h_n(y)$, for $n = 0, 1, 2, \cdots$

First, $\psi_0(x) = a_0 e^{-y^2/2}$ for some constant a_0.

Know that $\psi_2(x) = a_2(y)e^{-y^2/2}$, $h_2(-y) = h_2(y)$ even function so $h_2(y)$ is of the from $Ay^2 + B$. By orthogonality,

$$\begin{aligned}
0 &= (\psi_0, \psi_2) \\
&= \int_{-\infty}^{\infty} \psi_0^* \psi_2 \, \mathrm{d}y \\
&= \int_{-\infty}^{\infty} a_0 \left(Ay^2 + B\right) e^{-y^2/2} \, \mathrm{d}y \\
&= a_0 \left(A\sqrt{2\pi} + B\sqrt{2\pi}\right)
\end{aligned}$$

Thus $A = -B$, and $\psi_2(x) = a_2(y^2 - 1)$ for some constant a_2. Similarly, can write $h_3 = Cy^3 + Dy$ as h_3 odd function. Letting $h_1(y) = a_1 y$ for some constant a_1 we have:

$$\begin{aligned}
0 &= (\psi_1, \psi_3) \\
&= \int_{-\infty}^{\infty} \psi_1^* \psi_3 \, \mathrm{d}y \\
&= \int_{-\infty}^{\infty} a_1 y \left(Cy^3 + Dy\right) e^{-y^2/2} \, \mathrm{d}y \\
&= a_1 \left(3C\sqrt{2\pi} + B\sqrt{2\pi}\right)
\end{aligned}$$

Thus $B = -3C$, and we can write $\psi_3(x) = a_3(y^3 - 3y)$.

Next, if the initial state can be written as $\Psi(x, 0) = \sum_{n=0}^{\infty} c_n\psi_n(x)$, then

$$\begin{aligned}
\Psi(x, t) &= \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar} \\
&= \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-i(n+\frac{1}{2})\omega t} \\
&=
\end{aligned}$$

QUESTION 5

SE is

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x)$$

Probability current given by

$$J(x) = -\frac{i\hbar}{2m}(\psi^*\psi' - (\psi^*)'\psi)$$

Differentiating with respect to x,

$$\begin{aligned}
\frac{\mathrm{d}J}{\mathrm{d}x} &= -\frac{i\hbar}{2m}\left[(\psi^*)'\psi' + \psi^*\psi'' - (\psi^*)''\psi - (\psi^*)'\psi'\right] \\
&= -\frac{i\hbar}{2m}\left[\psi^*\psi'' - (\psi^*)''\psi\right] \\
&= -\frac{i\hbar}{2m}\left[\psi^*\left(-\frac{2m}{\hbar^2}(E-V)\psi\right) - \left(-\frac{2m}{\hbar^2}(E-V)\psi^*\right)\psi\right] \\
&= 0
\end{aligned}$$

Probability current as $x \to -\infty$, $\psi(x) \sim e^{ikx} + Be^{-ikx}$ given by:

$$\begin{aligned}
J &= -\frac{i\hbar}{2m}\left[(e^{-ikx} + B^*e^{ikx})(ike^{ikx} - ikBe^{-ikx}) - (-ike^{-ikx} + ikB^*e^{ikx})(e^{ikx} + Be^{-ikx})\right] \\
&= -\frac{i\hbar}{2m}\left[ik - ikBe^{-2ikx} + ikB^*e^{2ikx} - ik|B|^2 - \left(-ik - ikBe^{-2ikx} + ikB^*e^{2ikx} + ik|B|^2\right)\right] \\
&= -\frac{i\hbar}{2m}\left[2ik - 2ik|B|^2\right] \\
&= \frac{\hbar k}{m}(1 - |B|^2)
\end{aligned}$$

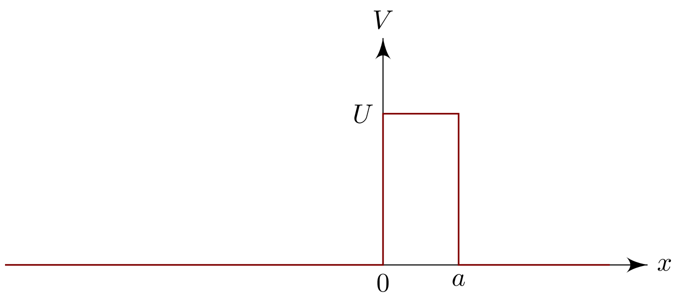
Probability current as $x \to \infty$, $\psi(x)Ce^{ikx}$ given by:

$$\begin{aligned}
J &= -\frac{i\hbar}{2m}\left[(C^*e^{-ikx})(ikCe^{ikx}) - (-ikC^*e^{-ikx})(Ce^{ikx})\right] \\
&= -\frac{i\hbar}{2m}\left[2ik|C|^2\right] \\
&= \frac{\hbar k}{m}|C|^2
\end{aligned}$$

As independent of x these two expressions are equal, thus $|B|^2 + |C|^2 = 1$

QUESTION 6

Take the potential to be



$$V(x) = \begin{cases} U & \text{if } 0 < x < a \\ 0 & \text{othewise} \end{cases}$$

where $U = 2E$. Set the constant

$$E = \frac{\hbar^2 k^2}{2m}$$

Then the Schrödinger equations become

$$\begin{aligned} \psi'' + k^2\psi &= 0 & x &< 0 \\ \psi'' - k^2\psi &= 0 & 0 < x &< a \\ \psi'' + k^2\psi &= 0 & x &> a \end{aligned}$$

So we get

$$\begin{aligned} \psi &= Ie^{ikx} + Re^{-ikx} & x &< 0 \\ \psi &= Ae^{kx} + Be^{-kx} & 0 < x &< a \\ \psi &= Te^{ikx} & x &> a \end{aligned}$$

(no e^{-ikx} term $\iff$ no particles sent from right)

Matching ψ and ψ' at $x = 0$ and a gives the equations

$$\begin{aligned} I + R &= A + B \\ ik(I - R) &= k(A - B) \\ Ae^{ka} + Be^{-ka} &= Te^{ika} \\ k(Ae^{ka} - Be^{ka}) &= ikTe^{ika}. \end{aligned}$$

We can solve these to obtain

$$\begin{aligned} I + \frac{k - ik}{k + ik}R &= Te^{ika}e^{-ka} \\ I + \frac{k + ik}{k - ik}R &= Te^{ika}e^{ka}. \end{aligned}$$

After ~~lots of~~ *some* algebra, we obtain

$$T = Ie^{-ika} (\cosh ka)^{-1}$$

To interpret this, we use the currents

$$j = j_{\text{inc}} + j_{\text{ref}} = (|I|^2 - |R|^2) \frac{\hbar k}{m}$$

for $x < 0$. On the other hand, we have

$$j = j_{\text{tr}} = |T|^2 \frac{\hbar k}{m}$$

for $x > a$. We can use these to find the transmission probability, and it turns out to be

$$P_{\text{tr}} = \frac{|j_{\text{tr}j}|}{|j_{\text{inc}}|} = \frac{|T|^2}{|I|^2} = \left[\cosh^2 ka\right]^{-1}.$$

This demonstrates *quantum tunneling*. There is a non-zero probability that the particles can pass through the potential barrier even though it classically does not have enough energy.

QUESTION 7

Time independent SE is

$$-\frac{\hbar^2}{2m}\psi'' - U\delta(x)\psi = E\psi$$

QUESTION 8

(i)

$$
\begin{aligned}
1 &= \int_0^a |\Psi|^2 \, \mathrm{d}x \\
&= C^2 \int_0^a x^2(a-x)^2 \, \mathrm{d}x \\
&= C^2 \frac{a^5}{30}
\end{aligned}
$$

So $C = \sqrt{30}a^{-5/2}$

(ii)

QUESTION 9

$Q\psi_n = 0 \; \forall \; n > 2 \Rightarrow$ zero is an eigenvalue. We are also given

$$Q\psi_1 = \psi_2, Q\psi_2 = \psi_1$$

Adding (and using linearity) gives $Q(\psi_1 + \psi_2) = \psi_1 + \psi_2$, thus 1 is an eigenvalue of Q. Similarly subtracting shows that $Q(\psi_1 - \psi_2) = -(\psi_1 - \psi_2)$, ie. -1 is an eigenvalue.

To find normalised eigenstates,

$$\begin{aligned}
1 &= \int |C|^2 |\psi_1 + \psi_2|^2 \, \mathrm{d}x \\
&= |C^2| \int (\psi_1 + \psi_2)^* (\psi_1 + \psi_2) \, \mathrm{d}x \\
&= |C^2| \int |\psi_1|^2 + |\psi_2|^2 \qquad \text{(by orthoganilty of eigenstates)} \\
&= 2|C^2| \quad \text{as } \psi_n \text{ normalised}
\end{aligned}$$

Thus $\chi_+ = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2)$, and similarly $\chi_- = \frac{1}{\sqrt{2}}(\psi_1 - \psi_2)$

$$\begin{aligned}
\langle H \rangle_{\chi_\pm} &= (\chi_\pm, H\chi_\pm) \\
&= \frac{1}{\sqrt{2}}((\psi_1 \pm \psi_2), H(\psi_1 \pm \psi_2) \\
&= \frac{1}{\sqrt{2}}((\psi_1, H\psi_1) \pm (\psi_2, H\psi_2) \\
&= \frac{1}{\sqrt{2}}(E_1 \pm E_2)
\end{aligned}$$

Measurement axioms $\Rightarrow$ at time zero, Q is in state χ_+. Have

$$\Psi(0) = \alpha_+ \chi_+ + \alpha_- \chi_- \qquad (\alpha_\pm = (\chi_\pm, \Psi(0)))$$

By linearity, the solution of the t-dep SE is

$$\begin{aligned}
\Psi(t) &= \alpha_+ \chi_+ e^{-iE_+ t/\hbar} + \alpha_- \chi_- e^{-iE_- t/\hbar} \\
&=
\end{aligned}$$

QUESTION 10

$$\begin{aligned}
\langle [H, A] \rangle_\psi &= \langle HA - AH \rangle_\psi \\
&= (\psi, (HA - AH)\psi) \\
&= (\psi, HA\psi) - (\psi, AH\psi) \\
&= (H\psi, A\psi) - (\psi, AH\psi)
\end{aligned}$$

QUESTION 11