QM HW4

Jiete XUE

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Problem 1 (Probability current)
By definition
$$\frac{\partial \rho}{\partial t} = \frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t}. \tag{1.1}$$
By Schrödinger equation,
$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m}\nabla^2\psi - \frac{iV}{\hbar}\psi. \tag{1.2}$$
$$\frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m}\nabla^2\psi^* + \frac{iV}{\hbar}\psi^*.^1 \tag{1.3}$$
Plug in (1.1),
$$\frac{\partial \rho}{\partial t} = \frac{i\hbar}{2m}\left[\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right] = \frac{i\hbar}{2m}\nabla\cdot\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right]. \tag{1.4}$$
Let
$$\boxed{\vec{j} = -\frac{i\hbar}{2m}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right].} \tag{1.5}$$
Then,
$$\frac{\partial \rho}{\partial t} + \nabla\cdot\vec{j} = 0. \tag{1.6}$$
Problem 2 (time-evolution)
(1)
$$\frac{\mathrm{d}\bar{O}}{\mathrm{d}t} = \frac{\partial}{\partial t}\langle\psi| O |\psi\rangle + \langle\psi| O \frac{\partial}{\partial t}|\psi\rangle. \tag{2.1}$$
The Schrödinger equation in bra-ket form is
$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle. \tag{2.2}$$
$$-i\hbar\frac{\partial}{\partial t}\langle\psi| = \langle\psi| H. \tag{2.3}$$

[1] $V^* = V$.

Then we can deduce that,

$$\boxed{\frac{\mathrm{d}\bar{O}}{\mathrm{d}t} = \frac{i}{\hbar}\langle\psi|[H,O]|\psi\rangle = 0.} \tag{2.4}$$

(2) Let E be the eigen-value of state $|\psi(t)\rangle$,then

$$\langle\psi|[H,O]|\psi\rangle = \langle\psi|EO|\psi\rangle - \langle\psi|OE|\psi\rangle = 0. \tag{2.5}$$

Therefore,

$$\boxed{\frac{\mathrm{d}\bar{O}}{\mathrm{d}t} = 0.} \tag{2.6}$$

Problem 3 (f-sum rule)
We calculate the commutator first.

$$[H,x] = \frac{1}{2m}\left[p^2,x\right] + [V(x),x] = -i\hbar\frac{p}{m}. \tag{3.1}$$

$$[[H,x],x] = -\frac{i\hbar}{m}[p,x] = -\frac{\hbar^2}{m}. \tag{3.2}$$

Then for any eigen state $|l\rangle$,

$$\langle l|[[H,x],x]|l\rangle = -\frac{\hbar^2}{m}. \tag{3.3}$$

One has

$$\langle l|[[H,x],x]|l\rangle = \sum_n\left[\langle l|[H,x]|n\rangle\langle n|x|l\rangle - \langle l|x|n\rangle\langle n|[H,x]|l\rangle\right]. \tag{3.4}$$

$$\langle l|[H,x]|n\rangle = E_l\langle l|x|n\rangle - \langle l|x|n\rangle E_n. \tag{3.5}$$

Hence,

$$-\frac{\hbar^2}{m} = 2\sum_n(E_l - E_n)\left|\langle n|x|l\rangle\right|^2, \tag{3.6}$$

$$\boxed{\sum_n(E_n - E_l)\left|\langle n|x|l\rangle\right|^2 = \frac{\hbar^2}{2m}.} \tag{3.7}$$

Problem 4 (The double δ-potential)
(1) By the conservation of current of probability, we can find the relation between R and S.

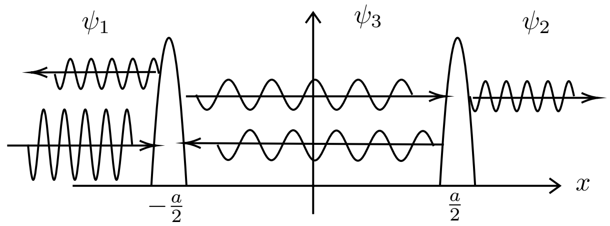
$$j_1 = \frac{k\hbar}{m}\left(1 - |R|^2\right). \tag{4.1}$$

$$j_2 = \frac{k\hbar}{m}|S|^2. \tag{4.2}$$

$j_1 = j_2$ leads to

$$\boxed{|R|^2 + |S|^2 = 1.} \tag{4.3}$$

(2) Suppose $\psi_3(x) = Ae^{ikx} + Be^{-ikx}$.



Since the wavefunction is continuous,

$$\psi_1\left(-\frac{a}{2}\right)=\psi_3\left(-\frac{a}{2}\right),\psi_3\left(\frac{a}{2}\right)=\psi_2\left(\frac{a}{2}\right). \tag{4.4}$$

Thus,

$$e^{-ik\frac{a}{2}}+Re^{ik\frac{a}{2}}=Ae^{-ik\frac{a}{2}}+Be^{ik\frac{a}{2}}, \tag{4.5}$$

$$Se^{ik\frac{a}{2}}=Ae^{ik\frac{a}{2}}+Be^{-ik\frac{a}{2}}. \tag{4.6}$$

Integrate the Schrödinger equation,

$$\lim_{\epsilon\to 0^+}\int_{x_0-\epsilon}^{x_0+\epsilon}\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)\right]\psi(x)\,\mathrm{d}x=\lim_{\epsilon\to 0^+}\int_{x_0-\epsilon}^{x_0+\epsilon}E\psi(x)\,\mathrm{d}x=0. \tag{4.7}$$

i.e.

$$\psi_3'\left(-\frac{a}{2}\right)-\psi_1'\left(-\frac{a}{2}\right)=\frac{2m\gamma}{\hbar^2}\psi\left(-\frac{a}{2}\right), \tag{4.8}$$

$$\psi_2'\left(\frac{a}{2}\right)-\psi_3'\left(\frac{a}{2}\right)=\frac{2m\gamma}{\hbar^2}\psi\left(\frac{a}{2}\right). \tag{4.9}$$

Then we can deduce that,

$$A=\frac{2(\sigma+2)}{\sigma^2\tau^4-\sigma^2+4},B=-\frac{2\sigma\tau^2}{\sigma^2\tau^4-\sigma^2+4}, \tag{4.10}$$

$$R=-\frac{\left[(\sigma+1)^2-1\right](\tau^4-1)}{\tau^2\left(\sigma^2\tau^4-\sigma^2+4\right)},S=\frac{4}{\sigma^2\tau^4-\sigma^2+4} \tag{4.11}$$

where

$$\tau=e^{ik\frac{a}{2}},\ \sigma=\frac{2m\gamma}{ik\hbar^2}. \tag{4.12}$$

When, $|S|=1$, $\tau^4=e^{i2ka}=1$, hence,

$$\boxed{ka=n\pi,\ n=1,2,3,\ldots} \tag{4.13}$$

(3) For bounded state, $\lim_{x\to-\infty}\exp(-ikx)=0$

$$k=i\kappa=i\sqrt{-\frac{2mE}{\hbar^2}}. \tag{4.14}$$

Let $\psi_1 = Ce^{\kappa x}, \psi_2 = Ae^{\kappa x} \pm Ae^{-\kappa x}, \psi_3 = \pm Ce^{-\kappa x}$.[2] Then,

$$C\tau = A\tau \pm \frac{A}{\tau}, \tag{4.15}$$

$$\left[C\tau - \left(A\tau \mp \frac{A}{\tau}\right)\right] = -\sigma C\tau. \tag{4.16}$$

So,

$$\sigma = \frac{2}{\pm\tau^2 - 1}. \tag{4.17}$$

That's exactly the condition to make the denominator of S and R equal to 0. That means the bounded state do not allow the wavefunction to have the form $\exp(-ikx)$.

Problem 5 (Bound states)
First, we clarify that if $V_1(x) < V_2(x),\ -\infty < x < +\infty$, then $E_{g1} < E_{g2}$.

$$\begin{aligned}
E_{g2} \left|\psi_{g2}\right\rangle =& \sum_n H_2 \left|\psi_{n1}\right\rangle \left\langle \psi_{n1} | \psi_{g2}\right\rangle & (5.1)\\
=& \sum_n \left[H_1 + (V_2 - V_1)\right] \left|\psi_{n1}\right\rangle \left\langle \psi_{n1} | \psi_{g2}\right\rangle & (5.2)\\
=& \sum_n E_{n1} \left|\psi_{g1}\right\rangle \left\langle \psi_{g1} | \psi_{g2}\right\rangle + (V_2 - V_1) \left|\psi_{g2}\right\rangle & (5.3)\\
\geq& E_{g1} \left|\psi_{g2}\right\rangle + (V_2 - V_1) \left|\psi_{g2}\right\rangle & (5.4)
\end{aligned}$$

Thus,

$$(E_{g1} - E_{g2}) \left|\psi_{g2}\right\rangle \leq \int_{-\infty}^{+\infty} (V_1 - V_2) \left|x\right\rangle \left\langle x | \psi_{g2}\right\rangle \mathrm{d}x < 0 \left|\psi_{g2}\right\rangle. \tag{5.5}$$

$$\boxed{E_{g1} < E_{g2}} \tag{5.6}$$

Now, let $V_2(x) = 0$, then,

$$\psi_2(x) = Ae^{-ikx} + Be^{ikx}, \tag{5.7}$$

where,

$$k = \sqrt{\frac{2mE}{\hbar^2}}. \tag{5.8}$$

If $E_{g2} < 0$, then k is an imaginary number. That contradicts to the finiteness of probability as $x \to \infty$. So $E_{g2} = 0$. By the lemma, we obtain:

$$\boxed{E_{g1} < 0.} \tag{5.9}$$

[2]We set the odd or even parity solution.