ϕ506 Problems

⑯ In Schrödinger's Eqtn for mass m in an external 3D potential $V(\mathbf{r},t)$, $i\hbar\,\partial\psi/\partial t = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi$, let V become complex: $V \to V - i\frac{\hbar}{2}\Gamma$, w/ $\Gamma = \Gamma(\mathbf{r},t)$ a real function. Retain the standard forms for the probability density & current, resp. $\rho = |\psi|^2$ & $\mathbb{J} = (\hbar/2im)[\psi^*\nabla\psi - \psi\nabla\psi^*]$.

(A) Find the effect of Γ on the continuity eqtn, i.e. $\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbb{J} \to$ what?

(B) Integrate the continuity eqtn of part (A) over all space to find the effect of Γ on the total probability $\mathcal{P} = \int_\infty \rho\, d^3r$. Interpret your result. What happens to $\mathcal{P}$ (and thus m) if Γ is a positive real cnst?

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⑰ Consider the 1D Schrödinger Eqtn for m in a complex potential: $i\hbar\frac{\partial\psi}{\partial t} = \left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + [V(x) - \frac{1}{2}i\hbar\Gamma]\right\}\psi$, w/ $V(x)$ real & time indept., and $\Gamma = \text{real cnst} \geqslant 0$.

(A) Carry out a separation of variables: $\Psi(x,t) = u(x)f(t)$, to find out how Γ affects the wavefcn Ψ. What happens as $t\to\infty$?

(B) Discuss the effect of Γ on the expectation values of m's Newtonian motion: $\langle p\rangle = m\frac{d}{dt}\langle x\rangle$, $\langle F\rangle = \frac{d}{dt}\langle p\rangle$. Interpret your results classically.

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⑱ Starting from the definition: $\int_\infty (Q\psi)^*\psi\,dx = \int_\infty \psi^*(Q\psi)\,dx$, for a Hermitian operator Q (in 1D), show--by direct integration--that the momentum operator $p = -i\hbar\,\partial/\partial x$, and the total energy operator $E = i\hbar\,\partial/\partial t$, are both Hermitian. What does this imply for the expectation values of p & E?

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⑲ (A) For a = complex cnst, and Q a general operator, show that the adjoint operator for aQ is: $(aQ)^\dagger = a^* Q^\dagger$.

(B) Consider Q as a product of operators q_i, i.e. $Q = q_1 q_2 q_3 \cdots q_n$. Show that the adjoint here is: $Q^\dagger = q_n^\dagger \cdots q_3^\dagger q_2^\dagger q_1^\dagger$ (reversed order!).

(C) Let A & B be arbitrary Hermitian operators. Show that the operator defined by: $iC = AB - BA$, is also Hermitian.

(16) Effect of a complex potential on probability conservation.

(A)
$$\psi^* \cdot \left\{ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + (V - \tfrac{1}{2} i\hbar\Gamma)\psi \right\}, \quad ①$$
$$\psi \cdot \left\{ -i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + (V + \tfrac{1}{2} i\hbar)\psi^* \right\}; \quad ②$$
$$\rightarrow i\hbar\left(\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t}\right) = -\frac{\hbar^2}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right) - i\hbar\Gamma\psi^*\psi; \quad (1)$$

so,
$$\underline{\underline{\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = -\Gamma\rho.}} \quad (2)$$

Write Sch. Eq. ① and its complex conjugate ②. Multiply ① on left by ψ^*, and ② on left by ψ. Subtract the eqtns to get Eq. (1). Identify $\rho = \psi^*\psi$ and $\mathbf{J}$ as given, and divide by $i\hbar$ to get Eq. (2). A non-zero Γ (i.e. potential with $\mathrm{Im}\,V \neq 0$) introduces a non-conservative term in Γ on the RHS of Eq. (2). This term will result in the non-conservation of particles.

(B) If $\mathcal{P} = \int_\infty \rho\, d^3r$ is the probability of finding m somewhere (anywhere) in space, then an integral $\int_\infty d^3r \cdot$ through Eq. (2) produces...

$$\rightarrow \frac{\partial \mathcal{P}}{\partial t} + \underbrace{\int_\infty \nabla \cdot \mathbf{J}\, d^3r} = -\int_\infty \Gamma\rho\, d^3r$$

convert to surface integral by Gauss' Thm: $\oint_\infty \mathbf{J} \cdot d\mathbf{S} \rightarrow 0$

$$\underline{\underline{\frac{\partial \mathcal{P}}{\partial t} = -\int_\infty \Gamma\rho\, d^3r}}, \quad \text{for general } \Gamma = \Gamma(\mathbf{r}, t). \quad (3)$$

$\rho = \psi^*\psi$ is (+) ve definite throughout the space, and if Γ is also, then (3) shows that $\mathcal{P}$ will decrease in time -- i.e. the probability of finding m somewhere (anywhere) in space will ultimately vanish. On the other hand, if Γ is (−) ve definite, then $\mathcal{P}$ increases in time and grows without bound. If Γ = (+) ve real cnst, then (3) yields...

$$\rightarrow \partial\mathcal{P}/\partial t = -\Gamma\mathcal{P} \Rightarrow \mathcal{P}(t) = \underline{\underline{\mathcal{P}(0)\exp(-\Gamma t).}} \quad (4)$$

Which is exponential decay of m. Clearly, in Schrödinger theory, we need a real potential V in order to conserve particles.

ϕ506 Solutions

(17) Effect of decay rate $\Gamma = \text{cnst} \geq 0$ on ψ(1D), and on Newton's Laws.

(A) Write the given 1D Schrödinger Eqtn with $\Gamma = \text{cnst} \geq 0$ as...

$$\rightarrow i\hbar\left(\frac{\partial}{\partial t} + \frac{\Gamma}{2}\right)\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi. \tag{1}$$

For separation of x (space) & t (time) variables, put $\psi(x,t) = u(x)f(t)$. Upon this substitution, and division by $1/uf$, we obtain...

$$\rightarrow \frac{i\hbar}{f}\left(\frac{\partial}{\partial t} + \frac{\Gamma}{2}\right)f = \frac{1}{u}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]u. \tag{2}$$

The LHS of (2) is a fcn of t only, while the RHS is a fcn of x only. Then (2) can be satisfied only if both sides are $\equiv$ some cnst W, indpt of x & t. So we get the separation [as in CLASS NOTES, p. Sch. 21, Eqs.(53)-(55)]...

$$\underline{i\hbar\left(\frac{\partial}{\partial t} + \frac{\Gamma}{2}\right)f = Wf} \; ; \; \underline{\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]u = Wu} \; ; \; W = \text{cnst}. \tag{3}$$

The solution to the first of Eqs.(3), for $\Gamma = \text{cnst} \geq 0$, is..

$$\underline{\underline{f(t) = e^{-\frac{i}{\hbar}(W - \frac{1}{2}i\hbar\Gamma)t} = e^{-(i/\hbar)Wt} \cdot e^{-(\Gamma/2)t}}} \tag{4}$$

Γ affects the system wavefcn $\psi = uf$ by introducing an <u>exponential decay factor</u>; $\psi^*\psi \sim e^{-\Gamma t} \rightarrow 0$, as $t \rightarrow \infty$. m <u>disappears</u> after $\Delta t \sim 1/\Gamma$!

(B) $\langle x \rangle = \int_\infty x|\psi|^2 dx \rightarrow e^{-\Gamma t}\int_\infty x|u|^2 dx$ also decays as a result of $\Gamma > 0$. The QM version of Newtonian momentum then finally vanishes, as...

$$\rightarrow \langle p \rangle = m\frac{d}{dt}\langle x \rangle = \langle p \rangle_0 - \Gamma m e^{-\Gamma t}\int_\infty x|u|^2 dx \;,\; \langle p \rangle_0 = \langle p \rangle|_{t=0}. \tag{5}$$

m not only disappears, but comes to a dead stop in the process. Classically, this is the effect of a <u>dissipative</u> (i.e. frictional) <u>force</u>. The force doing this is//

$$\rightarrow \langle F \rangle = \frac{d}{dt}\langle p \rangle = \Gamma^2 m e^{-\Gamma t}\int_\infty x|u|^2 dx = \Gamma(\langle p \rangle_0 - \langle p \rangle). \tag{6}$$

⑱ Show $p_{op} = -i\hbar\,\partial/\partial x$ and $E_{op} = i\hbar\,\partial/\partial t$ are Hermitian directly.

1. For p_{op}, calculate...

$$\rightarrow \int_\infty \psi^*(p_{op}\psi)\,dx = -i\hbar\int_\infty \psi^*\left(\frac{\partial\psi}{\partial x}\right)dx \overset{\text{partial integrate}}{=} -i\hbar\left\{\underbrace{\cancel{\psi^*\psi\Big|_{-\infty}^{+\infty}}}_{0\ (\psi\to 0\text{ as }|x|\to\infty)} - \int_\infty\left(\frac{\partial\psi^*}{\partial x}\right)\psi\,dx\right\}$$

$$= \int\left(i\hbar\frac{\partial}{\partial x}\psi^*\right)\psi\,dx = \int_\infty (p_{op}\psi)^*\psi\,dx. \qquad (1)$$

So: $\langle\psi|p_{op}\psi\rangle = \langle p_{op}\psi|\psi\rangle$, and this is the requirement for a Hermitian operator. Thus $p_{op} = -i\hbar\,\partial/\partial x$ is Hermitian.

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2. For E_{op}, calculate...

$$\rightarrow \int_\infty \psi^*(E_{op}\psi)\,dx = i\hbar\int_\infty \psi^*\left(\frac{\partial\psi}{\partial t}\right)dx = i\hbar\int_\infty\left[\frac{\partial}{\partial t}(\psi^*\psi) - \left(\frac{\partial\psi^*}{\partial t}\right)\psi\right]dx$$

$$= \underbrace{i\hbar\frac{\partial}{\partial t}\int_\infty\psi^*\psi\,dx}_{0,\text{ because }\int_\infty\psi^*\psi\,dx = \text{cnst (cons}^{\text{x}}\text{n of probability)}} + \int_\infty\left(-i\hbar\frac{\partial}{\partial t}\psi^*\right)\psi\,dx = \int_\infty (E_{op}\psi)^*\psi\,dx. \qquad (2)$$

So, by direct integration, $\langle\psi|E_{op}\psi\rangle = \langle E_{op}\psi|\psi\rangle$, and E_{op} is Hermitian.

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3. The expectation value of operator Q is $\langle Q\rangle = \langle\psi|Q\psi\rangle$, so that

$$\rightarrow \langle Q\rangle^* = \langle\psi|Q\psi\rangle^* = \langle Q\psi|\psi\rangle. \qquad (3)$$

But for Q Hermitian, this last integral $\equiv \langle\psi|Q\psi\rangle = \langle Q\rangle$. So Hermitian operators have <u>real</u> expectation values: $\langle Q\rangle^* = \langle Q\rangle$. Thus it will be the case for p_{op} & E_{op} tested above that $\langle p_{op}\rangle$ & $\langle E_{op}\rangle$ are both real.

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(19) Ref. CLASS NOTES, p. Prop. 4, Eq. (10). The operator $Q^\dagger$ adjoint to operator Q is -- by definition -- such that: $\langle f|Q^\dagger g\rangle \equiv \langle Qf|g\rangle$.

→ (A) The adjoint for aQ, a = cnst, will obey...

$$\langle f|(aQ)^\dagger g\rangle = \langle (aQ)f|g\rangle = a^*\langle Qf|g\rangle = a^*\langle f|Q^\dagger g\rangle$$

$$= \langle f|(a^*Q^\dagger)g\rangle, \text{ So } \underline{\underline{(aQ)^\dagger = a^*Q^\dagger}}. \quad \text{QED} \qquad (1)$$

(B) Transfer the q's, one at a time, from ket to bra...

$$\rightarrow \langle f|(q_n^\dagger q_{n-1}^\dagger \cdots q_1^\dagger)g\rangle = \langle f|q_n^\dagger[(q_{n-1}^\dagger \cdots q_1^\dagger)g]\rangle \quad \text{1st step}$$

$$= \langle (q_n f)|q_{n-1}^\dagger[(q_{n-2}^\dagger \cdots q_1^\dagger)g]\rangle \quad \text{2nd step}$$

$$= \langle q_{n-1}(q_n f)|q_{n-2}^\dagger[(q_{n-3}^\dagger \cdots q_1^\dagger)g]\rangle \quad \text{3rd step}$$

$$= \langle (q_{n-2}q_{n-1}q_n)f|q_{n-3}^\dagger[(q_{n-4}^\dagger \cdots q_1^\dagger)g]\rangle \quad \text{etc.}$$

$$\vdots$$

$$= \underline{\underline{\langle (q_1 q_2 \cdots q_n)f|g\rangle}}, \text{ after } n \text{ steps.}$$

Comp. first & last eqtns to see: $\underline{\underline{q_n^\dagger \cdots q_1^\dagger = (q_1 \cdots q_n)^\dagger}}$. QED. (2)

(C) For: $iC = AB - BA$, take the adjoint for both sides. Use above rules

$$\Rightarrow (iC)^\dagger = -iC^\dagger = (AB-BA)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger$$

$$\xrightarrow{\text{So}} iC^\dagger = A^\dagger B^\dagger - B^\dagger A^\dagger = AB - BA = iC, \text{ So } \underline{\underline{C^\dagger = C}}. \quad \text{QED.} \qquad (3)$$

But A & B both Hermitian means they are <u>self-adjoint</u> (p. Prop. 5, #(E)), so $A^\dagger \equiv A$ & $B^\dagger \equiv B$... this explains the next-to-last step in (3). The last step implies $C^\dagger \equiv C$; C is self-adjoint and thus Hermitian.