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Problem 1. Consider a particle in a complex potential $V(\vec{r}) = U(\vec{r}) + iW(r)$, where $U(\vec{r})$ and $W(\vec{r})$ are real functions.
(a) Derive the continuity equation for the time-dependent Schrödinger equation for a particle of mass m in the above complex potential.
(b) What is the integral form of the continuity equation?
(c) What is the condition on $W(\vec{r})$ for it to describe a source? What is the condition on $W(\vec{r})$ for it to describe a sink?

Solution: (a) The Shrödinger equation

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t)+V(\vec{r},t)\psi(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t)+[U(\vec{r},t)+iW(\vec{r},t)]\psi(\vec{r},t) \quad (1)$$

Complex conjugate of the Shrödinger equation

$$-i\hbar\frac{\partial\psi^*(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^*(\vec{r},t) + [U(\vec{r},t) - iW(\vec{r},t)]\psi^*(\vec{r},t) \quad (2)$$

Multiplying the Shrödinger equation with $\psi^*(\vec{r},t)$

$$i\hbar\psi^*\frac{\psi}{\partial t} = -\frac{\hbar^2}{2m}\psi^*\nabla^2\psi + (V+iW)\psi^*\psi \quad (3)$$

Mutiplying the complex conjugate of the Shrödinger equation with $\psi(\vec{r},t)$

$$-i\hbar\psi\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\psi\nabla^2\psi^* + [V-iW]\psi\psi^* \quad (4)$$

Substracting the two resultant equation

$$i\hbar(\psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t}) = -\frac{\hbar^2}{2m}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*) + 2iW\psi\psi^* \quad (5)$$

$$\Longrightarrow i\hbar\frac{\partial}{\partial t}(\psi^*\psi) = -\frac{\hbar^2}{2m}\nabla\cdot(\psi^*\nabla\psi - \psi\nabla\psi^*) + 2iW\rho \quad (6)$$

Defining the probability current density as

$$\vec{J} = \frac{\hbar}{2im}[\psi^*(\vec{r},t)\nabla\psi(\vec{r},t) - \psi(\vec{r},t)\nabla\psi^*(\vec{r},t)] \quad (7)$$

Continuity equation

$$\frac{\partial\rho}{\partial t} + \nabla\vec{J} = \frac{2W}{\hbar}\rho \quad (8)$$

(b) Integrating the continuity equation over Ω

$$\int_\Omega\frac{\partial\rho}{\partial t}d^3r + \int_\Omega\nabla\cdot\vec{J} = \frac{2W}{\hbar}\int_\Omega\rho d^3r \quad (9)$$

$$\Longrightarrow \frac{\partial}{\partial t}\int_\Omega\rho d^3r + \int_\Sigma\vec{J}\cdot d\vec{S} = \frac{2W}{\hbar}\int_\Omega\rho d^3r \quad (10)$$

(c) The continuity equation describes a source if $W(\vec{r}) > 0$.
The continuity equation describes a sink if $W(\vec{r}) < 0$. □

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Problem 2. Show that

$$\hat{\vec{p}}^2 = \frac{1}{r^2}\hat{\vec{L}}^2 - \hbar^2 \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})$$

Solution: Due to

$$\hat{\vec{p}} = -i\hbar\nabla \tag{11}$$

left side of the equation

$$\begin{aligned}\hat{\vec{p}}^2 =& -\hbar^2\nabla^2\\ =& -\hbar^2[\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}] - \hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})\end{aligned} \tag{12}$$

Due to

$$\hat{\vec{L}} = -i\hbar\vec{r}\times\nabla \tag{13}$$

right side of the equation

$$\begin{aligned}&\frac{1}{r^2}\hat{\vec{L}}^2 - \hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})\\ =& -\frac{\hbar^2}{r^2}(\vec{r}\times\nabla)\cdot(\vec{r}\times\nabla) - \hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})\\ =& -\hbar^2[\hat{r}\times(\frac{\partial}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial}{\partial\theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\hat{\varphi})]\cdot[\hat{r}\times(\frac{\partial}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial}{\partial\theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\hat{\varphi})] - \hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})\\ =& -\hbar^2(\frac{1}{r}\frac{\partial}{\partial\theta}\hat{\varphi} - \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\hat{\theta})\cdot(\frac{1}{r}\frac{\partial}{\partial\theta}\hat{\varphi} - \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\hat{\theta}) - \hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})\\ =& -\hbar^2[\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}] - \hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})\end{aligned} \tag{14}$$

Therefore

$$\hat{\vec{p}}^2 = \frac{1}{r^2}\hat{\vec{L}}^2 - \hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) \tag{15}$$

□

Problem 3. (a) Find the Taylor expansion of $\hat{f}(\lambda) = e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}}$ with respect to λ about $\lambda = 0$. Here the operators $\hat{A}$ and $\hat{B}$ may not commute.
(b) Setting $\lambda = 1$ in the above Taylor expansion of $\hat{f} = e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}}$, derive an expansion for $e^{\hat{A}}\hat{B}e^{-\hat{A}}$.
(c) Using the expansion of $e^{\hat{A}}\hat{B}e^{-\hat{A}}$, evaluate $e^{i\hat{L}_y\theta/\hbar}\hat{L}_z e^{i\hat{L}_y\theta/\hbar}$.

Solution:
(a) The first-order derivative of $\hat{f}(\lambda)$ with respect to λ about $\lambda = 0$

$$\frac{df}{d\lambda}\Big|_{\lambda=0} = \left(e^{\lambda\hat{A}}\hat{A}\hat{B}e^{-\lambda\hat{A}} - e^{\lambda\hat{A}}\hat{B}\hat{A}e^{-\lambda\hat{A}}\right)\Big|_{\lambda=0} = \left\{e^{\lambda\hat{A}}[\hat{A},\hat{B}]e^{-\lambda\hat{A}}\right\}\Big|_{\lambda=0} = [\hat{A},\hat{B}] \tag{16}$$

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The second-order derivative of $\hat{f}(\lambda)$ with respect to λ about $\lambda = 0$

$$\left.\frac{d^2\hat{f}}{d\lambda^2}\right|_{\lambda=0} = \left\{e^{\lambda\hat{A}}\hat{A}[\hat{A},\hat{B}]e^{-\lambda\hat{A}} - e^{\lambda\hat{A}}[\hat{A},\hat{B}]\hat{A}e^{-\lambda\hat{A}}\right\}\Big|_{\lambda=0} = [\hat{A},[\hat{A},\hat{B}]] \tag{17}$$

$$\cdots\cdots$$

The Taylor expansion of $\hat{f}(\lambda)$ about $\lambda = 0$

$$\hat{f}(\lambda) = \hat{B} + \frac{1}{1!}[\hat{A},\hat{B}]\lambda^1 + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]]\lambda^2 + \frac{1}{3!}[\hat{A},[\hat{A},[\hat{A},\hat{B}]]]\lambda^3 + \cdots \tag{18}$$

(b) The n th-order derivative of $\hat{f}(\lambda)$ with respect to λ about $\lambda = 1$

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + \frac{1}{1!}[\hat{A},\hat{B}]\lambda^1 + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]]\lambda^2 + \frac{1}{3!}[\hat{A},[\hat{A},[\hat{A},\hat{B}]]]\lambda^3 + \cdots \tag{19}$$

(c)

$$e^{i\hat{L}_y\theta/\hbar}\hat{L}_z e^{i\hat{L}_y\theta/\hbar} = \hat{L}_z + \frac{i\theta}{1!\hbar}[\hat{L}_y,\hat{L}_z] + \frac{i^2\theta^2}{2!\hbar^2}[\hat{L}_y,[\hat{L}_y,\hat{L}_z]] + \frac{i^3\theta^3}{3!\hbar^3}[\hat{L}_y,[\hat{L}_y,[\hat{L}_y,\hat{L}_z]]] + \cdots \tag{20}$$

Due to $[\hat{\lambda}_\alpha, \hat{L}_\beta] = i\hbar\sum_{\gamma=x,y,z}\varepsilon_{\alpha\beta\gamma}\hat{L}_\gamma$

$$e^{i\hat{L}_y\theta/\hbar}\hat{L}_z e^{i\hat{L}_y\theta/\hbar} = \sum_{n=0}^{\infty}\frac{\theta^n}{n!}\begin{cases}\hat{L}_z, & n \bmod 4 = 0\\ \hat{L}_x, & n \bmod 4 = 1\\ -\hat{L}_z, & n \bmod 4 = 2\\ -\hat{L}_x, & n \bmod 4 = 3\end{cases} \tag{21}$$

Due to $\cos\theta = \sum_{k=0}^{\infty}\frac{(-1)^k\theta^{2k}}{(2k)!}, \sin\theta = \sum_{k=0}^{\infty}\frac{(-1)^{2k+1}\theta^k}{(2k+1)!}$

$$e^{i\hat{L}_y\theta/\hbar}\hat{L}_z e^{i\hat{L}_y\theta/\hbar} = \hat{L}_z\cos\theta + \hat{L}_x\sin\theta \tag{22}$$

□

Problem 4. The operators $\hat{A}$ and $\hat{B}$ do not commute, $[\hat{A},\hat{B}] = \hat{C} \neq 0$, but they both commute with their commutator $\hat{C}$, $[\hat{A},\hat{C}] = [\hat{B},\hat{C}] = 0$. Show that

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\hat{C}/2} = e^{\hat{B}}e^{\hat{A}}e^{\hat{C}/2}$$

Solution: Let

$$\hat{f}(\lambda) = e^{-\lambda\hat{B}}e^{-\lambda A}e^{\lambda(\hat{A}+\hat{B})} \tag{23}$$

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The derivative of $\hat{f}(\lambda)$

$$\begin{aligned}\frac{d\hat{f}}{d\lambda} =& - e^{-\lambda\hat{B}}\hat{B}e^{-\lambda\hat{A}}e^{\lambda(\hat{A}+\hat{B})} - e^{-\lambda\hat{B}}e^{-\lambda\hat{A}}\hat{A}e^{\lambda(\hat{A}+\hat{B})} + e^{-\lambda\hat{A}}e^{-\lambda\hat{B}}e^{\lambda(\hat{A}+\hat{B})}(\hat{A}+\hat{B}) \\ =& - e^{-\lambda\hat{B}}\hat{B}e^{-\lambda\hat{A}}e^{\lambda(\hat{A}+\hat{B})} + e^{-\lambda\hat{B}}e^{-\lambda\hat{A}}\hat{B}e^{\lambda(\hat{A}+\hat{B})} \\ =& - \hat{B}\hat{f}(\lambda) - e^{-\lambda\hat{B}}(e^{-\lambda\hat{A}}\hat{B}e^{\lambda\hat{A}})e^{-\lambda\hat{A}}e^{\lambda(\hat{A}+\hat{B})} \end{aligned} \tag{24}$$

where

$$e^{-\lambda\hat{A}}\hat{B}e^{\lambda\hat{A}} = \hat{B} - \frac{1}{1!}[\hat{A},\hat{B}]\lambda^1 + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]]\lambda^2 - \frac{1}{3!}[\hat{A},[\hat{A},[\hat{A},\hat{B}]]]\lambda^3 + \cdots \tag{25}$$

Due to $[\hat{A},\hat{B}] = \hat{C}, [\hat{A},\hat{C}] = [\hat{B},\hat{C}] = 0$

$$e^{-\lambda\hat{A}}\hat{B}e^{\lambda\hat{A}} = \hat{B} - \hat{C}\lambda \tag{26}$$

so

$$\frac{d\hat{f}}{d\lambda} = - \hat{B}\hat{f}(\lambda) + e^{-\lambda\hat{B}}(\hat{B} - \hat{C}\lambda)e^{-\lambda}\hat{A}e^{\lambda(\hat{A}+\lambda\hat{B})} \tag{27}$$

$$= - \lambda\hat{C}\hat{f}(\lambda) \tag{28}$$

integrate to get

$$\hat{f}(\lambda) = e^{-\lambda^2\hat{C}/2} \tag{29}$$

$$\Longrightarrow e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\hat{C}/2} \tag{30}$$

Similarly, let

$$\hat{g}(\lambda) = e^{-\hat{A}}e^{-\hat{B}}e^{\hat{A}+\hat{B}} \tag{31}$$

$$\Longrightarrow \frac{dg}{d\lambda} = -\hat{A}\hat{g}(\lambda) + e^{-\lambda\hat{A}}(e^{-\lambda\hat{B}}\hat{A}e^{\lambda\hat{B}})e^{-\lambda\hat{B}}e^{\lambda(\hat{A}+\hat{B})} = -\hat{A}\hat{g}(\lambda) + e^{-\lambda\hat{A}}(\hat{A} - \lambda\hat{C})e^{-\lambda\hat{B}}e^{\lambda(\hat{A}+\hat{B})} \tag{32}$$

$$\Longrightarrow \hat{g}(\lambda) = e^{\lambda^2\hat{C}/2} \tag{33}$$

$$\Longrightarrow e^{\hat{A}+\hat{B}} = e^{\hat{B}}e^{\hat{A}}e^{\hat{C}/2} \tag{34}$$

$\square$

Problem 5. Consider a particle of mass m subject to a potential $V(x) = \lambda|x|^n$ with λ a constant, $n \neq -2$, and $-\infty < x < \infty$. The energy of the particle is given by $E = \frac{p^2}{2m} + \lambda|x|^n$.

(a) Making use of $|p| \sim \Delta p$, $\Delta x\Delta p \sim \hbar$, and $|x| \sim \Delta x/2$, express E in terms of Δx.

(b) To obtain the ground-state energy, minimize E with respect to Δx. Find the value of Δx in the ground state.

(c) What is the expression of the ground-state energy?

Solution: (a) E in terms of Δx

$$E = \frac{p^2}{2m} + \lambda|x|^n = \frac{\hbar^2}{2m\Delta x^2} + \lambda(\frac{\Delta x}{2})^n \tag{35}$$

(b) The derivative of E about Δx

$$\frac{dE}{d\Delta x} = -\frac{\hbar^2}{m\Delta x^3} + \frac{n\lambda}{2}(\frac{\Delta x}{2})^{n-1} \tag{36}$$

Let

$$\frac{dE}{d\Delta x} = 0 \tag{37}$$

$$\Longrightarrow \Delta x = \left(\frac{2^n\hbar^2}{nm\lambda}\right)^{1/(n+2)} \tag{38}$$

(c) The expression of the ground-state energy

$$E_0 = \frac{\hbar^2}{2m}\left(\frac{2^n\hbar^2}{nm\lambda}\right)^{-2/(n+2)} + \lambda\left(\frac{2^n\hbar^2}{nm\lambda}\right)^{n/(n+2)} \tag{39}$$

□