



Quantum Mechanics

Solutions to the Problems in Homework Assignment 02

Fall, 2018

1. Consider a particle in a complex potential $V(\vec{r}) = U(\vec{r}) + iW(\vec{r})$, 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?

- (a) The time-dependent Schrödinger equation and its complex conjugate for a particle of mass m in the given complex potential are respectively given by

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

Multiplying the equation for ψ with ψ^* and the equation for ψ^* with ψ , we have

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

Subtracting the second equation from the first one yields

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

The above equation can be rewritten as

$$\frac{\partial(\psi^* \psi)}{\partial t} = -\frac{\hbar}{2im} \vec{\nabla} \cdot (\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^*) + \frac{2}{\hbar} W(\vec{r}) \psi^* \psi.$$

Introducing

$$\begin{aligned} \rho(\vec{r}, t) &= \psi^* \psi = |\psi|^2, \\ \vec{J}(\vec{r}, t) &= \frac{\hbar}{2im} (\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^*), \end{aligned}$$

we can put the above equation into the following form

$$\frac{\partial \rho(\vec{r}, t)}{\partial t} = -\vec{\nabla} \cdot \vec{J}(\vec{r}, t) + \frac{2}{\hbar} W(\vec{r}) \rho(\vec{r}, t).$$

The above equation is the continuity equation for the time-dependent Schrödinger equation for a particle of mass m in the given complex potential. Because of the presence of the second term on the right hand side, the probability is no longer conserved.

- (b) Integrating both sides of the above-derived continuity equation for the time-dependent Schrödinger equation over the region Ω whose surface is Σ and making use of the divergence theorem to the term that contains $\vec{\nabla} \cdot \vec{J}(\vec{r}, t)$, we have

$$\frac{d}{dt} \int_{\Omega} d^3r \rho(\vec{r}, t) = - \int_{\Sigma} d\vec{A} \cdot \vec{J}(\vec{r}, t) + \frac{2}{\hbar} \int_{\Omega} d^3r W(\vec{r}) \rho(\vec{r}, t).$$

The above equation is the integral form of the continuity equation. Assume that ψ is normalized. The term on the left hand of the above equation is the rate of increase of the total probability within the region Ω . The first term on the right hand side is the probability flowing into the region Ω through the surface per unit time; the second term on the right hand side is the generation of the probability per unit time if it is greater than zero or the reduction of the probability per unit time if it is smaller than zero.

- (c) A source implies that the probability is generated in the region Ω while a sink implies that the probability is reduced in the region Ω . The condition for $W(\vec{r})$ to describe a source is that

$$\int_{\Omega} d^3r W(\vec{r})\rho(\vec{r}, t) > 0.$$

Note that the above condition ensures that $W(\vec{r})$ describes a net source in Ω . If $W(\vec{r}) > 0$ at every point in Ω , then $W(\vec{r})$ describes a source at every point in Ω .

The condition for $W(\vec{r})$ to describe a sink is that

$$\int_{\Omega} d^3r W(\vec{r})\rho(\vec{r}, t) < 0.$$

Note that the above condition ensures that $W(\vec{r})$ describes a net sink in Ω . If $W(\vec{r}) < 0$ at every point in Ω , then $W(\vec{r})$ describes a sink at every point in Ω .

2. Show that

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

The identity for the product $(\hat{A} \times \hat{B}) \cdot (\hat{C} \times \hat{D})$ is given by

$$(\hat{A} \times \hat{B}) \cdot (\hat{C} \times \hat{D}) = \sum_{\alpha\beta} \hat{A}_{\alpha} \hat{B}_{\beta} \hat{C}_{\alpha} \hat{D}_{\beta} - \sum_{\alpha\beta} \hat{A}_{\alpha} \hat{B}_{\beta} \hat{C}_{\beta} \hat{D}_{\alpha}.$$

Because the components of the operators \hat{A} , \hat{B} , \hat{C} , and \hat{D} may not commute, their order given on the left hand side is maintained on the right hand side.

From the definition of \hat{L} , \hat{L}^2 can be written as

$$\hat{L}^2 = (\hat{\vec{r}} \times \hat{\vec{p}}) \cdot (\hat{\vec{r}} \times \hat{\vec{p}}).$$

Making use of the above-given identity, we have

$$\begin{aligned} \hat{L}^2 &= \sum_{\alpha\beta} x_{\alpha} p_{\beta} x_{\alpha} p_{\beta} - \sum_{\alpha\beta} x_{\alpha} p_{\beta} x_{\beta} p_{\alpha} = \sum_{\alpha\beta} x_{\alpha} (x_{\alpha} p_{\beta} - i\hbar \delta_{\alpha\beta}) p_{\beta} - \sum_{\alpha\beta} x_{\alpha} (x_{\beta} p_{\beta} - i\hbar) p_{\alpha} \\ &= r^2 \hat{p}^2 - i\hbar \vec{r} \cdot \hat{\vec{p}} - \sum_{\alpha\beta} x_{\alpha} x_{\beta} p_{\beta} p_{\alpha} + 3i\hbar \vec{r} \cdot \hat{\vec{p}} = r^2 \hat{p}^2 + 2i\hbar \vec{r} \cdot \hat{\vec{p}} - \sum_{\alpha\beta} x_{\alpha} (p_{\alpha} x_{\beta} + i\hbar \delta_{\alpha\beta}) p_{\beta} \\ &= r^2 \hat{p}^2 + 2i\hbar \vec{r} \cdot \hat{\vec{p}} - (\vec{r} \cdot \hat{\vec{p}})^2 - i\hbar \vec{r} \cdot \hat{\vec{p}} = r^2 \hat{p}^2 - (\vec{r} \cdot \hat{\vec{p}})^2 + i\hbar \vec{r} \cdot \hat{\vec{p}}. \end{aligned}$$

Making use of

$$\hat{\vec{p}} = -i\hbar \vec{\nabla} = -i\hbar \left(\frac{\partial}{\partial r} \vec{e}_r + \frac{1}{r} \frac{\partial}{\partial \theta} \vec{e}_{\theta} + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \vec{e}_{\phi} \right),$$

we have

$$\begin{aligned} \vec{r} \cdot \hat{\vec{p}} &= -i\hbar r \frac{\partial}{\partial r}, \\ i\hbar \vec{r} \cdot \hat{\vec{p}} &= \hbar^2 r \frac{\partial}{\partial r}, \\ (\vec{r} \cdot \hat{\vec{p}})^2 &= -\hbar^2 r \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) = -\hbar^2 \left(r^2 \frac{\partial^2}{\partial r^2} + r \frac{\partial}{\partial r} \right). \end{aligned}$$

We thus have

$$\hat{L}^2 = r^2 \hat{p}^2 + \hbar^2 \left(r^2 \frac{\partial^2}{\partial r^2} + r \frac{\partial}{\partial r} \right) + \hbar^2 r \frac{\partial}{\partial r} = r^2 \hat{p}^2 + \hbar^2 \left(r^2 \frac{\partial^2}{\partial r^2} + 2r \frac{\partial}{\partial r} \right) = r^2 \hat{p}^2 + \hbar^2 \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right)$$

from which it follows that

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

Another way to solve this problem is to utilize

$$\begin{aligned} \nabla^2 &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}, \\ \hat{L}^2 &= -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]. \end{aligned}$$

We have

$$\begin{aligned} \hat{p}^2 &= -\hbar^2 \nabla^2 = -\hbar^2 \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \\ &= -\hbar^2 \frac{1}{r^2} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] - \hbar^2 \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \\ &= \frac{1}{r^2} \hat{L}^2 - \hbar^2 \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right). \end{aligned}$$

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 $\hat{f}(\lambda) = e^{\lambda \hat{A}} \hat{B} e^{-\lambda \hat{A}}$, 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 $e^{-i\hat{L}_y \theta / \hbar} \hat{L}_z e^{i\hat{L}_y \theta / \hbar}$.

(a) For $\hat{f}(\lambda) = e^{\lambda \hat{A}} \hat{B} e^{-\lambda \hat{A}}$, we have

$$\begin{aligned} \hat{f}(0) &= \hat{B}, \\ \left. \frac{d\hat{f}(\lambda)}{d\lambda} \right|_{\lambda=0} &= (e^{\lambda \hat{A}} \hat{A} \hat{B} e^{-\lambda \hat{A}} - e^{\lambda \hat{A}} \hat{B} \hat{A} e^{-\lambda \hat{A}})_{\lambda=0} = e^{\lambda \hat{A}} [\hat{A}, \hat{B}] e^{-\lambda \hat{A}} \Big|_{\lambda=0} = [\hat{A}, \hat{B}], \\ \left. \frac{d^2 \hat{f}(\lambda)}{d\lambda^2} \right|_{\lambda=0} &= (e^{\lambda \hat{A}} \hat{A} [\hat{A}, \hat{B}] e^{-\lambda \hat{A}} - e^{\lambda \hat{A}} [\hat{A}, \hat{B}] \hat{A} e^{-\lambda \hat{A}})_{\lambda=0} = e^{\lambda \hat{A}} [\hat{A}, [\hat{A}, \hat{B}]] e^{-\lambda \hat{A}} \Big|_{\lambda=0} = [\hat{A}, [\hat{A}, \hat{B}]], \\ \left. \frac{d^3 \hat{f}(\lambda)}{d\lambda^3} \right|_{\lambda=0} &= [\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]], \\ &\vdots \end{aligned}$$

The Taylor expansion of $\hat{f}(\lambda) = e^{\lambda \hat{A}} \hat{B} e^{-\lambda \hat{A}}$ with respect to λ about $\lambda = 0$ is then given by

$$\hat{f}(\lambda) = e^{\lambda \hat{A}} \hat{B} e^{-\lambda \hat{A}} = \hat{B} + [\hat{A}, \hat{B}] \lambda + \frac{1}{2!} [\hat{A}, [\hat{A}, \hat{B}]] \lambda^2 + \frac{1}{3!} [\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]] \lambda^3 + \dots$$

(b) Setting $\lambda = 1$ in the above Taylor expansion of $\hat{f}(\lambda) = e^{\lambda \hat{A}} \hat{B} e^{-\lambda \hat{A}}$, we have

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

(c) For $e^{-i\hat{L}_y\theta/\hbar}\hat{L}_ze^{i\hat{L}_y\theta/\hbar}$, we have

$$\hat{A} = -\frac{i\theta}{\hbar}\hat{L}_y, \quad \hat{B} = \hat{L}_z.$$

Making use of the commutation relations between the component operators of the orbital angular momentum, we have

$$\begin{aligned} [\hat{A}, \hat{B}] &= -\frac{i\theta}{\hbar}[\hat{L}_y, \hat{L}_z] = \theta\hat{L}_x, \\ [\hat{A}, [\hat{A}, \hat{B}]] &= -\frac{i\theta^2}{\hbar}[\hat{L}_y, \hat{L}_x] = -\theta^2\hat{L}_z, \\ [\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]] &= \frac{i\theta^3}{\hbar}[\hat{L}_y, \hat{L}_z] = -\theta^3\hat{L}_x, \\ [\hat{A}, [\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]]] &= \frac{i\theta^4}{\hbar}[\hat{L}_y, \hat{L}_x] = \theta^4\hat{L}_z, \\ &\vdots \end{aligned}$$

We thus have

$$\begin{aligned} e^{-i\hat{L}_y\theta/\hbar}\hat{L}_ze^{i\hat{L}_y\theta/\hbar} &= \hat{L}_z + \theta\hat{L}_x - \frac{1}{2!}\theta^2\hat{L}_z - \frac{1}{3!}\theta^3\hat{L}_x + \frac{1}{4!}\theta^4\hat{L}_z + \dots \\ &= \left(1 - \frac{1}{2!}\theta^2 + \frac{1}{4!}\theta^4 - \dots\right)\hat{L}_z + \left(\theta - \frac{1}{3!}\theta^3 + \dots\right)\hat{L}_x \\ &= \cos\theta\hat{L}_z + \sin\theta\hat{L}_x \end{aligned}$$

where we have made use of the Taylor expansions of $\cos\theta$ and $\sin\theta$,

$$\begin{aligned} \cos\theta &= 1 - \frac{1}{2!}\theta^2 + \frac{1}{4!}\theta^4 - \dots = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!}\theta^{2n}, \\ \sin\theta &= \theta - \frac{1}{3!}\theta^3 + \dots = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!}\theta^{2n+1}. \end{aligned}$$

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

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

To prove that $e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\hat{C}/2}$, we consider

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

Differentiating $\hat{f}(\lambda)$ with respect to λ yields

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

Making use of $[\hat{A}, \hat{C}] = [\hat{B}, \hat{C}] = 0$ and

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

we have

$$\begin{aligned}\frac{d\hat{f}(\lambda)}{d\lambda} &= -\hat{B}\hat{f}(\lambda) + e^{-\lambda\hat{B}}(\hat{B} - [\hat{A}, \hat{B}]\lambda)e^{-\lambda\hat{A}}e^{\lambda(\hat{A}+\hat{B})} \\ &= -\hat{B}\hat{f}(\lambda) + e^{-\lambda\hat{B}}(\hat{B} - \lambda\hat{C})e^{-\lambda\hat{A}}e^{\lambda(\hat{A}+\hat{B})} \\ &= -\lambda\hat{C}\hat{f}(\lambda).\end{aligned}$$

Note that \hat{C} commutes with $\hat{f}(\lambda)$. Integrating both sides of the above equation from $\lambda = 0$ to λ and making use of $\hat{f}(0) = 1$, we obtain

$$\ln \hat{f}(\lambda) = -\frac{1}{2}\lambda^2\hat{C}.$$

We thus have

$$\hat{f}(\lambda) = e^{-\lambda\hat{B}}e^{-\lambda\hat{A}}e^{\lambda(\hat{A}+\hat{B})} = e^{-\lambda^2\hat{C}/2}.$$

Setting $\lambda = 1$ in the above equation yields

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

which can be also written as

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

To prove that $e^{\hat{A}+\hat{B}} = e^{\hat{B}}e^{\hat{A}}e^{\hat{C}/2}$, we consider

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

Comparing $\hat{g}(\lambda)$ with $\hat{f}(\lambda)$, we see that the difference between them lies in the exchange of \hat{A} and \hat{B} in their expressions. We thus have from the above result for $\hat{f}(\lambda)$

$$\hat{g}(\lambda) = e^{-\lambda\hat{A}}e^{-\lambda\hat{B}}e^{\lambda(\hat{A}+\hat{B})} = e^{\lambda^2\hat{C}/2}.$$

Setting $\lambda = 1$ in the above equation yields

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

which can be also written as

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

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 $E = \frac{p^2}{2m} + \lambda|x|^n$.

- 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 .
- To obtain the ground-state energy, minimize E with respect to Δx . Find the value of Δx in the ground state.
- What is the expression of the ground-state energy?

(a) From $\Delta x \Delta p \sim \hbar$, we have $\Delta p = \frac{\hbar}{\Delta x}$. Inserting $|x| = \frac{1}{2}\Delta x$ and $|p| = \Delta p = \frac{\hbar}{\Delta x}$ into $E = \frac{p^2}{2m} + \lambda|x|^n$ yields

$$E = \frac{1}{2m} \left(\frac{\hbar}{\Delta x} \right)^2 + \lambda \left(\frac{1}{2}\Delta x \right)^n = \frac{\hbar^2}{2m(\Delta x)^2} + \frac{\lambda}{2^n}(\Delta x)^n.$$

(b) To minimize E , differentiating E with respect to Δx and setting the result to zero, we obtain

$$-\frac{\hbar^2}{m(\Delta x)^3} + \frac{n\lambda}{2^n}(\Delta x)^{n-1} = 0.$$

Solving for Δx from the above equation, we have

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

(c) Inserting

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

into

$$E = \frac{\hbar^2}{2m(\Delta x)^2} + \frac{\lambda}{2^n}(\Delta x)^n,$$

we obtain the following expression for the ground-state energy

$$E_0 = \frac{\hbar^2}{2m} \left(\frac{nm\lambda}{2^n \hbar^2} \right)^{2/(n+2)} + \frac{\lambda}{2^n} \left(\frac{2^n \hbar^2}{nm\lambda} \right)^{n/(n+2)} = (n+2) \left[\frac{\hbar^2 \lambda^{2/n}}{2^{(3n+2)/n} nm} \right]^{n/(n+2)}.$$