

Problem 1 – Chapter 3 # 4)

The time-dependent Schrödinger equation of a charged particle in an electromagnetic field reads

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \left\{ \frac{1}{2m} \left[-i\hbar \vec{\nabla} - \frac{q}{c} \vec{A}(\vec{r}, t) \right]^2 + qU(\vec{r}, t) \right\} \Psi(\vec{r}, t) \quad (1)$$

where $U(\vec{r}, t)$ and $\vec{A}(\vec{r}, t)$ are the (real) scalar and vector potential, respectively, c is the speed of light, and q is the charge of the particle. Show that the probability density $\rho(\vec{r}, t)$ and the probability current density $\vec{j}(\vec{r}, t)$ are given in this case by

$$\rho(\vec{r}, t) = |\Psi(\vec{r}, t)|^2 \quad (2)$$

$$\vec{j}(\vec{r}, t) = \frac{\hbar}{2mi} \left[\Psi^*(\vec{r}, t) \vec{\nabla} \Psi(\vec{r}, t) - \Psi(\vec{r}, t) \vec{\nabla} \Psi^*(\vec{r}, t) \right] - \frac{q}{mc} \vec{A}(\vec{r}, t) |\Psi(\vec{r}, t)|^2 \quad (3)$$

with

$$\frac{\partial}{\partial t} \rho(\vec{r}, t) + \vec{\nabla} \cdot \vec{j}(\vec{r}, t) = 0. \quad (4)$$

As in our previous derivations of ρ and \vec{j} we define $\rho(\vec{r}, t) = |\Psi|^2$, and \vec{j} such that $\frac{\partial \rho}{\partial t} = -\vec{\nabla} \cdot \vec{j}$. Taking the time derivative of ρ , we have

$$\frac{\partial \rho}{\partial t} = \Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t}. \quad (5)$$

Again, we get the time-derivative of the wave function from S.E. (which requires a bit more massaging than in the previous cases):

$$\begin{aligned} \frac{\partial \Psi}{\partial t} &= \frac{1}{2mi\hbar} \left[-\hbar^2 \nabla^2 + \frac{i\hbar q}{c} \vec{\nabla} \cdot \vec{A} + \frac{i\hbar q}{c} \vec{A} \cdot \vec{\nabla} + \frac{q^2}{c^2} \vec{A}^2 \right] \Psi + \frac{q}{i\hbar} U \Psi \\ &= -\frac{\hbar}{2mi} \nabla^2 \Psi + \frac{q}{2mc} \underbrace{\left[\vec{\nabla} \cdot \vec{A} \Psi + \vec{A} \cdot \vec{\nabla} \Psi \right]}_{\Psi \vec{\nabla} \cdot \vec{A} + 2\vec{A} \cdot \vec{\nabla} \Psi} + \frac{q^2}{2mi\hbar c} \vec{A}^2 \Psi + \frac{q}{i\hbar} U \Psi. \end{aligned} \quad (6)$$

Observe that the last two terms are purely imaginary, and therefore cancel in Eq. (5),

leaving us with¹

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= - \left\{ \vec{\nabla} \cdot \frac{\hbar}{2mi} [\Psi^* \vec{\nabla} \Psi - \Psi \vec{\nabla} \Psi^*] + \frac{q}{mc} [|\Psi|^2 \vec{\nabla} \cdot \vec{A} + \vec{A} \cdot (\Psi^* \vec{\nabla} \Psi + \Psi \vec{\nabla} \Psi^*)] \right\} \\ &= - \vec{\nabla} \cdot \underbrace{\left\{ [\Psi^* \vec{\nabla} \Psi - \Psi \vec{\nabla} \Psi^*] + \frac{q}{mc} \vec{A} |\Psi|^2 \right\}}_{\vec{j}(\vec{r}, t)} \end{aligned} \quad (7)$$

It is manifest then that

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0. \quad (8)$$

Problem 2 – Chapter 3 # 8)

Consider a particle in a potential $V(\vec{r})$ with associated wave function satisfying the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \Psi(\vec{r}, t). \quad (9)$$

(a) Show that

$$\frac{d}{dt} \langle \vec{r}(t) \rangle = \int d^3 \vec{r} \, \vec{j}(\vec{r}, t), \quad (10)$$

where $\langle \vec{r}(t) \rangle$ is the average position of the particle (notation as in notes) and $\vec{j}(\vec{r}, t)$ is the probability current density. Using the definition of $\vec{j}(\vec{r}, t)$, show that the equation above can also be written as

$$m \frac{d}{dt} \langle \vec{r}(t) \rangle = \langle \vec{p}(t) \rangle. \quad (11)$$

(b) Show that

$$\begin{aligned} \frac{d}{dt} \langle \vec{p}(t) \rangle &= - \langle \vec{\nabla} V \rangle = - \int d^3 \vec{r} \, \Psi^*(\vec{r}, t) [\vec{\nabla} V(\vec{r})] \Psi(\vec{r}, t) \\ &= \int d^3 \vec{r} \, \Psi^*(\vec{r}, t) \vec{F}(\vec{r}) \Psi(\vec{r}, t), \end{aligned} \quad (12)$$

where we have introduced the force $\vec{F}(\vec{r})$.

¹We use the fact that $\vec{\nabla} \cdot \vec{A} |\Psi|^2 = |\Psi|^2 \vec{\nabla} \cdot \vec{A} + \vec{A} \cdot \vec{\nabla} |\Psi|^2 = |\Psi|^2 \vec{\nabla} \cdot \vec{A} + \vec{A} \cdot (\Psi^* \vec{\nabla} \Psi + \Psi \vec{\nabla} \Psi^*)$.

Hint: Consider, say, the x -component and, by using the Schrödinger equation and its complex conjugate, obtain

$$\begin{aligned} \frac{d}{dt} \langle p_x(t) \rangle = & -\frac{\hbar^2}{2m} \int d^3\vec{r} \left[(\nabla^2 \Psi^*) \frac{\partial \Psi}{\partial x} - \Psi^* \nabla^2 \frac{\partial \Psi}{\partial x} \right] \\ & + \int d^3\vec{r} \left[V \Psi^* \frac{\partial \Psi}{\partial x} - \Psi^* \frac{\partial (V \Psi)}{\partial x} \right], \end{aligned} \quad (13)$$

where the dependence on \vec{r} and t on the r.h.s. has been suppressed for brevity. Next examine these two terms.

(c) The equation above looks like Newton's second law but for average values. As a matter of fact if $\langle \vec{F} \rangle = \vec{F}(\langle \vec{r} \rangle)$, then $\langle \vec{r}(t) \rangle$ changes in time as the position of a classical particle under the action of the force $\vec{F}(\vec{r})$. Under what condition(s) can this happen? Obtain $\langle \vec{r}(t) \rangle$ and $\langle \vec{p}(t) \rangle$ for a particle in a harmonic potential

$$V(\vec{r}) = \frac{m\omega^2}{2} \vec{r}^2. \quad (14)$$

(a) Observe that

$$\boxed{\frac{d}{dt} \langle \vec{r}(t) \rangle = \int d^3\vec{r} \frac{\partial}{\partial t} \rho(\vec{r}, t) = - \int d^3\vec{r} \vec{j}(\vec{r}, t)}, \quad (15)$$

where we have used the continuity equation for the probability density and current density.

Using $\vec{j} = (\hbar/2mi)[\Psi^* \vec{\nabla} \Psi - \Psi \vec{\nabla} \Psi^*]$, we can also rewrite Eq. (15) as

$$\boxed{m \frac{d}{dt} \langle \vec{r}(t) \rangle = \frac{1}{2} \int d^3\vec{r} [\Psi \vec{p} \Psi^* + \Psi^* \vec{p} \Psi] = \int d^3\vec{r} \Psi^* \vec{p} \Psi = \langle \vec{p}(t) \rangle}. \quad (16)$$

Note that we have used the fact that \vec{p} is hermitian to rewrite $\Psi \vec{p} \Psi^* = \Psi^* \vec{p} \Psi$ under the integral sign.

(b) We can do this as follows:

$$\begin{aligned}
\frac{d}{dt} \langle \vec{p}(t) \rangle &= -i\hbar \int d^3\vec{r} \frac{\partial}{\partial t} \Psi^* \vec{\nabla} \Psi \\
&= -i\hbar \int d^3\vec{r} \left[\frac{\partial \Psi^*}{\partial t} \vec{\nabla} \Psi + \Psi^* \vec{\nabla} \frac{\partial \Psi}{\partial t} \right] \\
&= -i\hbar \int d^3\vec{r} \left[-\frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \nabla^2 \Psi^* + V \Psi^* \right) \vec{\nabla} \Psi + \frac{1}{i\hbar} \Psi^* \vec{\nabla} \left(-\frac{\hbar^2}{2m} \nabla^2 \Psi + V \Psi \right) \right] \quad (17) \\
&= \int d^3\vec{r} \left\{ -\frac{\hbar^2}{2m} [(\nabla^2 \Psi^*)(\vec{\nabla} \Psi) - \Psi^* \vec{\nabla}(\nabla^2 \Psi)] + [V \Psi^* \vec{\nabla} \Psi - \Psi^* \vec{\nabla}(V \Psi)] \right\} \\
&= \boxed{\langle -\vec{\nabla} V \rangle = \langle \vec{F} \rangle}.
\end{aligned}$$

Notice that the integral

$$\int d^3\vec{r} [(\nabla^2 \Psi^*)(\vec{\nabla} \Psi) - \Psi^* \vec{\nabla}(\nabla^2 \Psi)] = \sum_{i=1}^3 \hat{x}_i \int d^3\vec{r} \left[(\nabla^2 \Psi^*) \frac{\partial \Psi}{\partial x_i} - \Psi^* \frac{\partial}{\partial x_i} (\nabla^2 \Psi) \right] \quad (18)$$

Let us focus on only the x -component since the result there applies also in the y and z components:

$$\begin{aligned}
\int d^3\vec{r} \left[(\nabla^2 \Psi^*) \frac{\partial \Psi}{\partial x} - \Psi^* \frac{\partial}{\partial x} (\nabla^2 \Psi) \right] &= \int d^3\vec{r} \left[(\nabla^2 \Psi^*) \frac{\partial \Psi}{\partial x} - \Psi^* \nabla^2 \frac{\partial \Psi}{\partial x} \right] \\
&= \int d^3\vec{r} \vec{\nabla} \cdot \left[(\vec{\nabla} \Psi^*) \frac{\partial \Psi}{\partial x} - \Psi^* \vec{\nabla} \frac{\partial \Psi}{\partial x} \right] \quad (19) \\
&= \int dS_\infty \left[(\vec{\nabla} \Psi^*) \frac{\partial \Psi}{\partial x} - \Psi^* \vec{\nabla} \frac{\partial \Psi}{\partial x} \right] = 0,
\end{aligned}$$

where we have used the divergence theorem to rewrite the volume integral as a surface integral. Note that S_∞ denotes the surface at infinity. It should be clear that $\Psi|_{S_\infty} = \partial_x \Psi|_{S_\infty} = 0$.

(c) The condition $\langle \vec{F} \rangle = \vec{F}(\langle \vec{r} \rangle)$ when $\vec{F} = \vec{F}_0 + F_1 \vec{r}$, where \vec{F}_0 and F_1 are a constant vector and scalar, respectively.

Now, we turn our attention to the harmonic potential $V(\vec{r}) = m\omega^2 r^2/2$. Observe that $F = -\vec{\nabla} V(\vec{r}) = -m\omega^2 \vec{r}$, which is linear in \vec{r} and falls under the special case we outlined above. Thus,

$$\frac{d}{dt} \langle \vec{r} \rangle = \frac{1}{m} \langle \vec{p} \rangle \quad (20)$$

$$\frac{d}{dt} \langle \vec{p}(t) \rangle = \langle F(\vec{r}) \rangle = -m\omega^2 \langle \vec{r} \rangle. \quad (21)$$

Notice that this is a set of coupled first-order differential equations. We can “decouple” these by differentiating Eq. (20), which gives

$$\frac{d^2}{dt^2} \langle \vec{r} \rangle = \frac{1}{m} \frac{d}{dt} \langle p \rangle = -\omega^2 \langle \vec{r} \rangle, \quad (22)$$

which is as expected the equation for a particle undergoing harmonic motion and has solution

$$\langle \vec{r} \rangle = \vec{A} \cos \omega t + \vec{B} \sin \omega t, \quad (23)$$

We also have then

$$\langle \vec{p} \rangle = m \frac{d}{dt} \langle \vec{r} \rangle = m\omega (\vec{B} \cos \omega t - \vec{A} \sin \omega t). \quad (24)$$

Note that \vec{A} and \vec{B} are constants of integration determined by initial or boundary conditions on $\langle \vec{r} \rangle$ and $\langle \vec{p} \rangle$. For example, if $\langle \vec{r}(0) \rangle$ and $\langle \vec{p}(0) \rangle$, which are the expectation values of \vec{r} and \vec{p} at $t = 0$ in the state Ψ , are given as initial conditions

$$\vec{A} = \langle \vec{r}(0) \rangle \quad \text{and} \quad \vec{B} = \frac{\langle \vec{p}(0) \rangle}{m\omega}. \quad (25)$$

Problem 3 – Chapter 4 # 1)

Consider the problem of a particle in an attractive δ -function potential given by

$$V(x) = -V_0 \delta(x) \quad V_0 > 0. \quad (26)$$

- (a) Obtain the energy and wave-function of the bound state. Sketch the wave function and provide an estimate for Δx .
- (b) Calculate the probability $dP(p)$ that a measurement of the momentum in this bound state will give a result included between p and $p + dp$. For what value of p is this probability largest? Provide an estimate for Δp and an order of magnitude for $\Delta x \Delta p$.

(a) The Schrödinger equation under this potential reads

$$\psi''(x) = -[v_0 \delta(x) - |\varepsilon|] \psi(x), \quad (27)$$

where $v_0 = 2mV_0/\hbar^2$ and $\varepsilon = 2mE/\hbar^2$. Note that we have explicitly written $|\varepsilon|$ since bound states may only exist for $E < 0$. This admits a solution of the form

$$\psi(x) = \Theta(-x)[A_- e^{\kappa x} + B_- e^{-\kappa x}] + \Theta(x)[A_+ e^{\kappa x} + B_+ e^{-\kappa x}], \quad (28)$$

where $\Theta(x)$ denotes the Heaviside step function and $\kappa = \sqrt{|\varepsilon|}$.

At this point, we need to determine the constants A_{\pm} , B_{\pm} which satisfy relevant boundary conditions. Firstly, we must have that the wave function is normalizable, which implies $\psi(x \rightarrow \pm\infty) = 0$ and therefore $A_+ = B_- = 0$. Secondly, we have the conditions on the wave function and its derivative at $x = 0$:

$$\psi(0^-) = \psi(0^+) \Rightarrow A_- = B_+ \quad (29)$$

$$\psi'(0^+) - \psi'(0^-) = v_0\psi(0) \Rightarrow \kappa[-B_+ - A_-] = -v_0A_-, \quad (30)$$

where we use the notation $\psi(0^{\pm}) = \lim_{x \rightarrow 0^{\pm}} \psi(x)$. Also, note that Eq. (30) comes from integrating the Eq. (27) in an infinitesimal region around $x = 0$. The first condition tells us that the wave function is symmetric about $x = 0$:

$$\psi(x) = \sqrt{\kappa}e^{-\kappa|x|}. \quad (31)$$

The second gives the energy of our bound state: $\epsilon = -(v_0/2)^2$.

A sketch of the wavefunction is given in Fig. 1. From the form of the wavefunction, we can estimate $\Delta x \sim 1/\sqrt{\kappa}$ ².

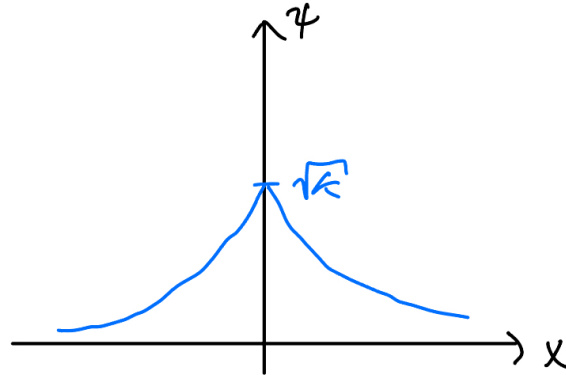


Figure 1: Sketch of bound state wave function in the potential $V(x) = -V_0\delta(x)$. Excuse the non-smooth behavior of the sketch, which demonstrates why I did not pursue any career requiring a steady hand!

(b) We now calculate the probability density of the momentum of a function in this potential by taking its Fourier transform:

$$\begin{aligned} \tilde{\psi}(p) &= \sqrt{\kappa} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} e^{-\kappa|x|} \\ &= \sqrt{\frac{\kappa}{2\pi\hbar}} \left[\int_{-\infty}^0 dx e^{(\kappa-ip/\hbar)x} + \int_0^{\infty} dx e^{-(\kappa+ip/\hbar)x} \right] \\ &= \sqrt{\frac{\kappa}{2\pi\hbar}} \left[\frac{1}{\kappa - ip/\hbar} + \frac{1}{\kappa + ip/\hbar} \right] = \sqrt{\frac{2\kappa}{\pi\hbar}} \frac{\kappa}{\kappa^2 + (p/\hbar)^2}. \end{aligned} \quad (32)$$

²Upon first glance, it may be tempting to estimate $\Delta x \sim 1/\kappa$, but $\Delta x = \sqrt{\langle x^2 \rangle} = \sqrt{[\int_{-\infty}^{\infty} e^{-|u|} du]/\kappa}$

The probability to find the particle with momentum in the interval $[p, p + dp]$ is then given as

$$\tilde{\rho}(p) = |\tilde{\psi}(p)|^2 = \frac{2}{\pi\hbar} \frac{\kappa^3}{[\kappa^2 + (p/\hbar)^2]^2} = \frac{2}{\pi\hbar\kappa} \frac{1}{[1 + (p/\kappa\hbar)^2]^2}. \quad (33)$$

Observe that the maximum of this probability density is peaked at $p = 0$ with a value of $2/(\pi\hbar\kappa)$.

From the form of the momentum-space wavefunction, we can also estimate that $\Delta p \sim \hbar\sqrt{\kappa}$ ³. Hence, we have $\Delta x \Delta p \sim \hbar$.

Problem 4 – Chapter 4 # 5)

Consider a particle in the one-dimensional potential $V(x)$, such that $V(x) = \infty$ for $x < 0$ and

$$V(x) = -V_0 \delta(x - a) \text{ for } x > 0 \quad (34)$$

where $V_0 > 0$. Determine whether this potential admits any bound states.

This potential does have the ability to admit bound states since $\min_{x \in \mathbb{R}} V(x) = -\infty$. For $E < 0$, the wave function would be of the form

$$\psi(x) = \begin{cases} 0 & x < 0 \\ Ae^{\kappa x} + Be^{-\kappa x} & 0 < x < a \\ Ce^{-\kappa x} & x > a, \end{cases} \quad (35)$$

where $\kappa^2 = 2m|E|/\hbar^2$. Note that we have used the fact that $\psi \rightarrow 0$ as $x \rightarrow \infty$ to rule out the solution $e^{\kappa x}$ in the region $x > a$.

The following boundary conditions must be respected:

$$\psi(0) = 0 \quad (36)$$

$$\psi(a^-) = \psi(a^+) \quad (37)$$

$$\psi'(a^+) - \psi'(a^-) = -\frac{2mV_0}{\hbar^2} \psi(a). \quad (38)$$

Translating this into an statement in terms of A , B , C , and κ , we have

$$A + B = 0 \quad (39)$$

$$Ae^{\kappa a} + Be^{-\kappa a} = Ce^{-\kappa a} \quad (40)$$

$$-Ce^{-\kappa a} - (Ae^{\kappa a} - Be^{-\kappa a}) = -\frac{v_0}{\kappa} Ce^{-\kappa a}, \quad (41)$$

³Again, this comes from the fact that $\Delta p = \sqrt{\langle p^2 \rangle} = \sqrt{\hbar^2 \kappa [(2/\pi) \int_{-\infty}^{\infty} u^2 / (1 + u^2)^2 du]}$

where we have defined $v_0 = 2mV_0/\hbar^2$. Remember that we also have the normalization condition, which imposes an additional constraint on these constants. Thus, for a non-trivial solution $\{A, B, C\}$, Eqs. (39)–(41) must be linearly dependent.

$$\begin{vmatrix} \sinh \kappa a & -e^{-\kappa a} \\ \cosh \kappa a & (1 - v_0/\kappa)e^{-\kappa a} \end{vmatrix} = e^{-\kappa a}[(1 + v_0/\kappa) \sinh \kappa a + \cosh \kappa a] = 0 \quad (42)$$

$$\tanh \kappa a = -\frac{1}{1 - v_0/\kappa} = \frac{1}{v_0/\kappa - 1}, \quad (43)$$

where we have used $B = -A$ to reduce the dimensionality (and therefore some complexity) of the problem. Also note that we have redefined $2A \rightarrow A$.

This is a transcendental equation for κ , so we cannot solve it directly, but notice that $\kappa a > 0$. Thus, $\tanh \kappa a > 0$, meaning that this equation may only have a solution if $v_0/\kappa > 1$, and hence, a bound state only under this condition. Additionally, $\tanh \kappa a < 1$ for all κa . We thus have a second condition on v_0/κ :

$$\frac{v_0}{\kappa} < 2, \quad (44)$$

and therefore, generally a bound state exists if and only if

$$1 < \frac{v_0}{\kappa} = \frac{V_0}{E} < 2 \Leftrightarrow \frac{V_0}{2} < E < V_0. \quad (45)$$