

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 the S.E.:

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

Observe that the last two terms are purely imaginary, and therefore cancel in Eq. (5), leaving us with¹

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

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

It is manifest then that

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

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 $\vec{F}(\vec{r})$.

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

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

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

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

where we have used the continuity equation for the probability density and current density. For this integration, it suffices to look at only one component and generalize to the other two:

$$\begin{aligned} \frac{d}{dt} \langle \vec{r}(t) \rangle &= - \sum_{i=1}^3 \int d^3\vec{r} x_i \vec{\nabla} \cdot \vec{j}(\vec{r}, t) \\ &= \sum_{i=1}^3 \int d^3\vec{r} [\vec{j}(\vec{r}, t) \cdot \vec{\nabla} x_i - \vec{\nabla} \cdot (x_i \vec{j}(\vec{r}, t))] \\ &= \sum_{i=1}^3 \left[\int d^3\vec{r} \vec{j}(\vec{r}, t) \cdot \hat{e}_i - \int dS_\infty x_i \vec{j}(\vec{r}, t) \right], \end{aligned} \quad (16)$$

where S_∞ is a surface at infinity. Notice that the second integral is zero since $|\vec{j}| \rightarrow 0$ as $|\vec{r}| \rightarrow \infty$ faster than $1/|\vec{r}|$ as a result of the normalizability of the wavefunction. Thus, we can write

$$\boxed{\frac{d}{dt} \langle \vec{r}(t) \rangle = \int d^3\vec{r} \vec{j}(\vec{r}, t)}. \quad (17)$$

Using $\vec{j} = (\hbar/2mi)[\Psi^* \vec{\nabla} \Psi - \Psi \vec{\nabla} \Psi^*]$, we can also rewrite Eq. (17) as

$$\boxed{m \frac{d}{dt} \langle \vec{r}(t) \rangle = \frac{1}{2} \int d^3\vec{r} [\Psi \vec{p} \Psi^* + \Psi^* \vec{p} \Psi] = \int d^3\vec{r} \Psi^* \vec{p} \Psi = \langle \vec{p}(t) \rangle}. \quad (18)$$

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

(b) We can do this as follows:

$$\begin{aligned} \frac{d}{dt} \langle \vec{p}(t) \rangle &= -i\hbar \int d^3\vec{r} \frac{\partial}{\partial t} \Psi^* \vec{\nabla} \Psi \\ &= -i\hbar \int d^3\vec{r} \left[\frac{\partial \Psi^*}{\partial t} \vec{\nabla} \Psi + \Psi^* \vec{\nabla} \frac{\partial \Psi}{\partial t} \right] \\ &= -i\hbar \int d^3\vec{r} \left[-\frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \nabla^2 \Psi^* + V \Psi^* \right) \vec{\nabla} \Psi + \frac{1}{i\hbar} \Psi^* \vec{\nabla} \left(-\frac{\hbar^2}{2m} \nabla^2 \Psi + V \Psi \right) \right] \\ &= \int d^3\vec{r} \left\{ -\frac{\hbar^2}{2m} [(\nabla^2 \Psi^*)(\vec{\nabla} \Psi) - \Psi^* \vec{\nabla}(\nabla^2 \Psi)] + [V \Psi^* \vec{\nabla} \Psi - \Psi^* \vec{\nabla}(V \Psi)] \right\} \\ &= \boxed{\langle -\vec{\nabla} V \rangle = \langle \vec{F} \rangle}. \end{aligned} \quad (19)$$

Notice that the integral

$$\int d^3\vec{r} [(\nabla^2\Psi^*)(\vec{\nabla}\Psi) - \Psi^*\vec{\nabla}(\nabla^2\Psi)] = \sum_{i=1}^3 \hat{x}_i \int d^3\vec{r} \left[(\nabla^2\Psi^*) \frac{\partial\Psi}{\partial x_i} - \Psi^* \frac{\partial}{\partial x_i} (\nabla^2\Psi) \right] \quad (20)$$

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

$$\begin{aligned} \int d^3\vec{r} \left[(\nabla^2\Psi^*) \frac{\partial\Psi}{\partial x} - \Psi^* \frac{\partial}{\partial x} (\nabla^2\Psi) \right] &= \int d^3\vec{r} \left[(\nabla^2\Psi^*) \frac{\partial\Psi}{\partial x} - \Psi^* \nabla^2 \frac{\partial\Psi}{\partial x} \right] \\ &= \int d^3\vec{r} \vec{\nabla} \cdot \left[(\vec{\nabla}\Psi^*) \frac{\partial\Psi}{\partial x} - \Psi^* \vec{\nabla} \frac{\partial\Psi}{\partial x} \right] \\ &= \int dS_\infty \left[(\vec{\nabla}\Psi^*) \frac{\partial\Psi}{\partial x} - \Psi^* \vec{\nabla} \frac{\partial\Psi}{\partial x} \right] = 0, \end{aligned} \quad (21)$$

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,

$$\frac{d}{dt} \langle \vec{r} \rangle = \frac{1}{m} \langle \vec{p} \rangle \quad (22)$$

$$\frac{d}{dt} \langle \vec{p}(t) \rangle = \langle F(\vec{r}) \rangle = -m\omega^2 \langle \vec{r} \rangle. \quad (23)$$

Notice that this is a set of coupled first-order differential equations. We can “decouple” these by differentiating Eq. (22), which gives

$$\frac{d^2}{dt^2} \langle \vec{r} \rangle = \frac{1}{m} \frac{d}{dt} \langle \vec{p} \rangle = -\omega^2 \langle \vec{r} \rangle, \quad (24)$$

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

$$\boxed{\langle \vec{r} \rangle = \vec{A} \cos \omega t + \vec{B} \sin \omega t}, \quad (25)$$

We also have then

$$\boxed{\langle \vec{p} \rangle = m \frac{d}{dt} \langle \vec{r} \rangle = m\omega (\vec{B} \cos \omega t - \vec{A} \sin \omega t)}. \quad (26)$$

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

$$\vec{A} = \langle \vec{r}(0) \rangle \quad \text{and} \quad \vec{B} = \frac{\langle \vec{p}(0) \rangle}{m\omega}. \quad (27)$$

Problem 3 – Chapter 4 # 1)

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

$$V(x) = -V_0\delta(x) \quad V_0 > 0. \quad (28)$$

- (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

$$\psi''(x) = -[v_0\delta(x) - |\epsilon|]\psi(x), \quad (29)$$

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

$$\psi(x) = \Theta(-x)[A_-e^{\kappa x} + B_-e^{-\kappa x}] + \Theta(x)[A_+e^{\kappa x} + B_+e^{-\kappa x}], \quad (30)$$

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

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 $x = 0$:

$$\psi(0^-) = \psi(0^+) \Rightarrow A_- = B_+ \quad (31)$$

$$\psi'(0^+) - \psi'(0^-) = v_0\psi(0) \Rightarrow \kappa[-B_+ - A_-] = -v_0A_-, \quad (32)$$

where we use the notation $\psi(0^{\pm}) = \lim_{x \rightarrow 0^{\pm}} \psi(x)$. Also, note that Eq. (32) comes from integrating Eq. (29) in an infinitesimal region around $x = 0$. The first condition tells us that the wave function is symmetric about $x = 0$. The second gives the energy of our bound state: $\epsilon = -(v_0/2)^2$, and normalization gives the overall constant such that:

$$\psi(x) = \sqrt{\kappa}e^{-\kappa|x|}. \quad (33)$$

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.

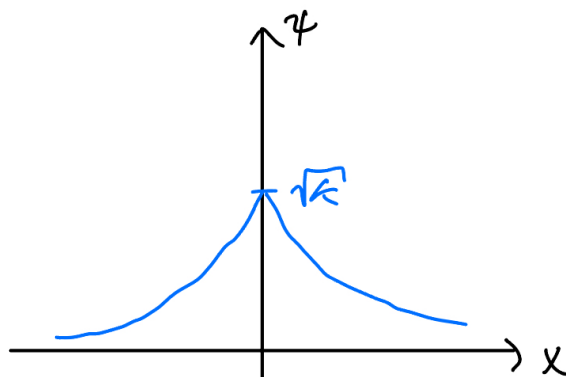


Figure 1: Sketch of the bound state wave function in the potential $V(x) = -V_0\delta(x)$.

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

$$\begin{aligned}
 \tilde{\psi}(p) &= \sqrt{\kappa} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} e^{-\kappa|x|} \\
 &= \sqrt{\frac{\kappa}{2\pi\hbar}} \left[\int_{-\infty}^0 dx e^{(\kappa - ip/\hbar)x} + \int_0^{\infty} dx e^{-(\kappa + ip/\hbar)x} \right] \\
 &= \sqrt{\frac{\kappa}{2\pi\hbar}} \left[\frac{1}{\kappa - ip/\hbar} + \frac{1}{\kappa + ip/\hbar} \right] = \sqrt{\frac{2\kappa}{\pi\hbar}} \frac{\kappa}{\kappa^2 + (p/\hbar)^2}.
 \end{aligned} \tag{34}$$

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

$$\tilde{\rho}(p) = |\tilde{\psi}(p)|^2 = \frac{2}{\pi\hbar} \frac{\kappa^3}{[\kappa^2 + (p/\hbar)^2]^2} = \frac{2}{\pi\hbar\kappa} \frac{1}{[1 + (p/\kappa\hbar)^2]^2}. \tag{35}$$

Observe that 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

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

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

$x < 0$ and

$$V(x) = -V_0 \delta(x - a) \text{ for } x > 0 \quad (36)$$

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

$$\psi(x) = \begin{cases} 0 & x < 0 \\ Ae^{\kappa x} + Be^{-\kappa x} & 0 < x < a \\ Ce^{-\kappa x} & x > a, \end{cases} \quad (37)$$

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:

$$\psi(0) = 0 \quad (38)$$

$$\psi(a^-) = \psi(a^+) \quad (39)$$

$$\psi'(a^+) - \psi'(a^-) = -\frac{2mV_0}{\hbar^2} \psi(a). \quad (40)$$

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

$$A + B = 0 \quad (41)$$

$$Ae^{\kappa a} + Be^{-\kappa a} = Ce^{-\kappa a} \quad (42)$$

$$-Ce^{-\kappa a} - (Ae^{\kappa a} - Be^{-\kappa a}) = -\frac{v_0}{\kappa} Ce^{-\kappa a}, \quad (43)$$

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. (41)–(43) must be linearly dependent.

$$\begin{vmatrix} \sinh \kappa a & -e^{-\kappa a} \\ \cosh \kappa a & (1 - v_0/\kappa)e^{-\kappa a} \end{vmatrix} = e^{-\kappa a} [(1 + v_0/\kappa) \sinh \kappa a + \cosh \kappa a] = 0 \quad (44)$$

$$\tanh \kappa a = -\frac{1}{1 - v_0/\kappa} = \frac{1}{v_0/\kappa - 1}, \quad (45)$$

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 :

$$\frac{v_0}{\kappa} < 2, \quad (46)$$

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

$$1 < \frac{v_0}{\kappa} = \frac{V_0}{E} < 2 \Leftrightarrow \frac{V_0}{2} < E < V_0. \quad (47)$$

The above analysis is not entirely correct. We can rewrite Eq. (43) to read

$$\tanh z = \frac{z}{z_0 - z}, \quad (48)$$

where $z = \kappa a$ and $z_0 = v_0 a$. In this case then, we have something like $f(z) = g(z)$. Clearly then, whether there is a solution depends on the value of z_0 .

Let us observe the following:

1. $z > 0$ (since $\kappa, a > 0$)
2. $0 < \tanh z < 1$
3. $z/(z_0 - z) > 0$ for $z \in [0, z_0)$
4. for $z \in [0, z_0)$, the function $z/(z_0 - z)$ is monotonically increasing
5. $\tanh 0 = 0$ and $0/(z_0 - 0) = 0$

Clearly, these functions always intersect at $E = 0$, but this is not interesting for this problem since ψ is not normalizable then and hence not a bound state. We can, however, state whether or not the transcendental equation has a solution (only one if any!). Since $z/(z_0 - z)$ is monotonically increasing, for a bound state to exist, we must have

$$\left. \frac{d}{dz} \tanh z \right|_{z=0} > \left. \frac{d}{dz} \frac{z}{z_0 - z} \right|_{z=0} \Rightarrow z_0 > 1. \quad (49)$$

If this condition is met, though, we must resort to some numerical scheme to determine the energy of the bound state.