

**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  $\rho$  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  $\rho$ , 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 with<sup>1</sup>

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

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

<sup>1</sup>We 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  $S_\infty$  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  $\Psi$ , 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  $\delta$ -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  $\Delta x$ .
- (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  $\Delta p$  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  $\Delta x \sim 1/\sqrt{\kappa}$ <sup>2</sup>.

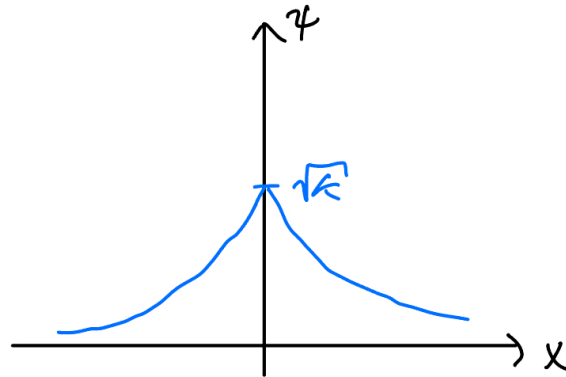


Figure 1: Sketch of bound state wave function in the potential  $V(x) = -V_0\delta(x)$ . Excuse the non-smooth behavior of the sketch, which demonstrates why I did not pursue any career requiring a steady hand!

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

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

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<sup>2</sup>Upon 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  $\Delta p \sim \hbar\sqrt{\kappa}$ <sup>3</sup>. 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  $\kappa$ , we have

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

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

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

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<sup>3</sup>Again, 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  $\kappa$ , 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  $\kappa a$ . We thus have a second condition on  $v_0/\kappa$ :

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

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

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

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

$$\tanh z = \frac{z}{z_0 - z}, \quad (46)$$

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  $\psi$  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

$$\left. \frac{d}{dz} \tanh z \right|_{z=0} > \left. \frac{d}{dz} \frac{z}{z_0 - z} \right|_{z=0} \Rightarrow z_0 > 1. \quad (47)$$

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