Problem 1 – Chapter 3 # 4)
The time-dependent Schrödinger equation of a charged particle in an electromagnetic field reads

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

where $U(\vec{\boldsymbol{r}},t)$ and $\vec{\boldsymbol{A}}(\vec{\boldsymbol{r}},t)$ 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 $\rho(\vec{\boldsymbol{r}},t)$ and the probability current density $\vec{\boldsymbol{j}}(\vec{\boldsymbol{r}},t)$ are given in this case by

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

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

with

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

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

$$\frac{\partial\rho}{\partial t}=\Psi^*\frac{\partial\Psi}{\partial t}+\Psi\frac{\partial\Psi^*}{\partial t}. \tag{5}$$

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

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

Observe that the last two terms are purely imaginary, and therefore cancel in Eq. (5), leaving us with[1]

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

It is then manifestly obvious that

$$\boxed{\frac{\partial \rho}{\partial t} + \vec{\boldsymbol{\nabla}} \boldsymbol{\cdot} \vec{\boldsymbol{j}} = 0}. \tag{8}$$

Problem 2 – Chapter 3 # 8)
Consider a particle in a potential $V(\vec{\boldsymbol{r}})$ with associated wave function satisfying the time-dependent Schrödinger equation

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

(a) Show that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \vec{\boldsymbol{r}}(t)\right\rangle = \int \mathrm{d}^3\vec{\boldsymbol{r}}\; \vec{\boldsymbol{j}}(\vec{\boldsymbol{r}}, t), \tag{10}$$

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

$$m\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \vec{\boldsymbol{r}}(t)\right\rangle = \left\langle \vec{\boldsymbol{p}}(t)\right\rangle. \tag{11}$$

(b) Show that

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

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

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

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

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

where the dependence on $\vec{\boldsymbol{r}}$ 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 $\left\langle\vec{\boldsymbol{F}}\right\rangle = \vec{\boldsymbol{F}}(\langle\vec{\boldsymbol{r}}\rangle)$, then $\langle\vec{\boldsymbol{r}}(t)\rangle$ changes in time as the position of a classical particle under the action of the force $\vec{\boldsymbol{F}}(\vec{\boldsymbol{r}})$. Under what condition(s) can this happen? Obtain $\langle\vec{\boldsymbol{r}}(t)\rangle$ and $\langle\vec{\boldsymbol{p}}(t)\rangle$ for a particle in a harmonic potential

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

(a) Observe that

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\vec{\boldsymbol{r}}(t)\right\rangle = \int \mathrm{d}^3\vec{\boldsymbol{r}}\,\frac{\partial}{\partial t}\rho(\vec{\boldsymbol{r}},t) = -\int \mathrm{d}^3\vec{\boldsymbol{r}}\,\vec{\boldsymbol{j}}(\vec{\boldsymbol{r}},t)}, \tag{15}$$

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

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

$$\boxed{m\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\vec{\boldsymbol{r}}(t)\right\rangle = \frac{1}{2}\int \mathrm{d}^3\vec{\boldsymbol{r}}\,[\Psi\vec{\boldsymbol{p}}\Psi^* + \Psi^*\vec{\boldsymbol{p}}\Psi] = \int \mathrm{d}^3\vec{\boldsymbol{r}}\,\Psi^*\vec{\boldsymbol{p}}\Psi = \langle\vec{\boldsymbol{p}}(t)\rangle}. \tag{16}$$

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

(b) We can do this as follows:

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

Notice that the integral

$$\int \mathrm{d}^3\vec{\boldsymbol{r}}\,\big[(\nabla^2\Psi^*)(\vec{\boldsymbol{\nabla}}\Psi) - \Psi^*\vec{\boldsymbol{\nabla}}\big(\nabla^2\Psi\big)\big] = \sum_{i=1}^{3}\hat{\boldsymbol{x}}_i\int \mathrm{d}^3\vec{\boldsymbol{r}}\,\Big[(\nabla^2\Psi^*)\frac{\partial\Psi}{\partial x_i} - \Psi^*\frac{\partial}{\partial x_i}\big(\nabla^2\Psi\big)\Big] \qquad (18)$$

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

$$\begin{aligned}
\int \mathrm{d}^3\vec{\boldsymbol{r}}\Big[(\nabla^2\Psi^*)\frac{\partial\Psi}{\partial x} - \Psi^*\frac{\partial}{\partial x}\big(\nabla^2\Psi\big)\Big] &= \int \mathrm{d}^3\vec{\boldsymbol{r}}\,\Big[(\nabla^2\Psi^*)\frac{\partial\Psi}{\partial x} - \Psi^*\nabla^2\frac{\partial\Psi}{\partial x}\Big]. \qquad (19) \\
&=
\end{aligned}$$

Problem 3 – Chapter 4 # 1)
Consider the problem of a particle in an attractive δ-function potential given by

$$V(x) = -V_0\delta(x) \quad V_0 > 0. \qquad (20)$$

(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 $\mathrm{d}P\,(p)$ that a measurement of the momentum in this bound state will give a result included between p and $p + \mathrm{d}p$. 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

$$\psi''(x) = -[v_0\delta(x) - |\varepsilon|]\psi(x), \qquad (21)$$

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

$$\psi(x) = \Theta(-x)[A_-e^{\kappa x} + B_-e^{-\kappa x}] + \Theta(x)[A_+e^{\kappa x} + B_+e^{-\kappa x}], \qquad (22)$$

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 $\psi(x \to \pm\infty) = 0$ and therefore $A_+ = B_- = 0$. Secondly, we have the conditions on the wave function and its derivative at $x = 0$:

$$\psi(0^-) = \psi(0^+) \Rightarrow A_- = B_+ \tag{23}$$

$$\psi'(0^+) - \psi'(0^-) = v_0\psi(0) \Rightarrow \kappa[-B_+ - A_-] = -v_0 A_-, \tag{24}$$

where we use the notation $\psi(0^\pm) = \lim_{x\to 0^\pm} \psi(x)$. Also, note that Eq. (24) comes from integrating the Eq. (21) in an infinitesimal region around $x = 0$. The first condition tells us that the wave function is symmetric about $x = 0$:

$$\psi(x) = \sqrt{\kappa} e^{-\kappa|x|}. \tag{25}$$

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:

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

$$\begin{aligned}
\tilde{\psi}(p) &= \sqrt{\kappa} \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} e^{-\kappa|x|} \\
&= \sqrt{\frac{\kappa}{2\pi\hbar}} \Big[\int_{-\infty}^{0} \mathrm{d}x\, e^{(\kappa - ip/\hbar)x} + \int_{0}^{\infty} \mathrm{d}x\, e^{-(\kappa + ip/\hbar)x} \Big] \\
&= \sqrt{\frac{\kappa}{2\pi\hbar}} \Big[\frac{1}{\kappa - ip/\hbar} + \frac{1}{\kappa + ip/\hbar} \Big] = \sqrt{\frac{2\kappa}{\pi\hbar}}\, \frac{\kappa}{\kappa^2 + (p/\hbar)^2}.
\end{aligned} \tag{26}$$

The probability to find the particle with momentum in the interval $[p, p + \mathrm{d}p]$ is then given as

$$\tilde{\rho}(p) = |\tilde{\psi}(p)|^2 = \frac{2}{\pi\hbar} \frac{\kappa^3}{[\kappa^2 + (p/\hbar)^2]^2} = \frac{2}{\pi\hbar\kappa} \frac{1}{[1 + (p/\kappa\hbar)^2]^2}. \tag{27}$$

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

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

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

Problem 4 – Chapter 4 # 5)
Consider a particle in the one-dimensional potential $V(x)$, such that $V(x) = \infty$ for $x < 0$ and

$$V(x) = -V_0\,\delta(x-a) \text{ for } x > 0 \tag{28}$$

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

$$\psi(x) = \begin{cases} 0 & x < 0 \\ Ae^{\kappa x} + Be^{-\kappa x} & 0 < x < a \\ Ce^{-\kappa x} & x > a, \end{cases} \tag{29}$$

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

The following boundary conditions must be respected:

$$\psi(0) = 0 \tag{30}$$
$$\psi(a^-) = \psi(a^+) \tag{31}$$
$$\psi'(a^+) - \psi'(a^-) = -\frac{2mV_0}{\hbar^2}\psi(a). \tag{32}$$

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

$$A + B = 0 \tag{33}$$
$$Ae^{\kappa a} + Be^{-\kappa a} = Ce^{-\kappa a} \tag{34}$$
$$Ae^{\kappa a} - Be^{-\kappa a} + Ce^{-\kappa a} = -v_0 Ce^{-\kappa a}, \tag{35}$$

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. (33)–(35) must be linearly dependent or

$$\begin{vmatrix} 1 & 1 & 0 \\ e^{2\kappa a} & 1 & -1 \\ e^{2\kappa a} & -1 & (1+v_0) \end{vmatrix} = [(1-v_0) - 1] - [e^{2\kappa a}(1+v_0) + e^{2\kappa a}] = 0 \tag{36}$$

$$e^{2\kappa a} = \frac{v_0}{2+v_0} \Rightarrow \kappa = \frac{1}{2a}\ln\left(\frac{v_0}{2+v_0}\right). \tag{37}$$

Thus, there is one bound state permitted under this potential.