

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):

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

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

leaving us with¹

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

It is then manifestly obvious 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 $\vec{\nabla} \cdot \vec{A} |\Psi|^2 = |\Psi|^2 \vec{\nabla} \cdot \vec{A} + \vec{A} \cdot \vec{\nabla} |\Psi|^2 = |\Psi|^2 \vec{\nabla} \cdot \vec{A} + \vec{A} \cdot (\Psi^* \vec{\nabla} \Psi + \Psi \vec{\nabla} \Psi^*)$ and $\Psi^* \vec{\nabla} \cdot \vec{A} \Psi = \vec{\nabla} \cdot \vec{A} |\Psi|^2 - \Psi \vec{A} \cdot \vec{\nabla} \Psi^*$.

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.

