Quantum A
Solution to Problem set 3

Problem 1

we want to show that both sides of equation (2) satisfy Schrödinger's equation given that $\psi(\vec{r},t)$ is a solution i.e

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)\right)\psi(\vec{r},t) = i\hbar\,\partial_t\psi(\vec{r},t) \qquad (3)$$

Eq (3) implies that

$$\left(\frac{\hbar^2}{2m}\nabla^2 + i\hbar\,\partial_t\right)\psi(\vec{r},t) = V(\vec{r},t)\,\psi(\vec{r},t)$$

Let us apply the operator $\hat{O} = \frac{\hbar^2}{2m}\nabla^2 + i\hbar\,\partial_t$ on the RHS of equation (2). The first term gives you zero immediately because of the definition of K through eq. 1. The second term of the RHS of Eq. 2 gives

$$\frac{1}{i\hbar}\int_{t_0}^{t} dt' \int d^3r' \left(\frac{\hbar^2}{2m}\nabla^2 + i\hbar\,\partial_t\right) K(\vec{r},t;\vec{r}\,',t')\,V(\vec{r}\,',t')\,\psi(\vec{r}\,',t')$$

$$+\frac{1}{i\hbar}(i\hbar)\int d^3r'\,K(\vec{r},t;\vec{r}\,',t)\,V(\vec{r}\,',t)\,\psi(\vec{r}\,',t)$$

we have used the identity

$$\frac{\partial}{\partial t}\int_{t_0}^{t} dt'\, F(t,t') = F(t,t) + \int_{t_0}^{t} dt' \frac{\partial}{\partial t} F(t,t')$$

Now, as shown in class, and this can be easily verified by solving Eq. 1 for $K(\vec{r},t;\vec{r}',t')$, the following is true

$$\lim_{t'\to t} K(\vec{r},t;\vec{r}',t') = \delta(\vec{r}-\vec{r}')$$

Therefore, after the application of the operator $\hat{O}$ on the RHS of Eq. 2 we obtain

$$V(\vec{r},t)\,\psi(\vec{r},t).$$

Therefore, when we apply $\hat{O}$ on both sides of Eq 2. we have

$$\hat{O}\,\psi(\vec{r},t) = V(\vec{r},t)\,\psi(\vec{r},t) \Rightarrow$$

$$\left(\frac{\hbar^2}{2m}\nabla^2 + i\hbar\frac{\partial}{\partial t}\right)\psi(\vec{r},t) = V(\vec{r},t)\,\psi(\vec{r},t)$$

which is Schrödinger's Equation.

Problem 2

(2.1) $$|\psi\rangle_t = \underbrace{\int \frac{d^3p}{(2\pi\hbar)^3} \, |p\rangle\langle p|}_{\hat{1}} \psi\rangle_t \Rightarrow$$

$$\langle \vec{r}|\psi\rangle_t = \int \frac{d^3p}{(2\pi\hbar)^3} \langle \vec{r}|\vec{p}\rangle \langle \vec{p}|\psi\rangle_t \Rightarrow$$

(2.2) $$\psi(\vec{r},t) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \, \phi(\vec{p},t)$$

where $\phi(p,t) \equiv \langle \vec{r}|\psi\rangle_t$ the amplitude to be in state $|p\rangle$.

Now, schrödinger eq. (3) (in problem set) and (2.2) give

$$i\hbar \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \frac{\partial \phi(\vec{p},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right) \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \phi(\vec{p},t)$$

The rhs of the above eq. becomes $\longrightarrow$

$$\text{r.h.s} = \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \frac{\hbar^2 p^2}{2m} \phi(\vec{p},t) + V(\vec{r}) \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \phi(\vec{p},t)$$

Now the operator $\vec{r}$ can be written as

$$\vec{r} \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \phi(\vec{p},t) = \int \frac{d^3p}{(2\pi\hbar)^3} \left(\frac{\hbar}{i} \vec{\nabla}_p e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}\right) \phi(\vec{p},t)$$

by integration by parts and by assuming the $\phi(\vec{p}\to\infty,t)\to 0$ we obtain

$$\vec{r} \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \phi(\vec{p},t) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \left(-\frac{\hbar}{i}\vec{\nabla}_p \phi(\vec{p},t)\right)$$

similarly for any power of $\vec{r}$

$$\vec{r}^{\,n} \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \phi(\vec{p},t) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \left(-\frac{\hbar}{i}\nabla_p\right)^n \phi(\vec{p},t)$$

and, therefore, by means of Taylor expansion, any Taylor expandable function $V(\vec{r})$ gives

$$V(\vec{r}) \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \phi(\vec{r},t) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} V(i\hbar\vec{\nabla}_p)\phi(\vec{p},t)$$

Therefore, Schrödinger's Eq. takes the form

$$\int \frac{d^3p}{(2\pi\hbar)^3}\, e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \left[i\hbar \frac{\partial}{\partial t} + \frac{p^2}{2m} - V(i\hbar\vec{\nabla}_p)\right] \phi(\vec{p},t) = 0$$

which implies (because this is $\forall\ \vec{r}$) that

$$\left[i\hbar \frac{\partial}{\partial t} - \frac{p^2}{2m} - V(i\hbar\vec{\nabla}_p)\right] \phi(\vec{p},t) = 0$$

Problem 3

We had discussed in class that the equality in the uncertainty principle

$$(\Delta x)(\Delta P_x) \geq \frac{\hbar}{2}$$

holds when our defined vector $|S\rangle = 0$ where $|S\rangle = |\Theta\rangle - e^{i\alpha}|\phi\rangle$ and with the choices of $|\phi\rangle = \frac{\hat{P}_x - \langle \hat{P}_x\rangle}{\Delta P_x}|\psi\rangle$ and $|\Theta\rangle = \frac{\hat{x} - \langle\hat{x}\rangle}{\Delta x}|x\rangle$ and $e^{i\alpha} = -i$ which we made in order to prove the uncertainty relation, this means that

$$\frac{\hat{x} - \langle \hat{x} \rangle}{\Delta x} |\psi\rangle + i \frac{\hat{P}_x - \langle \hat{P}_x \rangle}{\Delta P_x} |\psi\rangle = 0$$

This implies that;

$$\frac{\langle \vec{r} | \hat{x} - \langle \hat{x} \rangle | \psi \rangle}{\Delta x} + i \frac{\langle \vec{r} | \hat{P}_x - \langle \hat{P}_x \rangle | \psi \rangle}{\Delta P_x} = 0$$

which means

$$\frac{x - \langle x \rangle}{\Delta x} \langle \vec{r} | \psi \rangle + i \frac{\left(-i\hbar \partial_x - \langle P_x \rangle\right)}{\Delta P_x} \langle \vec{r} | \psi \rangle = 0$$

which can be rewritten as follows.

$$\Delta P_x \left[\frac{x - \langle x \rangle}{\Delta x} - i \frac{\langle P_x \rangle}{\Delta P_x} \right] \psi(x,y,z) = -\hbar \frac{\partial \psi(x,y,z)}{\partial x}$$

which can be integrated with respect to the variable x to give

$$\psi(x,y,z) = e^{\frac{i \langle P_x \rangle}{\hbar} x - \frac{1}{2} \frac{\Delta P_x}{\hbar \Delta x} (x - \langle x \rangle)^2} g(y,z)$$

above $g(y,z)$ is a constant of integration which is independent of x, but, in general, a function of y, z.

in this case $\qquad \Delta x \, \Delta p_x = \hbar/2 \Rightarrow \Delta p_x = \dfrac{\hbar}{2\Delta x}$,

thus

$$\psi(x,y,z) = e^{i\frac{\langle p_x\rangle}{\hbar}x - \frac{1}{4}\frac{(x-\langle x\rangle)^2}{(\Delta x)^2}} g(y,z)$$

Problem 4

The equation

$$\frac{\partial}{\partial t}\rho + \vec{\nabla}\cdot\vec{J} = 0 \qquad (4.1)$$

with $\rho = |\psi(\vec{r},t)|^2$ and $J = \frac{-i\hbar}{2m}\left(\psi^*\nabla\psi - (\nabla\psi^*)\psi\right)$

can be equivalently written as

$$\psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t} + \left(-\frac{i\hbar}{2m}\right)\left[\cancel{\nabla\psi^*\cdot\nabla\psi} + \psi^*\nabla^2\psi - \nabla^2\psi^*\psi - \cancel{\nabla\psi^*\nabla\psi}\right] = 0$$

$$\psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t} = +\frac{i\hbar}{2m}\left[\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right]$$

or $\quad \psi^*\left(i\hbar\frac{\partial\psi}{\partial t}\right) + \psi\left(-i\hbar\frac{\partial\psi}{\partial t}\right)^* = -\frac{\hbar^2}{2m}\left[\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right] \quad (4.2)$

Therefore, (4.1) $\Leftrightarrow$ (4.2) (i.e, we can go back and forth from (4.1) to (4.2)).

Eq 4.2, however, can be easily derived from Schrödinger's Equation

$$i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \quad (4.3)$$

by, first multiplying both sides by ψ^*

$$\psi^*\left(i\hbar\frac{\partial}{\partial t}\psi\right) = -\frac{\hbar^2}{2m}\psi^*\nabla^2\psi + \psi^* V\psi, \quad (4.4)$$

then, taking the complex conjugate of both sides

$$\psi\left(i\hbar\frac{\partial\psi}{\partial t}\right)^* = -\frac{\hbar^2}{2m}\psi\nabla^2\psi^* + \psi V\psi^* \quad (4.5)$$

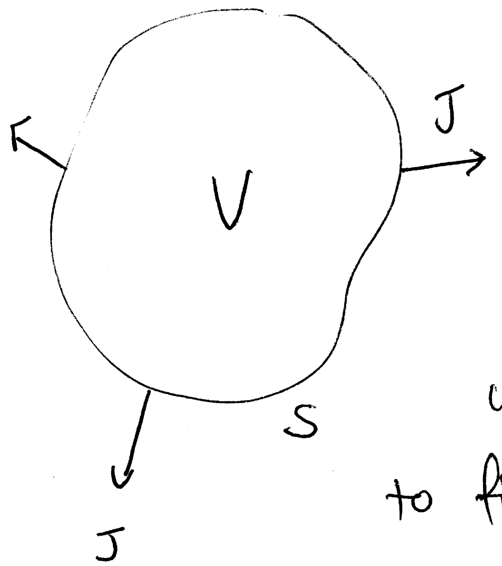
and substracting (4.5) from (4.4) we obtain

$$\psi^*\left(i\hbar\frac{\partial}{\partial t}\psi\right) - \psi\left(i\hbar\frac{\partial\psi}{\partial t}\right)^* = -\frac{\hbar^2}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right)$$

The term which contains the potential is $V|\psi|^2$ in both cases and cancels.

By integrating the continuity equation over a volume

V and applying Gauss's theorem, we find



$$-\oint_S \vec{J}\cdot d\vec{s} = \frac{\partial}{\partial t}\int_V |\psi|^2 d^3\vec{r}$$

which means that the probability to find a particle inside this arbitrary volume V has changed because of the flux of probability through the surface S which encloses the volume V.

Problem 5

The Hamiltonian is

$$H = \frac{1}{2m}\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)^2 + e\phi + V \qquad (5.1)$$

and Schrödinger's eq is

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{i\hbar e}{2mc}\vec{\nabla}\cdot\vec{A}\,\psi + \frac{i\hbar e}{2mc}\vec{A}\cdot\nabla\psi + \frac{e^2}{2mc^2}\vec{A}^2\psi + V\psi + e\phi\psi = i\hbar\frac{\partial\psi}{\partial t} \qquad (5.2)$$

We want to show that

$$\psi(\vec{r},t) = \exp\left[-\frac{ie}{\hbar c}\lambda(\vec{r},t)\right]\psi^{(0)}(\vec{r},t) \qquad (5.3)$$

where $\psi^{(0)}(\vec{r},t)$ is the solution to the schrödinger equation for the case of $\lambda(\vec{r},t)=0$

i.e

$$-\frac{\hbar^2}{2m}\nabla^2\psi^{(0)}(\vec{r},t) + V\psi^{(0)}(\vec{r},t) = i\hbar\partial_t\psi^{(0)}(\vec{r},t) \quad (5.4)$$

We substitute (5.3) in (5.2) and after straightforward algebra we obtain (5.4).

i.e,

$$e^{-\frac{ie}{\hbar c}\lambda(\vec{r},t)}\left(-\frac{\hbar^2}{2m}\nabla^2\psi^{(0)}(\vec{r},t) + V\psi^{(0)}(\vec{r},t)\right) = e^{-\frac{ie}{\hbar c}\lambda(\vec{r},t)}\, i\hbar\frac{\partial\psi^{(0)}}{\partial t}$$

In the case where $\lambda(\vec{r},t)$ is independant of $\vec{r}$ we have

$$\vec{A}=0, \qquad \varphi(\vec{r},t) = \frac{1}{c}\frac{\partial\lambda}{\partial t}$$

and so $\lambda = c\int_{-\infty}^{t} dt'\,\varphi(t')$ and thus

$$\psi(\vec{r},t) = e^{-\frac{ie}{\hbar}\int_{-\infty}^{t}\varphi(t')dt'}\,\psi^{(0)}(\vec{r},t)$$

Problem 6

1. For this problem we can use the result of the previous problem (Problem 5), i.e.

$$\psi(\vec{r},t) = e^{-\frac{ie}{\hbar}\int_{-\infty}^{t}\phi(t')dt'}\,\psi^{(0)}(\vec{r},t)$$

and

$$\psi^{(0)}(\vec{r},t) = e^{\frac{i}{\hbar}\left(\vec{p}\cdot\vec{r} - E_p t\right)}$$

and so

$$\psi_A(\vec{r},t) = e^{-\frac{ie}{\hbar}V_A(t_1-t_0)}\,e^{\frac{i}{\hbar}\left(\vec{p}\cdot\vec{r}_A - E_p t\right)}$$

$$\psi_B(\vec{r},t) = e^{-\frac{ie}{\hbar}V_B(t_1-t_0)}\,e^{\frac{i}{\hbar}\left(\vec{p}\cdot\vec{r}_B - E_p t\right)}$$

The total amplitude at a given point z on the screen is

$$\psi(x,y,z,t) = \psi_A(\vec{r},t) + \psi_B(\vec{r},t) = \psi_A(\vec{r},t)\left(1 + e^{+i\Delta\phi}\right)$$

where $\Delta\phi = -\frac{e}{\hbar}(V_A - V_B)(t_1 - t_0) + \frac{p_z}{\hbar}\Delta z$

where Δz is the path difference along the z direction and, thus, the shift in the diffraction pattern, ΔZ, is given from

$$k_z \Delta Z = \frac{e}{\hbar}(V_A - V_B)(t_1 - t_0) \rightarrow$$

$$\Delta Z = \frac{e(V_A - V_B)(t_1 - t_0)}{\hbar \; k_z} = \frac{10^{-6}\,eV \times 10^{-9}\,sec}{6.6\;10^{-16}\,eVs\,10^{4}}\ cm$$

$$= 1.5\;10^{-4}\ cm$$