Lecture 10

From last discussion, QM has both wave and fluid aspects, is there a connection betwen these 2?
Consider a state in the $\vec{r}$ representation (plane wave) to be

$$\psi(\vec{r}) = A(\vec{r})e^{iS(\vec{r})/\hbar}, \tag{1}$$

were $A(\vec{r}) = A$ and $S(\vec{r}) = S$ are taken to be real functions. Consider also Schrödinger's equation with a potential $V(\vec{r})$:

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

and plug-in the ansatz:

$$\begin{aligned} i\hbar\left[\dot{A}e^{\frac{i}{\hbar}S} + \frac{i}{\hbar}A\dot{S}e^{\frac{i}{\hbar}S}\right] &= -\frac{\hbar^2}{2m}\nabla\left[\nabla\cdot Ae^{\frac{i}{\hbar}S} + \frac{i}{\hbar}A\nabla Se^{\frac{i}{\hbar}S}\right] + VAe^{\frac{i}{\hbar}S} \\ &= -\frac{\hbar^2}{2m}\left[\nabla^2Ae^{\frac{i}{\hbar}S} + \frac{2i}{\hbar}e^{\frac{i}{\hbar}S}\nabla A\cdot\nabla Se^{\frac{i}{\hbar}S} + \frac{i}{\hbar}A\nabla^2Se^{\frac{i}{\hbar}S} - \frac{1}{\hbar^2}A(\nabla S)^2e^{\frac{i}{\hbar}S}\right] + VAe^{\frac{i}{\hbar}S} \\ i\hbar\left[\dot{A} + \frac{i}{\hbar}A\dot{S}\right] &= -\frac{\hbar^2}{2m}\left[\nabla^2A + \frac{2i}{\hbar}\nabla A\cdot\nabla S + \frac{i}{\hbar}A\nabla^2S - \frac{1}{\hbar^2}A(\nabla S)^2\right] + VA \end{aligned} \tag{2}$$

Since A and S are real functions, every term is either real or imaginary.
Equate first all imaginary terms, this gives:

$$\begin{aligned} i\hbar\dot{A} &= -\frac{i\hbar}{m}\nabla A\cdot\nabla S - \frac{i\hbar}{2m}A\nabla^2S \\ \dot{A} &= -\frac{1}{m}\nabla A\cdot\nabla S - \frac{1}{2m}A\nabla^2S, \end{aligned}$$

multiplying both sides by $2A$

$$2A\dot{A} = -\frac{2A}{m}\nabla A\cdot\nabla S - \frac{1}{m}A^2\nabla^2S,$$

allows to rewrite the expression in the following way

$$\frac{\partial A^2}{\partial t} = -\frac{1}{m}\nabla\left(A^2\nabla S\right). \tag{3}$$

This expression seems neat but what does it represent? Note first that $|\psi|^2 = A^2$ is the probability density ρ; then, what is ∇S? it can be regarded as momentum, since S for a free particle is $S = \vec{p} \cdot \vec{r}$. Then $A^2 \nabla S$ is the current density [1]. So Eq. 3 simply restates the continuity equation

$$\frac{\partial \rho}{\partial t} = -\nabla \vec{J}$$

which we know to be correct.
Equate now all the real terms in eq.(2), this gives

$$\begin{aligned} -A\dot{S} &= -\frac{\hbar^2}{2m}\left(\nabla^2 A - \frac{1}{\hbar^2} A (\nabla S)^2\right) + VA \\ &= -\frac{\hbar^2}{2m}\nabla^2 A + \frac{1}{2m} A (\nabla S)^2 + VA \end{aligned}$$

An approximation is to be made in here. *Assume that the first term can be ingored*, since it is the only term that contains $\hbar$ (and even squared). This is equivalent to asking the gradient of A to change really slow over 1 wavelength, or the envelope to be more less linear over several wavelengths. Then

$$\begin{aligned} -A\dot{S} &= \frac{1}{2m} A (\nabla S)^2 + VA \\ \dot{S} &= -\frac{1}{2m} (\nabla S)^2 - V \\ &= -\frac{m}{2} (\vec{v})^2 - V \end{aligned}$$

the first term looks like the kinetic energy. How is this equation interpreted? Take the gradient of the whole equation:

$$\nabla \dot{S} = -m(\vec{v} \cdot \nabla)\vec{v} - \nabla V$$

$$\frac{d\vec{p}}{dt} = \left.\frac{\partial \vec{p}}{\partial t}\right|_{position} + \vec{v} \cdot \nabla \vec{p},$$

this is the convective derivative, the second term tells how the momentum of a given point (tiny volume) within the fluid is changing as the point moves in the direction of $\vec{v}$. Thus Schrödinger equation tells that momentum follows Newton's law. The probability density behaves like a fluid following Newton's law. We've started with a wave picture of QM and checked how it supports a fluid picture.

Wigner function

Phase space

In classical mechanics, for a point particle you need to know both its initial position *and* its initial momentum to know how it will move in the future. This

[1] This can also be proven exactly by applying the definition of the probability current density to our Ansatz for the wave function, Eq. 1.

corresponds to a point in 6-dimensional phase space. Similarly, for a fluid (an infinite number of "point particles"), just knowing the (probability) density $\rho(\vec{r})$ doesn't tell you its future state. You need to know also the flow which is proportional to the momentum, i.e. you need the 6 dimensional phase space density $\rho(\vec{r},\vec{p})$.

For a particle, Hamilton's equations of motion completely specify its trajectory in phase space, whereas for a fluid, we can pick a (small) volume in phase space and then Hamilton's equation will tell us how it will evolve in the future. Louville's theorem states the following:

The volume occupied by a "fluid" in phase space is conserved if the Hamiltonian is independent of time .

This theorem is for instance important for accelerator design and optics (where one can reduce the spatial extend of a light beam, but only by simultaneously increasing its divergence).

Is it then possible to introduce a function $\rho(\vec{r},\vec{p}) \to W(\vec{r},\vec{p})$ (Wigner function), so that it gives the probability to find a particle with $\vec{r}$ and $\vec{p}$? This seems to be in conflict with QM, since one cannot measure momentum and position with simultaneously with arbitrary position. However, it is still useful to have a Wigner function that mimics *some* of the aspects of a true probability distribution, in particular for the calculation of expectation values (both of commuting and non-commuting pairs of operators).

The Wigner function is now defined in 3-dim (3 coordinates and 3 momenta):

$$W(\vec{r},\vec{p}) = \frac{1}{(2\pi\hbar)^3} \iiint_{\text{Phase Space}} d\vec{r}' e^{-i\vec{p}\cdot\vec{r}'\hbar} \psi^* \left(\vec{r} - \frac{\vec{r}}{2}\right) \psi \left(\vec{r} + \frac{\vec{r}'}{2}\right)$$

but lets work on it in just 1-dim (1 spatial coordinate and 1 momentum):

$$W(x,p) = \frac{1}{2\pi\hbar} \int dx' e^{-ipx'/\hbar} \psi^* \left(x - \frac{x'}{2}\right) \psi \left(x + \frac{x'}{2}\right).$$

What should this function satisfy if it is to be taken as a joint probability density?

- It should be real: $W = W^*$

This is already satisfied, for taking the complex conjugate gives

$$W(x,p) = \frac{1}{2\pi\hbar} \int dx' e^{ipx'/\hbar} \psi \left(x - \frac{x'}{2}\right) \psi^* \left(x + \frac{x'}{2}\right)$$

and it is always possible to take $x'' = -x'$, in which case we have $W = W^*$.

- $W(p,x)$ should be positive definite (Probability should range in $0 < \rho < 1$).

This is not true, since Wigner function can also be negative, but we just ignore this fact.
Integrate now the Wigner function over all momenta

$$\int_{-\infty}^{\infty} dpW(x,p) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dpe^{-ipx'/\hbar}\psi\left(x - \frac{x'}{2}\right)\psi^*\left(x + \frac{x'}{2}\right).$$

Recall that

$$\int_{-\infty}^{\infty} dpe^{-ipx'/\hbar} = 2\pi\hbar\delta(x'),$$

then it is found

$$\int_{-\infty}^{\infty} dpW(x,p) = \psi\left(x\right)\psi^*\left(x\right) = \left|\psi(x)\right|^2,$$

which is in fact the probability density in configuration space.

Integrate now the Wigner function over all coordinates

$$\int_{-\infty}^{\infty} dxW(x,p) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dxe^{-ipx'/\hbar}\psi\left(x - \frac{x'}{2}\right)\psi^*\left(x + \frac{x'}{2}\right)$$

this is not straightforward since ψ and ψ^* also depend on x. Introduce, however, the following change of variables

$$\begin{aligned} x_1 &= x + \frac{x'}{2} \\ x_2 &= x - \frac{x'}{2} \end{aligned}$$

the inverse transformation is then

$$\begin{aligned} x' &= x_1 - x_2 \\ x &= \frac{1}{2}(x_1 + x_2) \end{aligned}$$

and the Jacobian for this transformation is

$$\left|\frac{\partial(x,x')}{\partial(x_1,x_2)}\right| = \left|\begin{array}{cc} \frac{\partial x}{\partial x_1} & \frac{\partial x}{\partial x_2} \\ \frac{\partial x'}{\partial x_1} & \frac{\partial x'}{\partial x_2} \end{array}\right| = \left|\begin{array}{cc} \frac{1}{2} & \frac{1}{2} \\ 1 & -1 \end{array}\right| = 1$$

thus $dxdx' = dx_1dx_2$ and

$$\begin{aligned} \int_{-\infty}^{\infty} dxW(x,p) &= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 e^{-ipx_1/\hbar}e^{ipx_2/\hbar}\psi^*(x_2)\psi(x_1) \\ &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx_1 e^{-ipx_1/\hbar}\psi(x_1)\cdot\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx_2 e^{ipx_2/\hbar}\psi^*(x_2) \\ &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx_1 e^{-ipx_1/\hbar}\psi(x_1)\cdot\left[\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx_2 e^{-ipx_2/\hbar}\psi(x_2)\right]^* \\ &= \tilde{\psi}(p)\tilde{\psi}^*(p) \\ &= \left|\tilde{\psi}(p)\right|^2 \end{aligned}$$

Given the Wigner function $W(x,p)$, it is possible to calculate $\langle p^n \rangle$ and $\langle x^n \rangle$. What is

$$\frac{1}{2\pi\hbar}\int dppW(x,p)?$$

Taking $W(x,p)$ as the joint probability density, this should give the expectation value of p at a specific point x:

$$\begin{aligned}
\frac{1}{2\pi\hbar}\int dppW(x,p) &= \frac{1}{2\pi\hbar}\int dp\int dx'\left[-\frac{\hbar}{i}\frac{\partial}{\partial x'}e^{-ipx'/\hbar}\psi^*\left(x-\frac{x'}{2}\right)\psi\left(x+\frac{x'}{2}\right)\right] \\
&= \frac{1}{2\pi\hbar}\frac{\hbar}{i}\int dx'\int dpe^{-ipx'/\hbar}\frac{\partial}{\partial x'}\psi^*\left(x-\frac{x'}{2}\right)\psi\left(x+\frac{x'}{2}\right) \\
&= \frac{1}{2\pi\hbar}\frac{\hbar}{i}\int dx'\int dpe^{-ipx'/\hbar}\left(-\frac{1}{2}\frac{\partial\psi^*}{\partial x}\psi\bigg|_{x-x'/2}+\frac{1}{2}\psi^*\frac{\partial\psi}{\partial x}\bigg|_{x+x'/2}\right)
\end{aligned}$$

where integration by parts was used in the second line. Integration over p gives again the delta function $2\pi\hbar\delta(x')$ and finally,

$$\begin{aligned}
\frac{1}{2\pi\hbar}\int dppW(x,p) &= \frac{\hbar}{2i}\left(-\frac{\partial\psi^*}{\partial x}\psi+\psi^*\frac{\partial\psi}{\partial x}\right) \\
&= mj(x) \\
&= p\cdot\rho(x)
\end{aligned}$$

where we apply the definition of the current density $j(x)$ and our interpretation of it in terms of local density times local momentum.