The first two problems almost made it to the midterm

5.1 Consider the state $e^{ip_0 X/\hbar}\,|p\rangle$ where $|p\rangle$ is an eigenstate of the momentum operator P, X is the position operator and p_0 is real. Show that this is also an eigenstate of P and find the eigenvalue. (3 points)

It is easiest to evaluate it in the coordinate basis (since the X operator appears in the exponential): We have $|\psi\rangle = e^{ip_0 X/\hbar}\,|p\rangle$ and therefore

$$\psi(x) = \langle x|e^{ip_0 X/\hbar}\,|p\rangle = e^{ip_0 x/\hbar}\,\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\,e^{ip_0 x/\hbar}\,e^{ipx/\hbar}$$

where we have used the expression for $\langle x|p\rangle$. Clearly, as we have seen numerous times this is an eigenfunction of $-i\hbar\partial/\partial x$ the momentum operator with eigenvalue $p + p_0$.

5.2 Consider the diffusion equation for the density $n(x,t)$ in one dimension

$$\frac{\partial n}{\partial t} = D\,\frac{\partial^2 n}{\partial x^2}$$

where D is the diffusion constant. You are given $n(x,0) = n_0\,a\,\delta(x)$. (Why is it convenient to write it in this form? What is the dimension of a? Shankar does something similar in Exercise 5.2.3) Find $n(x,t)$; in particular determine how the width of the density profile evolves in time. (8 points)

We are considering a problem in one dimension. We know that the eigenfunctions of $\partial/\partial x^2$ are e^{ikx} with eigenvalues $-k^2$ and if we let $k \in (-\infty, +\infty)$ we have a complete set. We write

$$n(x,t) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\,\hat{n}(k,t)\,e^{ikx}\,.$$

We substitute it into the diffusion equation and obtain

$$\int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} e^{ikx}\,\frac{\partial \hat{n}(k,t)}{\partial t} = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} (-Dk^2 \hat{n}(k,t))\,e^{ikx}\,.$$

We deduce, therefore[1]

$$\frac{\partial \hat{n}(k,t)}{\partial t} = -Dk^2\,\hat{n}(k,t)\,.$$

[1] Be absolutely clear why you can do this. Be prepared to explain this and demonstrate this with an explicit calculation if necessary.

This is an easy equation to solve and we have

$$\hat{n}(k,t) \;=\; \hat{n}(k,0)\, e^{-Dk^2 t}\,.$$

If we know $\hat{n}(k,0)$ we can find $\hat{n}(k,t)$ and Fourier transform it back to obtain $n(x,t)$. Sine we know $n(x.0) \;=\; n_0 a \delta(x)$ we have

$$\hat{n}(k,0) \;=\; \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} n(x,0)\, e^{-ikx} \;=\; \frac{n_0 a}{\sqrt{2\pi}}\,.$$

So we obtain

$$n(x,t) \;=\; \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} e^{ikx}\, e^{-Dk^2 t}\, \frac{n_0 a}{\sqrt{2\pi}}\,.$$

Doing the Gaussian integral using

$$\int_{-\infty}^{\infty} dk\, e^{-bk^2+ikx} \;=\; e^{-\frac{x^2}{4b}} \sqrt{\frac{\pi}{b}} \quad \text{for} \quad \Re[b] \;>\; 0\,.$$

we have

$$n(x,t) \;=\; \frac{n_0 a}{\sqrt{4\pi D t}}\, e^{-\frac{x^2}{4Dt}}\,.$$

Note that the delta function density spreads and becomes Gaussian with a width given by $\sigma^2 \;=\; 2Dt$. **The fact that the width (a length) increases as $\sqrt{t}$ is one of the most important results of classical physics.** It is useful in astrophysics, condensed matter physics, material science, biology, ecology, finance, you get the picture.

5.3 Find the transcendental equation that determines the energy eigenvalues of the odd bound states for a potential well of depth $-V_0$ and width a symmetrically disposed about the origin considered in the lecture. You are urged to do this problem starting from the form of the wave functions in the different regions without looking at your notes or any book. Consider an electron in a well of width $a \;=\; 1nm$. What is the minimum well depth at which the first odd bound state appears? (5 points)

For even wave functions $\psi(x)$ for positive values of x is given by

$$\begin{aligned} \psi(x) \;&=\; F\, e^{-\kappa x} \quad \text{for} \quad x \geq a/2 &(1)\\ &=\; D\, \sin(qx) \quad \text{for} \quad 0 \leq x \leq a/2 &(2) \end{aligned}$$

where

$$q \;=\; \frac{\sqrt{2m(E+V_0)}}{\hbar} \quad \text{and} \quad \kappa \;=\; \frac{\sqrt{-2mE}}{\hbar}\,. \qquad (3)$$

Now apply boundary condition at $x = a/2$. We equate the logarithmic derivative to obtain

$$\frac{d}{dx} \log e^{-\kappa x} \Big|_{x=a/2} = \frac{d}{dx} \log[D \sin qx] \Big|_{x=a/2} .$$

This yields

$$-\cot(qa/2) = \frac{\kappa}{q} \Rightarrow \tan(qa/2) = -q/\kappa.$$

Note that there are three energy scales in the problem, E, V_0, and an energy scale set by the kinetic energy of a particle with wavevector equal to the inverse of the width of the well, $\epsilon_0 \equiv \hbar^2/(2ma^2)$. Let us define $\boxed{v_0 \equiv V_0/\epsilon_0}$. We can write

$$\frac{qa}{2} = \sqrt{\frac{2ma^2}{\hbar^2}\frac{1}{4}(E + V_0)} = \sqrt{\frac{v_0}{4}\left(1 + \frac{E}{V_0}\right)}$$

In terms of the energies (writing $E = -|E|$) we have

$$\tan\left[\sqrt{\frac{v_0}{4}\left(1 - \frac{|E|}{V_0}\right)}\right] = -\sqrt{-1 + \frac{V_0}{|E|}} .$$

Clearly, $|E| < V_0$ for the square root to be real and it vanishes as $|E| \to V_0$. Note that the right-hand side is negative while the tangent for arguments less than $\pi/2$ is positive. The bound state appears at zero energy first and for this $\sqrt{v_0/4} \geq \pi/2$, i.e., $V_0/\epsilon_0 > \pi^2$. **Please check my algebra (I did not) and put in the numbers.** When you evaluate $\hbar^2/(2ma^2)$ use the Bohr radius a_B and write it as

$$\frac{\hbar^2}{2ma^2} = \frac{\hbar^2}{2ma_B^2} \times \frac{a_B^2}{a^2} = 13.6\, eV \times \frac{a^2}{(0.053nm)^2}$$

You can avoid a calculator by taking the Bohr radius $a_B = 0.05nm$. You should memorize the hydrogenic numbers.

Simple trigonometric puzzle: For what range of values of v_0 does one obtain exactly n bound states (even and odd)?

5.4 Exercise 5.2.3 on page 163. (6 points)
If you did not do the problem on the midterm fully please find the momentum distribution function and its width. (2 points)

Consider the potential

$$V(x) \; = \; - \, aV_0 \, \delta(x) \tag{4}$$

We integrate the Schrödinger equation across the origin where the potential is singular from $-\epsilon$ to $+\epsilon$ to obtain

$$- \frac{\hbar^2}{2m} \left[\, \psi'(\epsilon) \; - \; \psi'(-\epsilon) \; = \; - \int_{-\epsilon}^{\epsilon} dx V(x) \psi(x) \tag{5}$$

since the term with E goes to zero as $\epsilon \longrightarrow 0$. We thus see that there is a discontinuity in the derivative of the wave function at the potential given by

$$\psi'(0^+) \; - \; \psi'(0^-) \; = \; - \, \frac{2ma}{\hbar^2} \, V_0 \, \psi(0) \tag{6}$$

where we remark that the wave function itself is continuous.

Assuming that the wave function has the form for $x < 0$ (Region I) and $x > 0$ (Region II)

$$\psi_I(x) \; = \; Ae^{\kappa x} \;\; \text{and} \;\; \psi_{II} \; = \; Be^{-\kappa x} \tag{7}$$

where $\boxed{\kappa \; = \; \sqrt{2m \mid E \mid /\hbar^2}}$. The continuity of the wave function implies $A = B$ and the wave function has even symmetry. The other boundary condition yields

$$-2A \, \kappa \; = \; - \, \frac{2ma}{\hbar^2} \, V_0 \, A \; \Rightarrow \; \kappa \; = \; \frac{ma}{\hbar^2} \, V_0 \, . \tag{8}$$

We use this to obtain

$$E \; = \; - \, \frac{\hbar^2 \kappa^2}{2m} \; = \; - \, \frac{ma^2}{2\hbar^2} \, V_0^2 \tag{9}$$

yielding just one bound state for any strength of the attractive potential. Note that the normalized wave function is

$$\psi_0(x) \; = \; \sqrt{\kappa} \, e^{-\kappa |x|} \tag{10}$$

where κ is given above. Please see the solutions to the midterm for the rest of the problem.

5.5 Given $\psi(x) \; = \; R(x) \, e^{i\phi(x)}$ where $R(x)$ and $\phi(x)$ are real-valued functions find the (probability) current density. The result is worth remembering. Generalize it to a three-dimensional wave function. We have suppressed the time dependence for convenience. (4 points)

The probability current density along x is given by

$$j_x = \frac{\hbar}{2im} \left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right] . \tag{11}$$

Let $\psi(x) = R(x)\, e^{i\phi(x)}$ where R is real and we obtain (denoting the derivative with respect to x as usual with a prime)

$$\psi^* \frac{\partial \psi}{\partial x} = R(x) e^{-i\phi(x)} [\, R' + iR\phi' \,]\, e^{i\phi(x)} = RR' + i\, R^2 \phi'(x)\, .$$

Complex conjugating we obtain

$$\psi \frac{\partial \psi^*}{\partial x} = RR' - i\, R^2 \phi'(x)\, .$$

Subtraction removes the first term and we obtain for the probability current density $\boxed{j_x = (\hbar/m)\, R^2\, \partial\phi/\partial x}$.

From symmetry one can obtain the y and z components and infer

$$\vec{j} = \frac{\hbar}{m} R^2(\vec{r})\, \vec{\nabla}\phi(\vec{r})\, .$$

If $\psi(x) = 0$ at some point the current vanishes. Or else we can write the current as

$$j = \frac{\hbar}{2im} \left[\psi^* \psi \left(\frac{1}{\psi} \frac{\partial \psi}{\partial x} \right) - \psi \psi^* \left(\frac{1}{\psi^*} \frac{\partial \psi^*}{\partial x} \right) \right] = . \tag{12}$$

This is clearly equal to

$$\frac{\hbar |\psi|^2}{2im} \left(\frac{\partial \log(\psi)}{\partial x} - \frac{\partial \log(\psi^*)}{\partial x} \right) = \frac{\hbar |\psi|^2}{2im} \frac{\partial \log(\psi/\psi^*)}{\partial x}$$

Substituting the given expression for ψ we have $\log(\psi/\psi^*) = 2i\phi(x)$ and this directly yields the answer.

The current is proportional to the gradient of the phase of the wave function.