Quantenmechanik I
Serie 3

HS 09
Tips!

Exercise 3.1 Wave packet in one dimension

The time dependent Schrödinger equation of a quantum system represented by the wave function $\Psi(t,\vec{x})$ and ruled by the Hamiltonian H is

$$i\hbar\frac{\partial}{\partial t}\Psi(t,\vec{x}) = H\Psi(t,\vec{x}).$$

When the Hamiltonian is time independent, the evolution of the wave function can be obtained by

$$\Psi(t,\vec{x}) = e^{\frac{-i(t-t_0)}{\hbar}H}\Psi(t_0,\vec{x}).$$

Finally, the Hamiltonian of a single particle moving in a time independent potential is given by

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}).$$

a) *Consider the wave function of a single particle in a time independent, one-dimensional potential,*

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x).$$

Prove that we have

$$\frac{d}{dt}\int_{-\infty}^{+\infty}\Psi^*(t,x)\Psi(t,x)dx = 0.$$

Tips:

1. Let us do it for the general case: The Schrödinger equations and its complex conjugate give us an expression for the time derivatives,

$$\frac{\partial}{\partial t}\Psi = -\frac{i}{\hbar}H\Psi \qquad \frac{\partial}{\partial t}\Psi^* = -\frac{i}{\hbar}H\Psi^*$$

b) *Consider a free particle in one dimension,*

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2},$$

with the initial wave function of Gaussian shape

$$\Psi(0,x) = \left(\pi{\Delta_0}^2\right)^{-\frac{1}{4}}\exp\left(\frac{ip_0x}{\hbar}\right)\exp\left(\frac{-x^2}{4{\Delta_0}^2}\right).$$

TYPO in the exercise sheet: $\frac{-x^2}{2{\Delta_0}^2} \rightarrow \frac{-x^2}{4{\Delta_0}^2}$

Show that, at generic instant t, the wave is still a Gaussian, of width

$$\Delta(t) = \Delta_0\sqrt{1+\frac{\hbar^2t^2}{m^2{\Delta_0}^4}}.$$

What happens to the mean position and mean momentum of the particle over time? And to the uncertainty on these quantities?

Tips:

To simplify the notation, let us use $\Delta \equiv \Delta_0$ and $k_0 = p_0/\hbar$,

$$\Psi(0,x) = \left(\pi\Delta^2\right)^{-\frac{1}{4}}\exp\left(ik_0x\right)\exp\left(\frac{-x^2}{4\Delta^2}\right).$$

1. Show the superposition of waves of the form

$$\Psi(t,x) = \int_{-\infty}^{+\infty}A(k)\exp\left(ikx - i\frac{\hbar k^2t}{2m}\right)$$

satisfies the Schrödinger equation of a one-dimensional free particle,

$$i\hbar\frac{\partial}{\partial t}\Psi(t,x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(t,x).$$

2. See that at instant $t = 0$ the wave function becomes

$$\Psi(0, x) = \int_{-\infty}^{+\infty} A(k) \exp(ikx)$$

and calculate the coefficient $A(k)$ via Fourier transform,

$$A(k) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \Psi(0, x) \exp(-ikx)\, dx,$$

using the expression for $\Psi(0, x)$ that is given.

3. Useful little thing:

$$\int_{-\infty}^{+\infty} e^{-ikx} e^{-\frac{x^2}{\alpha}} dx = \frac{\sqrt{\pi\alpha}}{2} \exp\left(\frac{\alpha k^2}{4}\right)$$

4. You will obtain **(I don't think this is the case, but a factor of 2 or $\sqrt{2}$ may be missing)**

$$A(k) = \frac{\sqrt{2}}{2\pi} \left(2\pi\Delta^2\right)^{\frac{1}{4}} \exp\left(-(k - k_0)^2 \Delta^2\right).$$

5. Introduce now the value of $A(k)$ in the expression for $\Psi(t, x)$ and calculate the dreadful integral.

6. Useful not so little thing:

$$\int_{-\infty}^{+\infty} e^{-ikx} e^{Bk} e^{k^2(C+iD)} dk = \frac{\sqrt{\pi}}{2\sqrt{C+iD}} \exp\left(-\frac{(B+ix)^2}{4(C+iD)}\right)$$

7. You will obtain

$$\Psi(t, x) = (2\pi\Delta^2)^{-\frac{1}{4}} \quad \frac{e^{-k_0^2\Delta^2}}{1 + i\hbar t/2m\Delta^2} \quad \exp\left(\frac{-x^2 + 4ik_0\Delta^2 x + 4{k_0}^2\Delta^4}{4L^2(1 + i\hbar t/2mL^2)}\right)$$

8. Play a bit with that expression to show that it has the form of a Gaussian of width (back to the notation Δ_0)

$$\Delta(t) = \Delta_0 \sqrt{1 + \frac{\hbar^2 t^2}{m^2 {\Delta_0}^4}}.$$

9. Now you have to calculate $\langle x \rangle$, $\langle \Delta x \rangle$, $\langle p \rangle$ and $\langle \Delta p \rangle$

c) *Suppose now that the particle feels the influence of a slowly varying potential $V(x)$. How does that affect the previous result?*
Extra challenge!

Exercise 3.2 Hydrogen atom and Rydberg constant

a) *Consider an atom formed by an electron orbiting a single proton. Use the fact that the electron is in a Coulomb potential of the form $U = -ke^2/r$ and Kepler's laws for the motion of classical rigid bodies in such potentials to derive the relation*

$$\nu(E) = \frac{1}{\pi e^2} \sqrt{\frac{2|E|^3}{m}},$$

where ν is the frequency of a given orbital and E the energy associated with that orbital. Recall Bohr's prediction for the energy of each level,

$$E_n = -hR\frac{1}{n^2}.$$

TYPO in the exercise sheet: $\hbar \to h$ *If we further consider Einstein's relation $E = \hbar\nu$, what is the expression for the frequency of the photons emitted when the electrons jumps from the energy level n to the $n - k$ one, in the limit $n \gg 1$? Relate these results to obtain the value of the Rydberg constant,*

$$R = \frac{2\pi^2 me^4}{h^3}.$$

Tips:

1. A bit ahead we will set $k = (4\pi\varepsilon_0) = 1$, by switching to the appropriate unit system. For now let us keep k.
2. We will also assume that the proton as infinite mass, ie., it does not move while the electron orbits it.
3. The potential energy between electron and proton is

$$E = k\frac{e^2}{r}.$$

4. Kepler's third law of planetary motion tells us that the square of the orbital period T of a planet is directly proportional to the cube of the semi-major axis of its orbit, R.
5. This is also true in the case of an electrical potential between two charges. For the general case of a Kepler orbit due to Coulomb forces, we have

$$T^2 = \frac{4\pi^2 m}{ke^2} R^3.$$

6. Now use that to calculate the total energy (kinetic + potential) of the orbital. It simplifies the problem if you consider uniform circular movement. As a challenge, you may try to do it for the general Kepler setting.
7. Now that you know the energy of the orbital, $E(R)$, insert it in Kepler's third law to obtain the expression for the frequency of the electron's orbit. Setting $k = 1$, it is given by

$$\nu_{orbit}(E) = \frac{1}{\pi e^2}\sqrt{\frac{2E^3}{m}}.$$

8. Why are we doing this? Because according to Rutherford's classical theory, the electron loses energy continually by emitting radiation. This radiation is a superposition of monochromatic waves, each of one has frequency $\nu_{orbit}(E)$ ore one of its harmonics.
9. Of course, the electron does not lose energy continually but rather by discrete jumps. What we will see is that, surprisingly, the energy lost in each of this jumps is equivalent to the energy of a photon of frequency $\nu_{orbit}(E)$.
10. Get the energy difference between two levels using Bohr's expression.
11. Obtain an expression for the frequency of a photon emitted when an electron jumps from the nth level to the $n-k$th level.
12. Evaluate the limit for large n and $k = 1$. You do not need to be very careful in the approximations, it is enough to get

$$\nu_{jump} = \frac{2R}{n^3}$$

13. We now say that for very large n this frequency is equivalent to the classical $\nu_{orbit}(E)$. Our justification for this is that the variation of quantum numbers between nearest energy levels is very small, so that the electron loses energy by a succession of many small quantum jumps. From each jump to the next one the energy of the emitted photon does not change much, and the emission spectrum is almost continuous, like in Rutherford's prediction. According to the correspondence principle, in the appropriate limit the quantum properties of a system must resemble the classical ones. We will see that this limit applies here.
14. Consider $\nu_{orbit} \approx \nu_{jump}$ and obtain an expression for the Rydberg constant,

$$R = \frac{2\pi^2 me^4}{h^3}.$$

15. Now the surprising part: the experimental value of R agrees with this naïve prediction - the results differ by less than a part in 10^4 .

b) *Explain why an experiment to observe the trajectory of an electron orbiting the nucleus of a hydrogen atom would not be realisable, without using Heisenberg's uncertainty principle.*
Tips:

1. Suppose you want to detect the electron by scattering with another particle (eg. a photon).
2. Which conditions would you have to impose on this particle in order to achieve resolution of the order of the radius of the atom? (quantify it!)
3. What would happen to an electron hit by a particle fulfilling those conditions?
4. Can you think of another way of following the trajectory of the electron?

Exercise 3.3 Spatial quantisation: the Stern-Gerlach experiment

TYPO in the exercise sheet: "electrons" → "atoms" (you know how the "electrons" key is so close to the "atoms" one in US keyboards....)

a) *Consider an uniform magnetic field* $\vec{B}$ *and the classical Hamiltonian*

$$H = -\vec{\mu} \cdot \vec{B},$$

with $\vec{\mu} = \mu_B \vec{L}$.
Use the classical Poisson bracket formalism to derive the result

$$\dot{\vec{L}} = \mu_B \vec{L} \times \vec{B}.$$

Tips:

1. $\vec{L} = (L_x, L_y, L_z)$ is the classical angular momentum, $\vec{L} = \vec{r} \times \vec{p}$.
2. As you know, the Poisson brackets are defined as

$$\{A, B\} = \sum_k \frac{\partial A}{\partial x_k}\frac{\partial B}{\partial p_k} - \frac{\partial A}{\partial p_k}\frac{\partial B}{\partial x_k}$$

   where $\{x_i\}_i$ are the spatial coordinates, $\{p_i\}_i$ the momentum components and A and B are functions of them.

3. Simple properties of Poisson brackets you might use ahead:

$$\{A + B, Z\} = \{A, Z\} + \{B, Z\}, \qquad \{AB, Z\} = B\{A, Z\} + A\{B, Z\}.$$

4. First you calculate the Poisson brackets of the angular momentum components, obtaining

$$\{L_i, L_j\} = \varepsilon_{ijl} L_l$$

5. Note that $\vec{B}$ is uniform, ie.,

$$\frac{\partial B_i}{\partial x_k} = \frac{\partial B_i}{\partial p_k} = 0, \forall i, k$$

6. Use the equations of motion,

$$\frac{dA}{dt} = \left(\frac{\partial A}{\partial t} - \{H, A\}\right)$$

   to derive an expression for $\dot{L}_i$.

7. Now obtain

$$\dot{\vec{L}} = \mu_B \vec{L} \times \vec{B}.$$

8. You may see that if $\vec{B} = B\hat{z}$, we have $\dot{L}_z = 0$.

b) *Consider now that the electron has to travel through a segment of length* l *along the* $\hat{x}$ *direction, where there is a field* $\vec{B} = B(x, y, z)\hat{z}$.
Using the relation $\vec{F} = -\nabla H$, *derive an expression for the angle between the velocity of the electron as it entered the field and its velocity after being deflected through by the magnetic field.*
What can you conclude about the nature of $\vec{\mu}$*?*

Tips:

1. In this case we have
$$H = -\vec{\mu} \times \vec{B} = -\mu_B L_z B_z.$$

2. Don't forget that L_z is still invariant!

3. Now
$$\vec{F} = -\nabla H = \mu_B \left(L_z \frac{\partial B_z}{\partial x}, L_z \frac{\partial B_z}{\partial y}, L_z \frac{\partial B_z}{\partial z} \right)$$
.

4. Now we are going to make some approximations just to get a qualitative idea of what would happen to particles in such a field. The approximations are:
$$\frac{\partial B_z}{\partial x}; \approx 0 \qquad \frac{\partial B_z}{\partial y}; \approx 0 \qquad \frac{\partial B_z}{\partial z} \approx \text{constant.}$$

5. In this case, we have $\vec{F} = F_z \hat{z} = \mu_z \frac{\partial B_z}{\partial z} \hat{z}$.

6. We want to have a rough idea of the deflection they suffer, so we want to calculate the angle that the velocity of the particles makes with the horizontal.

7. The particles take time $T = l/v_0$ to cross the field.

8. The z-component of velocity after leaving the field is given by
$$v_z = \int_0^T a_z dt = \frac{1}{m} \int_0^T \mu_z \frac{\partial B_z}{\partial z} dt$$

9. You will get
$$v_z = \frac{l}{m v_0} \mu_z \frac{\partial B_z}{\partial z}.$$

10. And then to get the angle do simply
$$\tan \alpha = \frac{v_z}{v_x} = \frac{l}{m {v_0}^2} \mu_z \frac{\partial B_z}{\partial z}$$

11. Conclusion: if the z-component of the magnetic moment of the particles could take any value (this is, this magnetic moment could have any orientation), the angle spectrum would be continuum. As only a limited number of spots are observed on the screen, μ_z can only take certain discrete values.