Quantum Mechanics

Problem Sheet 2 - Time evolution

Basics

1. Time evolution of the expectation value of a time-independent operator.
2. Same as above, but now the operator has a parametric dependence on t. In both problems, use Schrödinger equation to find the time derivative of the expectation value.
3. Definition of the exponential of an operator. Useful to practice elementary manipulations involving operators and wave functions.
4. Some properties of the momentum operator. Try to get familiar with the momentum operator, and its action of wave functions. It will reappear very frequently in the rest of the course!
5. Time-evolution of the two-state system.
6. Energy eigenstates for the infinite potential well. Properties of the eigenfunctions.
7. Action of the momentum and position operators in momentum space.

Further problems

1. A box partitioned in two, with a finite probability for tunnelling through the partition, is described as a two-state system.
2. A simple quantum mechanical model for an ideal gas. The ideal gas law is derived by combining the energy levels of the quantum system with some elementary thermodynamics.
3. The Feynman-Hellmann theorem yields the variation of expectation values with respect to external parameters.
4. Constant shift in the potential energy.
5. A first look at the probability current.

Basics

1. Consider an operator $\hat{f}$ such that

$$\left[\hat{f}, \hat{H}\right] = 0\,, \tag{1}$$

show that the expectation value $\langle \hat{f} \rangle$ is a constant for any wave function $\Psi(x,t)$.

Note that the operator does not have an explicit dependence on time, and therefore the time dependence is entirely due to the fact that the wave function evolves according to Schrödinger equation.

2. Let us consider an operator $\hat{O}(t)$ corresponding to some observable, where we have considered now the possibility of having a parametric dependence on time t. The expectation value of $\hat{O}(t)$ will evolve with time:

$$\langle \hat{O}(t) \rangle = \langle \Psi(t) | \hat{O}(t) | \Psi(t) \rangle\,. \tag{2}$$

The time evolution is due to *both* the parametric dependence on t, and the fact that the wave function evolves in time.
Show that the expectation value in Eq. (2) evolves according to:

$$\frac{d}{dt}\langle \hat{O}(t) \rangle = \langle \Psi(t) | \left(\frac{\partial}{\partial t}\hat{O}(t) + \frac{1}{i\hbar}\left[\hat{O}, \hat{H}\right] \right) | \Psi(t) \rangle\,. \tag{3}$$

3. The time-evolution operator $\hat{U}(t) = \exp\left[-i\hat{H}t/\hbar\right]$ is defined via the Taylor expansion of the exponential:

$$\hat{U}(t) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{-i}{\hbar}\right)^n \hat{H}^n t^n\,. \tag{4}$$

If $|\psi\rangle$ is an eigenstate of $\hat{H}$ with eigenvalue E, show that

$$\hat{U}(t)|\psi\rangle = e^{-iEt/\hbar}|\psi\rangle\,. \tag{5}$$

4. Using the fact that $\hat{P} = -i\hbar\frac{d}{dx}$, compute:

$$\hat{P}\hat{X}^n\psi(x) \tag{6}$$

$$\hat{X}^n\hat{P}\psi(x)\,. \tag{7}$$

Deduce that

$$\left[\hat{P}, \hat{X}^n\right] = -i\hbar n\hat{X}^{n-1}\,. \tag{8}$$

The operator $\hat{V} = V(\hat{X})$ is defined via the Taylor expansion of the function V

$$\hat{V} = V(\hat{X}) = \sum_k \frac{1}{k!}V^{(k)}(0)\hat{X}^k \tag{9}$$

where $V^{(k)}(0)$ are the coefficients of the expansion, i.e. they are numbers computed by evaluating the k-th derivative of the function V at $x = 0$. Show that

$$\left[\hat{P}, \hat{V}\right] = -i\hbar\frac{d}{dx}V(\hat{X})\,. \tag{10}$$

5. Consider the two-state system described in **B**6 in problem sheet 1. At $t = 0$ the system is in the state:

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}|1\rangle + \frac{i}{\sqrt{2}}|2\rangle\,. \tag{11}$$

Determine the probability $P_1(t)$ that the system is found in the state $|1\rangle$ at time t. Make a sketch of the function $P_1(t)$.

6. Consider a particle in an infinite potential well:

$$V(x) = \begin{cases} 0, & \text{for}|x| < a\,, \\ \infty, & \text{otherwise}\,. \end{cases} \tag{12}$$

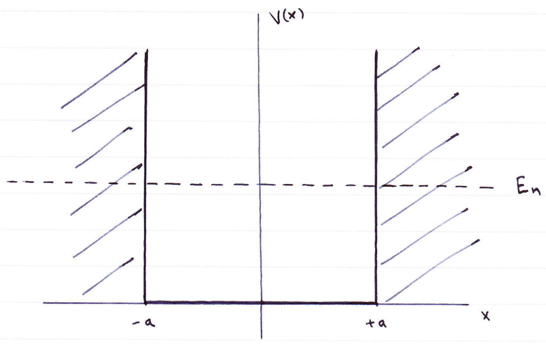

Figure 1: Infinite well potential described of size $2a$.

Physically this potential confines the particle to the region $|x| < a$, and therefore its wave function must vanish identically outside this region. Hence the solution of the Schrödinger equation must satisfy the boundary condition:

$$\psi(-a) = \psi(a) = 0\,. \tag{13}$$

Verify that the wave function

$$\psi(x,t) = \begin{cases} A\sin\left[\frac{\pi x}{a}\right] e^{-iEt/\hbar} & \text{if } -a < x < a\,, \\ 0 & \text{if } |x| > a \end{cases} \tag{14}$$

is a solution to the Schrödinger equation. Calculate the energy of this first excited state and the probability density P(x) to find the particle at a given x. Does P(x) differ from the corresponding result in classical mechanics?

Find all the energy eigenstates for this system.

Check the number of nodes (i.e. zeroes of the wave function) for the first three energy eigenstates.

7. The momentum space wave function can be defined as:

$$\tilde{\psi}(p) = \int dx e^{-ipx/\hbar}\psi(x)\,. \tag{15}$$

A generic operator $\hat{O}$ acts on $\psi(p)$ according:

$$\hat{O}\psi(p) = \int dx e^{-ipx/\hbar} \hat{O}\psi(x) \,. \tag{16}$$

Find the action of the momentum operator $\hat{P}$, and the position operator $\hat{X}$ on $\tilde{\psi}(p)$. Check that this new representation of $\hat{X}$ and $\hat{P}$ satisfies the canonical commutation relation.

Further problems

1. A box containing a particle is divided into a left and a right compartment by a thin partition. Suppose that the amplitude for particle being on the left side of the box is $\Psi_1(x,t)$ and the amplitude for being on the right side of the box is $\Psi_2(x,t)$. We will neglect the spatial dependence of the wave functions inside the two halves of the box. Suppose that the particle can tunnel through the partition, and that the rate of change of the amplitude on the right is $K/(i\hbar)$ times the amplitude on the left, where K is real:
$$i\hbar \frac{d}{dt}\Psi_2(t) = K\Psi_1(t)\,. \tag{17}$$
What is the equation of motion for Ψ_1? Write the Hamiltonian for this system.

2. Consider now a gas of quantum particles in a box of size a. We can model this system as a set of N particles in an infinite well. Note that compared to **B**6, here the size of the well is a and not $2a$!

   The possible values for the energy levels are:
$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2 = An^2\,, \tag{18}$$
write down the expression for A.

   Let us now compress the box, so that the size shrinks from a to $a-\delta a$. Show that the energy variation is:
$$E_n(a-\delta a) - E_n(a) = \frac{\hbar\pi^2 n^2}{ma^3}\delta a + \mathcal{O}(\delta a^2)\,. \tag{19}$$
The pressure P exerted by the particle on the wall is defined as:
$$\delta E_n = P\delta a\,. \tag{20}$$
Show that the pressure is: $P = (2/a)E_n$.

   For a gas in equilibrium at temperature T, the energy distribution is given by the Boltzmann distribution:
$$P_n \propto e^{-E_n/kT}\,, \tag{21}$$
where k is the Boltzmann constant.

   Write down the expression for the mean value of the energy.

   Evalutate the mean value in the limits $A/(kT) \to 0$, and $kT \to 0$.

   If we neglect their interactions, the total energy of a gas of N particles is simply $U = N\langle E\rangle$. Compute the total energy in the two limits above, and the total pressure in the box in the limit where $A/(kT) \to 0$.

3. *Feynman-Hellman theorem.* Let us consider a system where the potential depends on an external parameter g, $\hat{V} = V(\hat{X}, g)$. Show that for the energy eigenvalues we have:
$$\frac{\partial E_n}{\partial g} = \langle \psi_n | \frac{\partial V}{\partial g} | \psi_n \rangle\,. \tag{22}$$
Remember that the eigenfunctions also depend on g!

4. Show that the eigenfunctions of the time-independent Schrödinger are unchanged if the potential is shifted by an arbitrary constant V_0. What does happen to the eigenvalues? What is the physical interpretation of this result? Does it have a classical analogue?

5. Show that for a stationary state, the current:

$$j(x) = \frac{\hbar}{2mi} \left(\Psi(x,t)^* \left(\frac{\partial}{\partial x} \Psi(x,t) \right) - \left(\frac{\partial}{\partial x} \Psi(x,t)^* \right) \Psi(x,t) \right)$$

is independent of both x and t.