QUANTUM MECHANICS I A (FYSA231), spring 2010

Exercise 2.

1. a) Linear operator $\hat{A}$ fulfills the following relation:

$$\hat{A}(c_1\psi_1 + c_2\psi_2) = c_1\hat{A}\psi_1 + c_2\hat{A}\psi_2$$

where c_1 and c_2 are arbitrary complex constants and ψ_1 are ψ_2 are arbitrary wave functions. Check which of the operators defined by the following relations are linear:

$$\hat{A}_1\psi(x) = x^3\psi(x),\ \hat{A}_2\psi(x) = x\frac{d}{dx}\psi(x)$$

$$\hat{A}_3\psi(x) = \frac{d}{dx}\psi(x) + a,\ \hat{A}_4\psi(x) = \int_{-\infty}^{x} dx'[\psi(x')x']$$

b) Show that arbitrary operators $\hat{A}$, $\hat{B}$ and $\hat{C}$ fulfills the following commutator relations

$[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$.

ii) $[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$.

iii) $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$.

2. a) An arbitrary state describing one dimensional movement is $\psi(t, x)$ and the expectation value for the momentum operator is

$$\langle\hat{p}\rangle = \int_{-\infty}^{\infty} \psi^*(t, x)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(t, x)dx.$$

Make partial integration. As a result you should get the definition of Hermitian operator (integral) and another term. State that this term must be zero, so that $\hat{p}$ is Hermitian. This result means common boundary condition for the wave functions – what is this? Note that imaginary i is necessary for the Hermicity.

b) Quantum mechanical equation of motion is time depended Schrödinger's equation

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

where $\hat{H}$ is energy operator or Hamilton's operator. H is Hermitian operator – why? Total probability, which is usually normalized to 1, is $\int \psi^*(t, \vec{x})\psi(t, \vec{x})d^3\vec{x}$ (integrated over the whole space). Assume in the beginning that integral is not necessarily constant in time. Show by using Schrödinger's equation that:

$$\frac{\partial}{\partial t}\int \psi^*(t, \vec{x})\psi(t, \vec{x})d^3\vec{x} = 0.$$

3. Particle that has been restricted in the area $|x| \leq a$ is described by the wave function

$$\psi(x) = N \cos\left(\frac{x\pi}{2a}\right),$$

where N is the normalization constant.

a) Calculate the value of N. Is this value unambiguous?

b) What is the probability that the particle is in the area between $0 \leq x \leq a$.

c) What is the probability that the particle is in the area between $-a/2 \leq x \leq a/2$.

4. Solve the infinitely deep potential well (wave function and energy levels), when potential V(x) is defined in the following way:

$$V(x) = \begin{cases} 0, \; if \; -a \leq x \leq a \\ \infty, \; otherwise \end{cases} .$$

Notice that now you have to solve even and odd states separately. Otherwise this calculation follows the example at the lectures.

5. Normalized wave function of the ground state of the hydrogen atom is

$$\psi(\vec{r}) = (\pi a_0^3)^{-1/2} e^{-r/a_0},$$

where $a_0 = 0.0529$ nm.

a) Calculate the probability that the electron is inside a sphere with radius a_0. Integrate numerically by using calculator or computer.

b) Calculate the expectation value of r.