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## Quantum Mechanics

## Homework Assignment 09

Fall, 2019

- 1. [C-T Exercise 3-4] Consider a free particle in one dimension.
  - (a) Show, applying Ehrenfest's theorem, that  $\langle \hat{x} \rangle$  is a linear function of time, the mean value  $\langle \hat{p}_x \rangle$  remaining constant.
  - (b) Write the equations of motion for the mean values  $\langle \hat{x}^2 \rangle$  and  $\langle \hat{x}\hat{p}_x + \hat{p}_x\hat{x} \rangle$ . Integrate these equations.
  - (c) Show that, with a suitable choice of the time origin, the root-mean square deviation  $\Delta x$  is given by

$$(\Delta x)^2 = \frac{1}{m^2} (\Delta p_x)_0^2 t^2 + (\Delta x)_0^2,$$

where  $(\Delta x)_0$  and  $(\Delta p_x)_0$  are the root-mean-square deviations at the initial time.

How does the width of the wave packet vary as a function of time? Give a physical interpretation.

- 2. [C-T Exercise 3-5] In a one-dimensional problem, consider a particle of potential energy  $\hat{V}(\hat{x}) = -f\hat{x}$ , where f is a positive constant  $[\hat{V}(\hat{x})]$  arises, for example, from a gravity field or a uniform electric field.
  - (a) Write Ehrenfest's theorem for the mean values of the position  $\hat{x}$  and the momentum  $\hat{p}_x$  of the particle. Integrate these equations; compare with the classical motion.
  - (b) Show that the root-mean-square deviation  $\Delta p_x$  does not vary over time.
  - (c) Write the Schrödinger equation in the  $\{|p_x\rangle\}$  representation. Deduce from it a relation between  $\frac{\partial}{\partial t} |\langle p_x | \psi(t) \rangle|^2$  and  $\frac{\partial}{\partial p_x} |\langle p_x | \psi(t) \rangle|^2$ . Integrate the equation thus obtained; give a physical interpretation.
- 3. [C-T Exercise 3-9] One wants to show that the physical state of a (spinless) particle is completely defined by specifying the probability density  $\rho(\vec{r}) = |\psi(\vec{r})|^2$  and the probability current  $\vec{J}(\vec{r})$ .
  - (a) Assume the function  $\psi(\vec{r})$  known and let  $\xi(\vec{r})$  be its argument,  $\psi(\vec{r}) = \sqrt{\rho(\vec{r})} e^{i\xi(\vec{r})}$ . Show that

$$\vec{J}(\vec{r}) = \frac{\hbar}{m} \rho(\vec{r}) \vec{\nabla} \xi(\vec{r}).$$

Deduce that two wave functions leading to the same density  $\rho(\vec{r})$  and current  $\vec{J}(\vec{r})$  can differ only by a global phase factor.

- (b) Given arbitrary functions  $\rho(\vec{r})$  and  $\vec{J}(\vec{r})$ , show that a quantum state  $\psi(\vec{r})$  can be associated with them only if  $\nabla \times \vec{v}(\vec{r}) = 0$ , where  $\vec{v}(\vec{r}) = \vec{J}(\vec{r})/\rho(\vec{r})$  is the velocity associated with the probability fluid.
- (c) Now assume that the particle is submitted to a magnetic field  $\vec{B}(\vec{r}) = \vec{\nabla} \times \vec{A}(\vec{r})$ . Show that

$$\begin{split} \vec{J}(\vec{r}) &= \frac{\rho(\vec{r}\,)}{m} \big[\,\hbar\vec{\nabla}\xi(\vec{r}\,) - q\vec{A}(\vec{r}\,)\,\big], \\ \vec{\nabla}\times\vec{v}(\vec{r}\,) &= -\frac{q}{m}\vec{B}(\vec{r}\,). \end{split}$$

- 4. [C-T Exercise 3-16] Consider a physical system formed by two particles (1) and (2), of the same mass m, which do not interact with each other and which are both placed in an infinite potential well of width a. Denote by  $\hat{H}(1)$  and  $\hat{H}(2)$  the Hamiltonians of each of the two particles and by  $|\varphi_n(1)\rangle$  and  $|\varphi_q(2)\rangle$  the corresponding eigenstates of the first and second particle, of energies  $n^2\pi^2\hbar^2/2ma^2$  and  $q^2\pi^2\hbar^2/2ma^2$ . In the state space of the global system, the basis chosen is composed of the states  $|\varphi_n\varphi_q\rangle$  defined by  $|\varphi_n\varphi_q\rangle = |\varphi_n(1)\rangle \otimes |\varphi_q(2)\rangle$ .
  - (a) What are the eigenstates and the eigenvalues of the operator  $\hat{H} = \hat{H}(1) + \hat{H}(2)$ , the total Hamiltonian of the system? Give the degree of degeneracy of the two lowest energy levels.
  - (b) Assume that the system, at time t = 0, is in the state

$$|\psi(0)\rangle = \frac{1}{\sqrt{6}} |\varphi_1\varphi_1\rangle + \frac{1}{\sqrt{3}} |\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{6}} |\varphi_2\varphi_1\rangle + \frac{1}{\sqrt{3}} |\varphi_2\varphi_2\rangle.$$

- i. What is the state of the system at time t?
- ii. The total energy  $\hat{H}$  is measured. What results can be found, and with what probabilities?
- iii. Same questions if, instead of measuring  $\hat{H}$ , one measures  $\hat{H}(1)$ .
- (c) i. Show that  $|\psi(0)\rangle$  is a tensor product state. When the system is in this state, calculate the following mean values:  $\langle \hat{H}(1)\rangle, \langle \hat{H}(2)\rangle$  and  $\langle \hat{H}(1)\hat{H}(2)\rangle$ . Compare  $\langle \hat{H}(1)\rangle\langle \hat{H}(2)\rangle$  with  $\langle \hat{H}(1)\hat{H}(2)\rangle$ ; how can this result be explained?
  - ii. Show that the preceding results remain valid when the state of the system is the state  $|\psi(t)\rangle$  calculated in (b).
- (d) Now assume that the state  $|\psi(0)\rangle$  is given by

$$|\psi(0)\rangle = \frac{1}{\sqrt{5}} |\varphi_1\varphi_1\rangle + \sqrt{\frac{3}{5}} |\varphi_1\varphi_2\rangle + \frac{1}{\sqrt{5}} |\varphi_2\varphi_1\rangle.$$

- i. Show that  $|\psi(0)\rangle$  cannot be put in the form of a tensor product. When the system is in this state, calculate the following mean values:  $\langle \hat{H}(1) \rangle$ ,  $\langle \hat{H}(2) \rangle$  and  $\langle \hat{H}(1) \hat{H}(2) \rangle$ . Compare  $\langle \hat{H}(1) \rangle \langle \hat{H}(2) \rangle$  with  $\langle \hat{H}(1) \hat{H}(2) \rangle$ ; how can this result be explained?
- ii. Show that the preceding results remain valid when the state of the system is the state  $|\psi(t)\rangle$  derived from the above-given  $|\psi(0)\rangle$ .
- (e) Write the matrix, in the basis of the vectors  $|\varphi_n\varphi_q\rangle$ , which represents the density matrix  $\rho(0)$  corresponding to the ket  $|\psi(0)\rangle$  given in (b). What is the density matrix  $\rho(t)$  at time t? Calculate, at the instant t=0, the partial traces  $\rho(1) = \text{Tr}_2 \rho$  and  $\rho(2) = \text{Tr}_1 \rho$ . Do the density operators  $\rho$ ,  $\rho(1)$  and  $\rho(2)$  describe pure states? Compare  $\rho$  with  $\rho(1) \otimes \rho(2)$ ; what is your interpretation?
- 5. [C-T Exercise 3-17] Let  $\hat{\rho}$  be the density operator of an arbitrary system, where  $|\chi_{\ell}\rangle$  and  $\pi_{\ell}$  are the eigenvectors and eigenvalues of  $\hat{\rho}$ . Write  $\hat{\rho}$  and  $\hat{\rho}^2$  in terms of the  $|\chi_{\ell}\rangle$  and  $\pi_{\ell}$ . What do the matrices representing these two operators in the  $\{|\chi_{\ell}\rangle\}$  basis look like first, in the case where  $\hat{\rho}$  describes a pure state and then, in the case of a statistical mixture of states? (Begin by showing that, in a pure case,  $\hat{\rho}$  has only one non-zero diagonal element, equal to 1, while for a statistical mixture,  $\hat{\rho}$  has several diagonal elements included between 0 and 1.) Show that  $\hat{\rho}$  corresponds to a pure case if and only if the trace of  $\hat{\rho}^2$  is equal to 1.