IF/UFRJ
Graduate Quantum Mechanics I
2023/2 – Raimundo

Problem Set #5

4/8/2023 - due by 11/8/2023 at 12:00 noon

1. *Optional.* Consider a particle of mass m subject to the potential

$$V(x) = \begin{cases} 0, & \text{if} \quad 0 \leq x \leq a \\ +\infty, & \text{if} \quad x < 0 \text{ or } x > a. \end{cases}$$

   Let $|\varphi_n\rangle$ be the eigenstates of the Hamiltonian $\mathcal{H}$ of the system, where n is a positive integer. Suppose that the state of the particle at time $t = 0$ is given by

$$|\psi(0)\rangle = a_1|\varphi_1\rangle + a_2|\varphi_2\rangle + a_3|\varphi_3\rangle + a_4|\varphi_4\rangle$$

   (a) From the boundary conditions (on the wave functions) alone, show that the energy levels are given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2},$$

   (b) When the energy of the particle is measured in the state $|\psi(0)\rangle$, what is the probability of finding a value smaller than $3\pi^2\hbar^2/ma^2$?

   (c) What are the mean value and the root-mean-square deviation of the energy of the particle in the state $|\psi(0)\rangle$?

   (d) Calculate the state vector $|\psi(t)\rangle$ at the instant t. Do the results found in (b) and (c) at $t = 0$ remain valid at an arbitrary t?

   (e) Suppose that when the energy is measured, the result $8\pi^2\hbar^2/ma^2$ is found. What is the state of the system after the measurement is made? What is the result if the energy is measured again?

2. (a) Use Ehrenfest's theorem to obtain the explicit time evolution of the width of a free packet; the mass of the particle is m and the wave function at $t = 0$ is assumed to be known.

(b) Apply your result to the function

$$\psi(x, t=0) = \frac{1}{(\sigma^2\pi)^{1/4}}\, e^{-x^2/2\sigma^2}\, \mathrm{e}^{ik_0 x}, \tag{1}$$

where σ and k_0 are constants. Comment on your results.

3. Consider a particle of mass m and charge q, moving along the x-axis, subject to a uniform electric field, $\mathbf{E} = E_0\,\hat{\mathbf{x}}$.

   (a) Integrate the Heisenberg equation of motion for the linear momentum operator, P.

   (b) From (a) determine an operator $\Pi_H(P)$ such that $d\,\Pi_H/dt \equiv 0$, where the subscript H denotes 'Heisenberg picture'.

   (c) Show that
   $$\mathrm{e}^{i\,\Pi_H a/\hbar} X \mathrm{e}^{-i\,\Pi_H a/\hbar} = X + a,$$
   with a a constant. Interpret physically.

4. Consider a free particle of mass m, and an operator

$$G_H = mX_H - P_H t, \tag{1}$$

where X_H and P_H are, respectively, the position and momentum operators in Heisenberg's picture, and t is the time.

   (a) Integrate the equation of motion for G_H. Interpret your result.

   (b) Calculate $[G_H, X_H]$ and $[G_H, P_H]$.

   (c) Consider now the operator

$$W \equiv \mathbb{1} - \frac{i}{\hbar}\, G_H\, \delta v, \tag{2}$$

   where $\mathbb{1}$ is the identity operator, and δv is a parameter with dimension of velocity, which can be considered small in the relevant scales of the problem. Obtain an expression for $\widetilde{X}_H = W^\dagger X_H W$, to first order in δv. Interpret your result.

5. In some systems, like in the KH_2PO_4 crystal, the hydrogen atom (H) may occupy either side of a double potential well (see Fig. 1); denote these states by $|L\rangle$ and $|R\rangle$, for left and right wells, respectively. The middle barrier is sufficiently small, so that the H atom may tunnel between these two positions.

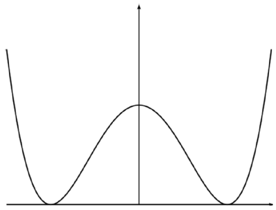

Figure 1: Problem 5 – Schematic representation of the potential felt by the H atom, in terms of a generalised coordinate.

The motion of the H atom in this double well may therefore be approximately described by the Hamiltonian

$$\mathcal{H} = \frac{\hbar\Omega}{2}\Big[|L\rangle\langle R| + |R\rangle\langle L|\Big], \tag{1}$$

where Ω is a constant.

(a) Express $\mathcal{H}$ in terms of Pauli matrices; use the representation in which σ^z is diagonal. Can you identify $|L\rangle$ and $|R\rangle$ as eigenvectors of one of the Pauli matrices? Comment.

(b) Write down the eigenvalues and eigenvectors of $\mathcal{H}$ in terms of $|L\rangle$ and $|R\rangle$.

(c) Write down the Heisenberg equations of motion for σ^z and σ^y.

(d) Integrate the Heisenberg equation of motion for σ^z.

(e) Suppose the H atom is on the left well at $t = 0$. Using explicitly your result from (d), write down the time dependence of the average value $\langle\sigma^z\rangle_t$.

(f) What is the physical interpretation of Ω?

6. The Hamiltonian for a one-dimensional quantum harmonic oscillator, of mass m and frequency ω, is

$$\mathcal{H} = \frac{1}{2m}P^2 + \frac{1}{2}m\omega^2 X^2. \tag{1}$$

(a) Integrate the Heisenberg equations of motion for X and P.

(b) From (a) write down the time dependence of the average values $\langle X\rangle_t$, $\langle P\rangle_t$ and $\langle X^2\rangle_t$. Suppose the initial wave function $\psi(x, t = 0)$ is known, so that it is legitimate to express these average values, and any others, in terms of the initial conditions $\langle\ldots\rangle_0$, whenever necessary.

(c) Show that when the wave function $\psi(x, t = 0)$ is even, one has $\langle X\rangle_0 = \langle P\rangle_0 = 0$. In addition, show that if the wave function is real, then $\langle XP + PX\rangle_0 = 0$.

(d) The harmonic oscillator eigenfunctions are of the form

$$\varphi_n(x) = A_n H_n(x)\ \mathrm{e}^{-(m\omega/2\hbar)\ x^2}, \tag{2}$$

where A_n is a normalisation constant, and $H_n(x)$ is a Hermite polynomial of degree n in x, and parity $(-1)^n$; for the ground state, in particular, one has $A_0 = (m\omega/\pi\hbar)^{1/4}$ and $H_0 = 1$. Assuming $\psi(x, t = 0) = \varphi_n(x)$, with n even, determine $\langle X \rangle_t$ and $\langle P \rangle_t$. Do these expectation values follow the classical trajectory? Comment.

(e) Evaluate the dispersion in position, $(\Delta X)_t^2 \equiv \langle (X^2 - \langle X \rangle^2) \rangle_t$, for $\psi(x, t = 0) = \varphi_0(x)$. Discuss the behaviour of the dispersion in position at short times, i.e., $t \ll 1/\omega$ Comment.