Quantum Mechanics 3 (Physics 4386)

First Assignment

Due: Wednesday, October 7, 2020

Dr. J. Sirker

29 September 2020

1. The Ehrenfest theorem and the classical limit (8 points)

In the lecture we have derived the Ehrenfest theorem

$$\frac{d\langle\vec{p}\rangle}{dt} = -\langle\nabla V(\vec{r})\rangle\,. \tag{1}$$

This equation is different from the classical equation of motion

$$\frac{d\langle\vec{p}\rangle}{dt} = -\nabla V(\vec{r})\,|_{\vec{r}=\langle\vec{r}\rangle} \tag{2}$$

because, in general, $\langle\nabla V(\vec{r})\rangle \neq \nabla V(\vec{r})\,|_{\vec{r}=\langle\vec{r}\rangle}$.

We want to consider in the following the validity of the classical approximation (2) and investigate the size of the quantum corrections. We restrict the discussion to one dimension where Eq. (1) simplifies to

$$\frac{d\langle p\rangle}{dt} = -\left\langle\frac{\partial V}{\partial x}\right\rangle\,. \tag{3}$$

Taylor expand $f(x) = -\frac{\partial V}{\partial x}$ around $x = \langle x\rangle$ to obtain an estimate for the quantum corrections. In which case does the classical approximation (2) for the expectation value—also restricted to one dimension—become exact?

2. The particle in a box using matrix methods (20 points)

Consider a free particle moving in the following one-dimension potential

$$V(x) = \begin{cases} \infty, & x < 0 \\ 0, & 0 \leq x \leq a \\ \infty, & x > a \end{cases}$$

a) (5 pts) Write the Hamiltonian in matrix form using a discretized position representation. Write a small computer program to calculate the lowest 5 eigenvalues and eigenstates by solving the discretized stationary Schroedinger equation. Plot the eigenstates.

b) (8 pts) Write the position operators $\hat{x}$ and $\hat{x}^2$ in matrix form and use the program to calculate $\langle\Psi_0(x)|\hat{x}|\Psi_0(x)\rangle$, $\langle\Psi_0(x)|\hat{x}^2|\Psi_0(x)\rangle$, as well as the variance $\Delta x = \sqrt{\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2}$ for the lowest eigenstate (ground state) $\Psi_0(x)$. Compare the results with the analytical results obtained by solving the Schroedinger equation directly.

c) (7 pts) Write the momentum operators $\hat{p}$ and $\hat{p}^2$ in matrix form and use the program to calculate $\langle\Psi_0(x)|\hat{p}|\Psi_0(x)\rangle$, $\langle\Psi_0(x)|\hat{p}^2|\Psi_0(x)\rangle$, as well as the variance $\Delta p = \sqrt{\langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2}$ for the lowest eigenstate (ground state) $\Psi_0(x)$. Compare the results with the analytical results obtained by solving the Schroedinger equation directly.

3. A three-dimensional problem (16 points)

Consider a potential $V(\vec{r})$ which can be written as a sum of three functions

$$V(\vec{r}) = V_1(x_1) + V_2(x_2) + V_3(x_3) \tag{4}$$

of the position vector $\vec{r} = (x_1, x_2, x_3)$.

a) (6 pts) Show that the three-dimensional stationary Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}\right) + V(\vec{r})\right]\Psi(\vec{r}) = E\Psi(\vec{r}) \tag{5}$$

is solved by the ansatz $\Psi(\vec{r}) = \psi_1(x_1)\psi_2(x_2)\psi_3(x_3)$ if the ψ_i fulfill the one-dimensional Schrödinger equation

$$-\frac{\hbar^2}{2m}\psi_i''(x_i) = [E_i - V(x_i)]\psi_i(x_i) \tag{6}$$

with eigenvalues

$$E = E_1 + E_2 + E_3 \,. \tag{7}$$

b) (6 pts) Consider now a particle moving in a three-dimensional box

$$V(x_i) = \begin{cases} 0 & ,0 \le x_i \le L_i \\ \infty & ,\text{else.} \end{cases} \tag{8}$$

Determine the eigenfunctions and eigenvalues of (5) using the one-dimensional solution. (*Note*: the solutions depend on three quantum numbers n_1, n_2, n_3; $n_i = 1, 2, 3, \cdots$.)

c) (4 pts) Calculate the the degeneracy of states with total quantum number $n^2 = \sum_{i=1}^{3} n_i^2 = 3$ and $n^2 = 6$.

4. Commutators (16 points)

Linear operators acting on the Hilbert space usually do not commute and

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{9}$$

is, in general, different from zero.

We want to summarize and proof some useful relations here.

a) (4 pts) Show that for operators $\hat{A}$, $\hat{B}$, $\hat{C}$ and a complex number α

$$\begin{aligned} [\alpha\hat{A}, \hat{B}] &= \alpha[\hat{A}, \hat{B}], \qquad [\hat{A} + \hat{B}, \hat{C}] = [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}] \\ [\hat{A}\hat{B}, \hat{C}] &= \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}. \end{aligned} \tag{10}$$

b) (6 pts) If $\hat{A}$ commutes with $[\hat{A}, \hat{B}]$, i.e., $[\hat{A}, [\hat{A}, \hat{B}]] = 0$, then $[\hat{A}^2, \hat{B}] = \hat{A}[\hat{A}, \hat{B}] + [\hat{A}, \hat{B}]\hat{A}$ can be simplified to $[\hat{A}^2, \hat{B}] = 2\hat{A}[\hat{A}, \hat{B}]$. Show by induction that for a polynomial $p(\hat{A})$ the following relation holds

$$[p(\hat{A}), \hat{B}] = p'(\hat{A})[\hat{A}, \hat{B}] \qquad \text{if } [\hat{A}, [\hat{A}, \hat{B}]] = 0\,. \tag{11}$$

Here $p'(x) = \frac{dp}{dx}$ is the derivative of $p(x)$.

c) (6 pts) Considering the polynomial in b) as part of a series in $\hat{A}$ we can also use this commutator relation for differentiable functions $f(\hat{A})$ instead of $p(\hat{A})$ (assuming convergence). Proof that

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] \qquad \text{if } [\hat{A}, [\hat{A}, \hat{B}]] = 0. \tag{12}$$