Exercises 18.05.2017: Questions

Problem 1

Calculate the following commutators:

a) $\left[\hat{H}, \hat{\mathbf{p}}\right]$,

b) $\left[\hat{H}, \hat{\mathbf{r}}\right]$,

where

$$\hat{H} = \frac{1}{2m}\hat{\mathbf{p}}^2 + V(\hat{\mathbf{r}}), \tag{1}$$

$\hat{\mathbf{p}}^2 = \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2$ and $V(\hat{\mathbf{r}}) = V(\hat{x}, \hat{y}, \hat{z})$ is an arbitrary good function.

Hint 1

First solve the problem 3 of the file "Exercises_11.05.2017".

Problem 2

Let $\hat{H}$ be the Hamiltonian of a system. Suppose that $\hat{H}$ has a degenerate eigenvalue E,

$$\hat{H}\psi_\alpha = E\psi_\alpha, \qquad (\alpha = 1, 2, \ldots, D), \tag{2}$$

where D is the degree of degeneracy of the energetic level E, that is D is the dimensionality of the subspace spanned by $\{\psi_\alpha\}$ and corresponding to the eigenvalue E. Let

$$\varphi_\beta = \sum_{\alpha=1}^{D} a_{\beta\alpha}\psi_\alpha, \qquad (\beta = 1, 2, \ldots, D), \tag{3}$$

be an *arbitrary* linear combination of the eigenfunctions ψ_α belonging to the *same* degenerate subspace of dimension D. It is evident that the functions φ_β are still eigenfunctions of $\hat{H}$ with the same eigenvalue E, namely

$$\begin{aligned}\hat{H}\varphi_\beta &= \sum_{\alpha=1}^{D} a_{\beta\alpha}\left(\hat{H}\psi_\alpha\right) \\ &= E\sum_{\alpha=1}^{D} a_{\beta\alpha}\psi_\alpha \\ &= E\varphi_\beta.\end{aligned} \tag{4}$$

Prove that it is possible to choose the set of new eigenfunctions $\{\varphi_\beta\}$ such that they are *orthonormal*, namely

$$\int \varphi_\alpha^*(q)\varphi_\beta(q)\,dq = \delta_{\alpha\beta}, \tag{5}$$

and that this can be done in infinitely many different ways.

Hint 2

Calculate the number of independent coefficients of the linear transformation $\psi_\alpha \to \varphi_\beta$, and the number of constraints implied by the orthonormality condition (5).

Problem 3

The probability density

$$\rho(\mathbf{r},t) \equiv |\psi(\mathbf{r},t)|^2\,, \tag{6}$$

and the probability current

$$\mathbf{j}(\mathbf{r},t) \equiv \frac{\hbar}{2m\,i}\big[\psi^*(\mathbf{r},t)\boldsymbol{\nabla}\psi(\mathbf{r},t) - \psi(\mathbf{r},t)\boldsymbol{\nabla}\psi^*(\mathbf{r},t)\big], \tag{7}$$

satisfy the *continuity equation*

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{j} = 0. \tag{8}$$

Calculate $\rho(\mathbf{r},t)$ and $\mathbf{j}(\mathbf{r},t)$ for

$$\psi(\mathbf{r},t) = A\exp\left(i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar} - i\frac{Et}{\hbar}\right) + B\exp\left(-i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar} - i\frac{Et}{\hbar}\right), \tag{9}$$

where

$$E = \frac{\mathbf{p}\cdot\mathbf{p}}{2m}, \tag{10}$$

and $A, B \in \mathbb{C}$. Verify that $\psi(\mathbf{r},t)$ satisfy Schrödinger's equation, check that $\rho(\mathbf{r},t)$ and $\mathbf{j}(\mathbf{r},t)$ fulfill the continuity equation (8) and discuss the results.

Solution 3

The wave function (9) is factorable in the product of a spatially-dependent function $f(\mathbf{r})$ and a time-dependent function $T(t)$, that is

$$\begin{aligned}\psi(\mathbf{r},t) &= \left[A\exp\left(i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right) + B\exp\left(-i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right)\right]\exp\left(-iEt/\hbar\right)\\ &\equiv f(\mathbf{r})T(t).\end{aligned} \tag{11}$$

Since

$$|T(t)|^2 = 1, \tag{12}$$

then the probability density $\rho(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2 = |f(\mathbf{r})|^2$ is automatically time independent and, therefore,

$$\frac{\partial \rho}{\partial t} = 0. \tag{13}$$

It is easy to see that $\psi(\mathbf{r}, t)$ satisfies the Schrödinger equation for a free particle,

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}, t), \tag{14}$$

because

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{r}, t) = i\hbar f(\mathbf{r})\frac{\partial}{\partial t}T(t) = i\hbar f(\mathbf{r})\left[-i\frac{E}{\hbar}T(t)\right] = E\psi(\mathbf{r}, t), \tag{15}$$

and

$$\boldsymbol{\nabla}\psi(\mathbf{r}, t) = T(t)\boldsymbol{\nabla} f(\mathbf{r}) = \frac{i\mathbf{p}}{\hbar}\left[A\exp\left(i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right) - B\exp\left(-i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right)\right]T(t), \tag{16}$$

and

$$\begin{aligned}\nabla^2\psi(\mathbf{r}, t) &= \boldsymbol{\nabla}\cdot[\boldsymbol{\nabla}\psi(\mathbf{r}, t)] \\ &= -\frac{\mathbf{p}\cdot\mathbf{p}}{\hbar^2}\left[A\exp\left(i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right) + B\exp\left(-i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right)\right]T(t) \\ &= -\frac{\mathbf{p}\cdot\mathbf{p}}{\hbar^2}\psi(\mathbf{r}, t).\end{aligned} \tag{17}$$

Therefore (14) becomes

$$\begin{aligned}E\psi(\mathbf{r}, t) &= -\frac{\hbar^2}{2m}\left[-\frac{\mathbf{p}\cdot\mathbf{p}}{\hbar^2}\psi(\mathbf{r}, t)\right] \\ &= \frac{\mathbf{p}\cdot\mathbf{p}}{2m}\psi(\mathbf{r}, t),\end{aligned} \tag{18}$$

which is indeed an equality if $E = \mathbf{p}\cdot\mathbf{p}/(2m)$.

The probability current is also time-independent because

$$\begin{aligned}\mathbf{j}(\mathbf{r}, t) &= \frac{\hbar}{2m\,i}\left[\psi^*(\mathbf{r}, t)\boldsymbol{\nabla}\psi(\mathbf{r}, t) - \psi(\mathbf{r}, t)\boldsymbol{\nabla}\psi^*(\mathbf{r}, t)\right] \\ &= \frac{\hbar}{2m\,i}\left[f^*(\mathbf{r})\boldsymbol{\nabla} f(\mathbf{r}) - f(\mathbf{r})\boldsymbol{\nabla} f^*(\mathbf{r})\right].\end{aligned} \tag{19}$$

Then, using (16) is easy to see that

$$\begin{aligned} f^*(\mathbf{r})\boldsymbol{\nabla} f(\mathbf{r}) = & \left[A^* \exp\left(-i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right) + B^* \exp\left(i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right)\right] \\ & \times \frac{i\mathbf{p}}{\hbar}\left[A \exp\left(i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right) - B \exp\left(-i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right)\right] \\ = & \frac{i\mathbf{p}}{\hbar}\left[|A|^2 - |B|^2 + AB^* \exp\left(2i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right) - A^*B \exp\left(-2i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right)\right], \end{aligned} \tag{20}$$

and that

$$-f(\mathbf{r})\boldsymbol{\nabla} f^*(\mathbf{r}) = \frac{i\mathbf{p}}{\hbar}\left[|A|^2 - |B|^2 + A^*B \exp\left(-2i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right) - AB^* \exp\left(2i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right)\right]. \tag{21}$$

Summing the last two equations and using (19), we obtain

$$\begin{aligned} \mathbf{j}(\mathbf{r},t) &= \frac{\hbar}{2m\,i}\left[\frac{i\mathbf{p}}{\hbar}\,2\left(|A|^2 - |B|^2\right)\right] \\ &= \frac{\mathbf{p}}{m}\left(|A|^2 - |B|^2\right). \end{aligned} \tag{22}$$

Clearly, from (22) it follows that $\mathbf{j}(\mathbf{r},t)$ is both time-independent and space-independent. Therefore, $\boldsymbol{\nabla}\cdot\mathbf{j} = 0$ and the continuity equation is satisfied because we already know that $\partial\rho/\partial t = 0$. It should be noticed that $\psi(\mathbf{r},t)$ is constructed as the sum of two counterpropagating waves with amplitudes A and B. When $|A| = |B|$ the two waves generates a *stationary* wave and $\mathbf{j} = 0$.

Problem 4

Consider a *classical* particle in a one-dimensional box, moving in the region $0 < x < a$ with constant speed v. Imagine to observe the motion of the particle during the time interval $t_0 \leq t \leq t_1 = t_0 + 2a/v$, with t_0 arbitrary. Calculate the probability to find the particle between x and $x + dx$ at time t_*, randomly peaked in the interval $[t_0, t_1]$. Compare your result with the quantum mechanical ones.

Hint 4

Plot the diagram position-vs-time to visualize the trajectory of the particle in the interval $[t_0, t_1]$. Assume that t_* is a value assumed by the *random variable* τ *uniformly* distributed in the interval $[t_0, t_1]$. Learn how to calculate the probability density function (p.d.f) of a given function of a uniformly distributed random variable.

Problem 5

Consider a classical particle of mass $m = 0.1\,\mathrm{g}$, moving at a constant speed $v = 1\,\mathrm{m/s}$ in a one-dimensional box of width $a = 1\,\mathrm{mm}$. Let E denotes the energy of this particle. Calculate the value of the index n such that the difference

$$|E - E_n| = \left| E - n^2 \frac{\hbar^2 \pi^2}{2ma^2} \right|, \tag{23}$$

is *minimum*.

Hint 5

Calculate the kinetic energy of the classical particle.

Problem 6

This problem is given in Gasiorowicz's book, Example 3-5. Consider a particle in a box of width a. Its wave function is given by

The probability density

$$\psi(x) = \begin{cases} A\,\frac{x}{a}, & 0 < x < a/2, \\ A\left(1 - \frac{x}{a}\right), & a/2 < x < a, \end{cases} \tag{24}$$

where A is the normalization constant. Calculate A and the probability that a measurement of the energy yields the eigenvalue E_n.

Problem 7

This problem is given in Griffiths's book, Problem 2.8. A particle in the infinite square well (the box) has the initial wave function

$$\psi(x, 0) = Ax(a - x), \tag{25}$$

where $A > 0$ is the normalization constant.

a) Normalize $\psi(x, 0)$. Graph it. Which stationary state does it most closely resemble? On that basis, guess the expectation value of the energy.

b) Compute $\langle \hat{x} \rangle$, $\langle \hat{p} \rangle$, and $\langle \hat{H} \rangle$, at $t = 0$. (*Note*: This time you cannot get $\langle \hat{p} \rangle$ by differentiating $\langle \hat{x} \rangle$, because you only know $\langle \hat{x} \rangle$ at one instant of time.) How does $\langle \hat{H} \rangle$ compare with your estimate in (a)?

c) Expand $\psi(x, 0)$ in terms of the eigenfunctions of $\hat{H}$. Plot the absolute square of the expansion coefficients as function of n.

Problem 8

A solution of the second-order ordinary differential equation

$$\frac{d^2u}{dx^2} + k^2 u = 0, \tag{26}$$

with $k > 0$, is

$$u(x) = Ae^{ikx} + Be^{-ikx}. \tag{27}$$

Given the boundary conditions for the "particle in a box" problem,

$$u(0) = 0, \qquad \text{and} \qquad u(a) = 0, \tag{28}$$

which determines *uniquely* the constants A and B, prove that there are not other *independent* solutions.

Hint 8

The linear independence of the solutions can be quantified calculating the Wronskian determinant.