6.728 Applied Quantum and Statistical Physics

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PROBLEM SET 3

Issued: 9-19-02 Due: 9-25-02, in-class

Problem 3.1

Let $\hat{A}$, $\hat{B}$, and $\hat{C}$ be operators.
A comutator of two operators that act on wavefunction ψ is the expression

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

(a) Show that

$$[\hat{A},\hat{B}\hat{C}]\,\psi = [\hat{A},\hat{B}]\hat{C}\,\psi + \hat{B}[\hat{A},\hat{C}]\,\psi$$

also written as

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

(b) Let $\hat{p}$ and $\hat{x}$ be operators satisfying $[\hat{x},\hat{p}] = i\hbar$ and let the Hamiltonian be

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2$$

Use the commutation relations and Ehrenfest's Theorem, $\frac{d}{dt}\langle \hat{A}\rangle = \frac{1}{i\hbar}\langle [\hat{A},\hat{H}]\rangle + \left\langle \frac{d\hat{A}}{dt}\right\rangle$

to find

$$\frac{d}{dt}\langle \hat{x}^2\rangle, \qquad \frac{d}{dt}\langle \hat{p}^2\rangle$$

and

$$\frac{d}{dt}\langle \hat{x}\,\sin(\omega_0 t)\rangle, \qquad \frac{d}{dt}\langle \hat{p}\,\cos(\omega_0 t)\rangle, \quad \text{where } \omega_0 \text{ is a constant.}$$

Problem 3.2

The probability amplitude $\psi(x,t)$ of an electron satisfies the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)$$

It is known that $\psi(x,t=0)$ is sinusoidal and real, and is given by

$$\psi(x,t=0) = A\cos(kx)$$

where A is a normalization constant.

(a) Describe the corresponding physical system in words; what does the wavefunction in this system correspond to?

(b) Compute $\psi(x,t)$ for $t > 0$.

(c) What is the expectation value of kinetic energy $\langle p^2/2m\rangle$ at $t = 0$ for this wavefunction? What is the kinetic energy $\langle p^2/2m\rangle$ for $t > 0$? If it has changed, explain what would cause the kinetic energy to change.

(d) What is the expectation value of momentum $\langle p\rangle$ at $t = 0$ for this wavefunction? Would you expect a <u>measurement</u> of the momentum in this case to result in $\langle p\rangle$? Why?

(e) A Gedanken experiment is considered where an electron is prepared initially such that it is described by this probability amplitude, and then the momentum is measured. Sketch a probable resulting histogram as a function of momentum if the experiment were repeated 1000 times.

Note: The expectation value for free solutions can be computed similarly as for localized states; For example

$$\langle p\rangle = \frac{\langle\psi(x,t)|(-i\hbar\frac{\partial}{\partial x})|\psi(x,t)\rangle}{\langle\psi(x,t)|\psi(x,t)\rangle}$$

Problem 3.3 Parseval's Theorem

Parseval's Theorem states that given two functions *f(x)* and *g(x)* with Fourier Transforms *F(k)* and *G(k)* defined through

$$F(k) = \int_{-\infty}^{\infty} f(x)\, e^{-ikx} dx$$
$$G(k) = \int_{-\infty}^{\infty} g(x)\, e^{-ikx} dx$$

that the following equality is valid:

$$\int_{-\infty}^{\infty} f^*(x)\, g(x)\, dx = \int_{-\infty}^{\infty} F^*(k)\, G(k)\, \frac{dk}{2\pi}$$

(a) Show that this identity is correct.

(b) Show that if

$$\psi(x) = \int_{-\infty}^{\infty} A(k)\, e^{ikx}\, \frac{dk}{2\pi}$$

then

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x)(-i\hbar \frac{d}{dx})\, \psi(x)\, dx = \int_{-\infty}^{\infty} A^*(k)\, \hbar k\; A(k)\, \frac{dk}{2\pi}$$

(c) Use this approach to find the operator $\hat{Q}(k)$ which satisfies

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x)\; x\; \psi(x)\, dx = \int_{-\infty}^{\infty} A^*(k)\, \hat{Q}(k)\; A(k)\, \frac{dk}{2\pi}$$

(d) The Schrödinger equation in *x*-space for the simple harmonic oscillator is

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + \frac{1}{2}m\omega^2 x^2\; \psi(x,t)$$

Recast this Schrödinger equation in *k*-space for *A(k,t)* which satisfies

$$\psi(x) = \int_{-\infty}^{\infty} A(k,t)\, e^{ikx}\, \frac{dk}{2\pi}$$

Problem 3.4 Spread of GaussianWave packet in time.

This problem uses the `Matlab` script files `ps3p1.m` and `cyclelines.m` which can be found in `/mit/6.728/www/script/locker`. Copy them over to your own `Matlab` directory. Read the `ps3p1.m` script carefully, and be sure that you understand what they are doing. You will be asked below to make some modifications of the scripts to solve new problems. (The `cyclelines.m` script is just for beautifying the graphs, and is not relevant to the "physics" of the problem.)

Note: If you prefer to use another graphing package feel free to rewrite the simulation

(a) Run script `ps3p1.m`. Explain the calculations being performed, and the resulting graphs. Also type the command `waterfall(psi_t_pdf')` to see another view of how the wave function changes in time. Also plot $A(q)$ vs. q.

(b) Modify the script `ps3p1.m` to study the time evolution of a wavepacket which at $t = 0$ has the form:

$$\psi(x,0) = \left(\frac{1}{\pi L^2}\right)^{1/4} e^{\left(\frac{-x^2}{2L^2}\right)} e^{\left(\frac{i\pi x}{4L}\right)}$$

with $L = 1$ nm. Suppress the plotting of the "analytic solution", which will otherwise clutter up your graphs (or, if you wish, modify the "analytic solution" so it matches the case you are working on). Also type the command `waterfall(psi_t_pdf')` to see another view of how the wave function changes in time. Plot the real part, the imaginary part and the magnitude of $A(q, t)$ and comment.

(c) Using the results from part (b), plot the expectation value of the displacement versus time (which, for a Gaussian, is the peak position) and determine the group velocity of the wave packet. Compare it to what you would predict analytically.