NTNU **Institutt for fysikk**

Contact during the exam:
Faglærer: Professor Arne Brataas
Kontakt under eksamen: Dr. Anh Kiet Nguyen
Telephone: 73593647

Exam in TFY4205 Quantum Mechanics
August, 2006
9:00–13:00

Allowed help: Alternativ C
Approved Calculator.
K. Rottman: *Matematische Formelsammlung*
Barnett and Cronin: *Mathematical formulae*

At the end of the problem set some relations are given that might be helpful.

This problem set consists of 6 pages.

Problem 1. Momentum Representation

A particle of mass m is subjected to a force $\mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r})$ such that the wave function $\phi(\mathbf{p})$ satisfies the momentum-space Schrödinger equation

$$\left(\frac{\mathbf{p}^2}{2m} - a\nabla_p^2\right)\phi(\mathbf{p},t) = i\hbar\frac{\partial}{\partial t}\phi(\mathbf{p},t)\,, \tag{1}$$

where a is a real constant and

$$\nabla_p^2 = \frac{\partial^2}{\partial p_x^2} + \frac{\partial^2}{\partial p_y^2} + \frac{\partial^2}{\partial p_z^2}\,. \tag{2}$$

Find the force $\mathbf{F}(\mathbf{r})$.

Solution

The coordinate and momentum representations of a wave function are related by

$$\psi(\mathbf{r},t) = \left(\frac{1}{2\pi\hbar}\right)^{3/2}\int d\mathbf{p}\phi(\mathbf{p},t)\exp i\mathbf{p}\cdot\mathbf{r}/\hbar\,, \tag{3}$$

$$\phi(\mathbf{p},t) = \left(\frac{1}{2\pi\hbar}\right)^{3/2}\int d\mathbf{r}\psi(\mathbf{r},t)\exp -i\mathbf{p}\cdot\mathbf{r}/\hbar\,. \tag{4}$$

Thus

$$\mathbf{p}^2\phi(\mathbf{p},t) \rightarrow -\hbar^2\nabla^2\psi(\mathbf{r},t)\,, \tag{5}$$

$$\nabla_p^2\phi(\mathbf{p},t) \rightarrow -r^2\psi(\mathbf{r},t)\,, \tag{6}$$

and the Schrödinger equation becomes in coordinate space

$$\left(-\frac{\hbar^2}{2m} + ar^2\right)\psi(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t)\,. \tag{7}$$

Hence the potential is

$$V(\mathbf{r}) = ar^2\,, \tag{8}$$

and the force is

$$\mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r}) = -\frac{\mathbf{r}}{r}\frac{d}{dr}V(r) = -2a\mathbf{r}\,. \tag{9}$$

Problem 2. Harmonic Oscillator

The Hamiltonian for a harmonic oscillator can be written in dimensionless units ($m = \hbar = \omega = 1$) as

$$\hat{H} = \hat{a}^\dagger\hat{a} + \frac{1}{2}\,, \tag{10}$$

where

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\hat{x} + i\hat{p}\right)\,, \hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\hat{x} - i\hat{p}\right)\,, \tag{11}$$

and $\hat{x}$ is the position operator and $\hat{p}$ is the momentum operator. One unnormalized energy eigenfunction is

$$\psi_a = \left(2x^3 - 3x\right)\exp -x^2/2\,. \tag{12}$$

a) Find two other (unnormalized) eigenfunctions which are closest in energy to ψ_a.

Hint: In the Fock representation of harmonic oscillation, $\hat{a}$ and $\hat{a}^\dagger$ are the annihilation and creation operators such that

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle\,, \tag{13}$$

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle\,, \tag{14}$$

where

$$\hat{H}|n\rangle = \left(n + \frac{1}{2}\right)|n\rangle\,. \tag{15}$$

Solution

Using the definitions for the operators $\hat{a}$ and $\hat{a}^\dagger$, we find

$$\hat{a}\hat{a}^\dagger|n\rangle = (n+1)\,|n\rangle\,. \tag{16}$$

As

$$\hat{a}\hat{a}^\dagger\psi_a = \frac{1}{2}\left(x + \frac{d}{dx}\right)\left(x - \frac{d}{dx}\right)\left(2x^3 - 3x\right)\exp -x^2/2\,, \tag{17}$$

$$= \frac{1}{2}\left(x + \frac{d}{dx}\right)\left(3x^4 - 12x^2 + 3\right)\exp -x^2/2\,, \tag{18}$$

$$= 4\left(2x^3 - 3x\right)\exp -x^2/2\,, \tag{19}$$

$$= (3+1)\,\psi_a\,, \tag{20}$$

we have $n = 3$. Hence the eigenfunctions closest in energy to ψ_a have $n = 2$ and $n = 4$, the unnormalized wave functions being

$$\psi_2 = \frac{1}{\sqrt{3}}\hat{a}\psi_a\,, \tag{21}$$

$$= \frac{1}{\sqrt{6}}\left(x + \frac{d}{dx}\right)\left(2x^3 - 3x\right)\exp -x^2/2\,, \tag{22}$$

$$\sim \left(2x^2 - 1\right)\exp -x^2/2\,, \tag{23}$$

and

$$\psi_4 = \frac{1}{2}\hat{a}^\dagger\psi_a\,, \quad (24)$$
$$= \frac{1}{2\sqrt{2}}\left(x - \frac{d}{dx}\right)\left(2x^3 - 3x\right)\exp -x^2/2\,, \quad (25)$$
$$\sim \left(4x^4 - 12x^2 + 3\right)\exp -x^2/2\,, \quad (26)$$

where the unimportant constant prefactors have been omitted.

b) We now reintroduce the dimensions and write the Hamiltonian using the momentum and position operators:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2\,. \quad (27)$$

Find the time dependence of the expectation values of the "initial position" and "initial momentum" operators

$$\hat{x}_0 = \hat{x}\cos\omega t - \frac{\hat{p}}{m\omega}\sin\omega t\,, \quad (28)$$
$$\hat{p}_0 = \hat{p}\cos\omega t + m\omega\hat{x}\sin\omega t\,. \quad (29)$$

Solution

Making use of the relation (in the Heisenberg representation)

$$\frac{d\hat{f}}{dt} = \frac{1}{i\hbar}\left[\hat{f},\hat{H}\right] + \frac{\partial\hat{f}}{\partial t}\,, \quad (30)$$

and

$$\frac{1}{i\hbar}\left[\hat{x},\hat{H}\right] = \frac{1}{2m}\frac{1}{i\hbar}\left[\hat{x},\hat{p}^2\right] = \frac{\hat{p}}{m} \quad (31)$$
$$\frac{1}{i\hbar}\left[\hat{p},\hat{H}\right] = \frac{1}{2}m\omega^2\frac{1}{i\hbar}\left[\hat{p},\hat{x}^2\right] = -m\omega^2\hat{x} \quad (32)$$
$$(33)$$

so that

$$\frac{d\hat{x}}{dt} = \frac{\hat{p}}{m}\,, \quad (34)$$
$$\frac{d\hat{p}}{dt} = -m\omega^2\hat{x}\,. \quad (35)$$

That means that for the expectation values, we have the two coupled differential equations

$$\frac{dx}{dt} = \frac{p}{m}\,, \quad (36)$$
$$\frac{dp}{dt} = -m\omega^2 p\,. \quad (37)$$

with the solutions

$$x(t) = x(t=0)\cos\omega t - \frac{p(t=0)}{m}\sin\omega t\,, \quad (38)$$
$$p(t) = p(t=0)\cos\omega t + m\omega x(t=0)\sin\omega t \quad (39)$$

We then have

$$\frac{dx_0(t)}{dt} = \frac{p(t)}{m}\cos\omega t - \omega x(t)\sin\omega t = 0\,, \quad (40)$$

$$\frac{d\hat{p}_0}{dt} = \frac{\hat{p}}{m}\cos\omega t + \omega\hat{x}\sin\omega t = 0\,. \quad (41)$$

c) Compute the commutator $[\hat{p}_0, \hat{x}_0]$. What is the significance for measurements theory?

Solution

Using the expression for $\hat{p}_0$ and $\hat{x}_0$, we find

$$[\hat{p}_0, \hat{x}_0] = \left[\hat{x}\cos\omega t - \frac{\hat{p}}{m\omega}\sin\omega t, \hat{p}\cos\omega t + m\omega\hat{x}\sin\omega t\right], \quad (42)$$

$$= \cos^2\omega t\,[\hat{x}, \hat{p}] - \sin^2\omega t\left[\frac{\hat{p}}{m\omega}, m\omega\hat{x}\right], \quad (43)$$

$$= [\hat{p}, \hat{x}] \quad (44)$$

$$= \frac{\hbar}{i}\,. \quad (45)$$

Thus, we have the same uncertainty as between the the operators $\hat{p}$ and $\hat{x}$, so that

$$\Delta p_0 \Delta x_0 \geq \frac{\hbar}{2}\,. \quad (46)$$

Problem 3. Particle in a Periodic Potential

A particle of mass m moves in one dimension in a periodic potential of of infinite exten. The potential is zero at most places, but in narrow regions of width b separated by spaces of length a ($b \ll a$) the potential is V_0, where V_0 is a large positive constant. One may think of the potential as a sum of Dirac delta functions:

$$V(x) = \sum_{n=-\infty}^{\infty} V_0 b\delta(x - na)\,. \quad (47)$$

a) Show that the appropriate boundary conditions to apply to the wave function are

$$\left(\frac{d\psi}{dx}\right)_{x=na+\epsilon} - \left(\frac{d\psi}{dx}\right)_{x=na-\epsilon} = 2\Omega\psi(na)\,, \quad (48)$$

where $\epsilon \to 0$ and $\Omega = mV_0 b/\hbar^2$, n is an integer, and

$$\psi(na + \epsilon) - \psi(na - \epsilon) = 0\,. \quad (49)$$

Solution

The Schrödinger equation is

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \sum_{n=-\infty}^{\infty} V_0 b\delta(x - na)\right]\psi(x) = E\psi(x)\,. \quad (50)$$

Integrating it from $x = a - \epsilon$ to $x = a + \epsilon$ and letting $\epsilon \to 0$, we get

$$\left(\frac{d\psi}{dx}\right)_{x=na+\epsilon} - \left(\frac{d\psi}{dx}\right)_{x=na-\epsilon} = 2\Omega\psi(na)\,. \tag{51}$$

The wave function must be continous since otherwise the kinetic energy would become infinitely large. Consequently,

$$\psi(na+\epsilon) - \psi(na-\epsilon) = 0\,. \tag{52}$$

b) Let the lowest energy of a wave that can propagate through this potential be $E_0 = \hbar^2 k_0^2$ (this defines k_0). Write down a transcendental equation (not a differential equation) that can be solved to give k_0 and thus E_0. (It is not necessary to solve the transcendental equation).

Solution

For $x \neq na$, there are two fundamental solutions to the Schrödinger equation:

$$u_1(x) = \exp ikx\,, u_2(x) = \exp ikx \tag{53}$$

the corresponding energy being

$$E = \frac{\hbar^2 k^2}{2m}\,. \tag{54}$$

Let

$$\psi(x) = A \exp ikx + B \exp -ikx\,,\; 0 \le x \le a\,. \tag{55}$$

According to Bloch's Theorem, in the region $a \le x \le 2a$

$$\psi(x) = \exp iKa \left[A \exp ik(x-a) + B \exp -ik(x-a)\right]\,, \tag{56}$$

where K is the Bloch wave number. The boundary condition give

$$e^{iKa}(A+B) = Ae^{ika} + Be^{-ika}\,, \tag{57}$$

$$ike^{iKa} + (A-B) = ik\left(Ae^{ika} - Be^{-ika}\right) + 2\Omega\left(Ae^{ika} + Be^{-ika}\right)\,. \tag{58}$$

For non-zero solutions of A and B we require

$$\begin{vmatrix} e^{iKa} - e^{ika} & e^{iKa} - e^{-ika} \\ ike^{iKa} - (ik+2\Omega)e^{ika} & -ike^{iKa} + (ik-2\Omega)e^{-ika} \end{vmatrix} = 0 \tag{59}$$

or

$$\cos ka + \frac{\Omega}{k}\sin ka = \cos Ka \tag{60}$$

which determines the Bloch wave number K. Consequently, the allowed values of k are limited to the range given by

$$\left|\cos ka + \frac{\Omega}{k}\sin ka\right| \le 1\,, \tag{61}$$

or

$$\left(\cos ka + \frac{\Omega}{k}\sin ka\right)^2 \le 1\,. \tag{62}$$

k_0 is the minimum of k that satisfy this inequality.

c) Write down the wave function at energy E_0 valid in the region $0 \le x \le a$. (For uniformity, let us choose normalization and phase such that $\psi(x = 0) = 1$). What happens to the wave function between $x = a$ and $x = a + b$?

Solution

For $E = E_0$,

$$\psi(x) = Ae^{ik_0x} + Be^{-ik_0x}\,,\ 0 \le x \le a\,, \tag{63}$$

where $k_0 = \sqrt{2mE_0/\hbar^2}$. A normalization choice, $\psi(x = 0) = 1$ gives

$$\psi(x) = 2iA \sin k_0x + e^{-ik_0x}\,,\ 0 \le x \le a\,, \tag{64}$$

The boundary conditions at $x = a$ give

$$e^{iKa} = 2iA \sin k_0a + e^{-ik_0a}\,, \tag{65}$$

or

$$2iA = \frac{\left(e^{iKa} - e^{-ik_0a}\right)}{\sin k_0a}\,. \tag{66}$$

So

$$\psi(x) = \left(e^{iKa} - e^{-ik_0a}\right)\frac{\sin k_0x}{\sin k_0a} + e^{-ik_0x}\,,\ 0 \le x \le a\,. \tag{67}$$

For x in the interval a to $a + b$, the wave function has the form $\exp \pm ik_1x$, where

$$k_1 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}\,. \tag{68}$$

d) Show that there are ranges of values of E, greater than E_0, for which there is no eigenfunction. Find (exactly) the energy at which the first such gap begins.

Solution

For $ka = n\pi + \delta$, where δ is a small positive number, we have

$$\left|\cos ka + \frac{\Omega}{k}\sin ka\right| = \left|\cos n\pi + \delta + \frac{\Omega}{k}\sin n\pi + \delta\right| \tag{69}$$

$$\approx \left|1 - \frac{\delta^2}{2} + \frac{\Omega}{k}\delta\right|\,. \tag{70}$$

When δ is quite small, the left side $\approx 1 + \Omega\delta/k \ge 1$. Therefore, in a certain region of $k > n\pi/a$, there is no eigenfunction. On the other hand, $ka = n\pi$ corresponds to eigenvalues. So the energy at which the first energy gap begins satisfies the relation $ka = \pi$,

$$E = \frac{\pi^2\hbar^2}{2ma^2}\,. \tag{71}$$