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### 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 $\psi_a$.

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 $\psi_a$ 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

$$\psi_4 \;=\; \frac{1}{2}\hat{a}^\dagger\psi_a\,, \tag{24}$$

$$=\; \frac{1}{2\sqrt{2}}\left(x - \frac{d}{dx}\right)\left(2x^3 - 3x\right)\exp{-x^2/2}\,, \tag{25}$$

$$\sim\; \left(4x^4 - 12x^2 + 3\right)\exp{-x^2/2}\,, \tag{26}$$

where the unimportant constant prefactors have been omitted.

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

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

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

$$\hat{x}_0 \;=\; \hat{x}\cos\omega t - \frac{\hat{p}}{m\omega}\sin\omega t\,, \tag{28}$$

$$\hat{p}_0 \;=\; \hat{p}\cos\omega t + m\omega\hat{x}\sin\omega t\,. \tag{29}$$

**Solution**

Making use of the relation (in the Heisenberg representation)

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

and

$$\frac{1}{i\hbar}\left[\hat{x},\hat{H}\right] \;=\; \frac{1}{2m}\frac{1}{i\hbar}\left[\hat{x},\hat{p}^2\right] = \frac{\hat{p}}{m} \tag{31}$$

$$\frac{1}{i\hbar}\left[\hat{p},\hat{H}\right] \;=\; \frac{1}{2}m\omega^2\frac{1}{i\hbar}\left[\hat{p},\hat{x}^2\right] = -m\omega^2\hat{x} \tag{32}$$

$$\tag{33}$$

so that

$$\frac{d\hat{x}}{dt} \;=\; \frac{\hat{p}}{m}\,, \tag{34}$$

$$\frac{d\hat{p}}{dt} \;=\; -m\omega^2\hat{x}\,. \tag{35}$$

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

$$\frac{dx}{dt} \;=\; \frac{p}{m}\,, \tag{36}$$

$$\frac{dp}{dt} \;=\; -m\omega^2 p\,. \tag{37}$$

with the solutions

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

$$p(t) = p(t=0)\cos\omega t + m\omega x(t=0)\sin\omega t \tag{39}$$

We then have

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

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

**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

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

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

$$= [\hat{p}, \hat{x}] \tag{44}$$

$$= \frac{\hbar}{i}\,. \tag{45}$$

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

$$\Delta p_0 \Delta x_0 \geq \frac{\hbar}{2}\,. \tag{46}$$

**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:

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

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

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

where $\epsilon \to 0$ and $\Omega = mV_0b/\hbar^2$, $n$ is an integer, and

$$\psi(na + \epsilon) - \psi(na - \epsilon) = 0\,. \tag{49}$$

**Solution**

The Schrödinger equation is

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

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

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

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

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

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

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

or

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

$k_0$ 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 $E = E_0$,

$$\psi(x) = Ae^{ik_0 x} + Be^{-ik_0 x} \,,\ 0 \le x \le a \,, \tag{63}$$

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

$$\psi(x) = 2iA \sin k_0 x + e^{-ik_0 x} \,,\ 0 \le x \le a \,, \tag{64}$$

The boundary conditions at $x = a$ give

$$e^{iKa} = 2iA \sin k_0 a + e^{-ik_0 a} \,, \tag{65}$$

or

$$2iA = \frac{\left(e^{iKa} - e^{-ik_0 a}\right)}{\sin k_0 a} \,. \tag{66}$$

So

$$\psi(x) = \left(e^{iKa} - e^{-ik_0 a}\right) \frac{\sin k_0 x}{\sin k_0 a} + e^{-ik_0 x} \,,\ 0 \le x \le a \,. \tag{67}$$

For $x$ in the interval $a$ to $a + b$, the wave function has the form $\exp \pm i k_1 x$, 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 $\delta$ 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 $\delta$ 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 $ka = \pi$,

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