NTNU Institutt for Fysikk

Final exam FY2045 Quantum Mechanics I Monday December 7, 2015

Exam time:4 hours (09.00 - 13.00)Allowed help:Karl Rottman, Matematisk formelsamling (any language)
Øgrim & Lian, Størrelser og enheter i fysikk og teknikk
Lian & Angell, Fysiske størrelser og enheter
Approved calculator

This exam consists of 4 problems, each of which counts 25% towards the result.

You may answer in Norwegian or English. I will visit twice during the exam, at approximately ten o'clock and twelve o'clock. Feel free to ask if you need help interpreting the questions.

Problem 1



a) The Figure shows the wavefunction of a particle with energy E, in a region where there is a potential V(x), given by

$$V(x) = \begin{cases} 0 & \text{if } x \leq L \\ V_0 & \text{if } -L < x \leq L \\ 0 & \text{if } L < x \end{cases}$$

Which of these statements is true?

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b) A particle is in a one-dimensional potential given by

$$V(x) = \begin{cases} \infty & \text{if } x \le 0\\ 0 & \text{if } 0 < x \le L\\ \infty & \text{if } L < x \end{cases}.$$

What is the normalised wave function of the first excited state?

A
$$\psi(x) = \sqrt{\frac{2}{L}} \sin(\pi x/L)$$

B $\psi(x) = \sqrt{\frac{2}{L}} \sin(2\pi x/L)$
C $\psi(x) = \sqrt{\frac{2}{L^2}} \sin(\pi x/L)$
D $\psi(x) = \sqrt{\frac{2}{\hbar}} \sin(\pi x/L)$
E $\psi(x) = \sqrt{\frac{\hbar}{L}} \sin(2\pi x/L)$

- c) The electron in a hydrogen atom has spin $\frac{1}{2}$, and is in a state with orbital angular momentum $|\mathbf{L}| = \hbar \sqrt{l(l+1)}$ with l = 2. The magnitude of the total angular momentum of the electron is given by $|\mathbf{J}| = \hbar \sqrt{j(j+1)}$. What are the possible values of j?
 - $\begin{array}{lll} {\rm A} & j=0,\pm 1,\pm 2 \\ {\rm B} & j=\pm \frac{1}{2},\pm \frac{3}{2} \\ {\rm C} & j=\frac{3}{2},\frac{5}{2} \\ {\rm D} & j=\pm \frac{\hbar}{2} \\ {\rm E} & j=\frac{1}{2} \end{array}$
- d) The Pauli matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

What is $[\sigma_x, \sigma_y]$?

 $\begin{array}{rll} \mathbf{A} & \mathbf{0} \\ \mathbf{B} & \mathrm{i}\hbar\sigma_z \\ \mathbf{C} & -2i\sigma_z \\ \mathbf{D} & 2i\sigma_z \\ \mathbf{E} & -2\sigma_z \end{array}$

e) The Fermi-Dirac distribution, which describes for example a gas of fermions in a box, is given by

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\frac{E-\mu}{k_B T}} + 1}.$$

What is the probability of finding an occupied state with energy $E = E_F$, where E_F is the Fermi energy? (Assume that $k_BT \ll E_F$, and hence that the chemical potential is equal to the Fermi energy.)

- $\begin{array}{rrr} \mathbf{A} & \mathbf{0} \\ \mathbf{B} & \mathbf{1/2} \\ \mathbf{C} & \mathbf{1} \\ \mathbf{D} & \frac{1}{\frac{2E_F}{\mathrm{e}^{k_BT}+1}} \\ \mathbf{E} & \frac{1}{\frac{-2E_F}{\mathrm{e}^{\frac{-2E_F}{k_BT}}+1}} \end{array}$
- **f)** For a particle with spin $\frac{1}{2}$, the operator \hat{S}_z , for the z component of the spin, has two eigenstates,

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

with eigenvalues $\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$. At t = 0, a particle is in the state

$$\chi = \frac{\sqrt{3}}{3} \begin{pmatrix} 1\\0 \end{pmatrix} - \frac{\sqrt{6}}{3} \begin{pmatrix} 0\\1 \end{pmatrix}.$$

What is the probability of measuring $S_z = \frac{1}{2}\hbar$ at t = 0?

 $\begin{array}{rrrr} A & 0 \\ B & 1 \\ C & \frac{\sqrt{3}}{3} \\ D & 1/3 \\ E & 2/3 \end{array}$

g) A particle is in a one-dimensional potential given by

$$V(x) = \begin{cases} \infty & \text{if} \quad x \le 0\\ 0 & \text{if} \quad 0 < x \le L\\ \infty & \text{if} \quad L < x \end{cases}$$

The discrete energy eigenstates of a particle in this potential are $\psi_n(x)$, and the associated energy eigenvalues are

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}.$$

At t = 0, the particle is in the (non-stationary) state

$$\psi(x) = \sqrt{\frac{1}{2}}\psi_1 - \sqrt{\frac{1}{2}}\psi_3.$$

What is the expectation value if the energy is measured at t = 0?

$$A \quad \frac{\pi^2 \hbar^2}{2mL^2}$$

$$B \quad \frac{3\pi^2 \hbar^2}{2mL^2}$$

$$C \quad \frac{5\pi^2 \hbar^2}{2mL^2}$$

$$D \quad \frac{9\pi^2 \hbar}{2mL^2}$$

$$E \quad \left(1 - \sqrt{3}\right) \frac{\pi^2 \hbar^2}{2mL^2}$$

Problem 2



A particle with mass m is moving in a one-dimensional potential given by

$$V(x) = \begin{cases} 2V_0 & \text{if} \quad x \le 0\\ 0 & \text{if} \quad 0 < x \le L\\ 4V_0 & \text{if} \quad L < x \end{cases},$$

where $V_0 = \hbar^2/(2ma_0^2)$. The width L is chosen such that the first excited state, $\psi_2(x)$, has an energy $E_2 = V_0$.

- a) Assume that the described system has at least two bound states. How many zeros does the wave function for the ground state, $\psi_1(x)$, and the first excited state, $\psi_2(x)$, have? You do not need to prove your answer.
- b) In the well region, that is for 0 < x < L, the wave function $\psi_2(x)$ can be written on the form $\psi_2(x) = A \sin(k_2(x-a))$, where A is a constant. Find the wave number k_2 , expressed in terms of a_0 .
- c) Show that $\psi_2(x)$ must have the form $\psi_2(x) = C e^{\kappa x}$ for x < 0, and the form $\psi_2(x) = C' e^{-\kappa' x}$ for x > L. Find κ and κ' .
- d) Use the continuity conditions for x = 0 to show that $k_2 a$ is equal to $3\pi/4$, and find the width of the well, L, expressed in terms of a_0 . Refer to the list of formulæ for some useful properties of the tangent function.
- e) Sketch $\psi_2(x)$. You don't have to get the magnitude right, only the approximate behaviour.
- f) For $E > 2V_0$, an energy eigenfunction for the potential V(x) can be written on the form

$$\psi_E(x) = \mathrm{e}^{ikx} + r\mathrm{e}^{-ikx} \quad \text{for} \quad x < 0,$$

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where

$$k = \frac{1}{\hbar}\sqrt{2m(E - 2V_0)}.$$

Show that this gives a probability density current

$$j(x) = \frac{\hbar k}{m}(1 - |r|^2),$$

in the region x < 0. Explain why all particles coming towards the well from the left, with energy $2V_0 < E < 4V_0$ will be reflected. Hint: Find the form of the energy eigenfunction in the region x > L, and calculate the probability density current in this region.

Problem 3



The figure shows a box, with edges $L_x = L_y = L_z = L$. Assume that the potential is 0 inside the box, and infinite outside. The energy eigenfunctions for a particle in the box can be written on the form

$$\psi_{n_x n_y n_z}(\mathbf{x}) = A \sin \frac{n_x \pi x}{L} \sin \frac{n_y \pi y}{L} \sin \frac{n_z \pi z}{L},$$

where A is some constant.

a) A particle of mass m is in the box, and is in the energy eigenstate $\psi_{211}(\mathbf{x})$. Find the energy eigenvalue of this state. b) Assume now that the box contains a particle of mass m, in the ground state. Show that the pressure in the box is given by

$$p = \frac{\hbar^2 \pi^2}{mL^5}.$$

You can for example proceed by considering the change in the energy of the particle if you change the volume of the box by changing L_x by an infinitesimal amount dL_x (while keeping L_y and L_z constant). You can assume that changing the volume in this way does not change the quantum numbers of the particle, that is, it will still be left in the ground state.

c) Assume now that the box contains 8 non-interacting spin $\frac{1}{2}$ particles, all with mass m, and that this system is in its ground state, that is the total energy is as small as possible. Calculate the pressure in the box.

Problem 4

Consider a potential, V(x), given by

$$V(x) = \begin{cases} \infty & \text{if } x \le 0\\ \lambda \delta(x - L/2) & \text{if } 0 < x \le L\\ \infty & \text{if } L < x \end{cases}$$

that is an infinite square well with a delta-function in the middle. In this problem we will study this system using time-independent perturbation theory. We will consider the infinite square well to be the unperturbed potential, where the delta-function is a weak perturbation, which disappears if $\lambda \to 0$.

The perturbed Hamiltonian, $H = H_0 + \lambda \delta(x)$, has stationary state solutions, which we will call $|\psi_n\rangle$, with associated energy eigenvalues, E_n . Assume that the energy eigenvalues of the perturbed Hamiltonian can be written as a series expansion in λ ,

$$E_n = E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$

and similarly for the eigenstates,

$$|\psi_n\rangle = |n\rangle + \lambda |\psi_n^{(1)}\rangle + \lambda^2 |\psi_n^{(2)}\rangle + \dots$$

a) Writing out the eigenvalue equation for the perturbed Hamiltonian, assume that this equation is satisfied order by order in λ , and show that the equations

for the zero and first order terms are

$$(H_0 - E_n^0) \left| \psi_n^0 \right\rangle = 0,$$

$$(H_0 - E_n^0) \left| \psi_n^{(1)} \right\rangle + \left(\delta(x - L/2) - E_n^{(1)} \right) \left| \psi_n^0 \right\rangle = 0.$$

b) Show that the first order correction to the energy eigenvalues is given by

$$\lambda E_n^{(1)} = \langle n | \lambda \delta(x - L/2) | n \rangle.$$

c) Given that

$$\psi_1(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L},$$

find the first order correction to the ground state energy, E_1 .

d) The first order correction to the energy of the state $|\psi_2\rangle$, and all other states where n is an even number, is 0. Argue on physical grounds why this is the case.

Formulæ

Schrödinger equation (time dependent)

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)=\hat{H}\Psi(\mathbf{r},t).$$

Schrödinger equation (time independent)

$$E\psi(\mathbf{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi(\mathbf{r}).$$

Trigonometry

$$\tan(3\pi/4) = -1, \quad \tan(5\pi/6) = \frac{-1}{\sqrt{3}},$$
 $\tan(x \pm \pi) = \tan(x), \quad \tan(-x) = -\tan(x).$

Probability current density

$$j(x) = \operatorname{Re}\left\{\psi^*(x)\frac{\hbar}{\mathrm{i}m}\frac{\partial}{\partial x}\psi(x)\right\}.$$

Delta function

$$\int f(x)\delta(x-a)\mathrm{d}x = f(a).$$