NTNU

Institutt for Fysikk — Contact during the exam: Tor Nordam

Final exam

FY2045 Quantum Mechanics I
Thursday December 14, 2017

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

In this problem, you do not have to show your reasoning or calculations. Just write what you think is the correct alternative for each question.

a) An electron is described by a wave-packet

$$\Psi(x,t) = \int_{-\infty}^{\infty} \phi(k) \mathrm{e}^{\mathrm{i}(kx-\omega t)}\,\mathrm{d}k,$$

where $\omega = \frac{\hbar k^2}{2m}$, and m is the electron mass. The coefficients $\phi(k)$ have a distribution

$$\phi(k) = \sqrt{\frac{\sigma}{2\pi^{3/2}}}\mathrm{e}^{-\sigma^2(k-k_0)^2/2},$$

where σ is a real constant larger than 0. This distribution has a large and narrow peak at $k = k_0$. The width of this peak is finite (i.e. larger than 0).

What are the expectation values of the variance of the position, $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$ and the momentum $\langle p_x\rangle$ of the wave packet?

A $\Delta x = 0$ $\quad\langle p_x\rangle = 0$
B $\Delta x = 0$ $\quad\langle p_x\rangle = \hbar k_0$
C $\Delta x = \sigma/\sqrt{2}$ $\quad\langle p_x\rangle = \hbar k_0 - \hbar\sigma$
D $\Delta x = \sigma/\sqrt{2}$ $\quad\langle p_x\rangle = \hbar k_0$
E $\Delta x = \sigma^2/\sqrt{2}$ $\quad\langle p_x\rangle = \hbar k_0$

b) Fermi's golden rule is related to transitions between states, and can be written in different forms. One of them is

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar} \left| \langle f|\hat{V}|i\rangle \right|^2 \rho,$$

where ρ is the density of final states.

What does $\Gamma_{i\to f}$ describe?

A The transition probability.
B The transition amplitude.
C The transition probability per unit time.
D The transition amplitude per unit time.
E The Fermi energy.

c) Consider a system of two non-interacting particles with spin 0. The first particle is in an eigenstate of its operator for the square of the total angular momentum, $\hat{\mathbf{L}}_{\mathbf{1}}^2$,

$$\hat{\mathbf{L}}_{\mathbf{1}}^2|l_1, m_1\rangle = \hbar^2 l_1(l_1+1)|l_1, m_1\rangle,$$

with $l_1 = 7$. The second particle is in an eigenstate of $\hat{\mathbf{L}}_{\mathbf{2}}^2$,

$$\hat{\mathbf{L}}_{\mathbf{2}}^2|l_2, m_2\rangle = \hbar^2 l_2(l_2+1)|l_2, m_2\rangle,$$

with $l_2 = 3$.

The possible values for the square of the total angular momentum of the two-particle system are then

$$\hbar^2 l(l+1),$$

where l is an integer that can take the values

A $l = -7, -6 \ldots, 6, 7$
B $l = 0, 1, 2, 3, 4, 5, 6, 7$
C $l = 0, 1, \ldots, 9, 10$
D $l = 3, 4, 5, 6, 7$
E $l = 4, 5, 6, 7, 8, 9, 10$

d) In the photoelectric effect, shining light onto a piece of metal can expel electrons from the metal into the vacuum surrounding the metal. A simple (but useful) model for the electrons in a metal, which can help us understand this effect, is to treat the metal as a system where the potential is 0 inside the metal, and V_0 outside. If the Fermi energy of the metal is E_F, what is the longest wavelength, λ_0, of light that will allow electrons to be liberated from the metal?

A $\lambda_0 = \frac{hc}{V_0 - E_F}$
B $\lambda_0 = \frac{\hbar\omega}{E_F}$
C $\lambda_0 = \frac{hc}{E_F}$
D $\lambda_0 = \frac{hf}{V_0 - E_F}$
E $\lambda_0 = \frac{hc}{V_0}$

e) It is common to represent spin states as two-component column vectors called spinors, where the inner product of two spinors χ_1 and χ_2 is given by $\chi_1^\dagger \chi_2$. Which of the following pairs of spinors do *not* make up an orthonormal basis?

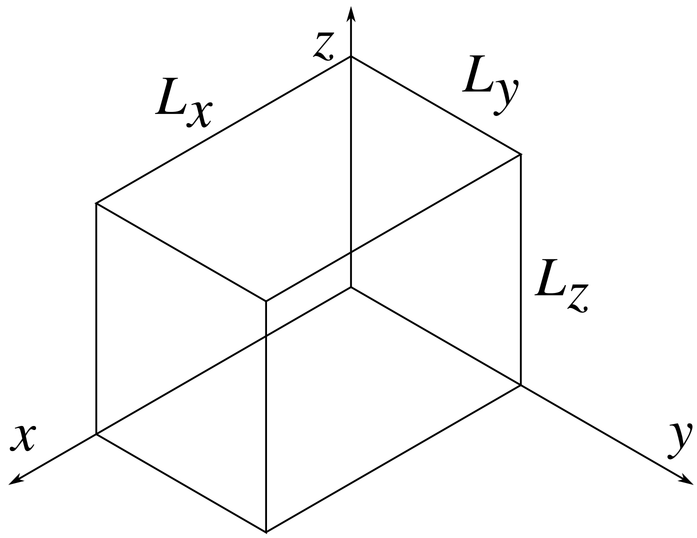
A $\chi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

B $\chi_1 = \frac{1}{2}\begin{pmatrix} \mathrm{i} \\ \sqrt{3} \end{pmatrix}, \quad \chi_2 = \frac{1}{2}\begin{pmatrix} -\mathrm{i} \\ \sqrt{3} \end{pmatrix}$

C $\chi_1 = \frac{1}{2}\begin{pmatrix} \mathrm{i} \\ \sqrt{3} \end{pmatrix}, \quad \chi_2 = \frac{1}{2}\begin{pmatrix} \sqrt{3} \\ \mathrm{i} \end{pmatrix}$

D $\chi_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \chi_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix}$

E $\chi_1 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1+\mathrm{i} \\ i \end{pmatrix}, \quad \chi_2 = \frac{1}{\sqrt{3}}\begin{pmatrix} i \\ 1-\mathrm{i} \end{pmatrix}$



f) A system consists of a rectangular box with sides $L_x = 2L$, $L_y = L$, and $L_z = \frac{3}{2}L$, and where the potential is 0 inside the box, and infinite outside the box, and where the box contains 5 identical non-interacting spin-$\frac{3}{2}$ particles. The energy eigenstates for a particle of mass m in this box are

$$\psi_{n_x n_y n_z} = A \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right) \sin\left(\frac{n_z \pi z}{L_z}\right),$$

where A is a normalisation constant, and n_x, n_y, and n_z are positive integers.

What is the Fermi energy, E_F, when the system is in the ground state?

A $\quad E_F = \frac{109}{36}\frac{\hbar^2\pi}{2mL^2}$

B $\quad E_F = \frac{109}{36}\frac{\hbar^2\pi^2}{2mL^2}$

C $\quad E_F = \frac{169}{36}\frac{\hbar^2\pi^2}{2mL^2}$

D $\quad E_F = \frac{11}{9}\frac{\hbar^2\pi^2}{mL^2}$

E $\quad E_F = \frac{\hbar^2\pi^2}{2mL^2}$

Problem 2

Consider a spherical box potential, given by

$$V(r) = \begin{cases} 0 & \text{if} \quad r \leq a \\ \infty & \text{if} \quad r > a \end{cases} .$$

For this potential, it can be shown that the stationary states are

$$\psi_{nlm}(\mathbf{r}) = \begin{cases} R_{nl}(r)Y_{lm}(\theta,\phi) & \text{for} \quad r \leq a \\ 0 & \text{for} \quad r > a \end{cases} ,$$

and the associated energies for particles of mass m_p are

$$E_{nl} = \frac{\left(\hbar\Pi_n^{(l)}\right)^2}{2m_p a^2}.$$

Here,

$$R_{nl}(r) = A_{nl} j_l\left(\Pi_n^{(l)}\frac{r}{a}\right),$$

where A_{nl} is a normalisation constant, $j_l(r)$ are the spherical Bessel functions, and $\Pi_n^{(l)}$ are the zeros of the spherical Bessel functions (see table in the Appendix). The quantum number n is an integer larger than 0, l is an integer larger than or equal to 0, and m is an integer between $-l$ and l.

a) If the box contains 18 identical, non-interacting spin-$\frac{1}{2}$ particles, show that the ground state energy of the system is approximately

$$473\frac{\hbar^2}{2ma^2}.$$

b) If the box contains 18 identical, non-interacting spin-$\frac{1}{2}$ particles, with the system in the ground state, what is the pressure on the inside of the box?

c) If the box contains 19 identical, non-interacting spin-$\frac{1}{2}$ particles, what is the ground state energy of the system?

Assume now that the spherical box contains a single particle, with mass m_p. Initially (at $t < 0$) the particle is in the ground state (that is, $\psi_{100}(\mathbf{r})$). Then, the system is subjected to a time-dependent perturbation of the form

$$\hat{V}(t) = -zp_0\delta(t).$$

After the perturbation, the state of the particle will be

$$\Psi(\mathbf{r}, t) = \sum_{nlm} a_{nlm} \psi_{nlm}(\mathbf{r}) \mathrm{e}^{-iE_n t/\hbar},$$

where a_{nlm} are time-independent amplitudes.

d) The first-order approximations to the amplitudes a_{nlm} are proportional to the matrix elements

$$V_{nlm,100}(t) = -p_0 \delta(t) \int \psi^*_{nlm}(\boldsymbol{r})\, z\, \psi_{100}(\boldsymbol{r})\, \mathrm{d}^3 r.$$

Show that the amplitudes are 0 for all transitions, except to states with $l = 1$ and $m = 0$. Hint: You may find it useful to recall that $z = r\cos\theta$, and to look at the spherical harmonics given in the appendix.

Problem 3

In this problem, you will calculate a first-order correction to the energy of the ground state of hydrogen, taking the finite size of the nucleus into account.

Assume that the nucleus consists of a single proton, and that the proton is a sphere with radius R, charge e, and a uniform charge distribution. This modifies the potential energy of the electron when $r < R$, which then becomes

$$V(r) = \frac{e^2}{4\pi\epsilon_0}\left(\frac{r^2}{2R^3} - \frac{3}{2R}\right) \quad \text{for} \quad r < R.$$

a) Show that taking the finite size of the proton into account, as described above, is equivalent to adding a time-independent perturbation

$$\hat{V}(r) = \begin{cases} 0 & \text{for} \quad r > R \\ \frac{e^2}{4\pi\epsilon_0}\left(\frac{r^2}{2R^3} - \frac{3}{2R} + \frac{1}{r}\right) & \text{for} \quad r \leq R \end{cases} \tag{1}$$

to the unperturbed Hamiltonian of the hydrogen atom.

b) Show that the first-order correction to the ground state energy of the perturbed system is

$$E_1^{(1)} = \frac{e^2}{\pi\epsilon_0 a_0^3}\int_0^R \mathrm{e}^{-2r/a_0}\left(\frac{r^2}{2R^3} - \frac{3}{2R} + \frac{1}{r}\right) r^2 \mathrm{d}r.$$

c) To evaluate this integral, we will first make a simplification. Since the proton radius is much, much smaller than the Bohr radius ($R/a_0 \approx 10^{-5}$) we see that r/a_0 is always going to be a very small number. As a good approximation, we can therefore replace the exponential with its Taylor series, and keep only the first term, that is

$$e^{-2r/a_0} \approx 1.$$

Using this approximation, calculate the first-order correction to the ground state energy, and express the answer as a multiple of the unperturbed ground state energy, $E_1^0 = -\frac{e^2}{8\pi\epsilon_0 a_0}$. (In other words, find x, in the equation $E_1^{(1)} = xE_1^0$).

d) In the unperturbed hydrogen atom, the energy E_n^0 of a state ψ_{nlm}^0 depends only on the quantum number n. Would you expect this to still be the case for the hydrogen atom with the perturbation described by equation (1)? Explain why or why not. You don't have to do any calculations to answer this question.

Problem 4

In the matrix representation, the operators for the components of the electron spin, $\hat{\mathbf{S}} = [\hat{S}_x, \hat{S}_y, \hat{S}_z]$, can be expressed as

$$\hat{S}_x = \frac{1}{2}\hbar\sigma_x, \quad \hat{S}_y = \frac{1}{2}\hbar\sigma_y, \quad \hat{S}_z = \frac{1}{2}\hbar\sigma_z,$$

where

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

are called the Pauli matrices. The electron spin can then be represented as a two-component column vector called a spinor:

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix},$$

where a and b can be functions of time. It is customary to define the two spinors

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

a) Verify that χ_+ and χ_- are eigenvectors of the operator $\hat{S}_z$, and find their corresponding eigenvalues.

b) Find the eigenvalues, $S_{\pm x}$, and eigenvectors, $\chi_{\pm x}$, of the $\hat{S}_x$ operator.

Assume now that an electron is placed in an external magnetic field, pointing in the x direction, given by

$$\mathbf{B} = B_0 \hat{\mathbf{x}}.$$

The energy of the interaction between the external field and the spin is dependent on the direction of the magnetic moment (and thus the spin) of the electron, relative to the external field. The Hamiltonian operator can be written

$$\hat{H} = g_e \frac{-e}{2m_e} \mathbf{B} \cdot \hat{\mathbf{S}},$$

where the constants g_e, e, and m_e are respectively the gyromagnetic factor, the elementary charge and the mass of the electron.

c) At $t = 0$, the electron is in an eigenstate of $\hat{S}_z$:

$$\psi(t = 0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

What state is the electron in at time $t = \frac{\pi}{2\omega}$, where $\omega = g_e \frac{eB_0}{m_e}$?

Hint: You may find it useful to recall that the differential equation

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} a(t) = -\omega^2 a(t)$$

has general solutions

$$a(t) = A_+ \mathrm{e}^{\mathrm{i}\omega t} + A_- \mathrm{e}^{-\mathrm{i}\omega t}$$

where A_+ and A_- are constants.

Appendix: Tables and Formulae

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)

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

Potential energy in hydrogen atom

$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$$

Radial part of the wave function for some hydrogen states

$$\begin{aligned}
R_{10} &= 2a_0^{-3/2}\mathrm{e}^{-r/a_0} \\
R_{20} &= \frac{1}{2\sqrt{2}}a_0^{-3/2}\left(2 - \frac{r}{a_0}\right)\mathrm{e}^{-r/(2a_0)} \\
R_{21} &= \frac{1}{2\sqrt{6}}a_0^{-3/2}\frac{r}{a_0}\mathrm{e}^{-r/(2a_0)}
\end{aligned}$$

Some spherical harmonics

$$\begin{aligned}
Y_{00} &= \sqrt{\frac{1}{4\pi}} \\
Y_{10} &= \sqrt{\frac{3}{4\pi}}\cos\theta
\end{aligned}$$

Thermodynamics

$$\mathrm{d}W = P\mathrm{d}V$$

Eigenvalues and eigenvectors

$$\det(A - \lambda I) = 0$$
$$(A - \lambda I)\,\boldsymbol{\xi} = 0$$

Some properties of the Dirac delta function

$$\int f(x)\delta(x-a)\mathrm{d}x = f(a).$$
$$\frac{1}{2\pi}\int e^{\mathrm{i}(k-k_0)x}\mathrm{d}x = \delta(k-k_0).$$

Some zeros of the spherical Bessel functions

j_0	j_1	j_2	j_3	j_4
$\Pi_1^{(0)} = \pi$	$\Pi_1^{(1)} = 4.4934$	$\Pi_1^{(2)} = 5.7635$	$\Pi_1^{(3)} = 6.9879$	$\Pi_1^{(4)} = 8.183$
$\Pi_2^{(0)} = 2\pi$	$\Pi_2^{(1)} = 7.7253$	$\Pi_2^{(2)} = 9.0950$	$\Pi_2^{(3)} = 10.417$	$\Pi_2^{(4)} = 11.705$
$\Pi_3^{(0)} = 3\pi$	$\Pi_3^{(1)} = 10.904$	$\Pi_3^{(2)} = 12.323$	$\Pi_3^{(3)} = 13.698$	$\Pi_3^{(4)} = 15.040$

Some constants

Bohr radius	$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} \approx 5.291 \cdot 10^{-11}$ m
Proton radius (approximate value)	$0.85 \cdot 10^{-15}$ m
Planck's constant	$h = 6.626070 \cdot 10^{-34}$ Js $= 4.135667 \cdot 10^{-15}$ eVs