**NTNU – Trondheim**
Norwegian University of
Science and Technology

NTNU, Department of Physics

# FY2045 Problem set 10 fall 2023

Professor Jens O. Andersen and Henning G. Hugdal

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## Problem 1

Consider the hydrogen atom in the ground state. The proton is not a point charge and we will now take into account the finite extent of it. Assume for simplicity that the charge of the proton $e$ is uniformly distributed inside it. The potential can then be shown to be

$$V(r) = \begin{cases} -\frac{e^2}{4\pi\epsilon_0 r}\,, & r \geq R \\ -\frac{e^2}{4\pi\epsilon_0 R}\left(\frac{3}{2} - \frac{r^2}{2R^2}\right), & r \leq R, \end{cases} \tag{1}$$

where $R$ is the radius of the proton. To get an idea of the scales involved, we express the potential $V(r)$ in terms of the unperturbed ground-state energy $E_0 = -\frac{e^2}{8\pi\epsilon_0 a_0}$, where $a_0 \approx 5.29 \times 10^{-11}\,\text{m}$ is the Bohr radius of hydrogen,

$$V(r) = \begin{cases} E_0 \frac{2a_0}{r}\,, & r \geq R \\ E_0 \frac{2a_0}{R}\left(\frac{3}{2} - \frac{r^2}{2R^2}\right), & r \leq R \end{cases}\,. \tag{2}$$

**a)** Explain why we can use non-degenerate perturbation theory in this case, despite the fact that the hydrogen atom is highly degenerate.

**b)** Use first-order perturbation theory to calculate the correction to the ground-state energy due to the finite size of the nucleus. The ground-state wavefunction is

$$\psi_{100}(r,\theta,\phi) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}.$$

Since the proton radius is of the order $10^{-15}$m, the ratio is $R/a_0 \sim 10^{-5}$. It therefore makes sense to expand the wavefunction in powers of $r/a_0$. Calculate to second order in $\frac{R}{a_0}$. Based on the results, is the finite size of the proton an important effect to include?
*Hint:* Convince yourself that to this order, we can approximate the exponential by unity.

## Problem 2

Consider the Hamiltonian

$$\hat{H} = V_0 \begin{pmatrix} 1-\epsilon & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix}, \tag{3}$$

where $V_0$ is a constant and $\epsilon$ is a small dimensionless number.

**a)** Set $\epsilon = 0$, find the eigenvectors and eigenvalues.

**b)** Find the exact eigenvectors and eigenvalues for nonzero $\epsilon$. Expand the eigenvalues to second order in $\epsilon$.

**c)** Calculate the correction to the non-degenerate eigenstate found in **a**) up to second order in $\epsilon$. How does it compare with the exact solution? Also calculate the first-order correction to the eigenvector and compare it to the exact solution.

**d)** Use first-order perturbation to calculate the energy shift of the two degenerate states found in **a**), and compare with the exact solution.

## Problem 3 — Bonus problem

Consider the Hamiltonian

$$H_0 = \frac{\hat{p}_x^2}{2m_e}, \tag{4}$$

a one-dimensional free electron gas in a box with length $L$.

**a)** Solve the Schrödinger equation to find the eigenenergies $E_n$ and eigenstates using periodic boundary conditions for the wavefunctions $\psi_n(x) = \langle x|\, n\rangle$ in position space.

Since $H_0$ has no spin-dependence, the eigenenergies have no spin-dependence, meaning that the levels $n$ are doubly degenerate in the free electron gas. Each level $n$ can thus be

filled by two electrons with opposite spin. In matrix notation for spin $\frac{1}{2}$, this amounts to writing the Hamiltonian as

$$H_0 = \begin{pmatrix} \frac{\hat{p}_x^2}{2m_e} & 0 \\ 0 & \frac{\hat{p}_x^2}{2m_e} \end{pmatrix} = \frac{\hat{p}_x^2}{2m_e}\mathbb{1}, \tag{5}$$

where $\mathbb{1}$ is an identity matrix in spin space. We can label states according to the energy and $S_z$ eigenvalues, $|n, m\rangle$,[1] where $m = \pm\frac{1}{2}$ for spin up or spin down along the $z$ direction.

**b)** Show that the combined position-spin space states

$$\Psi_{n+} = \begin{pmatrix} \psi_n(x) \\ 0 \end{pmatrix} = \psi_n(x)\chi_+ \equiv \begin{pmatrix} \left\langle x, +\frac{1}{2} \middle| \, n, +\frac{1}{2} \right\rangle \\ \left\langle x, -\frac{1}{2} \middle| \, n, +\frac{1}{2} \right\rangle \end{pmatrix}, \tag{6a}$$

$$\Psi_{n-} = \begin{pmatrix} 0 \\ \psi_n(x) \end{pmatrix} = \psi_n(x)\chi_- \equiv \begin{pmatrix} \left\langle x, +\frac{1}{2} \middle| \, n, -\frac{1}{2} \right\rangle \\ \left\langle x, -\frac{1}{2} \middle| \, n, -\frac{1}{2} \right\rangle \end{pmatrix}, \tag{6b}$$

with spin up and spin down spinors

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

and

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

are eigenstates of $H_0$ in eq. (5) with the same energy $E_n$, confirming that the energy levels of $H_0$ are doubly degenerate due to the two possible spin states.

A constant magnetic field is now applied to the system, resulting in an additional term in the system Hamiltonian,[2]

$$H_B = -\boldsymbol{\mu}_e \cdot \mathbf{B} = \frac{e}{m_e}\mathbf{S} \cdot \mathbf{B} = \frac{\hbar e}{2m_e} \begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix}, \tag{7}$$

where we in the last equality have expressed the spin operator in the matrix formulation in terms of the Pauli matrices, $\mathbf{S} = \frac{\hbar}{2}[\sigma_x\hat{x} + \sigma_y\hat{y} + \sigma_z\hat{z}]$, and written $\mathbf{B} = B_x\hat{x} + B_y\hat{y} + B_z\hat{z}$. The prefactor in the last equation is known as the Bohr magneton,

$$\mu_B = \frac{\hbar e}{2m_e}, \tag{8}$$

a natural unit for the magnetic moment of the electron.

[1] We do not include the quantum number $s$ in the state label since it is always equal to $\frac{1}{2}$.

[2] This term is often called the Zeeman term. A constant magnetic field also gives rise to other terms in the Hamiltonian, but we do not consider these here.

**c)** Use degenerate perturbation theory to find the first order correction to level $n$ in the case when $B_z = B$, and $B_x = B_y = 0$. What happens to the energy levels?

*Hint:* You will need to calculate the matrix elements

$$V_{mm'} \equiv \langle n, m|H_B|n, m'\rangle, \tag{9}$$

for different $m, m' = \pm\frac{1}{2}$. There are (at least) two ways to do this. (i) Use $S_z|n, m\rangle = \hbar m|n, m\rangle$ in eq. (9) directly, or (ii) use the matrix formulation for spin, and calculate the matrix elements using the position-spin space expressions in eqs. (6) and (7) together with

$$V_{mm'} = \int dx\ \Psi^\dagger_{nm}(x) H_B \Psi_{nm'}(x). \tag{10}$$

**d)** This problem can also be solved exactly, even when all $B_i \neq 0$. Using the position-spin space formulation, we get the eigenvalue equation

$$\begin{aligned} H\Psi(x) = (H_0 + H_B)\Psi(x) &= \begin{pmatrix} -\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2} + \mu_B B_z & \mu_B B_x - i\mu_B B_y \\ \mu_B B_x + i\mu_B B_y & -\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2} - \mu_B B_z \end{pmatrix} \begin{pmatrix} \Psi_1(x) \\ \Psi_2(x) \end{pmatrix} \\ &= E \begin{pmatrix} \Psi_1(x) \\ \Psi_2(x) \end{pmatrix} = E\Psi(x), \end{aligned} \tag{11}$$

where $\Psi$ is a position-dependent spinor. Show that by using $\Psi_1(x) = A_1\psi_n(x)$ and $\Psi_2(x) = A_2\psi_n(x)$, where $\psi_n(x)$ are the wavefunctions found in **a)**, we get the eigenenergies

$$E_{n\pm} = E_n \pm \mu_B|\mathbf{B}|. \tag{12}$$

Does this agree with the perturbation theory result in **c)**?

**e)** If we fill our system with $N$ electrons, the ground state of the free electron gas in the case $|\mathbf{B}| = 0$ has the same number of spin up and spin down electrons, $N_+ = N_- = N/2$. Based on the above results, how do you expect this to change when a magnetic field is applied to the system?