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FY2045 Solutions Problem set 10 fall 2023

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Problem 1

a) Since the perturbation is spherically symmetric and independent of spin, it commutes with all the operators that commute with the unperturbed Hamiltonian H_0 for the hydrogen atom. There is thus no mixing between the degenerate states and we can make this shortcut.

b) We notice that the potential is equal to the Coulomb potential for $r > R$, so we only have to take $r < R$ into account. Moreover, the perturbation term δV is given by the new potential minus the Coulomb potential,

$$\delta V(r) = V(r) - V_{\text{Coulomb}}(r) = \begin{cases} 0, & r \geq R, \\ E_0 \frac{2a_0}{R}\left(\frac{3}{2} - \frac{r^2}{2R^2}\right) - E_0\frac{2a_0}{r}, & r \leq R. \end{cases} \tag{1}$$

The first-order energy shift is then $E_0^{(1)} = \langle\psi_0|\delta V|\psi_0\rangle$. Integrating over angles gives us 4π and the energy shift is given by the radial integral

$$E_0^{(1)} = -\frac{8\pi E_0 a_0}{\pi a_0^3}\int_0^R \left[\frac{r^2}{2R^3} - \frac{3}{2R} + \frac{1}{r}\right] e^{-2r/a_0} r^2 dr\,. \tag{2}$$

To order $\frac{R^2}{a_0^2}$, the exponential can be set to unity, which greatly simplifies the integrals. Using $E_0 = -\frac{e^2}{8\pi\epsilon_0 a_0}$, we find

$$\begin{aligned} E_0^{(1)} &= -\frac{8}{a_0^2} E_0^{(0)} \left[\frac{R^5}{10R^3} - \frac{R^3}{2R} + \frac{R^2}{2} \right] \\ &= \underline{\underline{-\frac{4R^2}{5a_0^2} E_0^{(0)}}} \sim -10^{-10} E_0^{(0)} \,, \end{aligned} \tag{3}$$

which is a very small correction indeed.

Problem 2

a) We find the eigenvalues and eigenvectors by solving the equation

$$\hat{H}|v\rangle = E|v\rangle, \tag{4}$$

or in matrix notation

$$V_0 \begin{pmatrix} 1-\epsilon & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} . \tag{5}$$

For $\epsilon = 0$ the Hamiltonian is diagonal and the eigenvalues can be read off directly,

$$E_1^{(0)} = E_2^{(0)} = \underline{\underline{V_0}} \,, \qquad E_3^{(0)} = \underline{\underline{2V_0}} \,. \tag{6}$$

The normalized eigenvectors are the three unit vectors,

$$|v_1^{(0)}\rangle = \underline{\underline{\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}}} \,, \qquad |v_2^{(0)}\rangle = \underline{\underline{\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}}} \,, \qquad |v_3^{(0)}\rangle = \underline{\underline{\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}}} \,. \tag{7}$$

b) We find the exact eigenvalues by requiring $\det(\hat{H} - E\mathbb{I}) = 0$, which results in the secular equation

$$[V_0(1-\epsilon) - E][(V_0 - E)(2V_0 - E) - V_0^2\epsilon^2] = 0, \tag{8}$$

which we solve for E, resulting in the eigenvalues

$$E_1 = \underline{\underline{V_0(1-\epsilon)}}, \tag{9a}$$

$$E_{2,3} = \underline{\underline{\frac{3V_0}{2} \mp \frac{V_0}{2}\sqrt{1+4\epsilon^2}}}, \tag{9b}$$

where the sign of the second term is chosen to coincide with the labels of the $\epsilon = 0$ solutions.

To find the eigenvectors, we insert the eigenvalues E_n into

$$\hat{H}|v_n\rangle = E_n|v_n\rangle,$$

with $|v_n\rangle = \begin{pmatrix}\alpha_n & \beta_n & \gamma_n\end{pmatrix}^T$ and solve for the elements of $|v_n\rangle$. We then get

$$(1-\epsilon)\alpha_n = \frac{E_n}{V_0}\alpha_n, \tag{10a}$$

$$\beta_n + \epsilon\gamma_n = \frac{E_n}{V_0}\beta_n, \tag{10b}$$

$$\epsilon\beta_n + 2\gamma_n = \frac{E_n}{V_0}\gamma_n. \tag{10c}$$

For $n = 1$ we get the same eigenvector as before ($\alpha_1 = 1$, $\beta_1 = \gamma_1 = 0$),

$$|v_1\rangle = \underline{\underline{\begin{pmatrix}1\\0\\0\end{pmatrix}}}, \qquad E_1 = \underline{\underline{(1-\epsilon)V_0}}\,. \tag{11}$$

For $n = 2, 3$ we get from eq. (10b)

$$\beta_n = -\frac{V_0\epsilon}{V_0 - E_n}\gamma_n,$$

which we insert into eq. (10c):

$$\gamma_n = -\frac{V_0\epsilon}{2V_0 - E_n}\beta_n = \frac{V_0^2\epsilon^2}{(V_0 - E_n)(2V_0 - E_n)}.$$

Form the secular equation eq. (8) we have $(V_0 - E_n)(2V_0 - E_n) = V_0^2\epsilon^2$, so that we find

$$\gamma_{2,3} = 1,$$
$$\beta_{2,3} = \frac{2\epsilon}{1 \mp \sqrt{1+4\epsilon^2}} = -\frac{1 \pm \sqrt{1+4\epsilon^2}}{2\epsilon}.$$

Hence, we find the normalized eigenvectors

$$|v_{2,3}\rangle = \underline{\underline{\frac{1}{\sqrt{2}}\left[1 \mp \frac{1}{\sqrt{1+4\epsilon^2}}\right]^{\frac{1}{2}}\begin{pmatrix}0\\ -\frac{1\pm\sqrt{1+4\epsilon^2}}{2\epsilon}\\1\end{pmatrix}}}.$$

By Taylor expanding eq. (9b), we find the eigenenergies to second order in ϵ

$$E_2 = \underline{\underline{(1-\epsilon^2)V_0}} + \mathcal{O}(\epsilon^3)\,, \qquad E_3 = \underline{\underline{(2+\epsilon^2)V_0}} + \mathcal{O}(\epsilon^3)\,. \tag{12}$$

c) The perturbation is

$$\hat{H}_1 \;=\; V_0 \begin{pmatrix} -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix} \tag{13}$$

The first-order energy correction to the non-degenerate state $|v_3\rangle$ is

$$E_3^{(1)} \;=\; \langle v_3^{(0)}|H_1|v_3^{(0)}\rangle = V_0 \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \underline{0}\,. \tag{14}$$

This is consistent with the fact that the correction is of order ϵ^2, cf. E_3 in Eq. (12). To calculate the second-order correction to the energy, we need the off-diagonal matrix elements. They are calculated as above, we find

$$\langle v_1^{(0)}|H_1|v_3^{(0)}\rangle \;=\; 0\,, \tag{15}$$

$$\langle v_2^{(0)}|H_1|v_3^{(0)}\rangle \;=\; \epsilon V_0\,. \tag{16}$$

This yields

$$\begin{aligned} E_3^{(2)} \;&=\; \sum_{j=1,2} \frac{|\langle v_3^{(0)}|H_1|v_j^{(0)}\rangle|^2}{E_3^{(0)} - E_j^{(0)}}\,, \\ &=\; \frac{\epsilon^2 V_0^2}{E_3^{(0)} - E_2^{(0)}} \\ &=\; \underline{\underline{\epsilon^2 V_0}}\,. \end{aligned} \tag{17}$$

This result is again consistent with the fact that the correction is of order ϵ^2, cf. E_3 in Eq. (12).

The first-order correction to the eigenvector is given by

$$|v_3^{(1)}\rangle = \sum_{j=1,2} \frac{\langle v_j^{(0)}|H_1|v_3^{(0)}\rangle}{E_3^{(0)} - E_j^{(0)}} |v_j^{(0)}\rangle = \epsilon |v_2^{(0)}\rangle. \tag{18}$$

Hence, to first order in ϵ

$$|v_3\rangle \approx \begin{pmatrix} 0 \\ \epsilon \\ 1 \end{pmatrix}, \tag{19}$$

which is in perfect agreement with the Taylor expansion of the exact solution

$$|v_3\rangle = \frac{1}{\sqrt{2}} \left[1 + \frac{1}{\sqrt{1+4\epsilon^2}}\right]^{\frac{1}{2}} \begin{pmatrix} 0 \\ -\frac{1-\sqrt{1+4\epsilon^2}}{2\epsilon} \\ 1 \end{pmatrix} \approx [1 + \mathcal{O}(\epsilon^2)] \begin{pmatrix} 0 \\ \epsilon + \mathcal{O}(\epsilon^3) \\ 1 \end{pmatrix} \approx \begin{pmatrix} 0 \\ \epsilon \\ 1 \end{pmatrix}.$$

d) In the degenerate subspace, we must diagonalize the perturbation. The matrix elements are

$$\langle v_1^{(0)}|H_1|v_2^{(0)}\rangle = 0\,, \tag{20}$$
$$\langle v_1^{(0)}|H_1|v_1^{(0)}\rangle = -\epsilon V_0\,, \tag{21}$$
$$\langle v_2^{(0)}|H_1|v_2^{(0)}\rangle = 0\,. \tag{22}$$

The perturbation is then

$$\hat{H}_1 = V_0 \begin{pmatrix} -\epsilon & 0 \\ 0 & 0 \end{pmatrix}\,. \tag{23}$$

The first-order corrections $E_{1,2}^{(1)}$ are given by eigenvalues of this matrix, which we find directly: $-\epsilon V_0$ and 0. This is consistent with the shift of E_1, cf. Eq. (11) and the shift in E_2, which is of order ϵ^2, E_2 in Eq. (12).

Problem 3

a) In position space, we get the Scrödinger equation

$$-\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2}\psi(x) = E\psi(x). \tag{24}$$

We try a solution of the form $\psi(x) = Ae^{ikx}$, which gives

$$\frac{\hbar^2 k^2}{2m_e}\psi(x) = E\psi(x). \tag{25}$$

From the periodic boundary conditions, $\psi(x) = \psi(x+L)$, we get the requirement $e^{ikL} = 1$. Hence, we have

$$k_n = \frac{2\pi n}{L}, \tag{26}$$

with $n = 0, \pm 1, \pm 2, \ldots$, and

$$E_n = \frac{\hbar^2 k_n^2}{2m_e}. \tag{27}$$

Finally, we determine the constant A by requiring normalization,

$$1 = \int_0^L dx\ \psi_n(x)^*\psi_n(x) = |A|^2 \int_0^L dx = L|A|^2. \tag{28}$$

Hence, choosing A real and positive, we get the normalized wavefunctions

$$\psi_n = \frac{1}{\sqrt{L}} e^{ik_n x}. \tag{29}$$

b) Using the matrix notation, we get

$$H_0\Psi_{n+}(x) = \begin{pmatrix} -\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2} & 0 \\ 0 & -\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2} \end{pmatrix} \begin{pmatrix} \psi_n(x) \\ 0 \end{pmatrix} = \begin{pmatrix} -\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2}\psi_n(x) \\ 0 \end{pmatrix} = \begin{pmatrix} E_n\psi_n(x) \\ 0 \end{pmatrix}$$
$$= E_n\Psi_{n+}(x). \tag{30}$$

Following the same procedure for Ψ_{n-}, we get

$$H_0\Psi_{n-}(x) = E_n\Psi_{n-}(x). \tag{31}$$

Hence, both $\Psi_{n\pm}$ are eigenstates of the Hamiltonian H_0 with eigenvalue E_n, as expected for a spin-independent H_0. In fact, *any* spinor is an eigenspinor of H_0, since H_0 is diagonal in spin space.

c) Since the level n is doubly degenerate, we have to use degenerate perturbation theory, which in general means we have to solve the matrix equation

$$\begin{pmatrix} V_{++} - E^{(1)}_{n\alpha} & V_{+-} \\ V_{-+} & V_{--} - E^{(1)}_{n\alpha} \end{pmatrix} \begin{pmatrix} U_{+\alpha} \\ U_{-\alpha} \end{pmatrix} = 0, \tag{32}$$

with label $\alpha = \pm$. To obtain non-trivial solutions we require a zero determinant, resulting in a secular equation with solutions

$$E^{(1)}_{n\pm} = \frac{V_{++} + V_{--}}{2} \pm \frac{1}{2}\sqrt{(V_{++} - V_{--})^2 + 4|V_{+-}|^2}, \tag{33}$$

where we have used $V_{+-} = V^*_{-+}$. We then calculate the matrix elements using either of the two approaches mentioned in the hint, with $H_B = \frac{2\mu_B}{\hbar}BS_z$.

(i) Using the states $|n, m\rangle$ directly, we get

$$V_{mm'} = \frac{2\mu_B B}{\hbar}\langle n, m|S_z|n, m'\rangle = \frac{2\mu_B B}{\hbar}\langle n, m|\hbar m'|n, m'\rangle = 2\mu_B B m\delta_{mm'}, \tag{34}$$

where the last equality follows from the orthonormality of the states $|n, m\rangle$. Hence, with $m = \pm\frac{1}{2}$, we have

$$V_{++} = +\mu_B B, \tag{35}$$
$$V_{--} = -\mu_B B, \tag{36}$$
$$V_{+-} = V_{-+} = 0. \tag{37}$$

(ii) In the matrix formulation for spin $\frac{1}{2}$, we defined the operator matrix for an operator $\hat{F}$ as

$$F = \begin{pmatrix} \langle +|\hat{F}|+\rangle & \langle +|\hat{F}|-\rangle \\ \langle -|\hat{F}|+\rangle & \langle -|\hat{F}|-\rangle \end{pmatrix}. \tag{38}$$

Hence, if we express H_B with $\mathbf{B} = B\hat{z}$ using spin operator matrix $S_z = \hbar\sigma_z/2$, we get

$$H_B = \mu_B \begin{pmatrix} B & 0 \\ 0 & -B \end{pmatrix}. \tag{39}$$

Using the formula given in the problem text[1] together with the above matrix, we get

$$V_{mm'} = \mu_B \int dx\ |\psi_n(x)|^2 \chi_m^\dagger \begin{pmatrix} B & 0 \\ 0 & -B \end{pmatrix} \chi_{m'} = 2\mu_B B m \delta_{mm'}, \tag{45}$$

where we have used the normalization of ψ_n. Since there is no position dependence in H_B, we could actually have read off the matrix elements $V_{mm'}$ directly from eq. (39) based on eq. (38), giving the same result as was found above.

Hence, we get the first order corrections,

$$E_{n\pm}^{(1)} = \pm\mu_B B. \tag{46}$$

To first order in perturbation theory, each level is split into two

$$E_{n\pm} = \frac{\hbar^2 k_n^2}{2m_e} \pm \mu_B B. \tag{47}$$

[1]For completeness, let's show how the position-spin space formula for $V_{mm'}$ is obtained. We have

$$V_{mm'} = \langle n, m|H_B|n, m'\rangle = \int dx \int dx' \sum_{l,l'=\pm\frac{1}{2}} \langle n, m||x, l\rangle\langle x, l|H_B|x', l'\rangle\langle x', l'||n, m'\rangle, \tag{40}$$

where we have inserted two completeness relations $1 = \int dx \sum_m |x, m\rangle\langle x, m|$. Keeping it general, with $H_B = H_B(\hat{x}, \hat{p}_x)$, we get

$$V_{mm'} = \int dx \int dx' \sum_{l,l'=\pm\frac{1}{2}} \langle n, m|x, l\rangle\langle l|H_B(x, -i\hbar\partial_x)|l'\rangle\delta(x - x')\langle x', l'|n, m'\rangle, \tag{41}$$

where we have used the formula $\langle x|\hat{F}(\hat{x}, \hat{p}_x)|x'\rangle = F(x, -i\hbar\partial_x)\delta(x - x')$. Performing the integral over x', we can write the above equation as

$$V_{mm'} = \int dx\ \begin{pmatrix} \langle n, m|x, +\rangle & \langle n, m|x, -\rangle \end{pmatrix} \begin{pmatrix} \langle +|H_B(x, -i\hbar\partial_x)|+\rangle & \langle +|H_B(x, -i\hbar\partial_x)|-\rangle \\ \langle -|H_B(x, -i\hbar\partial_x)|+\rangle & \langle -|H_B(x, -i\hbar\partial_x)|-\rangle \end{pmatrix} \begin{pmatrix} \langle x, +|n, m'\rangle \\ \langle x, -|n, m'\rangle \end{pmatrix}. \tag{42}$$

Comparing this with the definition for the states $\Psi_{n\pm}$ in the problem set, and the matrix notation in eq. (38), we see that we can write the above as

$$V_{mm'} = \int dx\ \Psi_{nm}^\dagger(x) H_B \Psi_{nm'}(x). \tag{43}$$

If H_B has no position dependence, the space and spin parts of the above equation separate completely, giving us the simplified expression for the matrix elements,

$$V_{mm'} = \chi_m^\dagger H_B \chi_{m'}. \tag{44}$$

Extra: This was not asked for in the problem text, but to determine the "limit" states, we could now insert these energy corrections into the matrix equation eq. (32). For $\alpha = +$ we get

$$\begin{pmatrix} 0 & 0 \\ 0 & -2\mu_B B \end{pmatrix} \begin{pmatrix} U_{++} \\ U_{-+} \end{pmatrix} = 0, \tag{48}$$

meaning we have $U_{-+} = 0$, and $U_{++} = 1$ due to normalization. The state corresponding to the energy E_{n+} to first order is therefore $|n, +\frac{1}{2}\rangle$. In the same way we find that the state corresponding to E_{n-} is $|n, -\frac{1}{2}\rangle$. Hence, the spin down state is lowered in energy compared to the spin up state when a magnetic field is applied in the positive z direction. We could, however, have realized this directly since the off-diagonal elements $V_{\pm\mp}$ where zero, indicating that the spin-up and -down states are the "good" or "limit" states.

d) Using the given ansatz, where we know that

$$-\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2}\psi_n(x) = E_n\psi_n(x), \tag{49}$$

we get the eigenvalue equation

$$\begin{pmatrix} E_n + \mu_B B_z & \mu_B B_x - i\mu_B B_y \\ \mu_B B_x + i\mu_B B_y & E_n - \mu_B B_z \end{pmatrix} \begin{pmatrix} A_1\psi_n \\ A_2\psi_n \end{pmatrix} = E \begin{pmatrix} A_1\psi_n \\ A_2\psi_n \end{pmatrix}. \tag{50}$$

Cancelling the overall factor of ψ_n, we are left with the matrix equation

$$\begin{pmatrix} E_n + \mu_B B_z - E & \mu_B B_x - i\mu_B B_y \\ \mu_B B_x + i\mu_B B_y & E_n - \mu_B B_z - E \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = 0. \tag{51}$$

Again, this is an eigenvalue equation, which we solve by requiring that the determinant must be zero, resulting in the secular equation

$$(E_n + \mu_B B_z - E)(E_n - \mu_B B_z - E) - \mu_B^2 B_x^2 - \mu_B^2 B_y^2 = (E_n - E)^2 - \mu_B^2 \mathbf{B}^2 = 0. \tag{52}$$

Hence, the exact energies are

$$E_{nm} = E_n \pm \mu_B |\mathbf{B}|. \tag{53}$$

The energy levels are spin-split due to the magnetic field — the electrons with spin direction opposite of $\mathbf{B}$ will have lower energy than the electrons with spin direction parallel to $\mathbf{B}$. In the case $\mathbf{B} = B_z\hat{z}$ this agrees exactly with the first order result obtained earlier.

e) Assuming for simplicity that $\mathbf{B} = B_z\hat{z}$, spin down electrons will have lower energy than spin up electrons. Hence, the total energy of the system will be minimized by having more electrons with spin down compared to spin up, that is $N_- > N_+$.

Extra, not asked for in the problem: It's possible to calculate the difference in occupation numbers based on an applied field B_z. When we studied the non-interacting fermion gas, we approximated the sum over $\mathbf{k}$ with an integral in the macroscopic limit, i.e. when the system size is large. The number of fermions in the system could be calculated by filling all $\mathbf{k}$ states up to $|\mathbf{k}| = k_F$. We can use the same approach now, but with a spin-dependent Fermi wavenumber, $k_{F\pm}$. For our 1D system, we get the particle numbers

$$N_\pm = \frac{L}{2\pi}\int_{-k_{F\pm}}^{k_{F\pm}} dk = \frac{k_{F\pm}L}{\pi}, \tag{54}$$

where $m = \pm$, and $L/(2\pi)$ is the density of states in k space. The total energy of all electrons with spin quantum number m is given by

$$\begin{aligned} E_\pm &= \frac{L}{2\pi}\int_{-k_{F\pm}}^{k_{F\pm}} dk\ E_\pm(k) = \frac{L}{\pi}\int_0^{k_{F\pm}} dk\ \left[\frac{\hbar^2 k^2}{2m_e} \pm \mu_B|\mathbf{B}|\right] \\ &= \frac{L}{\pi}\left[\frac{\hbar^2 k_{F\pm}^3}{6m_e} \pm \mu_B|\mathbf{B}|k_{F\pm}\right]. \end{aligned} \tag{55}$$

The total system energy is then

$$E_{\text{tot}} = E_+ + E_- = \frac{\hbar^2 L}{6\pi m_e}[k_{F+}^3 + k_{F-}^3] + \frac{\mu_B|\mathbf{B}|L}{\pi}[k_{F+} - k_{F-}] \tag{56}$$

For a given particle number N we must have $N_+ + N_- = N$. Hence,

$$\frac{L}{\pi}[k_{F+} + k_{F-}] = N \quad \rightarrow k_{F-} = \pi\rho - k_{F+}, \tag{57}$$

where we have defined the particle density $\rho = N/L$. We now minimize the total energy with respect to k_{F+} using the above constraint:

$$\begin{aligned} &\frac{\partial E_{\text{tot}}}{\partial k_{F+}} = \frac{\hbar^2 L}{2\pi m_e}\left[k_{F+}^2 - (\pi\rho - k_{F+})^2\right] + \frac{2\mu_B|\mathbf{B}|L}{\pi} = 0, \\ \Rightarrow\quad &2\pi\rho k_{F+} - (\pi\rho)^2 + \frac{4m_e\mu_B|\mathbf{B}|}{\hbar^2} = 0, \\ \Rightarrow\quad &k_{F+} = \frac{\pi\rho}{2} - \frac{2m_e\mu_B|\mathbf{B}|}{\pi\rho\hbar^2}, \end{aligned}$$

Hence, we get the particle numbers

$$N_\pm = \frac{k_{F+}L}{\pi} = \frac{N}{2} \mp \frac{2m_e\mu_B|\mathbf{B}|L^2}{\pi^2\hbar^2 N}, \tag{58}$$

showing that as the field increases the number of particles with spin opposite to the field increases, while the number of particles with spin parallel to the field decreases in the ground state. This was done in 1D, but a similar analysis could be done also in 3D.