Note: These are examples of former P414 exam questions, with two for each chapter that we’ve discussed to date.

C5: (25 pts.) Consider the ground state of a system consisting of $N$, free, non-interacting, non-relativistic, spin-1/2 Fermions of mass $m$, where $N$ is a very large number. In class (and our textbook), we confined the particles to a cubical volume with sides of length $L$ and impenetrable walls. Now assume the particles are confined in a cubical volume with sides of length $L$, but obeying “periodic boundary conditions” (i.e., $\psi$ and its first derivative must both be periodic in all three directions, with period $L$). Calculate the Fermi momentum for this case. (Note: Just stating the answer without justification will earn zero points.)

C5: (25 pts.) An extremely simple (maybe “simplistic”?!?) model for an isolated metal atom is a single electron which is free to move within a cubical box with sides of length $a$. (Note: This is NOT a hydrogen atom!) Assume the electron in the isolated atom is in the ground state. Now consider the case where very many (e.g., Avogadro’s number) such atoms are placed in a three-dimensional cubic lattice so they don’t overlap but their surfaces just touch. Assume that, in this case, the electrons are no longer localized to a single atom, but become free to move (without interactions) throughout the entire volume associated with all of the atoms. Calculate the binding energy per atom when the atoms are placed next to each other.

C7: In addition to the Coulomb and fine-structure interactions, the electron and proton in the hydrogen atom interact via the spin-spin interaction $H’ = \beta \mathbf{S}_e \cdot \mathbf{S}_p$, where $\beta$ is a very small positive constant. Define the energy of the hydrogen ground state after considering the Coulomb and fine-structure interactions to be $E = 0$.

(a) (13 pts) What are the energies, quantum numbers, and (remaining, if any) degeneracies of the hydrogen ground state system after the additional effects introduced by $H’$ are also included?

(b) (12 pts) Now place each of the states from part (a) in a very weak external magnetic field $\mathbf{B} = B_0 \hat{z}$. How does this further change the energy of each state that you found in part (a)?

C7: A hydrogen-like atom in its ground state consists of a spinless particle with mass $m_\text{e}$ and charge $-e$ orbiting an infinitely heavy, spinless particle with charge $+e$. The atom is placed in a weak, uniform magnetic field $\mathbf{B} = B_0 \hat{z}$.

(a) (6 pts.) Show that the leading-order correction to the ground state energy is proportional to $B_0^2$.

(b) (13 pts.) Calculate the leading-order correction to the ground state energy due to the magnetic field.

(c) (6 pts.) Show that your result from part (b) can be interpreted that the hydrogen-like atom develops a magnetic moment when placed in the magnetic field, and determine the corresponding effective magnetic moment. Note: This is the quantum mechanical origin of diamagnetism.

C8: Consider the lowest lying excited states of the neutral helium atom.

(a) (4 pts.) Specify the occupied electron orbitals and the angular momentum (in Russell-Saunders notation) for the first and second excited states. Be sure to indicate which is which.

(b) (10 pts.) Give the best approximation that you can for the actual wave functions of the first and second excited states of the neutral helium atom without doing a detailed calculation. Describe how you would use the variational method to improve the wave functions that you
have specified, and whatever difficulties would arise in doing so, but don’t actually carry out
the calculations.

c) (9 pts.) If you have done parts (a) and (b) correctly, then in first-order perturbation theory you
can write the energies of your first and second excited states in the form \( E_1 + I_1 \pm I_2 \), where \( E_1 \)
is a constant and \( I_1 \) and \( I_2 \) are integrals. Calculate the constant \( E_1 \), and give explicit integral
expressions for \( I_1 \) and \( I_2 \). To make the definition of \( I_2 \) unambiguous, assign the lower (minus)
sign to the first excited state and the upper (plus) sign to the second excited state. Do not
perform the integrations.

d) (2 pts.) Indicate whether each of the integrals \( I_1 \) and \( I_2 \) will end up being positive or negative
and give physical reasons (not numerical calculations) to justify your answers.

C8: NOTE: We have not yet covered the material that is relevant to part (c) of this problem. We’ll get to it in Griffiths, Chapter 11.
The ground and low-lying states of the neutral \( N \) atom have the electronic configuration
\( 1s^22s^22p^3 \).

(a) (10 pts.) Determine the possible quantum numbers of the low-lying states of the \( N \) atom in
Russell-Saunders notation. Which state would you expect to be the ground state?

(b) (5 pts.) The low-lying states of the \( O \) atom (one electron more than \( N \)) are seen to have the \( ^1S \),
\( ^3P \), and \( ^1D \) configurations. What are the possible quantum numbers (in Russell-Saunders
notation) of the excited states of the \( N \) atom that have the electronic configuration \( 1s^22s2p^4 \)?

(c) (10 pts.) Assume that all of the states that you gave in part (b) are higher in energy than those
that you gave in part (a). Which pairs of states from parts (a) and (b) would you expect to
have fast \( E1 \) transitions?

C9: (25 pts.) A particle with mass \( m \) and total energy \( E = 0 \) is moving in one dimension under the
influence of a potential given by:

\[
V(x) = V_0 \left( 1 - \frac{x^2}{a^2} \right)
\]

where \( V_0 \) and \( a \) are positive constants. Assume the particle is incident from the region \( x < -a \).
Find the approximate transmission coefficient for the particle to end up in the region \( x > a \).
What conditions need to hold for your approximation to be valid?

C9: A particle of mass \( m \) is free to move in one dimension under the influence of the potential

\[
V(x) = V_0 |x|/a
\]

where \( V_0 \) and \( a \) are positive constants.

(a) (20 pts) Use the WKB approximation to estimate the energy of the \( n \)th state. Assume the
states are numbered such that the ground state has \( n = 0 \).

(b) (5 pts) Now assume the same particle is moving in three dimensions under the influence of
the potential

\[
V(r) = V_0 r/a.
\]
What are the allowed WKB energies of the s-wave states?
Mid-Term Exam, Problem 1

Wave functions for free particles are sinusoidal. For period $L$, we need

$$k_{x, y, z} = \frac{2\pi n}{L}$$

Perhaps most convenient is:

$$4 \sim \exp \left\{ \frac{2\pi n_x}{L} x + \frac{2\pi n_y}{L} y + \frac{2\pi n_z}{L} z \right\} \quad \text{with}$$

$$k^2 = \left( \frac{2\pi}{L} \right)^2 (n_x^2 + n_y^2 + n_z^2) \quad \text{and} \quad 2 \text{ states (spin)} \quad \text{per volume}$$

$$\left( \frac{2\pi}{L} \right)^3 \text{ in } k\text{-space}. \quad \text{Thus, to have } N \text{ unique states we need:}$$

$$N = 2 \cdot \frac{4 \pi^2 k_F^3}{(2\pi)^3} = \frac{4}{3} \cdot \frac{\rho}{L^3} \quad \Rightarrow \quad k_F^3 = 3\pi^2 \frac{N}{L^3}$$

$$k_F = \left( \frac{3\pi^2 \rho}{L^3} \right)^{1/3} \quad \text{or} \quad \rho_F = \frac{1}{L} \left( \frac{3\pi^2 \rho}{L^3} \right)^{1/3}$$

same as in class with different boundary conditions.
Mid-Term Exam: Problem 1

The binding energy of the 1D infinite square well ground state is \( \frac{\epsilon^2}{2m^2} \). In 3D, \( k^2 = k_x^2 + k_y^2 + k_z^2 \Rightarrow E_{gs} = \frac{3}{2} \frac{\hbar^2}{2m} \)

In the final state, \( \langle E \rangle = \frac{3}{5} \epsilon F = \frac{3}{5} \frac{\hbar^2 n_F^2}{2m} \) with \( k_F = (3\pi^2 n_F)^{1/3} \). For this case, \( \rho = \frac{1}{a^3} \Rightarrow E = \frac{3}{10} \frac{\hbar^2}{m \frac{a^2}{\pi^2}} \)

The binding energy is \( 3\pi^2 \frac{\hbar^2}{2m^2} - 3 \frac{(3\pi^2)^{2/3}}{5} \frac{\hbar^2}{2m^2} \)

\( = 3\pi^2 - \frac{3}{5} (3\pi^2)^{2/3} \frac{\hbar^2}{2m^2} \)

Note: If I take \( a = 4 \) Å, which is not a crazy guess, then this gives 5.7 eV/atom, which is good to a factor of a couple. Not bad for an incredible simplistic model!
Final Exam, Problem 1

(a) $H'$ commutes with $\mathbf{S}_{\text{tot}}^2$, so the eigenfunctions are the singlet and triplet states.

\[
\mathbf{S}^2 = S_e^2 + 2 \mathbf{S}_e \cdot \mathbf{S}_p + S_p^2 \Rightarrow S_e \cdot S_p = \frac{1}{2} \left[ S^2 - S_e^2 - S_p^2 \right]
\]

⇒ Singlet: $4 = \frac{1}{\sqrt{2}} \left( |\uparrow_e \downarrow_p \rangle - |\downarrow_e \uparrow_p \rangle \right)$, $S^2_{\text{tot}} = 0$, $S_{\text{tot}} = 0$

\[
E = \langle H' \rangle = \frac{1}{2} \beta \left[ \begin{array}{c} 0 \ - \ 1 \left( \frac{3}{2} \right) \ - \ 1 \left( \frac{3}{2} \right) \ + \ \frac{3}{2} \end{array} \right] = -\frac{3}{4} \beta
\]

⇒ Triplet: $4 = \frac{3}{\sqrt{2}} \left( |\uparrow_e \uparrow_p \rangle + |\downarrow_e \downarrow_p \rangle \right)$, with $S^2_{\text{tot}} = 2h^2$, $S_{\text{tot}} = 1$

\[
E = \langle H' \rangle = \frac{1}{2} \beta \left[ \begin{array}{c} 1 \left( \frac{1}{2} \right) \ - \ \frac{1}{2} \left( \frac{3}{2} \right) \ - \ \frac{1}{2} \left( \frac{3}{2} \right) \ - \ \frac{1}{2} \end{array} \right] = +\frac{1}{4} \beta
\]

3-fold degenerate

(b) $H = -\frac{e^2}{m} \mathbf{S_e} \cdot \mathbf{B}$ (neglecting the very small proton contribution)

⇒ $H = \frac{e^2}{m} \frac{S_e^2}{h} B_\theta$ ⇒

Singlet: $\Delta E = 0$

Triplet: $|\uparrow_e \uparrow_p \rangle$: $\Delta E = +\frac{1}{2} \frac{e B \hbar}{m}$

$\frac{1}{2} \left( |\uparrow_e \downarrow_p \rangle + |\downarrow_e \uparrow_p \rangle \right)$: $\Delta E = 0$

$|\downarrow_e \downarrow_p \rangle$: $\Delta E = -\frac{1}{2} \frac{e B \hbar}{m}$

All degeneracies have been broken.
Final Exam: Problem 4

(a) \( \vec{L} = 0 \) for the ground state, while there is no spin in this problem. Therefore, the part of the Hamiltonian that is linear in \( B \) is \( \frac{e^2}{2m} \vec{B} \cdot (\vec{L} \times \vec{S}) = 0 \). The leading-order effect then comes from the term:

\[
\frac{\hbar^2}{2m} \vec{A}^2 = \frac{e^2 \hbar^2}{2m} \left( \frac{1}{2} \vec{B}^2 \right) = \frac{e^2 \hbar^2}{8m} \frac{r^2 \sin^2 \theta}{r}
\]

and is quadratic in \( B_0 \), as requested.

(b) \( \psi = \frac{2}{\sqrt{\pi a^3}} e^{-\frac{r}{a}} \frac{1}{\sqrt{4\pi}} = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a^2}} \Rightarrow \psi = \frac{2\pi}{a^3} \int e^{-\frac{r}{a^2}} e^{-\frac{5}{a^2}} \, dr \int \sin^2 \theta (\sin \theta \, d\theta) \)

\[
\Delta E \approx \frac{e^2 B_0^2}{8m} \frac{1}{\pi a^3} \int_0^\infty e^{-\frac{r}{a^2}} e^{-\frac{5}{a^2}} \, dr \int_0^{\pi/2} \sin^2 \theta (\sin \theta \, d\theta)
\]

\[
= \frac{e^2 B_0^2}{8m} \frac{2\pi}{3\pi a^3} \int_0^\infty e^{-\frac{r}{a^2}} (\frac{1}{4} \, dr) = \frac{e^2 B_0^2}{4ma^3} \left( \frac{a^2}{3} \right)
\]

\[
= \frac{e^2 B_0^2}{3ma^3} \frac{r^2 \sin \theta}{r} = \frac{e^2 B_0^2}{4m}
\]

(c) \( \vec{E} = -\vec{r} \times \vec{B} = -\vec{r} \times \vec{B}_0 \hat{r} \Rightarrow \vec{E} = -\frac{e^2 a^2}{4m} \vec{B}_0 \hat{r} \)

points in the opposite direction from \( \vec{B} \) = diamagnetic!

Note: Electrons have spin. But this same approach will work for real atoms with all filled shells, so \( L = 0 \) and \( S = 0 \).
Mid-Term Exam, Problem 4

(a) First excited state: \(1s^2 2s^3 S_1\)

Second excited state: \(1s^2 2s^1 S_0\)

(b) 1st excited:
\[
\psi_{1s^2 2s} = \frac{4}{(r_1 r_2)} \sum_{l_1, l_2, m_1, m_2} \left( \begin{array}{c} l_1 \, l_2 \, m_1 \, m_2 \\ 1 \, 2 \, 0 \, 0 \end{array} \right) \chi_{l_1, m_1} \chi_{l_2, m_2}
\]

2nd excited:
\[
\psi_{1s^2 2s} = \frac{4}{(r_1 r_2)} \sum_{l_1, l_2, m_1, m_2} \left( \begin{array}{c} l_1 \, l_2 \, m_1 \, m_2 \\ 1 \, 2 \, 1 \, -1 \end{array} \right) \chi_{l_1, m_1} \chi_{l_2, m_2}
\]

These could be improved by treating \(Z = 1 + Z = 2\) as variational parameters and minimizing \(\langle H \rangle\). This is straightforward for the 1st excited state. However, for the 2nd excited state, extreme care is necessary to avoid falling into the ground state.

(c) The "clearest" approach sets \(E_i = \langle 4 | H_1 + H_2 | 4 \rangle\), where \(H_1 + H_2\) are the He atom single particle Hamiltonians and identify \(I_1 + I_2 = \langle 4 | \frac{e^2}{4 \pi \epsilon_0} \frac{1}{r_{12}} | 4 \rangle\). For \(E_{1s}\) we have:

Electron in \(1s\) for \(Z = 2\) \(\Rightarrow E = -Z^2 \frac{13.6 \text{eV}}{n^2} = (-4)(13.6 \text{eV})\).

Electron in \(2s\) for \(Z = 1\) has
\[
E = \langle \mathbf{T} \rangle + \langle V \rangle = \langle \mathbf{T} \rangle + 2Z^2 \langle V \rangle
\]
\[
= 13.6 \text{eV} + 2 \cdot 2 \cdot \frac{(-13.6 \text{eV})}{4} = -\frac{3}{4} (13.6 \text{eV}) \Rightarrow E = -\frac{3}{4} (13.6 \text{eV})
\]
Then $I_1 + I_2 = \frac{e^2}{4\pi\varepsilon_0} N_1^2 \left( \langle \phi_{15, 2=1}^{+} \phi_{25, 2=1}^{+} \rangle \pm \langle \phi_{15, 2=2}^{+} \phi_{25, 2=2}^{+} \rangle \right) \frac{1}{r_{12}} \ldots$

\[ = N_1^2 \frac{e^2}{4\pi\varepsilon_0} 2 \left[ \langle \phi_{15, 2=1}^{+} \phi_{25, 2=1}^{+} \rangle \frac{1}{r_{12}} \langle \phi_{15, 2=2}^{+} \phi_{25, 2=2}^{+} \rangle \right] \]

\[ \pm \langle \phi_{15, 2=2}^{+} \phi_{25, 2=1}^{+} \rangle \frac{1}{r_{12}} \langle \phi_{15, 2=1}^{+} \phi_{25, 2=2}^{+} \rangle \]

Thus, $I_1 = \frac{2 N_1^2 e^2}{4\pi\varepsilon_0} \langle \phi_{15, 2=2}^{+} \phi_{25, 2=1}^{+} \rangle \frac{1}{r_{12}} \langle \phi_{15, 2=1}^{+} \phi_{25, 2=2}^{+} \rangle$

and $I_2 = \frac{2 N_1^2 e^2}{4\pi\varepsilon_0} \langle \phi_{15, 2=1}^{+} \phi_{25, 2=2}^{+} \rangle \frac{1}{r_{12}} \langle \phi_{15, 2=2}^{+} \phi_{25, 2=1}^{+} \rangle$

(b) $I_2 > 0$ since the singlet state energy is larger.

Meanwhile, $I_1 > I_2 > 0$ since $\langle \frac{e^2}{4\pi\varepsilon_0} \frac{1}{r_{12}} \rangle$ must be positive (repulsive) for the first excited state.

Alternative approach

(c) $E_1 = -(z^2) \left( \frac{13.6\text{ eV}}{1^2} - (z) \left( \frac{13.6\text{ eV}}{2^2} \right) \right) = -(4\pi) \left( \frac{13.6\text{ eV}}{4} \right)$

In this case, $I_1$ above picks up an extra factor of $-\frac{1}{2} (13.6\text{ eV})$ from the remaining piece of the single-particle $\langle V \rangle$.

(d) The screening of the outer electron is only partial $\Rightarrow I_1 < 0$. 
Mid-Term Exam, Problem 3

(a) \[ \begin{array}{ccccccc}
m_L = +1 & m_L = 0 & m_L = -1 & m_L = -1 & m_L = 0 & m_S = \frac{3}{2} & \Rightarrow ^4S \\
\uparrow & \uparrow & \uparrow & \uparrow & \uparrow & 0 & \Rightarrow \ ^2D \\
\uparrow\downarrow & \uparrow & \downarrow & \uparrow & \downarrow & \Rightarrow \ ^2P \\
\uparrow & \downarrow & \uparrow & \downarrow & \uparrow & \Rightarrow \ ^2P \\
\uparrow & \uparrow & \downarrow & \uparrow & \Rightarrow \ ^2P \\
\Rightarrow \ ^4S_{3/2}, \ ^2D_{3/2, 5/2}, \text{and} \ ^2P_{1/2, 3/2} \\
The possible states are \( ^4S_{3/2}, \ ^2D_{3/2, 5/2} \), and \( ^2P_{1/2, 3/2} \).

(b) Combining the unpaired electron with \( ^1S \Rightarrow \ ^2S_{1/2} \)
Combining the unpaired electron with \( ^3P \Rightarrow \ ^2P_{1/2, 3/2} \)
Combining it with \( ^1D \Rightarrow \ ^2D_{3/2, 5/2} \)
\Rightarrow \text{Possibilities are} \( \ ^2S_{1/2}, \ ^2P_{1/2, 3/2}, \ ^4P_{1/2, 3/2, 3/2}, \text{and} \ ^2D_{3/2, 5/2} \).

(c) \( ^2S_{1/2} \rightarrow ^2P_{1/2, 3/2} \)
\( ^2P_{1/2, 3/2} \rightarrow ^2D_{3/2, 5/2} \) (but not \( ^2D_{5/2} \))
\( ^2P_{1/2, 3/2} \rightarrow ^2P_{1/2, 3/2} \)
\( ^2P_{1/2, 3/2} \rightarrow ^2P_{1/2, 3/2} \)
\( ^4P_{1/2, 3/2, 5/2} \rightarrow ^4S_{3/2} \)
\( ^2D_{3/2, 5/2} \rightarrow ^2P_{1/2, 3/2} \) (but not \( ^2D_{5/2} \))
Final Exam: Problem 1

The WKB approximation gives:

\[ T = e^{-2y} \text{ with } y = \frac{1}{\hbar} \int_{x_1}^{x_2} |p(x)| \, dx = \frac{1}{\hbar} \int_{-a}^{a} \sqrt{2mV_0(1 - \frac{k^2}{a^2})} \, dx \]

\[ = \frac{\pi}{\hbar} \sqrt{\frac{2mV_0}{a^2}} \int_{0}^{a} \sqrt{x^2 - k^2} \, dx = \frac{\pi}{\hbar} \sqrt{2mV_0} \left[ \frac{x}{2} \sqrt{x^2 - k^2} - \frac{k^2}{2} \log \left( x + \sqrt{x^2 - k^2} \right) \right]_{0}^{a} \]

\[ = \frac{\pi}{\hbar} \sqrt{\frac{2mV_0}{a^2}} \left( \frac{a}{2} \sqrt{a^2 - k^2} - \frac{k^2}{2} \log \left( a + \sqrt{a^2 - k^2} \right) \right) \]

\[ T \approx \exp \left\{ \frac{\pi}{\hbar} \sqrt{\frac{2mV_0a^2}{k^2}} \right\} \]

For this to hold, \(|p(x)|\) needs to vary slowly within the barrier. This is equivalent to the requirement that \(T \ll 1\).
Final Exam, Problem 2

(a) WKB requires \( \frac{1}{\hbar} \int_{k_n}^{k_n'} p(x) dx' = (n+\frac{1}{2}) \pi \), with \( E_n = V_0 \frac{k_n}{\alpha} \) \( \Rightarrow \)

\[
(n+\frac{1}{2}) \pi = \frac{2}{\hbar} \int_{0}^{x_n} \sqrt{2m(E_n - V_0 \frac{k'}{\alpha})} \, dk'
\]

\[
= \frac{2}{\hbar} \sqrt{2mV_0} \int_{0}^{x_n} \sqrt{x_n - k'} \, dk' = \sqrt{\frac{8mV_0}{\hbar^2 \alpha}} \int_{0}^{x_n} \sqrt{x'} \, dx'
\]

\[
= \sqrt{\frac{8mV_0}{\hbar^2 \alpha}} \frac{2}{3} x_n^{3/2} \Rightarrow x_n = \left[ \frac{9 \hbar^2 a (n+\frac{1}{2})^2 \pi^2 z^2}{32 \pi V_0} \right]^{1/3}
\]

\[
E_n = \frac{V_0}{\alpha} \left[ \frac{9 \hbar^2 V_0^2 (n+\frac{1}{2})^2 \pi^2 z^2}{32 m V_0} \right]^{1/3} = \left[ \frac{9 \hbar^2 V_0^2 (n+\frac{1}{2})^2 \pi^2 z^2}{32 m V_0} \right]^{1/3}
\]

with \( n = 0, 1, 2, \ldots \)

(b) The \( l=0 \) wave equation for \( u(r) = r R(r) \) has

\[
V_{\text{eff}}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} = V(r) \quad \text{[for s-wave]}, \text{ so it's identical to the 1-d wave equation. But the boundary condition for } u \text{ is } u(r=0) = 0 \Rightarrow \text{ only the odd eigenfuns from above are acceptable. } \Rightarrow \text{ Energies are the same, but } n \text{ is restricted to } 1, 3, 5, \ldots \]