Quantum Mechanics: Worksheet 8

Fine structure: spin-orbit interaction

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1 Kramers' relation

Consider the hydrogen-like atom. Derive Kramers' relation:

$$\frac{s}{4}\left[(2l+1)^2 - s^2\right] a_0^2 \langle r^{s-2}\rangle - Z\,(2s+1)\,a_0 \langle r^{s-1}\rangle + Z^2 \frac{s+1}{n^2}\langle r^s\rangle = 0.$$

(a) Consider a function $u = u(r)$. Show that, assuming the boundary terms vanish,

$$\int dr\, u r^s u' = -\frac{s}{2}\int dr\, u r^{s-1} u,$$

and use this result to show that

$$\int dr\, u' r^s u' = -\frac{2}{s+1}\int dr\, u' r^{s+1} u''.$$

(b) The radial equation of the hydrogen-like atom can be written as

$$u'' = \left[\frac{l(l+1)}{r^2} - \frac{2Z}{a_0 r} + \frac{Z^2}{n^2 a_0^2}\right] u,$$

where $u(r) = rR_{nl}(r)$. Prove this, and then use it to express $\int dr\, u r^s u''$ in terms of $\langle nl|r^s|nl\rangle$, $\langle nl|r^{s-1}|nl\rangle$, and $\langle nl|r^{s-2}|nl\rangle$.

(c) Now integrate $\int dr\, u r^s u''$ assuming the boundary terms vanish, and using the results of (a) and the radial equation from (b) to express it again (but differently) in terms of $\langle r^s\rangle$, $\langle r^{s-1}\rangle$, and $\langle r^{s-2}\rangle$.

(d) Equate the two different expressions for $\int dr\, u r^s u''$ and collect like terms to arrive at Kramers' relation.

2 Spin-orbit interaction

The spin-orbit interaction for a spherically-symmetric potential is given by

$$H_{so} = \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\boldsymbol{L}\cdot\boldsymbol{S}.$$

(a) Show that for the hydrogen-like atom with nuclear charge Ze,

$$H_{so} = \frac{Ze^2}{2m_e^2c^2}\frac{1}{r^3}\boldsymbol{L}\cdot\boldsymbol{S}.$$

(b) Use Kramers' relation together with your results from the previous worksheet to evaluate $\langle nl|r^{-3}|nl\rangle$.

The first-order correction due to spin-orbit interaction is harder to calculate because the operator $\boldsymbol{L}\cdot\boldsymbol{S}$ is not diagonal in each degenerate subspace. Note that

$$\boldsymbol{L}\cdot\boldsymbol{S} = \frac{1}{2}\left(L_+S_- + L_-S_+\right) + L_zS_z,$$

so that the only nonzero off-diagonal elements are between states $|l,m\rangle$ and $|l,m\pm1\rangle$ with different spin. This simplifies the calculation because it block diagonalizes the degenerate subspace. Use degenerate perturbation theory to calculate the correction for $l = 0, 1$.

(c) Show that there is no spin-orbit correction for $l = 0$.

(d) Calculate the matrix elements of $\boldsymbol{L} \cdot \boldsymbol{S}$ in the degenerate subspace for $l = 1$, which is spanned by the basis states

$$\{|p_+\rangle|\uparrow\rangle, |p_+\rangle|\downarrow\rangle, |p_0\rangle|\uparrow\rangle, |p_0\rangle|\downarrow\rangle, |p_-\rangle|\uparrow\rangle, |p_-\rangle|\downarrow\rangle\}.$$

(e) Find the eigenvalues and the corresponding eigenstates of $\boldsymbol{L} \cdot \boldsymbol{S}$ for $l = 1$. Label the eigenstates with the quantum numbers l, s, j, and $m_j = m_l + m_s$.

(f) Combine this result with the outcome of (b) for the radial part of the spin-orbit interaction to find the first-order spin-orbit correction to the energy levels for $l = 1$.

3 Fine structure

Combine your results for the kinetic energy correction, the Darwin term, and the spin-orbit interaction to find the total first-order fine-structure correction for $l = 0, 1$.

Angular-momentum ladder operators

$$L_+|l,m\rangle = \hbar\sqrt{(l-m)\,(l+m+1)}|l,m+1\rangle$$
$$L_-|l,m\rangle = \hbar\sqrt{(l+m)\,(l-m+1)}|l,m-1\rangle$$