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5.1. **Matrix formulation of angular momentum addition**

This problem will give some math behind the perturbation theory results we have been using so far. Consider a system of spin one-half operators \( \hat{s}_1, \hat{s}_2, \) and \( \hat{s}_3. \) Consider also the Hamiltonian

\[
\hat{H} = \alpha \hat{s}_1 \cdot \hat{s}_2 + \beta \hat{s}_2 \cdot \hat{s}_3.
\]

(a) Use the basis spanned by the vectors \( |\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\uparrow\down\rangle, \) and \( |\down\down\rangle. \) Write out the \( 8 \times 8 \) Hamiltonian matrix. Remember how to turn the dot product into a sum of \( z \) operators and raising/lowering operators. Show that it is block-diagonal in groups of \( 1 \times 1 \) and \( 3 \times 3 \) matrices.

(b) Write out one of the \( 1 \times 1 \) matrices. What is it’s eigenvalue. Yes, this is easy. Note that the answer is linear in \( \alpha \) and \( \beta. \)

(c) Write out one of the \( 3 \times 3 \) matrices explicitly (they should be the same so whichever). Find it’s spectrum (this means the eigenvalues). The sub-problems below help you to do this, but use whatever method you like.

i. From part 5.1b we know what one of the eigenvalues must be. This is because the eigenvalue form part 5.1b corresponds to a state with \( J_{\text{total}} = 3/2. \) Therefore, this eigenvalue must occur in the spectrum of our \( 3 \times 3 \) matrix as well, since it must have components with total \( z \) momentum at \( 3/2,1/2, -1/2, \) and \( 3/2. \)

ii. Write out the characteristic polynomial for the \( 3 \times 3 \) matrix. Use sums of powers of \( (\alpha + \beta) \) and \( (\alpha - \beta) \) for the coefficients. Or don’t, and it will be harder. Your choice.

iii. Since you know one of the factors, factor the characteristic polynomial down to a quadratic equation and use the quadratic formula.

(d) Assume \( \alpha \gg \beta. \) Find the first order Taylor expansion in terms of the small quantity \( \beta/\alpha \) (i.e. generate a power series and keep terms of order \( \alpha \) and \( \beta, \) but not \( \beta^2/\alpha). \)

(e) Now, we can do this whole process much more easily! Show that the eigenvalues of the Hamiltonian \( \hat{H}_0 = \alpha \hat{s}_1 \cdot \hat{s}_2 \) are \( \alpha/4 \) and \( -3\alpha/4. \) You will define the operator

\( \hat{J}_{12} = \hat{s}_1 + \hat{s}_2. \)
(f) As argued in class, the only term which is rotationally invariant, and commutes with $\hat{H}_0$, is $\hat{H}_C' = \hat{J}_{12} \cdot \hat{s}_3$. Find the eigenvalues of this matrix for the case $\alpha/4$ (the other case has $\hat{J}_{12} = 0$).

(g) The first order spectrum can be determined now, if we know the prefactor for $\hat{H}_C'$. Use this to find the first order approximation to the spectrum. Show that it matches your Taylor expansion.

(h) Now let $\hat{s}_1$ be a spin-one operator instead. Find the spectrum with the same Hamiltonian to first order in $\beta$. Wasn’t that easy? Imagine having to write out all the matrices. Yuck!

5.2. Breit-Rabi Formula

We are going to continue our work from class and derive a complete formula for the energies of a ground state alkali atom $J = S = 1/2$ with nuclear spin $I$. Recall that the Hamiltonian is (assuming a vertical field)

$$\hat{H} = g_s \mu_B B \hat{J}_z - g_I \mu_N B \hat{I}_z + A_{HF} \hat{I} \cdot \hat{J}.$$ 

(a) Expand out the dot product $\hat{I} \cdot \hat{J}$ into a sum of over $x$, $y$ and $z$, and then convert the answer to raising and lowering operators.

(b) Write a two by two matrix for the Hamiltonian in the basis of states with total projected spin $m_F$. (Hint: the two allowed states are $|I, m_I, J, m_J\rangle = |I, m_F - 1/2, 1/2, 1/2\rangle$ and $|I, m_F + 1/2, 1/2, -1/2\rangle$.) Show that the answer can be written in the form:

$$\begin{pmatrix} c_1 + c_2 & c_3 \\ c_3 & c_1 - c_2 \end{pmatrix},$$

and find the values $c_1$, $c_2$, and $c_3$.

(c) Diagonalize the matrix to find the eigenvalues.

(d) Consider the limiting case that $B = 0$. Does the result agree with the interval rule? Does the result depend on $m_F$? Why or why not?

(e) Consider the case of small $B$, perform a Taylor expansion around $B = 0$ to obtain the first non-zero correction. How does the result depend on $m_F$ (linear, quadratic, etc.)? Compare to the perturbation theory result from class.

(f) Consider the contrary limit that $A_{HF} = 0$.

(g) Expand for small values of $A_{HF}$ to obtain the first non-zero correction. Does the correction depend on $B$? Why or why not? (Again, compare to the perturbation theory result form class).