2.27: The Hyperfine Interaction in the Deutrium Atom

This tutorial is an addendum to the immediately preceeding one dealing with the hyperfine splitting in the hydrogen atom. It represents an alternative version of material that can be found in section 18.6 of Volume III of *The Feynman Lectures on Physics*.

The deuterium isotope of hydrogen consists of an electron, and a proton and neutron in the nucleus (a deuteron). All three fundamental particles are spin-1/2 fermions. However, the proton and the neutron in the nucleus collectively behave like a spin-1 particle in their magnetic interaction with the extra-nuclear electron. The spin-spin interaction between the electron and the nucleus is given below, where the superscript d refers to the proton-neutron nucleus.

$$\hat{H}_{SpinSpin} = A\left(J^d \sigma^e\right) = A\left(J_x^d \sigma_x^e + J_x^d \sigma_y^e + J_z^d \sigma_z^e\right)$$

The spin-1/2 and spin-1 operators required for this Hamiltonian are given below. The spin-1/2 operators are the familiar Pauli matrices. For a derivation of the spin-1 operators see *Quantum Mechanics Demystified* by David McMahon, chapter 10.

$$\sigma_x = \tfrac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \tfrac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \tfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$J_x = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad J_y = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad J_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Tensor multiplication is now used to represent the spin-spin operator in matrix format. In the interest of mathematical clarity the constant A a is set equal to unity.

$$H_{SpinSpin} = \text{kronecker}\left(J_x,\ \sigma_x\right) + \text{kronecker}\left(J_y,\ \sigma_y\right) + \text{kronecker}\left(J_x,\ \sigma_z\right)$$

We know ask Mathcad to calculate the eigenvalues and eigenvectors of the spin-spin operator. These results are displayed by constructing a matrix which contains the eigenvalues in the top row, and their eigenvectors in the columns below the eigenvalues.

$$\text{E} = \text{eigenvals}\left(H_{SpinSpin}\right) \qquad \text{EigenvalEigenvec} = \text{rsort}\left(\text{stack}\left(E^T,\ \text{eigenvecs}\left(H_{SpinSpin}\right)\right),\ I\right)$$

$$\text{EigenvalEigenvec} = \begin{pmatrix} -1 & -1 & 0.5 & 0.5 & 0.5 & 0.5 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & -0.816 & 0 & 0.577 & 0 & 0 \\ 0 & 0.577 & 0 & 0.816 & 0 & 0 \\ 0.577 & 0 & 0.816 & 0 & 0 & 0 \\ -0.816 & 0 & 0.577 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

These results are in agreement with Tables 18-5 and 18-6 in Feynman's text, a ground J = 1/2 state and an excited J = 3/2 state. We can go forward, as we did in the previous tutorial, by writing the electron and deuteron spin wavefunctions in vector format.

The spin states in vector format:

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The deuteron spin states in vector format (see McMahon):

$$|d_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad |d_0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad |d_{-1}\rangle \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Next we write the six electron-deuteron spin states in tensor format.

$$|+d_1\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\\0\end{pmatrix} = \begin{pmatrix}1\\0\\0\\0\\0\\0\end{pmatrix} \quad |+d_0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\\0\end{pmatrix} = \begin{pmatrix}0\\1\\0\\0\\0\\0\end{pmatrix} \quad |+d_{-1}\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\0\\1\end{pmatrix} = \begin{pmatrix}0\\0\\1\\0\\0\\0\end{pmatrix}$$

$$|-d_1\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\\0\end{pmatrix} = \begin{pmatrix}0\\0\\0\\1\\0\\0\end{pmatrix} \quad |-d_0\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\\0\end{pmatrix} = \begin{pmatrix}0\\0\\0\\0\\1\\0\end{pmatrix} \quad |-d_{-1}\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\0\\1\end{pmatrix} = \begin{pmatrix}0\\0\\0\\0\\0\\1\end{pmatrix}$$

These spin states are given the following labels to facilitate the calculation of energy matrix.

$$\mathrm{a} = \begin{pmatrix}1\\0\\0\\0\\0\\0\end{pmatrix} \quad \mathrm{b} = \begin{pmatrix}0\\1\\0\\0\\0\\0\end{pmatrix} \quad \mathrm{c} = \begin{pmatrix}0\\0\\1\\0\\0\\0\end{pmatrix} \quad \mathrm{d} = \begin{pmatrix}0\\0\\0\\1\\0\\0\end{pmatrix} \quad \mathrm{e} = \begin{pmatrix}0\\0\\0\\0\\1\\0\end{pmatrix} \quad \mathrm{f} = \begin{pmatrix}0\\0\\0\\0\\0\\1\end{pmatrix}$$

$$\mathrm{H} = \mathrm{H}_{SpinSpin}$$

$$\mathrm{eigenvals}\left(\begin{pmatrix} \mathrm{a}^T\mathrm{H}\,\mathrm{a} & \mathrm{a}^T\mathrm{H}\,\mathrm{b} & \mathrm{a}^T\mathrm{H}\,\mathrm{c} & \mathrm{a}^T\mathrm{H}\,\mathrm{d} & \mathrm{a}^T\mathrm{H}\,\mathrm{e} & \mathrm{a}^T\mathrm{H}\,\mathrm{f} \\ \mathrm{b}^T\mathrm{H}\,\mathrm{a} & \mathrm{b}^T\mathrm{H}\,\mathrm{b} & \mathrm{b}^T\mathrm{H}\,\mathrm{c} & \mathrm{b}^T\mathrm{H}\,\mathrm{d} & \mathrm{b}^T\mathrm{H}\,\mathrm{e} & \mathrm{b}^T\mathrm{H}\,\mathrm{f} \\ \mathrm{c}^T\mathrm{H}\,\mathrm{a} & \mathrm{c}^T\mathrm{H}\,\mathrm{b} & \mathrm{c}^T\mathrm{H}\,\mathrm{c} & \mathrm{c}^T\mathrm{H}\,\mathrm{d} & \mathrm{c}^T\mathrm{H}\,\mathrm{e} & \mathrm{c}^T\mathrm{H}\,\mathrm{f} \\ \mathrm{d}^T\mathrm{H}\,\mathrm{a} & \mathrm{d}^T\mathrm{H}\,\mathrm{b} & \mathrm{d}^T\mathrm{H}\,\mathrm{c} & \mathrm{d}^T\mathrm{H}\,\mathrm{d} & \mathrm{d}^T\mathrm{H}\,\mathrm{e} & \mathrm{d}^T\mathrm{H}\,\mathrm{f} \\ \mathrm{e}^T\mathrm{H}\,\mathrm{a} & \mathrm{e}^T\mathrm{H}\,\mathrm{b} & \mathrm{e}^T\mathrm{H}\,\mathrm{c} & \mathrm{e}^T\mathrm{H}\,\mathrm{d} & \mathrm{e}^T\mathrm{H}\,\mathrm{e} & \mathrm{e}^T\mathrm{H}\,\mathrm{f} \\ \mathrm{f}^T\mathrm{H}\,\mathrm{a} & \mathrm{f}^T\mathrm{H}\,\mathrm{b} & \mathrm{f}^T\mathrm{H}\,\mathrm{c} & \mathrm{f}^T\mathrm{H}\,\mathrm{d} & \mathrm{f}^T\mathrm{H}\,\mathrm{e} & \mathrm{f}^T\mathrm{H}\,\mathrm{f} \end{pmatrix}\right) = \begin{pmatrix}-1\\0.5\\0.5\\-1\\0.5\\0.5\end{pmatrix}$$

$$\mathrm{eigenvecs}\left(\begin{pmatrix} \mathrm{a}^T\mathrm{H}\,\mathrm{a} & \mathrm{a}^T\mathrm{H}\,\mathrm{b} & \mathrm{a}^T\mathrm{H}\,\mathrm{c} & \mathrm{a}^T\mathrm{H}\,\mathrm{d} & \mathrm{a}^T\mathrm{H}\,\mathrm{e} & \mathrm{a}^T\mathrm{H}\,\mathrm{f} \\ \mathrm{b}^T\mathrm{H}\,\mathrm{a} & \mathrm{b}^T\mathrm{H}\,\mathrm{b} & \mathrm{b}^T\mathrm{H}\,\mathrm{c} & \mathrm{b}^T\mathrm{H}\,\mathrm{d} & \mathrm{b}^T\mathrm{H}\,\mathrm{e} & \mathrm{b}^T\mathrm{H}\,\mathrm{f} \\ \mathrm{c}^T\mathrm{H}\,\mathrm{a} & \mathrm{c}^T\mathrm{H}\,\mathrm{b} & \mathrm{c}^T\mathrm{H}\,\mathrm{c} & \mathrm{c}^T\mathrm{H}\,\mathrm{d} & \mathrm{c}^T\mathrm{H}\,\mathrm{e} & \mathrm{c}^T\mathrm{H}\,\mathrm{f} \\ \mathrm{d}^T\mathrm{H}\,\mathrm{a} & \mathrm{d}^T\mathrm{H}\,\mathrm{b} & \mathrm{d}^T\mathrm{H}\,\mathrm{c} & \mathrm{d}^T\mathrm{H}\,\mathrm{d} & \mathrm{d}^T\mathrm{H}\,\mathrm{e} & \mathrm{d}^T\mathrm{H}\,\mathrm{f} \\ \mathrm{e}^T\mathrm{H}\,\mathrm{a} & \mathrm{e}^T\mathrm{H}\,\mathrm{b} & \mathrm{e}^T\mathrm{H}\,\mathrm{c} & \mathrm{e}^T\mathrm{H}\,\mathrm{d} & \mathrm{e}^T\mathrm{H}\,\mathrm{e} & \mathrm{e}^T\mathrm{H}\,\mathrm{f} \\ \mathrm{f}^T\mathrm{H}\,\mathrm{a} & \mathrm{f}^T\mathrm{H}\,\mathrm{b} & \mathrm{f}^T\mathrm{H}\,\mathrm{c} & \mathrm{f}^T\mathrm{H}\,\mathrm{d} & \mathrm{f}^T\mathrm{H}\,\mathrm{e} & \mathrm{f}^T\mathrm{H}\,\mathrm{f} \end{pmatrix}\right)$$

$$= \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0.577 & -0.816 & 0 & 0 \\ 0 & 0 & 0.816 & 0.577 & 0 & 0 \\ 0.577 & 0.816 & 0 & 0 & 0 & 0 \\ -0.816 & 0.577 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Appendix

While it's not directly pertinent to the subject of this tutorial, the interaction of two spin-1 systems is calculated below.

$$H_{SpinSpin} = (\mathrm{kronecker}\,(J_x,\ J_x) + \mathrm{kronecker}\,(J_y,\ J_y) + \mathrm{kronecker}\,(J_z,\ J_z))$$

$$H_{SpinSpin} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

We know ask Mathcad to calculate the eigenvalues and eigenvectors of the spin-spin operator.

$$\mathrm{E} = \mathrm{eigenvals}\left(H_{SpinSpin}\right) \quad \mathrm{EigenvalEigenvec} = \mathrm{rsort}\left(\mathrm{stack}\left(E^{T},\ \mathrm{eigenvecs}\left(H_{SpinSpin}\right)\right),\ 1\right)$$

$$\mathrm{EigenvalEigenvec} = \begin{pmatrix} -2 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0.707 & 0 & 0 & -0.707 & 0 & 0 & 0 & 0 \\ 0.577 & 0 & 0 & -0.707 & 0 & -0.408 & 0 & 0 & 0 \\ 0 & -0.707 & 0 & 0 & -0.707 & 0 & 0 & 0 & 0 \\ -0.577 & 0 & 0 & 0 & 0 & -0.816 & 0 & 0 & 0 \\ 0 & 0 & -0.770 & 0 & 0 & 0 & 0.707 & 0 & 0 \\ 0.577 & 0 & 0 & 0.707 & 0 & -0.408 & 0 & 0 & 0 \\ 0 & 0 & 0.707 & 0 & 0 & 0 & 0.707 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

These results are in agreement with Table 18-7 of Feynman's text. Reading from the left we have a singly degenerate J = 0 state, a triply degenerate J = 1 state, and a five-fold degenerate J = 2 state.
