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Two identical spin- $\frac{1}{2}$ particles interact via the Hamiltonian

$$H = J (S_1^x S_2^x + S_1^y S_2^y + K S_1^z S_2^z) + \mu (S_1^z + S_2^z) B$$

(a) Find the energy levels of this system assuming that the particles are in an anti-symmetric spatial wave function.

The total wave function for electrons must be anti-symmetric, so, if the spatial part is anti-symmetric, then the spin part must be symmetric to preserve the symmetry.

Now, let's rewrite the Hamiltonian into a more user friendly form.

$$S^2 = (S_1 + S_2)^2 = S_1^2 + S_2^2 + 2S_1 \cdot S_2 = S_1^2 + S_2^2 + 2(S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z)$$

$$\Rightarrow S_1^x S_2^x + S_1^y S_2^y = \frac{1}{2} (S^2 - S_1^2 - S_2^2) - S_1^z S_2^z$$

So, then the Hamiltonian becomes

$$H = J \left[\frac{1}{2} (S^2 - S_1^2 - S_2^2) + (K-1) S_1^z S_2^z \right] + \mu B (S_1^z + S_2^z)$$

note $S_i^2 = S_i(S_i+1) = \frac{1}{2}(\frac{1}{2}+1) = \frac{3}{4}$

so,

$$H = J \left[\frac{1}{2} S^2 - \frac{3}{4} + (K-1) S_1^z S_2^z \right] + \mu B (S_1^z + S_2^z)$$

what are the possible values of S ?

$$|S_1 - S_2| \leq S \leq |S_1 + S_2|$$

$$|\frac{1}{2} - \frac{1}{2}| \leq S \leq |\frac{1}{2} + \frac{1}{2}|$$

$$0 \leq S \leq 1$$

$$\Rightarrow S = 0 \text{ or } 1$$

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For $S=0$, $m_s=0$ and the only state possible is

$$|00\rangle = \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} \quad (1)$$

note: $|00\rangle$ is anti-symmetric ... if you let $\uparrow \rightarrow \downarrow$ and $\downarrow \rightarrow \uparrow$, you get back $-|00\rangle$

For $S=1$, $m_s = -1, 0, 1$ and the 3 states are

$$|1, -1\rangle = |\downarrow\downarrow\rangle$$

$$|1, 0\rangle = \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \quad (2)$$

$$|1, 1\rangle = |\uparrow\uparrow\rangle$$

note: all these states are symmetric. let $\uparrow \rightarrow \downarrow$ and $\downarrow \rightarrow \uparrow$ in $|1, 0\rangle$ and you get back $|1, 0\rangle$... The other two are trivially symmetric, so, for part (c), we want to find the energy levels of the $S=1$ (symmetric spin part).

So, we have

$$\langle 1, -1 | \langle H | H | 1, -1 \rangle = J \left[\frac{1}{2} S(S+1) - \frac{3}{4} + (K-1) S_1^z S_2^z \right] + \mu_B (S_1^z + S_2^z) \Big|_{S=1}$$

$$= J \left[1 - \frac{3}{4} + (K-1) \left(-\frac{1}{2}\right) \left(-\frac{1}{2}\right) \right] + \mu_B \left(-\frac{1}{2} + -\frac{1}{2}\right)$$

$$= J \left[\frac{1}{4} + \frac{K}{4} - \frac{1}{4} \right] - \mu_B$$

$$\therefore \boxed{E_{1,-1} = \frac{JK}{4} - \mu_B}$$

$$\begin{aligned}
 \langle 11,0 \rangle | < 101 | H | 110 \rangle &= \frac{1}{2} \left[J \left(\frac{1}{2} \cdot 2 - \frac{3}{4} + (K-1) \left(\frac{1}{2} \right) \left(-\frac{1}{2} \right) \right) + \mu B \left(\frac{1}{2} - \frac{1}{2} \right) + \right. \\
 &\quad \left. + J \left(1 - \frac{3}{4} + (K-1) \left(-\frac{1}{2} \right) \left(\frac{1}{2} \right) \right) + \mu B \left(-\frac{1}{2} + \frac{1}{2} \right) \right] \\
 &= \frac{1}{2} \left[J \left(\frac{1}{4} - \frac{K}{4} + \frac{1}{4} \right) + J \left(\frac{1}{4} - \frac{K}{4} + \frac{1}{4} \right) \right] \\
 &= \frac{2J}{2} \left(\frac{1}{2} - \frac{K}{4} \right)
 \end{aligned}$$

$$\therefore \boxed{E_{10} = J \left(\frac{1}{2} - \frac{K}{4} \right)}$$

$$\begin{aligned}
 \langle 11,1 \rangle | < 1,1 | H | 11,1 \rangle &= J \left[\frac{1}{4} + (K-1) \left(\frac{1}{4} \right) \right] + \mu B \left(\frac{1}{2} + \frac{1}{2} \right) \\
 &= J \left(\frac{K}{4} \right) + \mu B
 \end{aligned}$$

$$\Rightarrow \boxed{E_{11} = \frac{JK}{4} + \mu B}$$

b) repeat for a symmetric spatial wave function

Now, we use the anti-symmetric spin part (eq (1)).

$$\begin{aligned}
 \langle 10,0 \rangle | < 001 | H | 100 \rangle &= \frac{J}{2} \left[-\frac{3}{4} + (K-1) \left(\frac{1}{2} \right) \left(-\frac{1}{2} \right) \right] + \frac{\mu B}{2} \left(\frac{1}{2} - \frac{1}{2} \right) \\
 &\quad - \frac{J}{2} \left[-\frac{3}{4} + (K-1) \left(-\frac{1}{2} \right) \left(\frac{1}{2} \right) \right] - \frac{\mu B}{2} \left(-\frac{1}{2} + \frac{1}{2} \right)
 \end{aligned}$$

$$\Rightarrow \boxed{E_{00} = 0}$$