

1. Apply the variational method to find the ground state of the generic hamiltonian

$$H = H_0 + V \quad (1)$$

using trial states of the form

$$|a_1, \dots, a_n\rangle = \sum_{j=1}^{\infty} a_j |E_j\rangle \quad (2)$$

in which the state $|E_j\rangle$ is an eigenstate of H_0

$$H_0 |E_j\rangle = E_j |E_j\rangle \quad (3)$$

with energy E_j . Interpret your result.

$$\bar{H} = \frac{\langle a | H | a \rangle}{\langle a | a \rangle} = \frac{\sum E_j |a_j|^2 + \sum_{j,k} a_j^* a_k \langle E_j | V | E_k \rangle}{\sum |a_j|^2}$$

So

$$0 = \frac{\partial \bar{H}}{\partial a_j^*} = \frac{E_j a_j + \sum_k a_k \langle E_j | V | E_k \rangle}{\sum |a_j|^2}$$

$$= \frac{\left(\sum E_j |a_j|^2 + \sum_{j,k} a_j^* a_k \langle E_j | V | E_k \rangle \right) a_j}{\left(\sum |a_j|^2 \right)^2}$$

Multiply both sides by $\sum |a_j|^2$:

$$= \left(\sum E_j |a_j|^2 + \sum_{j,k} a_j^* a_k \langle E_j | V | E_k \rangle \right)$$

Get

$$E_j a_j + \sum_K a_K \langle E_j | V | E_K \rangle = \bar{H} a_j$$

So if \hat{H}_0 is the truncated diagonal matrix

$$\hat{H}_0 = \begin{pmatrix} E_1 & 0 & \dots & 0 \\ 0 & E_2 & & \\ \vdots & & \ddots & \\ 0 & & & E_n \end{pmatrix}$$

and \hat{V} is the $n \times n$ matrix with entries

$$\hat{V}_{jk} = \langle E_j | V | E_k \rangle$$

then the vector of coefficients

$$\psi = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

is an eigenvector of $\hat{H}_0 + \hat{V}$

$$(\hat{H}_0 + \hat{V}) \psi = \bar{H} \psi$$

with eigenvalue \bar{H} .

So: If one can compute all the matrix elements

$$\langle E_j | V | E_k \rangle$$

then one may use numerical programs to find the eigenvalues and eigenvectors of the truncated hamiltonian

$$\hat{H}_0 + \hat{V}.$$

This truncated-hamiltonian method works very well as long as there are not too many states $|E_k\rangle$ that are relevant and as long as one can compute the matrix elements $\langle E_j | V | E_k \rangle$.

2. Suppose two identical spin-one particles are both in s-states in some potential. If they also have the same value of the principal quantum number n , i.e., they are in the same space state, what are the possible values of the total angular momentum j ?

The identical particles are bosons, so the state must be symmetric under interchange of their labels. The space state is symmetric, so the spin state also must be symmetric.

The states with $j=2$ are symmetric because they are obtained by S_- from the state

$$|2,2\rangle = |1, m=1, 2, m=1\rangle + |1, m=2, 1, m=0\rangle$$

For instance,

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

The states with $j=1$ descend via S_- from

$$|1,1\rangle = \frac{1}{\sqrt{2}} (|1,0\rangle - |0,1\rangle)$$

and are antisymmetric. For instance

$$\frac{1}{\sqrt{2}} |1,0\rangle = S_- |1,1\rangle = \frac{1}{\sqrt{2}} (S_{1-} |1,0\rangle + S_{2-} |1,0\rangle - S_{1-} |0,1\rangle - S_{2-} |0,1\rangle)$$

$$= (|0,0\rangle + |1,-1\rangle - |-1,1\rangle - |0,0\rangle) \hbar$$

$$= (|1,-1\rangle - |-1,1\rangle) \hbar \quad \text{so}$$

$$|1,0\rangle = \frac{1}{\sqrt{2}} (|1,-1\rangle - |-1,1\rangle).$$

So the state with $j=0$ must be

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

which is symmetric; it can't have a $|0,0\rangle$ piece because then it would overlap with $|2,0\rangle$.

3. Consider two identical spin-one-half particles in an box of side L with a potential V_0 that is zero inside the box and infinite outside it. (a) If the particles do not interact, what are the energies and wave-functions (space and spin)? (b) Suppose now the potential is

$$V(\mathbf{r}_1, \mathbf{r}_2) = V_0(\mathbf{r}_1, \mathbf{r}_2) + a^2 \delta^{(3)}(\mathbf{r}_1 - \mathbf{r}_2) \quad (4)$$

in which \mathbf{r}_1 and \mathbf{r}_2 are the positions of the two particles. Show that the triplet states (i.e., those of total spin \hbar) are unaffected by the change in the potential.

The space wave functions for a single spin- $\frac{1}{2}$ particle are

$$\psi(x, y, z, \sigma) = \left(\frac{2}{L}\right)^{\frac{3}{2}} \sin n_1 \frac{x\pi}{L} \sin n_2 \frac{y\pi}{L} \sin n_3 \frac{z\pi}{L} \left|\frac{1}{2}, \sigma\right\rangle.$$

If the spin state is $|0, 0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$, then the space state must be symmetric. The 2-particle state then is

$$\frac{1}{\sqrt{2}} (|\vec{n}_1, \vec{n}_2\rangle + |\vec{n}_2, \vec{n}_1\rangle) |0, 0\rangle$$

with energy $E = \frac{\hbar^2 \pi^2}{2mL^2} (\vec{n}_1^2 + \vec{n}_2^2)$.

If the spin state is one of the triplet states $|1, m_s\rangle$, which are symmetric, then the space state must be antisymmetric. The states are

$$\frac{1}{\sqrt{2}} (|\vec{n}, \vec{m}\rangle - |\vec{m}, \vec{n}\rangle) |1, m_s\rangle \quad -1 \leq m_s \leq 1.$$

with the same energy $E = \frac{\hbar^2 \pi^2}{2mL^2} (\vec{n}^2 + \vec{m}^2), \vec{n} \neq \vec{m}.$

The potential annihilates the triplet states because

$$\begin{aligned} & \langle \vec{r}_1, \vec{r}_2 | \delta(\vec{r}_1 - \vec{r}_2) \left(\frac{1}{\sqrt{2}} (|m, m\rangle - |m, -m\rangle) \right) |1, m_s\rangle \\ &= \frac{1}{\sqrt{2}} \left[\psi_m(r_1) \psi_m(r_2) - \psi_m(r_1) \psi_{-m}(r_2) \right] \delta(r_1 - r_2) |1, m_s\rangle \\ &= \frac{\delta(r_1 - r_2)}{\sqrt{2}} \left[\psi_m(r_1) \psi_m(r_1) - \psi_m(r_1) \psi_{-m}(r_1) \right] |1, m_s\rangle = 0. \end{aligned}$$

So the potential does not change the energy levels of the triplet states.