Two Spin-1/2 Particles in a Double-Well Potential: Computational Approach

Although it is one of the oldest physical phenomena known to us, magnetism and magnetic materials are by far one of the most difficult and challenging subjects in physics. This is in part due to that understanding of magnetism requires many disciplines of physics: electrodynamics, statistical physics, and quantum mechanics. Further, when we consider the origin of magnetism in magnetic materials, it is necessary to discuss two ingredients: formation of a local magnetic moment and effective exchange interactions between local spin moments. To understand such concepts, we need to get some background knowledge in quantum mechanics.

I assume that most students in this camp are not familiar with the terms "spin moment" as well as "exchange interactions" as they are a sort of quantum mechanical jargon. Further, to understand the "interactions" between spin moments, one has to catch some idea about the quantum mechanics of not just one but many particles. Here I like to suggest a little project, through which you can figure out the essential mechanism of magnetism and magnetic interaction. Have fun!

Problem:

Consider a double-well potential in a typical "quantum mechanics" text book. The only difference here is that we like to consider not one but two spin-1/2 particles. To describe this system, one may use a two-particle Schrödinger's equation as follows:

$$\mathcal{H}_2\psi_2(x_1, s_1; x_2, s_2) = E\psi_2(x_1, s_1; x_2, s_2)$$

where the two particle Hamiltonian $\mathcal{H}_2$ is given by

$$\mathcal{H}_2 = \sum_{i=1}^{2} h_i + V_2(x_1,x_2)$$

$$h_i = -\frac{1}{2}\frac{d^2}{dx_i^2} + V_1(x_i)$$

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Here we use $\hbar \equiv 1$ and s_i represents either $\uparrow$ or $\downarrow$. The one-particle potential V_1 describes a double-well potential,

$$V_1(x) = \begin{cases} \infty, & |x| > a + d/2 \\ 0, & d/2 < |x| < a + d/2 \\ V_0, & |x| < d/2 \end{cases}$$

and the two-particle potential V_2 represents a repulsive interaction, which mimics a screened Coulomb interaction acting within a range of the distance a,

$$V_2(x_1, x_2) = V_C\theta(a - |x_1 - x_2|).$$

The objectives are to *calculate numerically* the ground states of the two spin-1/2 particles in the double-well potential *as a function of parameters: the separation d, the potential barrier height*

V_0, and the interaction strength V_C, and to investigate the physics of a local moment formation and effective spin exchange interactions.

Things to be explored:

- Setting up the Hamiltonian matrix:
  The construction of the Hamiltonian matrix requires a set of basis functions, *i.e.*, one-particle eigenfunctions. To solve this problem with two particles, you need to make up a set of two-particle wave functions out of the one-particle functions. But, this is not a trivial matter even if you have a powerful computer to do the calculations. Obviously you can not deal with the infinite size. In this regard, one has to choose a finite size. *What would be the best way to do?*

- Two-particle correlation:
  A simple representation of the two-particle wave function is a Slater's determinant of individual one-particle eigenfunctions. However, when we consider several extreme limits of the parameters, we can find alternative solutions. For instances, when $V_0 \to \infty$ (assuming d is fixed), it is obvious that a particle, once trapped in one side of the wells, is *not* likely to tunnel to the other side of the barrier. Similarly, for $V_C \to \infty$, once a particle occupies one side of the wells, then the second particle favors the occupancy of the other side. This kind of behavior is due to the so-called "two-particle correlation", which will disappear as $V_C \to 0$. *What would be the best set of two-particle basis in each extreme limit?*

- Broken symmetry solution:
  Considering the symmetry of the Hamiltonian, e.g., the inversion symmetry of $(x \leftrightarrow -x)$, one may expect the ground state $|\psi_G\rangle$ should preserve the same symmetry. For an example, the ground state of a simple harmonic oscillator is also an even function of x. Should it be valid for one-particle solutions in this problem? If not, what wrong with it?

- Effective spin Hamiltonian:
  Considering the limiting cases of either $V_0 \to \infty$ or $V_C \to \infty$, one can presume that the particles stop moving, which corresponds to the situation of so-called "frozen charge fluctuation". Then the remaining degrees of freedom become the "spins" of the particles. One can map out the effective spin Hamiltonian by removing the spatial degrees of freedom, i.e., by projecting the Hilbert space into the subspace $|\psi_G(s_1, s_2)\rangle$:

  $$\langle\psi_G(s_1, s_2)|\mathcal{H}|\psi_G(s_1', s_2')\rangle = [\mathcal{H}_{\text{eff}}(\vec{\mathbf{s}}_1, \vec{\mathbf{s}}_2)]_{(s_1,s_2;s_1',s_2')} \approx [J\vec{\mathbf{s}}_1 \cdot \vec{\mathbf{s}}_2]_{(s_1,s_2;s_1',s_2')}$$

  Compare the solution of the effective Hamiltonian with that of matrix diagonalization in this limit.