Phys 487 Discussion 2 – Symmetrization and the Exchange Force

It is considered a **postulate** of quantum mechanics that the wavefunction for n **identical particles** must be either **symmetric** (S,+) or **antisymmetric** (A,–) under the **exchange** of any two particles:

$\psi(\vec{r}_2,\vec{r}_1)=\pm\psi(\vec{r}_1,\vec{r}_2)$ if particle 1 and particle 2 are indistinguishable.

Problem 1 : Fermi, Bose, and Pauli

There is one more part to the postulate, which we mentioned at the end of last semester.

- 2-**Fermion** wavefunctions are **A**ntisymmetric under exchange → $\psi(\vec{r}_2,\vec{r}_1) = -\psi(\vec{r}_1,\vec{r}_2)$.
- 2-**Boson** wavefunctions are **S**ymmetric under exchange → $\psi(\vec{r}_2,\vec{r}_1) = +\psi(\vec{r}_1,\vec{r}_2)$.

where

- a **Fermion** is a particle with **half-integer spin** (e.g. electrons, protons, neutrons)
- a **Boson** is a particle with **integer spin** (e.g. photons, many nuclei)

(a) What if we have a system composed of one of each, e.g. a spin-1 deuterium nucleus (boson) and a spin-½ electron (fermion)? What is the symmetry of *that* under exchange? (Hint: No calculations required, and you will *laugh* when you realize the answer.)

(b) Show that it is impossible for two fermions to occupy exactly the same state: show that you cannot build a wavefunction $\psi(\vec{r}_1,\vec{r}_2)$ with the necessary symmetry properties when particle 1 and particle 2 have the exact same *individual* wavefunctions.

FYI: This result is the **Pauli Exclusion Principle**. It is an immediate consequence of the anti-symmetrization requirement on the wavefunctions of indistinguishable fermions, and is essential for understanding the periodic table – i.e. the chemical behavior of the various elements — as it means each available quantum state $\left| n\, l\, m_l\, s\, m_s \right\rangle$ is occupied by one and only one electron. The available states fill up one by one, which would *not* be the case if the electron were a boson.

Problem 2 : The Exchange Force

The purely quantum mechanical symmetrization principle for identical particles produces a purely quantum mechanical effect that has no analogue in classical mechanics (and therefore takes some getting used to) : the effective "**exchange force**".

Two particles move in 1D only (just for simplicity) and are described by the position coordinates x_1 and x_2 respectively. Let's calculate the <distance^2> between the two particles,

$$\text{<distance}^2\text{>} \equiv \left\langle (x_1-x_2)^2 \right\rangle = \left\langle x_1^2 \right\rangle + \left\langle x_2^2 \right\rangle - 2\left\langle x_1 x_2 \right\rangle$$

in different scenarios.

(a) If the particles are **D**istinguishable (not identical), we can given them a nice factorized wavefunction

$\psi_D(x_1,x_2)=\psi_a(x_1)\,\psi_b(x_2)$ where state a and state b are normalized and orthogonal to each other.[1]

This ψ_D has no particular exchange-symmetry properties. Calculate the expected separation^2, $\left\langle (x_1-x_2)^2 \right\rangle$, in terms of the single-particle/single-wavefunction expectation values $\langle x\rangle_a, \langle x\rangle_b, \langle x^2\rangle_a$, and/or $\langle x^2\rangle_b$.

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[1] Why make ψ_a and ψ_b orthogonal to each other? For convenience / simplicity, that's all. There is nothing profound about this requirement. We will remove it in part (d).

(b) Now suppose the particles are inditinguishable (identical). We must **S**ymmetrize or **A**ntisymmetrize the 2-particle wavefunction:

$$\psi_{S,A}(x_1,x_2) = \frac{1}{\sqrt{2}}\left[\ \psi_a(x_1)\,\psi_b(x_2)\ \pm\ \psi_b(x_1)\,\psi_a(x_2)\ \right]$$

Calculate the expected separation², $\left\langle (x_1 - x_2)^2 \right\rangle$, for this wavefunction. Your answer will again involve the single-particle/single-wavefunction expectation values $\langle x\rangle_a, \langle x\rangle_b, \langle x^2\rangle_a$, and/or $\langle x^2\rangle_b$ *and one other term*.

(c) Which of the cases **D**, **A**, or **S** produces the largest separation between the two particles and which produces the smallest?

THINK ABOUT THAT for a second! → Anti-symmetrizing a wavefunction actually *"pushes" the particles apart*, while symmetrization *"pulls" them closer together*. This effect actually behaves like an effective force / pseudo-force, and is sometimes called the **exchange force**. You do need to add it to your intuition to understand chemistry, most especially the bonding of molecules. Think of it like this: relatively speaking,

- identical fermions are "repelled" from each other more than you would think, and
- identical bosons are "attracted" to each other more than you would think.

"More than you would think" means "more than if you mentally take into account only *actual* forces", like electromagnetism or the strong force. Hence, a pseudo-force. **"ANTI-SYMMETRIC means APART"** helps me to internalize this effect because an antisymmetric wavefunction can *never* have the two particles *at the same place*. (You thought through this in Problem 1b = the Pauli Exclusion Principle!) That simple fact shows that anti-symmetrization produces some sort of repulsive pseudo-force for fermions.

(d) We started this problem with the wavefunction $\psi_D(x_1,x_2) = \psi_a(x_1)\,\psi_b(x_2)$ "where ψ_a and ψ_b are normalized and orthogonal to each other." *Normalizing* the individual, single-particle wavefunctions is a natural thing to require (so that there are no unknown normalization constants to worry about) … but why make the *a* and *b* states *orthogonal* to each other? Answer: it makes the normalization of the (anti)-symmetrized 2-particle wavefunction $\psi_{S,A}(x_1, x_2)$ easier, that's all! If states *a* and *b* are *not necessarily* orthogonal to each other, then the (anti)-symmetrized 2-particle wavefunction must be written

$$\psi_{S,A}(x_1,x_2) = C\left[\ \psi_a(x_1)\,\psi_b(x_2)\ \pm\ \psi_b(x_1)\,\psi_a(x_2)\ \right]$$

where the normalization constant C has to be determined as it is not necessarily $1/\sqrt{2}$. Calculate what constant C is necessary to make the norm $\left\langle \psi_{S,A} \middle| \psi_{S,A} \right\rangle$ of the above wavefunction equal to 1 in the following cases:

(i) if state *a* and state *b* are orthogonal to each other, as before

(ii) if state *a* and state *b* are the same.

Continue to assume that $\psi_a(x)$ and $\psi_b(x)$ are *individually* normalized, because why would you not. ☺

Problem 3 : Identical Particles in an Infinite Well

The infinite 1D well ($V(x) = 0$ for $0 < x < a$ and $V(x) = \infty$ elsewhere) is the perfect sandbox for testing new bits of physics because it is an easy system to play with. If you drop in one particle, its energy eigenstates are

$$\psi_n(x) = \sqrt{2/a}\,\sin(n\pi x/a) \quad \text{with corresponding eigenvalues} \quad E_n = n^2 K \quad (\text{where } K \equiv \pi^2\hbar^2/2ma^2).$$

To make our sandbox as delightful as possible, let's use distance units where $\underline{a = \pi}$. Whee! ☺

(a) If you drop in two **D**istinguishable particles that don't interact with each other, the energy eigenstates are simply $\psi_{n_1 n_2}(x_1, x_2) = \psi_{n_1}(x_1)\,\psi_{n_2}(x_2)$. Use the convenient symbol K defined above to answer these questions:

(i) What is the energy $E_{n_1 n_2}$ of such a 2-particle eigenstate in terms of n_1 and n_2?

(ii) Find the energy and the degeneracy of the ground state(s).

(iii) Find the energy and the degeneracy of the first excited state(s).

(b) Clear out the well, then drop in two identical **bosons**. (Again, they don't interact with each other, only with the well's walls.) This time, all 2-particle wavefunctions have to be **S**ymmetric under 1 <—> 2 exchange!

(i) What is the wavefunction of the ground state (≡ lowest-energy eigenstate)?

(ii) Find the energy and the degeneracy of the ground state(s).

(iii) Find the energy and the degeneracy of the first excited state(s).

(c) Clear out the well, then drop in two identical **fermions** (that don't interact with each other). This time, the 2-particle wavefunctions must be **A**nti-symmetric under 1 <—> 2 exchange.

(i) What is the wavefunction of the ground state (≡ lowest-energy eigenstate)?

(ii) Find the energy and the degeneracy of the ground state(s).

(iii) Find the energy and the degeneracy of the first excited state(s).