

Phys 487 Discussion 1 – Identical Particles

Problem 0 : The Sixth Axiom

Last semester, we presented the five axioms of quantum mechanics. (There is no standard numbering, or even number, some people write them as four axioms, some as seven axioms, but the content is always the same.) We start this semester by introducing *one more*. This axiom only shows up when you consider systems with *more than one particle*. More exactly, it only matters for systems with two or more particles that are **identical**, which means that they have **identical intrinsic¹ properties**: same charge, same rest-mass, same size, same spin, etc. If you place two electrons in a box, you have a system with two identical particles.

Now it turns out that, for quantum mechanics to describe nature properly, it must take the notion of identical particles very seriously indeed. The sixth axiom of QM states that any wavefunction involving two identical particles must make them **completely indistinguishable**, so that no experiment can ever tell which one is which. Let's take an example using our most excellent sandbox system, the 1-dimensional infinite well. Say we have two electrons, one called Alice and one called Bob. Alice's position coordinate is x_A and Bob's position coordinate is x_B . Let's place Alice in the 1D ∞ well and set her up so that she is in the ground state:

$$\psi(x_A) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x_A}{L}\right)$$

Let's drop in Bob, but we will put him in the 1st excited state instead:

$$\psi(x_B) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x_B}{L}\right)$$

(a) To visualize all this, and as a warmup after our long break, please make a quick sketch. The infinite well runs from $x = 0$ to $x = L$. Using your coloured crayons ☺ (e.g. a pen and a pencil), sketch Alice's wavefunction in one colour and Bob's wavefunction in another colour.

(b) Something important to remember from 486: wavefunctions! are! not! physical! observables! What you just sketched is *not* something that we can measure ... rather, wavefunctions *encode* measurable information. How to extract this information? We will review the complete answer to that question in class tomorrow; for now we need only the first technique you learned: $\rho(x) = \psi(x)^* \psi(x)$ gives you probability distribution vs position. Please sketch the probability distribution for Alice and that for Bob.

(c) Now we will construct a **multi-particle wavefunction** for the first time.. It's nothing grand, just a wavefunction that depends on the coordinates of more than one particle at a time. The combined wavefunction for the two-particle Alice-and-Bob system is:

$$\psi(x_A, x_B) = \frac{2}{L} \sin\left(\frac{\pi x_A}{L}\right) \sin\left(\frac{2\pi x_B}{L}\right)$$

Here's a question: are we sure we normalized this thing correctly? Write down the normalization condition that this two-particle wavefunction must satisfy, then satisfy yourself that it is, in fact normalized.

Hint: you have already worked with wavefunctions that depend on more than one coordinate and you knew how

¹ An **intrinsic** property is a defining property of a particle. An electron's intrinsic properties are those that make it an electron. Roughly speaking, an intrinsic property is one that cannot be changed by an external force ... so NOT velocity, position, momentum, kinetic energy, angular momentum, etc but rather charge, rest-mass, spin-magnitude (spin-orientation can certainly be changed by an external force), etc.

to normalize those ... this is just another multi-dimensional wavefunction, the only new bit is that the coordinates refer to different particles.

(d) The 2-dimensional probability distribution for our 2-dimensional wavefunction is still $\rho = \psi^* \psi$: $\rho(x_A, x_B) = \psi(x_A, x_B)^* \psi(x_A, x_B)$. Find some way to sketch what it looks like as a 2D plot (contour plot, e.g.)

(e) OK, have a look at your 2D probability plot, you will see that one of the particles likes to hang around the middle of the infinite well while the other prefers two positions closer to the sides. By setting up our two particles in the same way and measuring their positions many, many times, we can measure this distribution ... and then we can say: “let’s call the electron that hangs out near the middle “Alice”, and let’s call the other one “Bob”, they clearly behave quite differently!” ... But oops, that would make them **DISTINGUISHABLE**, and since they are two **IDENTICAL PARTICLES** — two electrons — the 6th axiom of QM says they must be **INDISTINGUISHABLE** by any and all experiments. The solution is to impose this restriction:

The wavefunction for n **identical particles** must be either **symmetric** (S,+) or **antisymmetric** (A,-) under the **exchange** of any two particles:

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

In other words, the wavefunction must remain the same *to within a sign* when you exchange the two particles. You create such a wavefunction by either **symmetrizing** or **anti-symmetrizing** your original two-particle wavefunction, as follows:

$$\begin{aligned} \psi_{\text{symmetrized}}(x_A, x_B) &= C [\psi(x_A, x_B) + \psi(x_B, x_A)] \\ \psi_{\text{anti-symmetrized}}(x_A, x_B) &= C [\psi(x_A, x_B) - \psi(x_B, x_A)] \end{aligned}$$

In words: swap the particles and either add or subtract the result. Please form the symmetrized version $\psi_S(x_A, x_B)$ and anti-symmetrized version $\psi_A(x_A, x_B)$ of the Alice-and-Bob wavefunction, and verify that the wavefunctions are now **EXACTLY THE SAME TO WITHIN A SIGN** when you **EXCHANGE** Alice and Bob. (About the overall sign: it does not affect any observable property of the two particles, we will remind ourselves about that in class tomorrow.)

Problem 1 : Fermi, Bose, and Pauli

There is one more part to the 6th axiom:

- **2-Fermion** wavefunctions are **Antisymmetric** under exchange $\rightarrow \psi(\vec{r}_2, \vec{r}_1) = -\psi(\vec{r}_1, \vec{r}_2)$.
- **2-Boson** wavefunctions are **Symmetric** under exchange $\rightarrow \psi(\vec{r}_2, \vec{r}_1) = +\psi(\vec{r}_1, \vec{r}_2)$.

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- $\frac{1}{2}$ 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

$|nlm_l s m_s\rangle$ 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 $\langle \text{distance}^2 \rangle$ between the two particles,

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

in different scenarios.

(a) If the particles are **Distinguishable** (not identical), we can give them a nice factorized wavefunction

$$\psi_D(x_1, x_2) = \psi_a(x_1) \psi_b(x_2) \quad \text{where state } a \text{ and state } b \text{ are normalized and orthogonal to each other.}^2$$

This ψ_D has no particular exchange-symmetry properties. Calculate the expected separation², $\langle (x_1 - x_2)^2 \rangle$, 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 $\langle x^2 \rangle_b$.

(b) Now suppose the particles are indistinguishable (identical). We must **Symmetrize** or **Antisymmetrize** the 2-particle wavefunction:

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

Calculate the expected separation², $\langle (x_1 - x_2)^2 \rangle$, 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.

² 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).

(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

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

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 $\langle \psi_{S,A} | \psi_{S,A} \rangle$ 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 $a = \pi$. Whee! ☺

(a) If you drop in two **Distinguishable** 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 **Symmetric** under 1 \longleftrightarrow 2 exchange!

- (i) What is the wavefunction of the ground state (\equiv 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 **Anti-symmetric** under 1 \longleftrightarrow 2 exchange.

- (i) What is the wavefunction of the ground state (\equiv 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).