Many-particle Systems, 1

Wavefunctions for more than one particle: distinguishable particles

Our previous examples of quantum mechanical wavefunction calculations involve a single particle moving about in a "magic" potential energy—e.g., a particle trapped inside a square well or an electron in a hydrogen atom. But, potential energy arises from interaction, so these situations must inevitably include more than one particle. Even the simplest atom—hydrogen—consists of two particles: the electron and the proton. So, how should the Schrödinger Equation be generalized to account for multiple particles?

The idea is to introduce a "system" wave equation, the solution of which is a "system" wavefunction. For concreteness, let's consider a system consisting of an electron and a proton in a 1D infinite square well. Let's assume the particles do not interact with one another (!) and the external potential energies arise only from the well's "walls." The system wave equation is then

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m_e}\left(\frac{\partial^2\Psi}{\partial x_e^2}\right) - \frac{\hbar^2}{2m_p}\left(\frac{\partial^2\Psi}{\partial x_p^2}\right).$$

The solution of this equation separates into a product of a time part and two space parts, i.e., $\Psi = e^{-Et/\hbar}\psi_e(x_e)\psi_p(x_p)$, where E is the *total energy of the system*. (If the electron and proton were allowed to interact electromagnetically, the potential energy of the electron-proton interaction would depend on both coordinates and the system wavefunction would not separate.) Neither the electron nor proton can be found outside the infinite well, so Ψ has to vanish when either coordinate is 0 or L. These boundary conditions produce two spatial quantum numbers– n_e and n_p–both of which are integers. The system wavefunction is labeled by these two quantum numbers:

$$\Psi = \Psi_{n_e n_p}\left(x_e, x_p, t\right) = Ae^{-iE_{n_e n_p}t/\hbar}\sin\left(\frac{n_e\pi x_e}{L}\right)\sin\left(\frac{n_p\pi x_p}{L}\right).$$

$\left|\Psi_{n_e n_p}\right|^2 dx_e dx_p$ is the probability of detecting an electron in state n_e in a small length dx_e centered on the position x_e (i.e., a small electron detector at x_e) *and simultaneously* at time t, detecting a proton in state n_p in a small length dx_p centered on the position x_p (a small proton detector). Assuming the system actually does consist of an electron and proton, then the integral of $\left|\Psi_{n_e n_p}\right|^2 dx_e dx_p$ over all values of both coordinates is 1. The system energy (which in this model is independent of spin) is

$$E_{n_e n_p} = \frac{\hbar^2\pi^2}{2L^2}\left(\frac{n_e^2}{m_e} + \frac{n_p^2}{m_p}\right).$$

More generally, if the system consists of N noninteracting distinguishable particles all moving in 3D, the system wavefunction will have an exponential time part involving the system total energy, and $3N$ spatial wavefunctions each depending on a spatial quantum number ($3N$ in all).

Indistinguishable, noninteracting particles

The example above deals with two *different* kinds of noninteracting particles (that is, *distinguishable* particles). When the proton detector clicks, it's certainly the proton that causes it, and the same for the electron. But now, suppose we replace the proton with a second electron. All electrons are identical. Electrons can't be painted or given little tags to carry around. If their wavefunctions overlap, as in the infinite well example above, they are *indistinguishable*. (If the particles are confined to be far from each other, such as in distant wells, they are distinguishable, i.e., particle 1 is definitely in well A, particle 2 is definitely in well B, etc. Their individual wave functions don't overlap.) Replace the proton detector with a second (identical) electron detector. If the electron wavefunctions fill up a single infinite well (i.e., they overlap), when one of the detectors clicks there's no way to tell which electron was detected. Now, the system wavefunction might be expected to look something like

$$\Psi_{n_1 m_{s1} n_2 m_{s2}}\left(x_1, x_2, t\right) = Ae^{-iE_{n_1 n_2}t/\hbar}\sin\left(\frac{n_1 \pi x_1}{L}\right)\sin\left(\frac{n_2 \pi x_2}{L}\right)\phi_{m_{s1}}\phi_{m_{s2}},$$

where the $\phi's$ represent spin directions measured in detectors 1 and 2. The labels "1" and "2" don't distinguish the electrons from one another, they simply convey the idea that there are two ns, two spins, and two places to put detectors. The quantity $\left|\Psi_{n_1 m_{s1} n_2 m_{s2}}\right|^2 dx_1 dx_2$ is the probability that *an* electron is detected at position x_1 and that *an* electron is detected at position x_2, and that the total quantum state of the pair is determined by n_1, m_{s1}, n_2, m_{s2}. It doesn't matter if we switch detector positions or if we switch the states measured in each detector; the system probability will be identical. In other words, $\left|\Psi_{n_1 m_{s1} n_2 m_{s2}}\left(x_1, x_2, t\right)\right|^2 = \left|\Psi_{n_2 m_{s2} n_1 m_{s1}}\left(x_1, x_2, t\right)\right|^2 = \left|\Psi_{n_1 m_{s1} n_2 m_{s2}}\left(x_2, x_1, t\right)\right|^2$. This string of equalities can be true provided $\Psi_{n_1 m_{s1} n_2 m_{s2}}\left(x_1, x_2, t\right) = \pm\Psi_{n_2 m_{s2} n_1 m_{s1}}\left(x_1, x_2, t\right)$ and $\Psi_{n_1 m_{s1} n_2 m_{s2}}\left(x_1, x_2, t\right) = \pm\Psi_{n_1 m_{s1} n_2 m_{s2}}\left(x_2, x_1, t\right)$. That is, the wavefunction can either be the same when states are switched or when detector positions are switched, or it can change sign. It turns out that **Nature employs both options and the consequences are astounding**.

A profound, but difficult to prove, theorem—the *Spin-Statistics Theorem*—stipulates that identical noninteracting **bosons (particles with integer spin)** have the same wavefunction under switch of state (i.e., quantum numbers) or position, while the wavefunction for identical noninteracting **fermions (particles with odd half-integer spin)** undergoes a sign change when state or position are switched. In other words, the proper wavefunction for two or more identical bosons is *symmetric* if two state labels or two positions are switched, but for fermions it is *antisymmetric*.

<u>Example</u>: Suppose two identical noninteracting spin-0 bosons are in a 1D infinite well. Suppose also that the spatial quantum numbers are 2 and 3. The proper wavefunction for the system is: $\Psi_{bosons} = A\left[\sin\left(\frac{2\pi x_1}{L}\right)\sin\left(\frac{3\pi x_2}{L}\right) + \sin\left(\frac{3\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right)\right]0_1 0_2$. The zeroes on the end are spin states, not numerical zeroes. Suppose now the particles are fermions with spin-1/2. Spin-1/2 can either be "up" (along a direction in space) or "down" (opposite that direction). For spin-1/2 fermions the spin functions ϕ can be represented by up or down pointing arrows. Two identical

fermions in spatial states 2 and 3 but with both spins up will have a system wavefunction $\Psi_{fermions} = A\left[\sin\left(\frac{2\pi x_1}{L}\right)\sin\left(\frac{3\pi x_2}{L}\right) - \sin\left(\frac{3\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right)\right]\uparrow_1\uparrow_2$.

The symmetry or antisymmetry of the wavefunction seems like a formal and unimportant detail, but it is anything but. Suppose in the previous example the two fermions are both in the spatial quantum number = 2 state, that is, they are in the same total spatial *and* spin state. Then the factor

$$\left[\sin\left(\frac{2\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right) - \sin\left(\frac{2\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right)\right]$$

vanishes. In other words, because of the antisymmetry of their system wavefunction, ***no two identical noninteracting fermions (whose individual wavefunctions overlap) can be in exactly the same single particle state***. This rule is often referred to as the **Pauli Exclusion Principle**; the atomic periodic table (as we see in a bit) is one direct consequence. The two fermions could be in the same n state if their spins were different, however. For example, suppose the fermions both have $n = 2$. Then, an antisymmetric system wavefunction could be

$$\Psi_{fermions} = A\sin\left(\frac{2\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right)\left[\uparrow_1\downarrow_2 - \downarrow_1\uparrow_2\right].$$

Often it is useful to construct wavefunctions for identical, noninteracting fermion systems by either antisymmetric combinations of products of spatial functions times symmetric spin combinations, or symmetric space combinations times antisymmetric spin combinations. (This isn't the only way to make such constructions.)

Example: Two indistinguishable fermions in an infinite square well in motion states n_1 and n_2 and spin states $\uparrow$ and $\downarrow$ might have wavefunctions

$$A[\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right) - \sin\left(\frac{n_2\pi x_1}{L}\right)\sin\left(\frac{n_1\pi x_2}{L}\right)[\uparrow_1\downarrow_2 + \downarrow_1\uparrow_2]$$

or

$$A[\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right) + \sin\left(\frac{n_2\pi x_1}{L}\right)\sin\left(\frac{n_1\pi x_2}{L}\right)[\uparrow_1\downarrow_2 - \downarrow_1\uparrow_2].$$

In either of the cases in this example, if two of the fermion detector positions are the same, so that two positions and two spins have the same indices (detectors measure spatial and spin quantum numbers), the wavefunction also vanishes: in other words, ***two identical fermions cannot occupy the same position in space at the same time***. The antisymmetry of the fermion wavefunction implies that **"fermions don't like one another." The antisymmetry of the wavefunction for identical fermions produces a kind of effective repulsive force**, one that manifests itself, for example, in the fact that solids are hard to compress. When you push on a solid it pushes back because in pushing you are trying to cause the solid's electrons to get "closer than they like to be."

Bosons are different. The symmetry of the wavefunction for identical bosons permits more than one boson to be in the same state and to occupy the same position in space. In fact, the probability that this happens is actually often greater than when they are in different states. This implies that **"bosons like one another"** and that **there is a kind of effective attractive force between them**. Bosonic attraction leads to the strange and practically important phenomena of superfluidity, superconductivity, and to the coherence of laser light. Identical photons in a laser beam are bosons that tend to travel together in the same state (see Fn2 p7). Bosonic attraction allows you to make a laser so you can scan your bag of chips! $(QM = \$)$

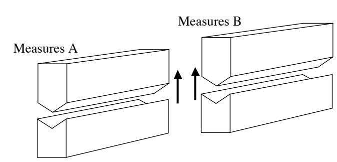
Example: Suppose the two particles in the previous example are identical, noninteracting bosons. The system wavefunction has to be completely symmetric under state or position switches. In this case, start with the product $\Psi_{s_1}(p_1)\Psi_{s_2}(p_2)$, where p is a position and s is a state. Then, leaving the state labels in place, permute the positions and add: $A[\Psi_{s_1}(p_1)\Psi_{s_2}(p_2)+\Psi_{s_1}(p_2)\Psi_{s_2}(p_1)]$. For larger systems do the same thing and permute the positions cyclically until all position arrangements have been constructed (e.g., $A[\Psi_{s_1}(p_1)\Psi_{s_2}(p_2)\Psi_{s_3}(p_3)+\Psi_{s_1}(p_2)\Psi_{s_2}(p_3)\Psi_{s_3}(p_1)+\Psi_{s_1}(p_3)\Psi_{s_2}(p_1)\Psi_{s_3}(p_2)]$).

Note that in either the fermion or boson case, the system wavefunction *is not* a simple product of single particle wavefunctions as it is when the particles are distinguishable. **The antisymmetry or symmetry requirement causes the single particle states to be strongly correlated**, and these correlations have powerful physical consequences, as we will see.

Appendix: No hidden variables (probably)

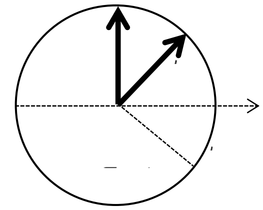
A more colorful expression for “strong correlation” of single particle wavefunctions is “entanglement.” If sufficiently strong, external interactions destroy entanglement (i.e., cause decoherence), producing, as a result, system wavefunctions that are simple products of single particle wavefunctions, with no symmetry or antisymmetry restrictions. Preventing this from occurring is a major research venture motivated by such hoped-for applications as quantum teleportation and quantum computing (both involving the manipulation of information encoded in quantum states, such as spin orientations).

Entanglement in two-particle systems has permitted stringent experimental tests of the nature of quantum reality. Quantum mechanics is a mathematical formalism that enables the possible outcomes of experiments to be calculated. It says nothing about which outcome actually emerges from a given measurement. One possible interpretation of this unpredictability is that quantum mechanics is an incomplete theory. In this view, every quantum system is described by more variables than those in the Schrödinger wavefunction, but they are “hidden” from us. If these hidden variables were known, a perfectly predictable (classical) theory could be constructed. An alternative interpretation is that quantum mechanics *is* complete, it’s just that when a measurement is performed all of the possible outcomes somehow “collapse” into a single reality. This suggests (maybe) the astonishing view that *there is no physical reality until one looks*! (See: http://whatis.techtarget.com/definition/Schrodingers-cat)



Here’s a cartoon description of an experiment that addresses these issues. Two spin-1/2 particles (A and B) are produced traveling in opposite directions with total spin = 0. The spins of the particles are measured by two separate Stern-Gerlach (S-G) devices (see Sc5, p3), arranged with their long axes on a common line; the devices measure particle deflections perpendicular to their long axes. See the figure to the right. Here the arrows indicate the classical magnetic field directions, z_A and z_B, not the spin directions. Provided the measurements are made before decoherence can muck things up, the spin of A along a given deflection direction (e.g., “up” along z_A) must be opposite to the spin of B along the same direction (i.e., “down” when $z_B = z_A$). The spin part of the two-particle wavefunction must be

$\uparrow_A \downarrow_B \pm \downarrow_A \uparrow_B$; no up-up or down-down. The situation becomes much more interesting when z_B and z_A do not point in the same direction.



The figure to right depicts looking down the common long axes of the two S-G devices. As shown, device B is rotated by an angle ϕ relative to device A. Suppose the two particles actually have well defined, oppositely pointing, spin vectors, and the direction of deflection in each device is determined by the sign of the dot product between the spin vectors and the respective z-axes. Suppose further that particle A deflects up. In this scenario, its spin vector must have been somewhere within the semi-circle above the x_A-axis. At the same time the spin vector of B must be somewhere within the semi-circle below the x_A-axis. If it were in the pie-shaped piece designated ϕ its dot product with z_B would be positive and it would deflect up along z_B. If it were in the pie-shaped piece designated $\pi - \phi$ its dot product with z_B would be negative and it would deflect down along z_B. If B's deflection is recorded over and over, but only when A deflects up, the average fraction of B's ups would be ϕ/π and downs would be $1-\phi/\pi$. Note that when $\phi = 0$, B always deflects down along z_B, as it should. Note also that when $\phi = \pi/2$, B deflects half the time "up" (in this case, to the right along x_A) and half the time "down." This is exactly what is observed when a particle after defecting one way in one device is passed through a second with deflection axis rotated by 90° relative to the first. The story spun here is an example of a hidden variable theory. In this story, the particles have well-defined spin vectors before any measurement is made, but we never know what they are, we only observe the resulting deflection.

Quantum mechanics predicts different fractions of up and down deflections for particle B. Let an up deflection correspond to a +1 output, down to –1. In the hidden variable scenario above, the average output value would be $O_{HV} = (+1)(\phi/\pi) + (-1)(1-\phi/\pi) = -1 + 2\phi/\pi$. Quantum mechanics says that measurement of B's deflections along z_B is equivalent to measurement along z_A a fraction of $\cos(\phi)$ of the time, and along x_A a fraction of $\sin(\phi)$ of the time. The average output value for the former is $(-1)\cos(\phi)$ while for the latter it is $(0)\sin(\phi)$. In other words, $O_{QM} = -\cos(\phi)$. If $\phi = 45^o$, for example, $O_{HV} = -0.500$ while $O_{QM} = -0.707$. In other words, not the same. Several sophisticated experimental tests of differing predictions of hidden variables versus quantum mechanics have been conducted over the last 20-30 years, and, to *extremely* high confidence (i.e., when you account for experimental uncertainties), quantum mechanics is always right. Sorry, dear reader: the bizarre behavior of quantum systems apparently cannot be accounted for by classical physics plus ignorance. **There apparently is no hidden reality; reality only emerges when measurements are made!**