## <u>Today</u>

- I. Last Time
- II. Two Particle Wave Functions in General
- III. Atoms: a beginning...

- I. Last time
- \* Zak's guest lecture on two particle systems. Symmetrized wave functions describe bosons and anti-symmetrize wave functions describe fermions. The symmetry is with respect to the exchange of the two particles. This requirement only arises because quantum mechanics allows for completely identical particles.
- \* Studied the combination of two angular momenta in general, and in particular, learned to use Clebsch-Gordan tables.

#### I. Addition of Angular Momentum

We've just identified a triplet of states  

$$\begin{cases}
|1 \ 1\rangle = |\uparrow\uparrow\rangle, s = 1 \text{ and } m = 1, \\
|1 \ 0\rangle = \frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle), s = 1 \text{ and } m = 0, \\
|1 \ -1\rangle = |\downarrow\downarrow\rangle, s = 1 \text{ and } m = -1
\end{cases}$$

These are a basis for the states with  $|s = 1 m\rangle$ . We can construct a fourth state by orthogonality:

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle).$$
$$\frac{1}{2}(\langle\uparrow\downarrow| - \langle\downarrow\uparrow|)(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle) = \frac{1}{2}(0+1-1-0) = 0.$$

This new 'singlet' state is

$$|0 0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$
, this is the  $s = 0$  (singlet)

# I. Final words on Addition of Angular Momentum

Suppose we now wanted to add up two general spins  $s_1$  and  $s_2$ , what possible results would we get? The strategy, which we won't carry out, is the same as in our example from last time: you pick the highest spin state and act lowering operators to construct all the intermediate states. The result is that you can get any spin in the following list:

$$s \in \{s_1 + s_2, s_1 + s_2 - 1, s_1 + s_2 - 2, \dots, |s_1 - s_2|\}.$$

In fact, this holds for the addition of any two angular momenta,  $j \in \{s + \ell, s + \ell - 1, ..., |\ell - s|\}.$ 

This is all summarized in so-called Clebsch-Gordan coefficients:  $|s \ m\rangle = \sum_{m_1+m_2=m} C_{m_1m_2m}^{s_1s_2s} |s_1 \ s_2 \ m_1 \ m_2\rangle$  I. Final words on Addition of Angular Momentum

This is all summarized in so-called Clebsch-Gordan coefficients:

$$|s m\rangle = \sum_{m_1+m_2=m} C^{s_1s_2s}_{m_1m_2m} |s_1 s_2 m_1 m_2\rangle.$$

Here's a small section of such a table



As an example, consider the state  $|3 0\rangle$  and ask how we make it out of two spins with  $s_1 = 2$  and  $s_2 = 1$ .

I. Final words on Addition of Angular Momentum

$$|s m\rangle = \sum C_{m_1m_2m}^{s_1s_2s} |s_1 s_2 m_1 m_2\rangle.$$

 $m_1 + m_2 = m$ 



$$|3 0\rangle = C_1 |2 1\rangle |1 - 1\rangle + C_2 |2 0\rangle |10\rangle + C_3 |2 - 1\rangle |1 1\rangle$$
$$= \frac{1}{\sqrt{5}} |2 1\rangle |1 - 1\rangle + \sqrt{\frac{3}{5}} |2 0\rangle |10\rangle + \frac{1}{\sqrt{5}} |2 - 1\rangle |1 1\rangle$$

The complete state of an electron puts together both the spatial dependence and the spin of the electron:

 $\psi(\vec{r})\chi.$ 

What happens when we put two particles together?

 $\psi(\vec{r}_1, \vec{r}_2)\chi(1,2).$ 

The symmetrization (or anti-sym.) axiom of quantum mechanics says that it is the *whole* wave function that has a definite symmetry type; e.g., for a fermion

$$\psi(\vec{r}_1, \vec{r}_2)\chi(1,2) = -\psi(\vec{r}_2, \vec{r}_1)\chi(2,1).$$

This means that we have to consider the full wave function when we are thinking about symmetrization.

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I can put two electrons in the same spatial wave function as long as I also require that the spin state is the singlet spin state!

We can formalize all of this mathematically. The idea is to introduce a new operator, called the exchange operator and denoted  $\hat{P}$ . The definition of this operator is that it interchanges two particles

 $\hat{P}|(1,2)\rangle = |(2,1)\rangle.$ 

This operator has a neat property  $\hat{P}^2 = 1$ , as a matrix this is the unit matrix with ones along the diagonal. This means that the eigenvalues of  $\hat{P}$  itself are ±1. Suppose we had two identical particles...

This means that the eigenvalues of  $\hat{P}$  itself are ±1. Suppose we had two identical particles..., then the Hamiltonian should treat them exactly the same  $m_1 = m_2$  and  $V(\vec{r}_1, \vec{r}_2) = V(\vec{r}_2, \vec{r}_1)$ , but then  $[\hat{P}, \hat{H}] = 0$ 

and hence are compatible observables. From the generalized Ehrenfest result we then have that

$$\frac{d\langle \hat{P} \rangle}{dt} = 0!$$

Any pair of particles that start out in a symmetrized state remain in that state for all time.

The **symmetrization axiom** states that not only do identical particles maintain their symmetrization, but they are required to be in such a state:  $|(1,2)\rangle = \pm |(2,1)\rangle$ .

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This is also true for *n* identical particles, they generally satisfy  $|(1,2,...,i,...,j,...,n) = \pm |(1,2,...,j,...,n)$ .

#### III. Atoms

All we'll do today is to write down the Hamiltonian and look at it.:

$$\hat{H} = \sum_{j=1}^{Z} \left\{ -\frac{\hbar^2}{2m} \nabla_j^2 - \left(\frac{1}{4\pi\epsilon_0}\right) \frac{Ze^2}{r_j} \right\} + \frac{1}{2} \left(\frac{1}{4\pi\epsilon_0}\right) \sum_{j\neq k}^{Z} \frac{e^2}{|\vec{r}_j - \vec{r}_k|}$$