

# Two-Particle Systems

Dylan McIntyre and Kenny Roffo

SUNY Oswego

April 23, 2015

# Changing from 1 to 2 Particles

- For a single particle, the wave function is

$$\Psi(\mathbf{r}, t)$$

# Changing from 1 to 2 Particles

- For a single particle, the wave function is

$$\Psi(\mathbf{r}, t)$$

- Adding a second particle to the system, we write

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t)$$

# Changing from 1 to 2 Particles

- For a single particle, the wave function is

$$\Psi(\mathbf{r}, t)$$

- Adding a second particle to the system, we write

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t)$$

- To use the Schrödinger equation we must use know the Hamiltonian:

$$H = -\frac{\hbar^2}{2m_1} \nabla_1^2 - \frac{\hbar^2}{2m_2} \nabla_2^2 + V(\mathbf{r}_1, \mathbf{r}_2, t)$$

# Changing from 1 to 2 Particles

- The probability of finding each particle in a given volume  $d^3\mathbf{r}_i$  is

$$\int |\Psi(\mathbf{r}_1, \mathbf{r}_2, t)|^2 d^3\mathbf{r}_1 d^3\mathbf{r}_2 = 1$$

# Changing from 1 to 2 Particles

- The probability of finding each particle in a given volume  $d^3\mathbf{r}_i$  is

$$\int |\Psi(\mathbf{r}_1, \mathbf{r}_2, t)|^2 d^3\mathbf{r}_1 d^3\mathbf{r}_2 = 1$$

- For time independent potentials, we have the general solution:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \psi(\mathbf{r}_1, \mathbf{r}_2) e^{-iEt/\hbar}$$

# Changing from 1 to 2 Particles

- The probability of finding each particle in a given volume  $d^3\mathbf{r}_i$  is

$$\int |\Psi(\mathbf{r}_1, \mathbf{r}_2, t)|^2 d^3\mathbf{r}_1 d^3\mathbf{r}_2 = 1$$

- For time independent potentials, we have the general solution:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \psi(\mathbf{r}_1, \mathbf{r}_2) e^{-iEt/\hbar}$$

- Here,  $\psi$  satisfies the time-independent Schrödinger wave equation:

$$-\frac{\hbar^2}{2m_1} \nabla_1^2 \psi - \frac{\hbar^2}{2m_2} \nabla_2^2 \psi + V\psi = E\psi$$

# The Difference Between 2 Particles

- Consider two objects. One in the state  $\psi_a$ , the other in the state  $\psi_b$



# The Difference Between 2 Particles

- Consider two objects. One in the state  $\psi_a$ , the other in the state  $\psi_b$
- Classically, we can tell these objects from one another

# The Difference Between 2 Particles

- Consider two objects. One in the state  $\psi_a$ , the other in the state  $\psi_b$
- Classically, we can tell these objects from one another
- In Quantum Mechanics, this is not the case

# The Difference Between 2 Particles

- Consider two objects. One in the state  $\psi_a$ , the other in the state  $\psi_b$
- Classically, we can tell these objects from one another
- In Quantum Mechanics, this is not the case
- Particles are inherently identical; there is no way to tell the difference between two electrons

# The Difference Between 2 Particles

- Consider two objects. One in the state  $\psi_a$ , the other in the state  $\psi_b$
- Classically, we can tell these objects from one another
- In Quantum Mechanics, this is not the case
- Particles are inherently identical; there is no way to tell the difference between two electrons
- With particles, we can only know that one of the two is in state  $\psi_a$ , and the other is in state  $\psi_b$ , but we cannot tell them apart

# The Difference Between 2 Particles

- Consider two objects. One in the state  $\psi_a$ , the other in the state  $\psi_b$
- Classically, we can tell these objects from one another
- In Quantum Mechanics, this is not the case
- Particles are inherently identical; there is no way to tell the difference between two electrons
- With particles, we can only know that one of the two is in state  $\psi_a$ , and the other is in state  $\psi_b$ , but we cannot tell them apart
- We represent this by a wave function which doesn't assume either particle is in a particular state:

$$\psi \pm (\mathbf{r}_1, \mathbf{r}_2) = A [\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) \pm \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)]$$

# Bosons and Fermions

$$\psi \pm (\mathbf{r}_1, \mathbf{r}_2) = A [\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) \pm \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)]$$

- Choosing + or – we have two types of particles

# Bosons and Fermions

$$\psi \pm (\mathbf{r}_1, \mathbf{r}_2) = A [\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) \pm \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)]$$

- Choosing + or – we have two types of particles
- **Bosons** are those particles for which we use +
- **Fermions** are those particles for which we use –

# Bosons and Fermions

$$\psi \pm (\mathbf{r}_1, \mathbf{r}_2) = A [\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) \pm \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)]$$

- Choosing + or – we have two types of particles
- **Bosons** are those particles for which we use +
- **Fermions** are those particles for which we use –
- It works out that Bosons are particles with integer spin, and Fermions are particles with half-integer spin.



# Bosons and Fermions

$$\psi \pm (\mathbf{r}_1, \mathbf{r}_2) = A [\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) \pm \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)]$$

- Choosing + or – we have two types of particles
- **Bosons** are those particles for which we use +
- **Fermions** are those particles for which we use –
- It works out that Bosons are particles with integer spin, and Fermions are particles with half-integer spin.
- As a consequence, we see we cannot have two Fermions cannot occupy the same state else  $\psi_a = \psi_b$  and

$$\psi_-(\mathbf{r}_1, \mathbf{r}_2) = A [\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) - \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2)] = 0$$

- This result is the famous *Pauli Exclusion Principle*

# Exchange Forces

- Let's take a look at a one-dimensional example

# Exchange Forces

- Let's take a look at a one-dimensional example
- Particle 1 is in state  $\psi_a(x)$  and particle 2 is in state  $\psi_b(x)$

# Exchange Forces

- Let's take a look at a one-dimensional example
- Particle 1 is in state  $\psi_a(x)$  and particle 2 is in state  $\psi_b(x)$
- The two states are orthogonal and normalized

# Exchange Forces

- Let's take a look at a one-dimensional example
- Particle 1 is in state  $\psi_a(x)$  and particle 2 is in state  $\psi_b(x)$
- The two states are orthogonal and normalized
- If the two are distinguishable, the combined wave function looks like:

# Exchange Forces

- Let's take a look at a one-dimensional example
- Particle 1 is in state  $\psi_a(x)$  and particle 2 is in state  $\psi_b(x)$
- The two states are orthogonal and normalized
- If the two are distinguishable, the combined wave function looks like:

$$\psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2) \quad (1)$$

# Exchange Forces

- Let's take a look at a one-dimensional example
- Particle 1 is in state  $\psi_a(x)$  and particle 2 is in state  $\psi_b(x)$
- The two states are orthogonal and normalized
- If the two are distinguishable, the combined wave function looks like:

$$\psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2) \quad (1)$$

- If they are identical bosons:

$$\psi_+(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_a(x_1)\psi_b(x_2) + \psi_b(x_1)\psi_a(x_2)] \quad (2)$$

# Exchange Forces

- Let's take a look at a one-dimensional example
- Particle 1 is in state  $\psi_a(x)$  and particle 2 is in state  $\psi_b(x)$
- The two states are orthogonal and normalized
- If the two are distinguishable, the combined wave function looks like:

$$\psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2) \quad (1)$$

- If they are identical bosons:

$$\psi_+(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_a(x_1)\psi_b(x_2) + \psi_b(x_1)\psi_a(x_2)] \quad (2)$$

- If they are identical fermions:

$$\psi_-(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_a(x_1)\psi_b(x_2) - \psi_b(x_1)\psi_a(x_2)] \quad (3)$$



# Exchange Forces: Distinguishable Particles

- Now calculating the expectation value of the particles' separation distance squared we get:

# Exchange Forces: Distinguishable Particles

- Now calculating the expectation value of the particles' separation distance squared we get:

$$\langle (x_1 - x_2)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2\langle x_1 x_2 \rangle$$

# Exchange Forces: Distinguishable Particles

- Now calculating the expectation value of the particles' separation distance squared we get:

$$\langle (x_1 - x_2)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2\langle x_1 x_2 \rangle$$

- Case 1: Distinguishable particles (using the wavefunction from 1)

# Exchange Forces: Distinguishable Particles

- Now calculating the expectation value of the particles' separation distance squared we get:

$$\langle (x_1 - x_2)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2\langle x_1 x_2 \rangle$$

- Case 1: Distinguishable particles (using the wavefunction from 1)

$$\langle x_1^2 \rangle = \int x_1^2 |\psi_a(x_1)|^2 dx_1 \int |\psi_b(x_2)|^2 dx_2 = \langle x^2 \rangle_a$$

# Exchange Forces: Distinguishable Particles

- Now calculating the expectation value of the particles' separation distance squared we get:

$$\langle (x_1 - x_2)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2\langle x_1 x_2 \rangle$$

- Case 1: Distinguishable particles (using the wavefunction from 1)

$$\langle x_1^2 \rangle = \int x_1^2 |\psi_a(x_1)|^2 dx_1 \int |\psi_b(x_2)|^2 dx_2 = \langle x^2 \rangle_a$$

$$\langle x_2^2 \rangle = \int |\psi_a(x_1)|^2 dx_1 \int x_2^2 |\psi_b(x_2)|^2 dx_2 = \langle x^2 \rangle_b$$

# Exchange Forces: Distinguishable Particles

- Now calculating the expectation value of the particles' separation distance squared we get:

$$\langle (x_1 - x_2)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2\langle x_1 x_2 \rangle$$

- Case 1: Distinguishable particles (using the wavefunction from 1)

$$\langle x_1^2 \rangle = \int x_1^2 |\psi_a(x_1)|^2 dx_1 \int |\psi_b(x_2)|^2 dx_2 = \langle x^2 \rangle_a$$

$$\langle x_2^2 \rangle = \int |\psi_a(x_1)|^2 dx_1 \int x_2^2 |\psi_b(x_2)|^2 dx_2 = \langle x^2 \rangle_b$$

$$\langle x_1 x_2 \rangle = \int x_1 |\psi_a(x_1)|^2 dx_1 \int x_2 |\psi_b(x_2)|^2 dx_2 = \langle x \rangle_a \langle x \rangle_b$$

# Exchange Forces: Distinguishable Particles

- Now calculating the expectation value of the particles' separation distance squared we get:

$$\langle (x_1 - x_2)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2\langle x_1 x_2 \rangle$$

- Case 1: Distinguishable particles (using the wavefunction from 1)

$$\langle x_1^2 \rangle = \int x_1^2 |\psi_a(x_1)|^2 dx_1 \int |\psi_b(x_2)|^2 dx_2 = \langle x^2 \rangle_a$$

$$\langle x_2^2 \rangle = \int |\psi_a(x_1)|^2 dx_1 \int x_2^2 |\psi_b(x_2)|^2 dx_2 = \langle x^2 \rangle_b$$

$$\langle x_1 x_2 \rangle = \int x_1 |\psi_a(x_1)|^2 dx_1 \int x_2 |\psi_b(x_2)|^2 dx_2 = \langle x \rangle_a \langle x \rangle_b$$

$$\langle (x_1 - x_2)^2 \rangle_d = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x \rangle_b$$

# Exchange Forces: Identical Particles

- Case 2: Identical Particles (using wavefunctions from 2 and 3)

$$\begin{aligned}\langle x_1^2 \rangle &= \frac{1}{2} \left[ \int x_1^2 |\psi_a(x_1)|^2 dx_1 \int |\psi_b(x_2)|^2 dx_2 \right. \\ &\quad + \int x_1^2 |\psi_b(x_1)|^2 dx_1 \int |\psi_a(x_2)|^2 dx_2 \\ &\quad \pm \int x_1^2 \psi_a(x_1)^* \psi_b(x_1) dx_1 \int \psi_b(x_2)^* \psi_a(x_2) dx_2 \\ &\quad \left. \pm \int x_1^2 \psi_b(x_1)^* \psi_a(x_1) dx_1 \int \psi_a(x_2)^* \psi_b(x_2) dx_2 \right] \\ &= \frac{1}{2} \left[ \langle x^2 \rangle_a + \langle x^2 \rangle_b \pm 0 \pm 0 \right] = \frac{1}{2} \left( \langle x^2 \rangle_a + \langle x^2 \rangle_b \right)\end{aligned}$$

- Just the same,

$$\langle x_2^2 \rangle = \frac{1}{2} \left( \langle x^2 \rangle_b + \langle x^2 \rangle_a \right)$$



# Exchange Forces: Identical Particles Continued

$$\begin{aligned}\langle x_1 x_2 \rangle &= \frac{1}{2} \left[ \int x_1 |\psi_a(x_1)|^2 dx_1 \int x_2 |\psi_b(x_2)|^2 dx_2 \right. \\ &\quad + \int x_1 |\psi_b(x_1)|^2 dx_1 \int x_2 |\psi_a(x_2)|^2 dx_2 \\ &\quad \pm \int x_1 \psi_a(x_1)^* \psi_b(x_1) dx_1 \int x_2 \psi_b(x_2)^* \psi_a(x_2) dx_2 \\ &\quad \left. \pm \int x_1 \psi_b(x_1)^* \psi_a(x_1) dx_1 \int x_2 \psi_a(x_2)^* \psi_b(x_2) dx_2 \right] \\ &= \frac{1}{2} (\langle x \rangle_a \langle x \rangle_b + \langle x \rangle_b \langle x \rangle_a \pm \langle x \rangle_{ab} \langle x \rangle_{ba} \pm \langle x \rangle_{ba} \langle x \rangle_{ab}) \\ &= \langle x \rangle_a \langle x \rangle_b \pm |\langle x \rangle_{ab}|^2,\end{aligned}$$

where

$$\langle x \rangle_{ab} \equiv \int x \psi_a(x)^* \psi_b(x) dx.$$

Evidently

$$\langle (x_1 - x_2)^2 \rangle_{\pm} = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x \rangle_b \mp 2|\langle x \rangle_{ab}|^2.$$

# Exchange Forces

- If we compare the results of the distinguishable particles and the identical, we see the only difference occurring in the last term:

$$\langle (\Delta x)^2 \rangle_{\pm} = \langle (\Delta x)^2 \rangle_d \mp 2|\langle x \rangle_{ab}|^2$$

# Exchange Forces

- If we compare the results of the distinguishable particles and the identical, we see the only difference occurring in the last term:

$$\langle(\Delta x)^2\rangle_{\pm} = \langle(\Delta x)^2\rangle_d \mp 2|\langle x\rangle_{ab}|^2$$

- Compared to distinguishable, in the same two states identical bosons tend to be closer together

# Exchange Forces

- If we compare the results of the distinguishable particles and the identical, we see the only difference occurring in the last term:

$$\langle(\Delta x)^2\rangle_{\pm} = \langle(\Delta x)^2\rangle_d \mp 2|\langle x\rangle_{ab}|^2$$

- Compared to distinguishable, in the same two states identical bosons tend to be closer together
- Identical fermions tend to be further apart

# Exchange Forces

- If we compare the results of the distinguishable particles and the identical, we see the only difference occurring in the last term:

$$\langle (\Delta x)^2 \rangle_{\pm} = \langle (\Delta x)^2 \rangle_d \mp 2|\langle x \rangle_{ab}|^2$$

- Compared to distinguishable, in the same two states identical bosons tend to be closer together
- Identical fermions tend to be further apart
- The term  $\langle x \rangle_{ab}$  vanishes if the two wave functions do not overlap

# Exchange Forces

- If we compare the results of the distinguishable particles and the identical, we see the only difference occurring in the last term:

$$\langle (\Delta x)^2 \rangle_{\pm} = \langle (\Delta x)^2 \rangle_d \mp 2|\langle x \rangle_{ab}|^2$$

- Compared to distinguishable, in the same two states identical bosons tend to be closer together
- Identical fermions tend to be further apart
- The term  $\langle x \rangle_{ab}$  vanishes if the two wave functions do not overlap
- If one state is zero where the another is nonzero, the integral becomes zero

# Exchange Forces

- If we compare the results of the distinguishable particles and the identical, we see the only difference occurring in the last term:

$$\langle (\Delta x)^2 \rangle_{\pm} = \langle (\Delta x)^2 \rangle_d \mp 2|\langle x \rangle_{ab}|^2$$

- Compared to distinguishable, in the same two states identical bosons tend to be closer together
- Identical fermions tend to be further apart
- The term  $\langle x \rangle_{ab}$  vanishes if the two wave functions do not overlap
- If one state is zero where the another is nonzero, the integral becomes zero
- Therefore, it's safe to say that if two electrons have nonoverlapping wave functions, they are in fact distinguishable

# Exchange Forces

- We're interested in when they overlap



# Exchange Forces

- We're interested in when they overlap
- We see that systems behave with an attractive force between identical bosons

# Exchange Forces

- We're interested in when they overlap
- We see that systems behave with an attractive force between identical bosons
- On the contrary, we see a repulsive force for identical fermions

# Exchange Forces

- We're interested in when they overlap
- We see that systems behave with an attractive force between identical bosons
- On the contrary, we see a repulsive force for identical fermions
- These forces are called exchange forces, though they are merely a consequence of geometry and not actual physical forces

# Exchange Forces

- We're interested in when they overlap
- We see that systems behave with an attractive force between identical bosons
- On the contrary, we see a repulsive force for identical fermions
- These forces are called exchange forces, though they are merely a consequence of geometry and not actual physical forces
- If we look at the  $H_2$  molecule as an example, we have one electron centered around nucleus 1 and another around nucleus 2

# Exchange Forces

- We're interested in when they overlap
- We see that systems behave with an attractive force between identical bosons
- On the contrary, we see a repulsive force for identical fermions
- These forces are called exchange forces, though they are merely a consequence of geometry and not actual physical forces
- If we look at the  $H_2$  molecule as an example, we have one electron centered around nucleus 1 and another around nucleus 2
- Since electrons are fermions, the electrons should tend toward the outer side of the molecule, pulling the protons apart (breaking the bond)

# Exchange Forces

- We're interested in when they overlap
- We see that systems behave with an attractive force between identical bosons
- On the contrary, we see a repulsive force for identical fermions
- These forces are called exchange forces, though they are merely a consequence of geometry and not actual physical forces
- If we look at the  $H_2$  molecule as an example, we have one electron centered around nucleus 1 and another around nucleus 2
- Since electrons are fermions, the electrons should tend toward the outer side of the molecule, pulling the protons apart (breaking the bond)
- However, this isn't the case because we've ignored spin!

# Exchange Forces

- We're interested in when they overlap
- We see that systems behave with an attractive force between identical bosons
- On the contrary, we see a repulsive force for identical fermions
- These forces are called exchange forces, though they are merely a consequence of geometry and not actual physical forces
- If we look at the  $H_2$  molecule as an example, we have one electron centered around nucleus 1 and another around nucleus 2
- Since electrons are fermions, the electrons should tend toward the outer side of the molecule, pulling the protons apart (breaking the bond)
- However, this isn't the case because we've ignored spin!
- The complete state is described by the electrons position and also a spinor:  $\psi(r)\chi(s)$

Thank you!