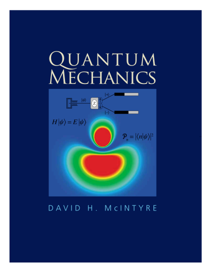
Enrico Fermi (1901-1954)

Identical Particles

Read McIntyre 13.1-2

PH451/551



Satyendra Nath Bose (1894-1974)

Reading Quiz

1. What is the spin of a boson?

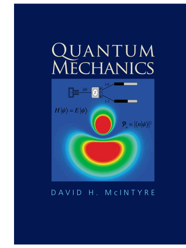
2. What is the spin of a fermion?

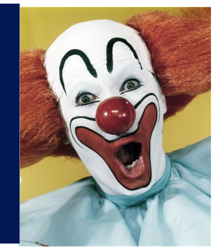
3. T/F? The wave function of a two-particle system of identical fermions is antisymmetric under particle interchange

Reading Quiz

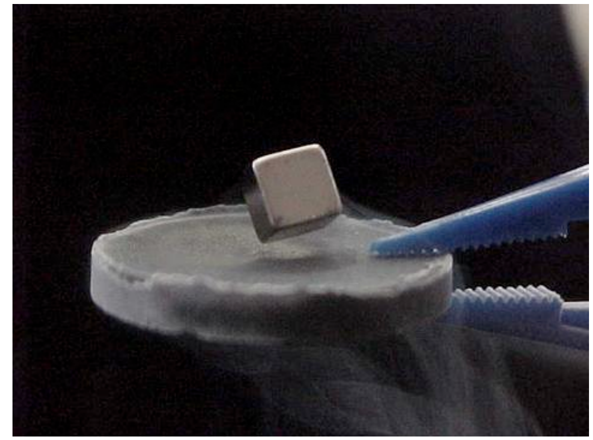
1. What is the spin of a boson?
   Integer : 0, 1, 2, 3 …
2. What is the spin of a fermion?
   Half-integer : ½, 3/2, ..
3. T/F? The wave function of a two-particle system of identical fermions is antisymmetric under particle interchange
   TRUE

Famous bosons

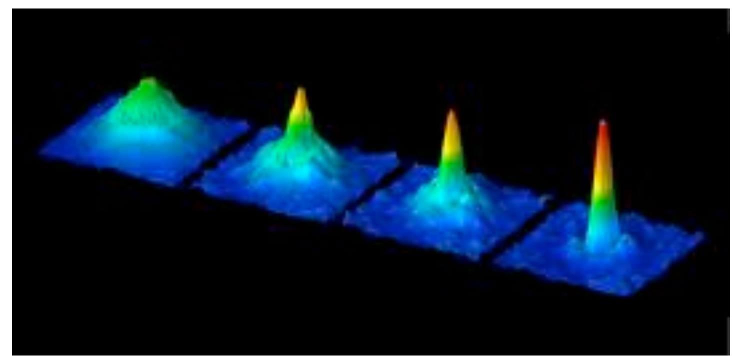




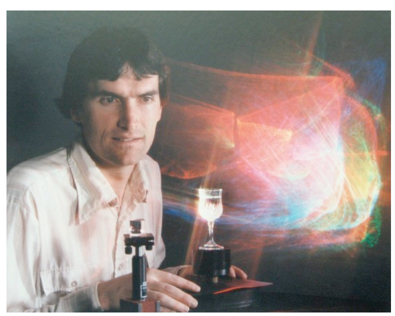
1. Superconductors:
   http://www.forcefieldmagnets.com/catalog/product_info.php?products_id=103



2. B-E condensate of atoms:
   http://www.mpq.mpg.de/cms/mpq/en/departments/quanten/homepage_cms/projects/bec/index.html



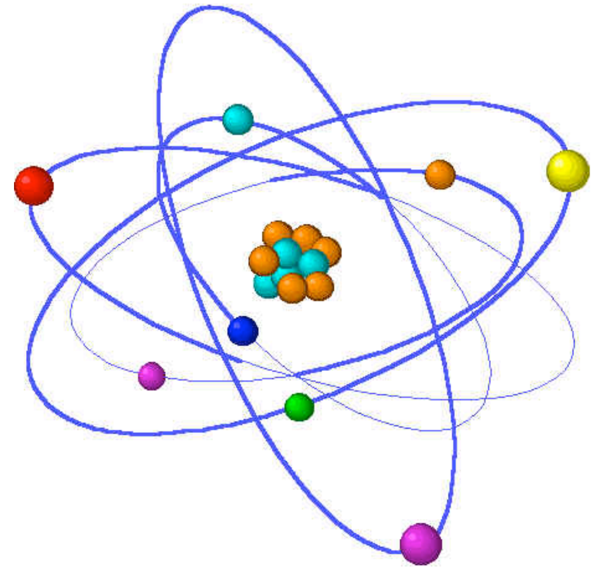
3. Photons:



4. Higgs

Famous fermions

1. Electrons:
   http://www.formulamedical.com/QA/Cholesterol/Free%20Radical.htm



2. Fundamental constituents of baryonic matter:
   http://physics.aps.org/synopsis-for/10.1103/PhysRevLett.108.181807

	I	II	III
Quarks	u	c	t
	d	s	b
Leptons	ν_e	ν_μ	ν_τ
	e	μ	τ

Symmetry under particle exchange

1. Exchange operator swaps the quantum numbers of the two particles.

$$P_{12}\left|s_1 s_2 m_1 m_2\right\rangle = \left|s_2 s_1 m_2 m_1\right\rangle$$

2. Exchange symmetry

$$\frac{1}{\sqrt{2}}\left[\left|+-\right\rangle + \left|-+\right\rangle\right] \xrightarrow[\text{exchange}]{} \frac{1}{\sqrt{2}}\left[\left|-+\right\rangle + \left|+-\right\rangle\right] = +\frac{1}{\sqrt{2}}\left[\left|+-\right\rangle + \left|-+\right\rangle\right]$$

$$\frac{1}{\sqrt{2}}\left[\left|+-\right\rangle - \left|-+\right\rangle\right] \xrightarrow[\text{exchange}]{} \frac{1}{\sqrt{2}}\left[\left|-+\right\rangle - \left|+-\right\rangle\right] = -\frac{1}{\sqrt{2}}\left[\left|+-\right\rangle - \left|-+\right\rangle\right]$$

Space & spin

1. State vectors have a space and a spin part that are usually separable.

$$|\psi\rangle = |\psi_{spatial}\rangle |\psi_{spin}\rangle$$

Bosons
(exch. symm.)

$$|\psi^{SS}_{boson}\rangle = |\psi^{S}_{spatial}\rangle |\psi^{S}_{spin}\rangle$$

$$|\psi^{AA}_{boson}\rangle = |\psi^{A}_{spatial}\rangle |\psi^{A}_{spin}\rangle$$

Fermions
(exch. antisymm.)

$$|\psi^{SA}_{fermion}\rangle = |\psi^{S}_{spatial}\rangle |\psi^{A}_{spin}\rangle$$

$$|\psi^{AS}_{fermion}\rangle = |\psi^{A}_{spatial}\rangle |\psi^{S}_{spin}\rangle$$

Two-particle system

(Hamiltonian, energies, states ..)

1. Each particle has its own coordinates that span the same range, but are independent of each other

$$H_{\text{single}} = \frac{p^2}{2m} + V(x) \rightarrow \boxed{H = \frac{p_1^2}{2m} + V(x_1) + \frac{p_2^2}{2m} + V(x_2)}$$

2. Eigenvalue equation (only ONE energy)

$$H\psi(x_1, x_2) = E\psi(x_1, x_2)$$

3. Probability to find particle #1 between x_1 and $x_1 + dx_1$ AND particle #2 between x_2 and $x_2 + dx_2$

$$\left|\psi(x_1, x_2)\right|^2 dx_1 dx_2 \qquad \iint \left|\psi(x_1, x_2)\right|^2 dx_1\, dx_2 = 1$$

Example 2-particle system – disting. particles (diff. *m*) – space only

1. Each particle has its own coordinates that span the same range, but are independent of each other

$$H=\frac{p_1^2}{2m_1}+\frac{1}{2}m_1\omega^2x_1^2+\frac{p_2^2}{2m_2}+\frac{1}{2}m_2\omega^2x_2^2$$

2. Hamiltonian separable in x_1 and x_2

$$\psi_{n_a,n_b}\left(x_1,x_2\right)=\varphi_{n_a}\left(x_1\right)\varphi_{n_b}\left(x_2\right)$$

3. Single particle states

$$\left(\frac{p_1^2}{2m_1}+\frac{1}{2}m_1\omega^2x_1^2\right)\varphi_{n_a}\left(x_1\right)=E_{n_a}\varphi_{n_a}\left(x_1\right)$$

$$\left(\frac{p_2^2}{2m_2}+\frac{1}{2}m_2\omega^2x_2^2\right)\varphi_{n_b}\left(x_2\right)=E_{n_b}\varphi_{n_b}\left(x_2\right)$$

Example (diff. *m*) - space part

1. 2-particle wf is PRODUCT of 1-particle wfs and energy is SUM of 1-particle energies

$$\left(\frac{p_1^2}{2m_1}+\frac{1}{2}m_1\omega^2x_1^2\right)\varphi_{n_a}(x_1)\varphi_{n_b}(x_2)=E_{n_a}\varphi_{n_b}(x_1)\varphi_{n_b}(x_2)$$

$$\left(\frac{p_2^2}{2m_2}+m_2\omega^2x_2^2\right)\varphi_{n_b}(x_2)\varphi_{n_a}(x_1)=E_{n_b}\varphi_{n_b}(x_2)\varphi_{n_a}(x_1)$$

$$\underbrace{\left(\frac{p_1^2}{2m_1}+\frac{1}{2}m_1\omega^2x_1^2+\frac{p_2^2}{2m_2}+m_2\omega^2x_2^2\right)}_{H}\underbrace{\varphi_{n_a}(x_1)\varphi_{n_b}(x_2)}_{\psi_{n_a,n_b}(x_1,x_2)}$$

$$=\underbrace{\left(E_{n_a}+E_{n_b}\right)}_{E}\underbrace{\varphi_{n_a}(x_1)\varphi_{n_b}(x_2)}_{\psi_{n_a,n_b}(x_1,x_2)}$$

Example (diff. *m*)- space part

1. 2-particle wave function is PRODUCT of 1-particle wave functions and state energy is SUM of 1-particle energies

$$\psi_{n_a,n_b}(x_1,x_2) = \varphi_{n_a}(x_1)\varphi_{n_b}(x_2)$$

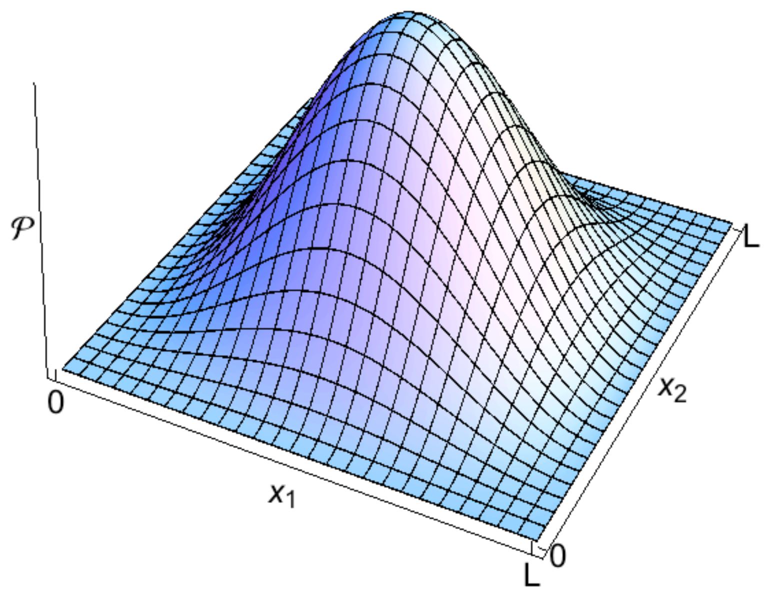
$$E_{n_a,n_b} = E_{n_a} + E_{n_b}$$

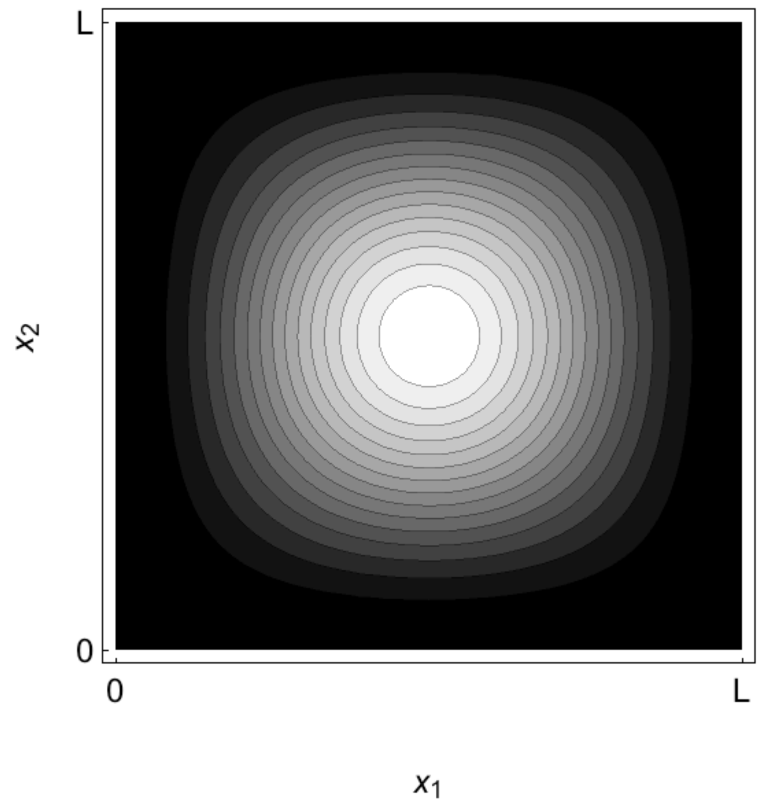
2. Language: The two-particle state labeled ($n_a n_b$)- e.g. (3,1) has particle #1 (with coordinate x_1) is in the single-particle state n_a (state 3 in this example) and particle #2 (with coordinate x_2) is in the single-particle state n_b (state 1 in this example).

   The energy of the two-particle state labeled ($n_a n_b$) is $E_{na,nb}$, and it is the sum of the energies of the single-particle states 3 and 1.

Example (diff. *m*)- space part

1. Probability density – 2 particle – distinguishable – ground state





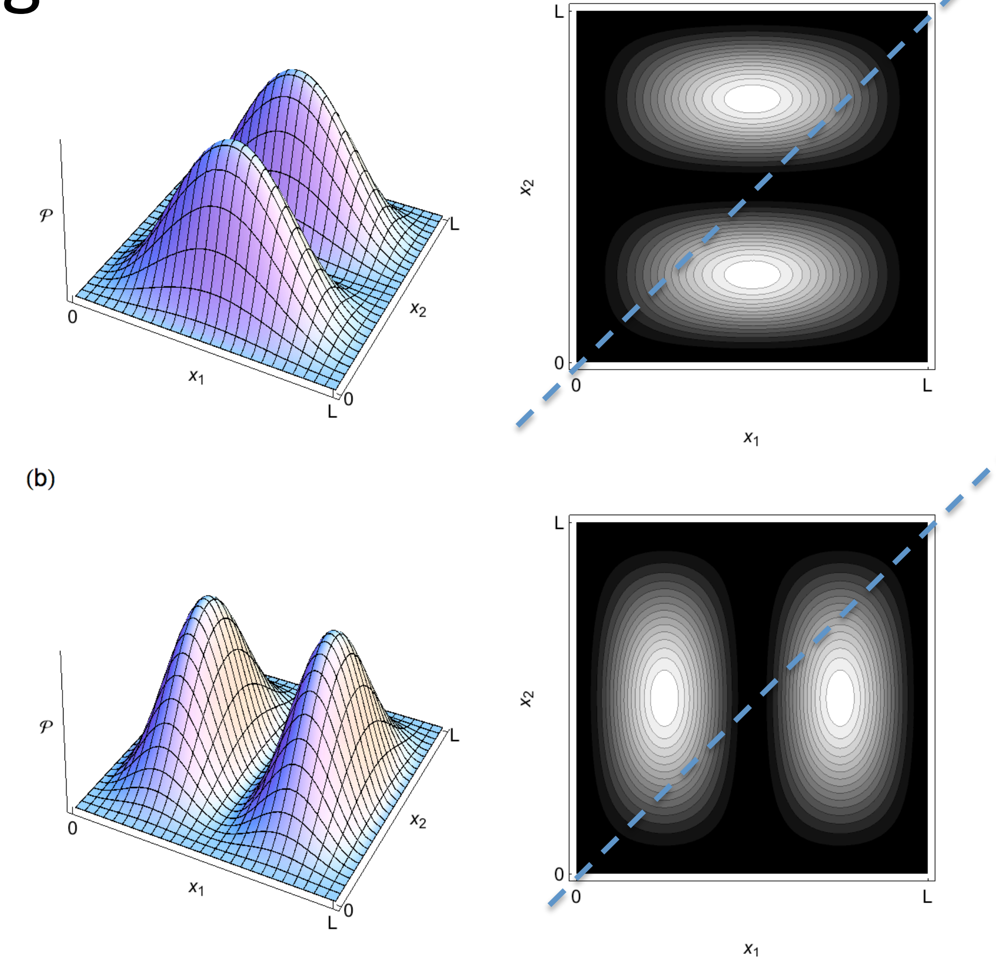
$$\psi_{n_a=1,\, n_b=1}\left(x_1, x_2\right) = \varphi_{n_a=1}\left(x_1\right)\varphi_{n_b=1}\left(x_2\right)$$

$$E = E_{n_a} + E_{n_b}$$

(symmetry under particle interchange – even though not required for distinguishable)

2 particle - distinguishable

1. Probability density – 2 particle – distinguishable – ground + 1st excited



$$\psi_{n_a=1,\, n_b=2}(x_1,x_2) = \varphi_{n_a=1}(x_1)\varphi_{n_b=2}(x_2)$$
$$E = E_1 + E_2$$

(no symmetry under particle interchange – but not required for distinguishable)

$$\psi_{n_a=2,\, n_b=1}(x_1,x_2) = \varphi_{n_a=2}(x_1)\varphi_{n_b=1}(x_2)$$
$$E = E_2 + E_1$$

Example -2 indistinguishable particles, with spin, lowest possible energy?

1. BOTH particles in single-particle ground state called n=1. Product wf already symmetric:

$$\psi^{Space,S}_{n_a=1,\,n_b=1}(x_1,x_2) = \varphi_{n_a=1}(x_1)\varphi_{n_b=1}(x_2)$$

$$E = E_{n_a} + E_{n_b}$$

2. Antisymmetric version is zero for both in single-particle ground state (boson or fermion)!

$$\psi^{Space,A}_{n_a=1,\,n_b=1}(x_1,x_2) = \varphi_{n_a=1}(x_1)\varphi_{n_b=1}(x_2) - \varphi_{n_a=1}(x_2)\varphi_{n_b=1}(x_1)$$

Example -2 indistinguishable spin-zero BOSONS, lowest possible energy

$$\left|\psi_{boson}^{SS}\right\rangle = \left|\psi_{spatial}^{S}\right\rangle \left|\psi_{spin}^{S}\right\rangle$$

$$\left|\psi_{boson}^{AA}\right\rangle = \cancel{\left|\psi_{spatial}^{A}\right\rangle} \left|\psi_{spin}^{A}\right\rangle$$

1. Need space part symm, because antisymmetric version is zero for both in single-particle ground state (boson or fermion). So spin part must be symm for bosons

$$\psi_{n_a=1,\, n_b=1}^{Space,S}\left(x_1,x_2\right)\left|\psi_{spin}^{S}\right\rangle =$$

$$\varphi_{n_a=1}\left(x_1\right)\varphi_{n_b=1}\left(x_2\right)\left|s=0,m_s=0,s_1=0,s_2=0\right\rangle_{coupled}$$

$$E = E_{n_a} + E_{n_b}$$

Example -2 indistinguishable spin-1/2 FERMIONS, lowest possible energy

$$\left|\psi^{SA}_{fermion}\right\rangle = \left|\psi^{S}_{spatial}\right\rangle \left|\psi^{A}_{spin}\right\rangle$$

$$\left|\psi^{AS}_{fermion}\right\rangle = \cancel{\left|\psi^{A}_{spatial}\right\rangle} \left|\psi^{S}_{spin}\right\rangle$$

1. Need space part symm, because antisymmetric version is zero for both in single-particle ground state (boson or fermion). So spin part must be antisymm for fermions (singlet)

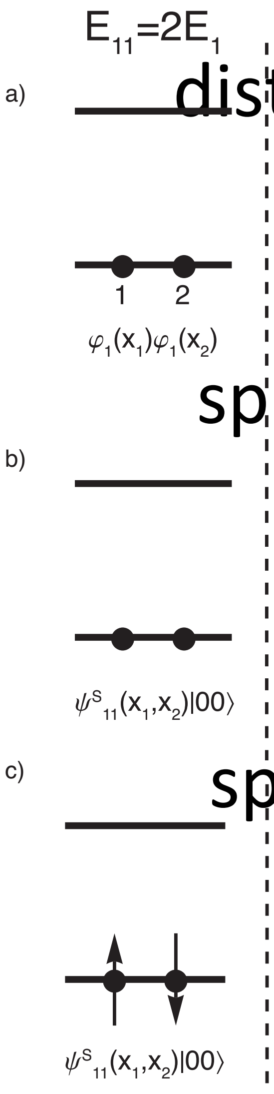
$$\psi^{Space,S}_{n_a=1,\,n_b=1}\left(x_1,x_2\right)\left|\psi^{A}_{spin}\right\rangle =$$

$$|0,0\rangle_{coupled} = |+,-\rangle_{unc} - |-,+\rangle_{unc}$$

$$\varphi_{n_a=1}\left(x_1\right)\varphi_{n_b=1}\left(x_2\right)\left|s=0,m_s=0,s_1=\tfrac{1}{2},s_2=\tfrac{1}{2}\right\rangle_{coupled}$$

$$E = E_{n_a} + E_{n_b}$$

2 particles – ground state



disting

$$\psi_{n_a=1,n_b=1}\left(x_1,x_2\right)=\varphi_{n_a=1}\left(x_1\right)\varphi_{n_b=1}\left(x_2\right)$$

$$E=E_1+E_1=2E_1$$

spin 0 bosons

$$\psi_{n_a=1,n_b=1}\left(x_1,x_2\right)=$$

$$\underbrace{\left(\varphi_{n_a=1}\left(x_1\right)\varphi_{n_b=1}\left(x_2\right)+\varphi_{n_a=1}\left(x_2\right)\varphi_{n_b=1}\left(x_1\right)\right)}_{symmetric}\underbrace{\left|00\right\rangle_{coupled}}_{symm}$$

$$E=2E_1$$

spin 1/2 fermions

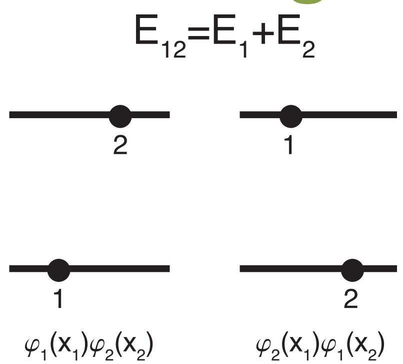
$$\psi_{n_a=1,n_b=1}\left(x_1,x_2\right)=$$

$$\underbrace{\left(\varphi_{n_a=1}\left(x_1\right)\varphi_{n_b=1}\left(x_2\right)+\varphi_{n_a=1}\left(x_2\right)\varphi_{n_b=1}\left(x_1\right)\right)}_{symmetric}\underbrace{\left|00\right\rangle_{coupled}}_{antisymm}$$

$$E=2E_1$$

2 particles – distinguishable; or spin-0 bosons – 1st excited state

1. Distinguishable (2-fold degenerate)



distinguishable particles

$$\psi_{n_a=1,n_b=2}(x_1,x_2)=\varphi_{n_a=1}(x_1)\varphi_{n_b=2}(x_2)$$

$$\psi_{n_a=2,n_b=1}(x_1,x_2)=\varphi_{n_a=2}(x_1)\varphi_{n_b=1}(x_2)$$

$$E=E_1+E_2$$

2. Bosons, spin 0 (non-degenerate)

bosons

$$\psi_{n_a=1,n_b=2}(x_1,x_2)=$$

$$\underbrace{\left(\varphi_{n_a=1}(x_1)\varphi_{n_b=2}(x_2)+\varphi_{n_a=1}(x_2)\varphi_{n_b=2}(x_1)\right)}_{symmetric}\underbrace{|00\rangle_{coupled}}_{symm}$$

$$E=E_1+E_2$$

2 particles: fermions – 1st excited state (4-fold degenerate)

3. Fermions, spin 1/2

$$\psi_{n_a=1,n_b=2}\left(x_1,x_2\right)=$$

$$\underbrace{\left(\varphi_{n_a=1}\left(x_1\right)\varphi_{n_b=2}\left(x_2\right)-\varphi_{n_a=1}\left(x_2\right)\varphi_{n_b=2}\left(x_1\right)\right)}_{antisymmetric}\underbrace{\left|1m_j\right\rangle_{\text{coupled basis}}}_{symm}$$

There are 3 possible symmetric spin states:

$$\left|1,1\right\rangle_{coupled}=\left|+,+\right\rangle_{unc}$$

$$\left|1,0\right\rangle_{coupled}=\left|+,-\right\rangle_{unc}+\left|-,+\right\rangle_{unc}$$

$$\left|1,-1\right\rangle_{coupled}=\left|-,-\right\rangle_{unc}$$

$$E=E_1+E_2$$

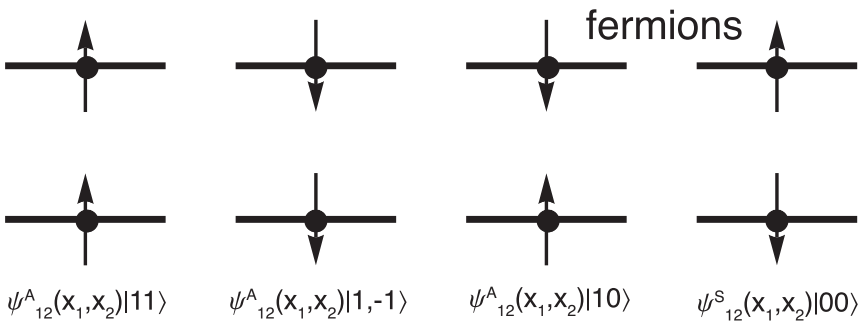
$$\psi_{n_a=1,n_b=2}\left(x_1,x_2\right)=$$

$$\underbrace{\left(\varphi_{n_a=1}\left(x_1\right)\varphi_{n_b=2}\left(x_2\right)+\varphi_{n_a=1}\left(x_2\right)\varphi_{n_b=2}\left(x_1\right)\right)}_{symmetric}\underbrace{\left|00\right\rangle_{\text{coupled basis}}}_{antisymm}$$

There is 1 possible antisymmetric spin state:

$$\left|0,0\right\rangle_{coupled}=\left|+,-\right\rangle_{unc}-\left|-,+\right\rangle_{unc}$$

$$E=E_1+E_2$$



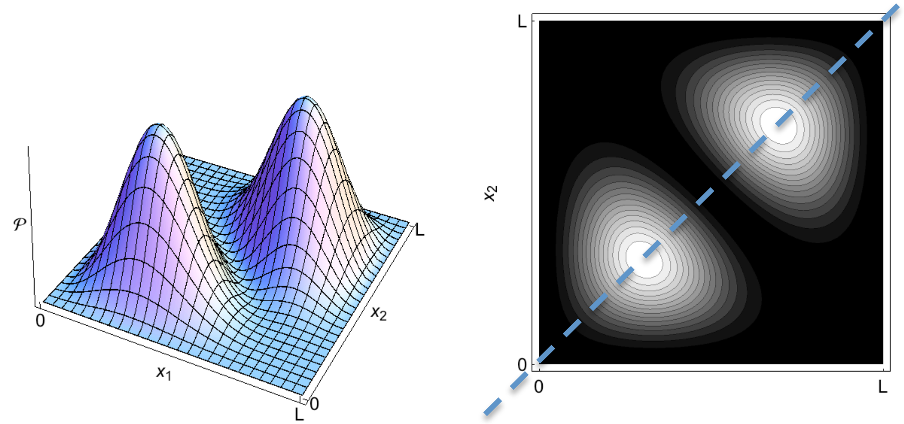
2 particle - indistinguishable

1. Configurations–1st excited

$$\psi^{S}{}_{n_a=1,n_b=2}(x_1,x_2)=\varphi_{n_a=1}(x_1)\varphi_{n_b=2}(x_2)+\varphi_{n_a=1}(x_2)\varphi_{n_b=2}(x_1)$$

$$E=E_{n_a}+E_{n_b}$$

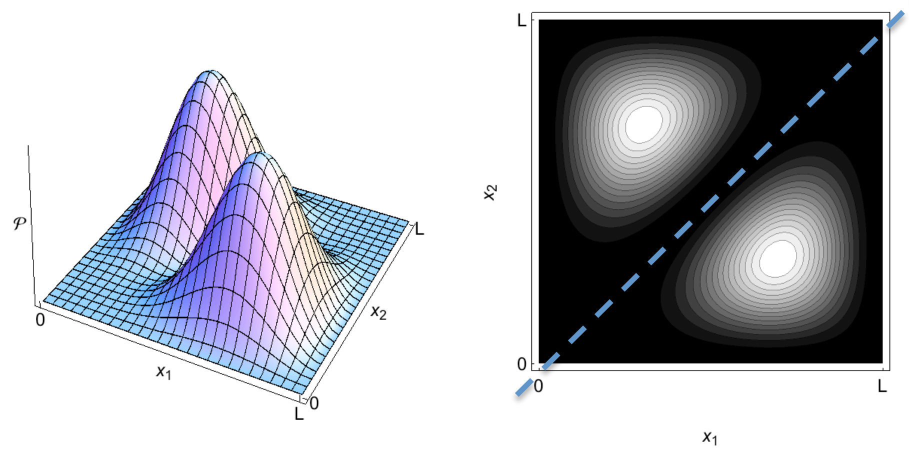
(c)



$$\psi^{A}{}_{n_a=1,n_b=2}(x_1,x_2)=\varphi_{n_a=1}(x_1)\varphi_{n_b=2}(x_2)-\varphi_{n_a=1}(x_2)\varphi_{n_b=2}(x$$

$$E=E_{n_a}+E_{n_b}$$

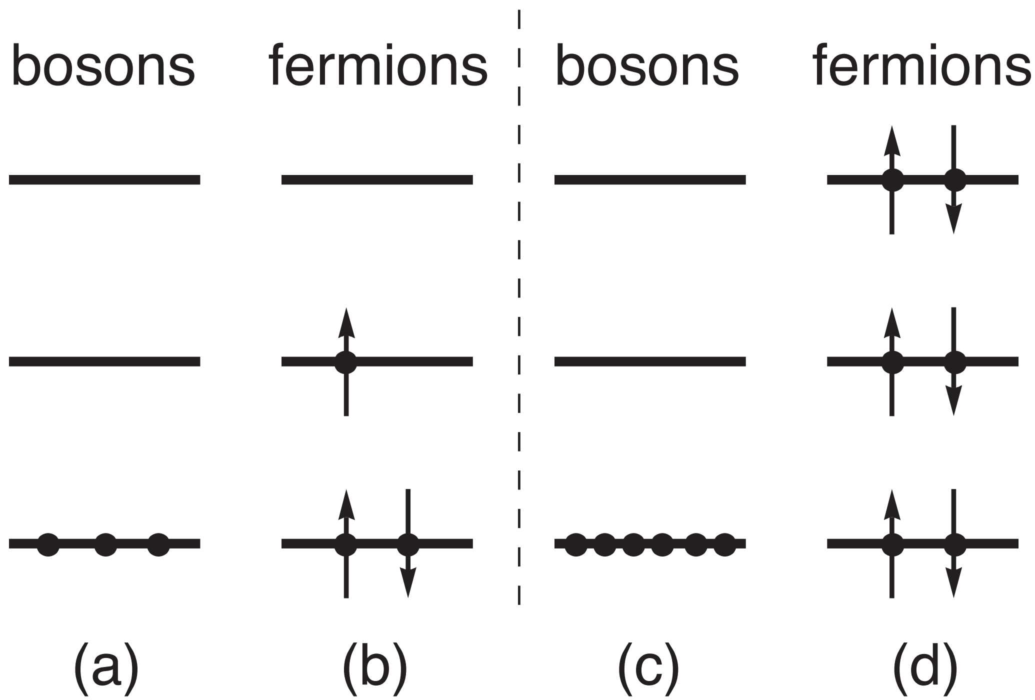
(d)



x1≠x2

many particle - indistinguishable

1. Ground state



2. Highest energy for fermions is called FERMI ENERGY

Exchange interaction

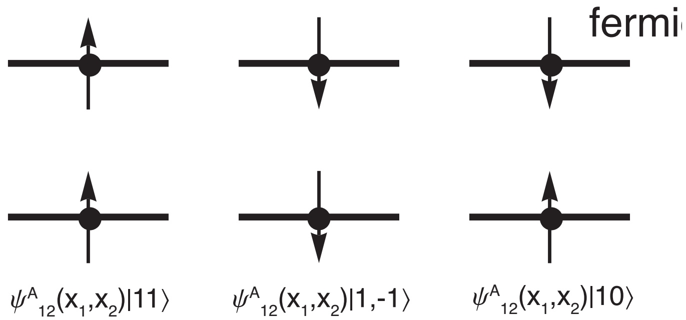
1. NON INTERACTING particles "seem to have an interaction" – exchange
2. Expectation value of particle separation

$$\left\langle \left(x_1 - x_2\right)^2 \right\rangle = \left\langle x_1^2 - 2x_1x_2 + x_2^2 \right\rangle$$

$$= \left\langle x_1^2 \right\rangle + \left\langle x_2^2 \right\rangle - 2\left\langle x_1 x_2 \right\rangle$$

$$\left|\psi_{12}^{AS}\right\rangle = \left|\psi_{12}^{A}\right\rangle \left|1M\right\rangle$$

3. Fermion triplet-spin

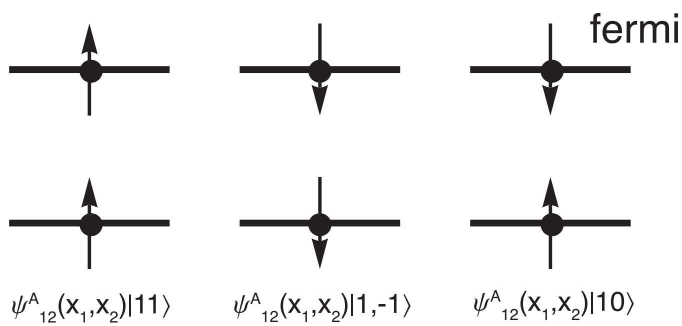


$$\left\langle x_1^2 \right\rangle = \left\langle \psi_{12}^{A} \middle| x_1^2 \middle| \psi_{12}^{A} \right\rangle \left\langle 1M \middle| 1M \right\rangle$$

Exchange interaction

1. Expectation value of particle separation
2. Fermion triplet-spin

$$\left\langle (x_1 - x_2)^2 \right\rangle = \left\langle x_1^2 - 2x_1x_2 + x_2^2 \right\rangle$$
$$= \left\langle x_1^2 \right\rangle + \left\langle x_2^2 \right\rangle - 2\left\langle x_1x_2 \right\rangle$$



$$\left\langle x_1^2 \right\rangle = \left\langle \psi_{12}^{A} \middle| x_1^2 \middle| \psi_{12}^{A} \right\rangle \left\langle 1M \middle| 1M \right\rangle$$

$$\left\langle x_1^2 \right\rangle = \frac{1}{\sqrt{2}}\left({}_1\langle 1|\,{}_2\langle 2| - {}_2\langle 1|\,{}_1\langle 2| \right) x_1^2 \frac{1}{\sqrt{2}}\left(|1\rangle_1 |2\rangle_2 - |1\rangle_2 |2\rangle_1 \right)$$

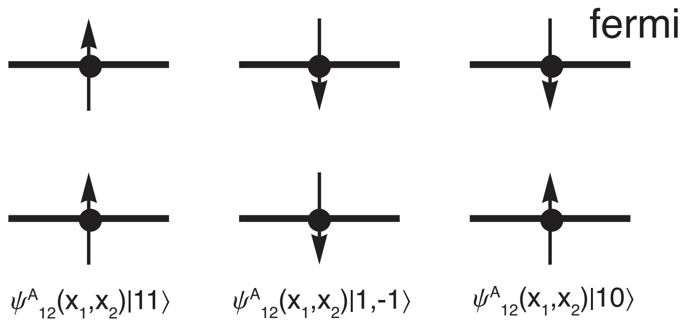
$$= \frac{1}{2}\Big\{ \left({}_1\langle 1|x_1^2|1\rangle_1 \right)\left({}_2\langle 2|2\rangle_2 \right) - \left({}_1\langle 1|x_1^2|2\rangle_1 \right)\left({}_2\langle 2|1\rangle_2 \right)$$

$$- \left({}_1\langle 2|x_1^2|1\rangle_1 \right)\left({}_2\langle 1|2\rangle_2 \right) + \left({}_1\langle 2|x_1^2|2\rangle_1 \right)\left({}_2\langle 1|1\rangle_2 \right) \Big\}$$

Exchange interaction

1. Expectation value of particle separation
2. Fermion triplet-spin

$$\left\langle (x_1 - x_2)^2 \right\rangle = \left\langle x_1^2 - 2x_1x_2 + x_2^2 \right\rangle$$
$$= \left\langle x_1^2 \right\rangle + \left\langle x_2^2 \right\rangle - 2\left\langle x_1x_2 \right\rangle$$



$$\left\langle x_2^2 \right\rangle = ?$$

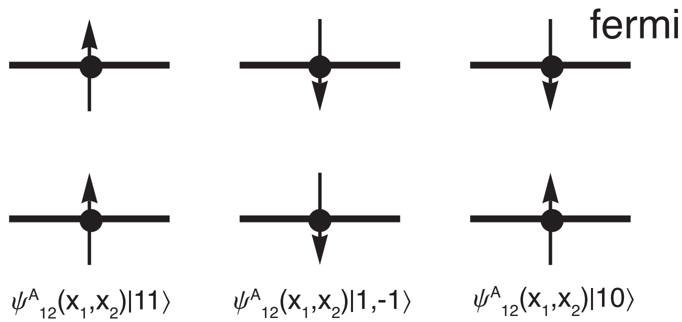
$$\left\langle x_1^2 \right\rangle = \frac{1}{2}\left\{\left({}_1\langle 1|\, x_1^2 \,|1\rangle_1 \right) + \left({}_1\langle 2|\, x_1^2 \,|2\rangle_1 \right)\right\}$$

$$\left\langle x_1^2 \right\rangle = \tfrac{1}{2}\int_{-\infty}^{\infty} \varphi_1^*(x_1) x_1^2 \varphi_1(x_1)\, dx_1 + \tfrac{1}{2}\int_{-\infty}^{\infty} \varphi_2^*(x_1) x_1^2 \varphi_2(x_1)\, dx_1$$

Exchange interaction

1. Expectation value of particle separation
2. Fermion triplet-spin

$$\left\langle (x_1 - x_2)^2 \right\rangle = \left\langle x_1^2 - 2x_1x_2 + x_2^2 \right\rangle$$
$$= \left\langle x_1^2 \right\rangle + \left\langle x_2^2 \right\rangle - 2\left\langle x_1x_2 \right\rangle$$



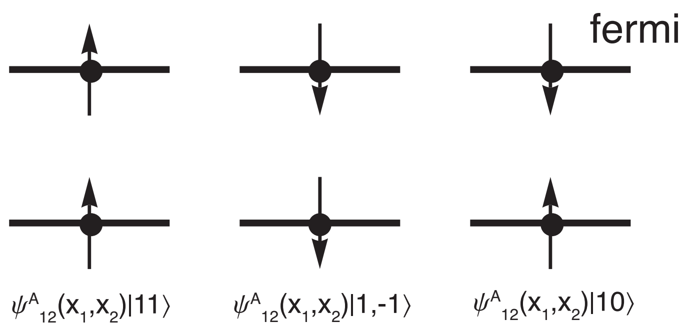
$$\left\langle x_1x_2 \right\rangle = \left\langle \psi_{12}^A \middle| x_1x_2 \middle| \psi_{12}^A \right\rangle \left\langle 1M \middle| 1M \right\rangle$$

$$\left\langle x_1x_2 \right\rangle = \frac{1}{\sqrt{2}}\left({}_1\langle 1|\, {}_2\langle 2| - {}_2\langle 1|\, {}_1\langle 2| \right) x_1x_2 \frac{1}{\sqrt{2}}\left(|1\rangle_1 |2\rangle_2 - |1\rangle_2 |2\rangle_1 \right)$$
$$= \frac{1}{2}\Big\{ \left({}_1\langle 1| x_1 |1\rangle_1 \right)\left({}_2\langle 2| x_2 |2\rangle_2 \right) - \left({}_1\langle 1| x_1 |2\rangle_1 \right)\left({}_2\langle 2| x_2 |1\rangle_2 \right)$$
$$- \left({}_1\langle 2| x_1 |1\rangle_1 \right)\left({}_2\langle 1| x_2 |2\rangle_2 \right) + \left({}_1\langle 2| x_1 |2\rangle_1 \right)\left({}_2\langle 1| x_2 |1\rangle_2 \right)\Big\}$$

Exchange interaction

1. Expectation value of particle separation
2. Fermion triplet-spin

$$\left\langle \left(x_1 - x_2\right)^2 \right\rangle = \left\langle x_1^2 - 2x_1x_2 + x_2^2 \right\rangle$$
$$= \left\langle x_1^2 \right\rangle + \left\langle x_2^2 \right\rangle - 2\left\langle x_1x_2 \right\rangle$$



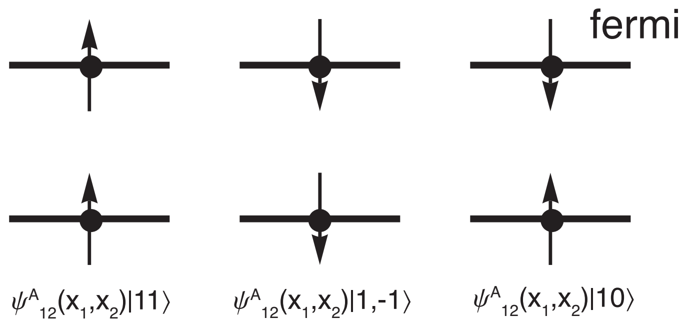
$$\left\langle x_1x_2 \right\rangle = \left\langle \psi_{12}^A \middle| x_1x_2 \middle| \psi_{12}^A \right\rangle \left\langle 1M \middle| 1M \right\rangle$$

$$\left\langle x_1x_2 \right\rangle = \int_{-\infty}^{\infty} \varphi^*{}_1\left(x_1\right)x_1\varphi_1\left(x_1\right)dx_1 \int_{-\infty}^{\infty} \varphi^*{}_2\left(x_2\right)x_2\varphi_2\left(x_2\right)dx_2$$

$$-\int_{-\infty}^{\infty} \varphi^*{}_1\left(x_1\right)x_1\varphi_2\left(x_1\right)dx_1 \int_{-\infty}^{\infty} \varphi^*{}_2\left(x_2\right)x_2\varphi_1\left(x_2\right)dx_2$$

Exchange interaction

1. Expectation value of particle separation
2. Fermion triplet-spin



$$\langle x_1 x_2 \rangle = \langle \psi_{12}^A | x_1 x_2 | \psi_{12}^A \rangle \langle 1M | 1M \rangle$$

$$\left\langle (x_1 - x_2)^2 \right\rangle = \int_{-\infty}^{\infty} \varphi^*{}_1(x) x^2 \varphi_1(x)\,dx + \int_{-\infty}^{\infty} \varphi^*{}_2(x) x^2 \varphi_2(x)\,dx$$

$$-2\int_{-\infty}^{\infty} \varphi^*{}_1(x) x \varphi_1(x)\,dx \int_{-\infty}^{\infty} \varphi^*{}_2(x) x \varphi_2(x)\,dx \underbrace{-2\left|\int_{-\infty}^{\infty} \varphi^*{}_1(x) x \varphi_2(x)\,dx\right|^2}_{EXTRA!!}$$

Exchange interaction

1. NON INTERACTING particles "seem to have an interaction" – exchange
2. Expectation value of particle separation

$$\left\langle \left(x_1 - x_2\right)^2 \right\rangle = \left\langle x_1^2 - 2x_1x_2 + x_2^2 \right\rangle$$

$$= \left\langle x_1^2 \right\rangle + \left\langle x_2^2 \right\rangle - 2\left\langle x_1x_2 \right\rangle$$

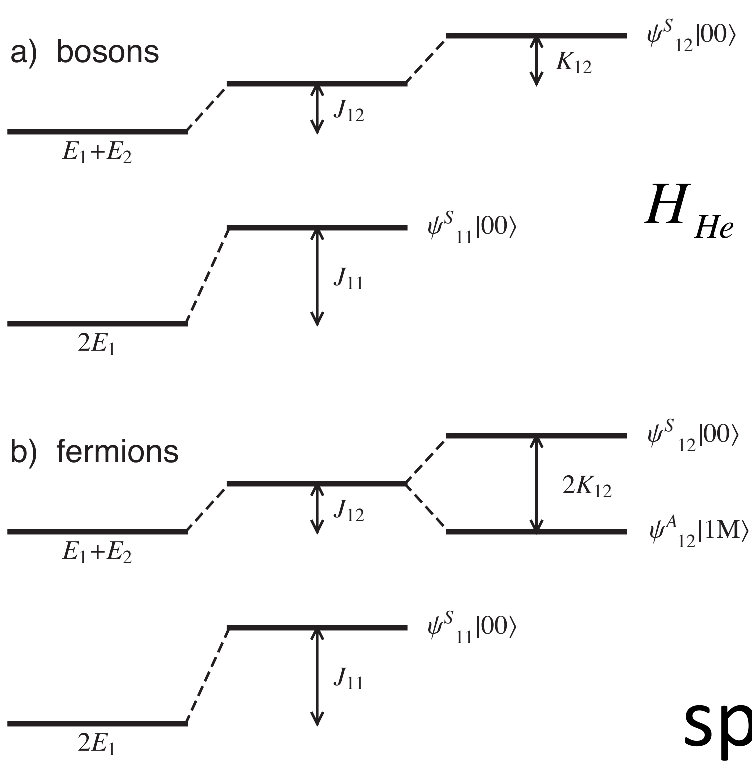
$$\sqrt{\left\langle \left(x_1 - x_2\right)^2 \right\rangle_S} = 0.20L$$

$$\sqrt{\left\langle \left(x_1 - x_2\right)^2 \right\rangle_D} = 0.32L$$

$$\sqrt{\left\langle \left(x_1 - x_2\right)^2 \right\rangle_A} = 0.41L$$

Interactions & exchange

1. INTERACTING particles also exhibit effects due to exchange … use perturbation theory



$$H' = V_{\text{int}}\left(x_1 - x_2\right)$$

$$H_{He} = \left(\frac{p_1^2}{2m} - \frac{2e^2}{4\pi\varepsilon_0 r_1}\right) + \left(\frac{p_2^2}{2m} - \frac{2e^2}{4\pi\varepsilon_0 r_2}\right) + \frac{e^2}{4\pi\varepsilon_0 r_{12}}$$

$$E^{(1)} = \left\langle \psi^{(0)} \middle| H' \middle| \psi^{(0)} \right\rangle$$

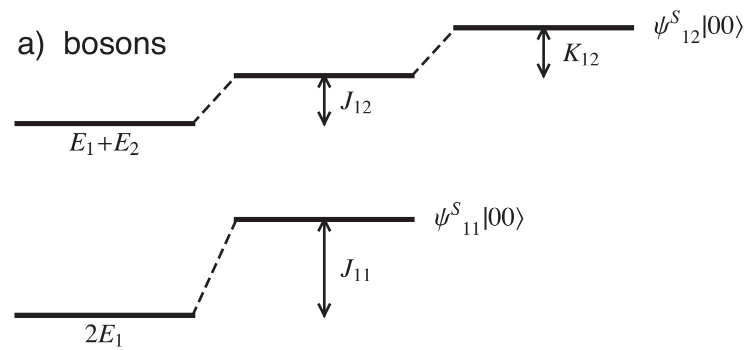
$$= \left\langle \psi_{spatial}{}^{(0)} \middle| H' \middle| \psi_{spatial}{}^{(0)} \right\rangle$$

spin state determines spatial wf!

Interactions & exchange- ground state

1. Ground state – 2 bosons/fermions – spatial part is symmetric

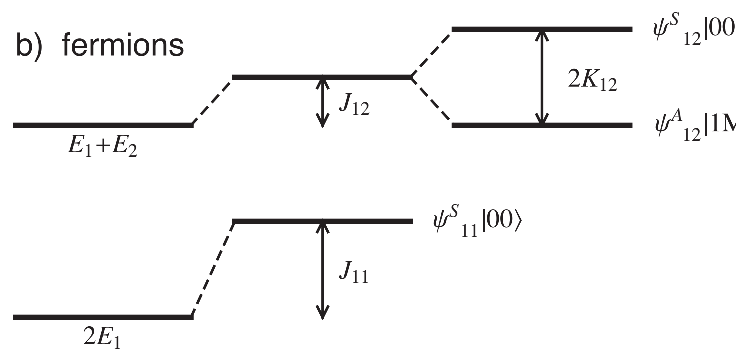
$$H' = V_{\text{int}}\left(x_1 - x_2\right)$$



$$E_{11}^{(1)} = \left\langle \psi^{(0)} \middle| V_{\text{int}} \middle| \psi^{(0)} \right\rangle$$

$$= \left({}_2\langle 1|_1\langle 1|\right) V_{\text{int}} \left(|1\rangle_1 |1\rangle_2\right)$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \varphi_1^*\left(x_2\right)\varphi_1^*\left(x_1\right) V_{\text{int}}\left(x_1 - x_2\right)\varphi_1\left(x_1\right)\varphi_1\left(x_2\right) dx_1 dx_2$$



$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left|\varphi_1^*\left(x_2\right)\right|^2 \left|\varphi_1^*\left(x_1\right)\right|^2 V_{\text{int}}\left(x_1 - x_2\right) dx_1\, dx_2$$

$$J_{nm} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left|\varphi_n\left(x_1\right)\right|^2 V_{\text{int}}\left(x_1 - x_2\right) \left|\varphi_m\left(x_2\right)\right|^2 dx_1\, dx_2$$

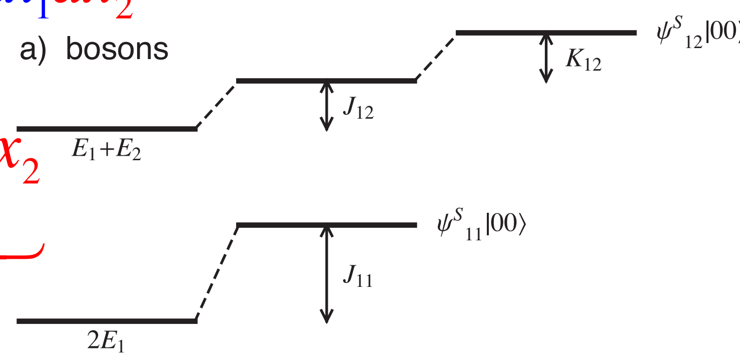
Direct integral

Exchange - excited symm state

$$E_{12}^{(1)} = \left\langle \psi^{(0)} \middle| V_{\text{int}} \middle| \psi^{(0)} \right\rangle$$

$$= \tfrac{1}{2}\left({}_1\langle 1|_2\langle 2| + {}_2\langle 1|_1\langle 2| \right) V_{\text{int}} \left(|1\rangle_1 |2\rangle_2 + |1\rangle_2 |2\rangle_1 \right)$$

$$= \tfrac{1}{2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left[\varphi_1^*(x_1)\varphi_2^*(x_2) + \varphi_1^*(x_2)\varphi_2^*(x_1) \right] V_{\text{int}}(x_1 - x_2) \left[\varphi_1(x_1)\varphi_2(x_2) + \varphi_1(x_2)\varphi_2(x_1) \right] dx_1 dx_2$$



$$= \underbrace{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left|\varphi_2^*(x_2)\right|^2 \left|\varphi_1^*(x_1)\right|^2 V_{\text{int}}(x_1 - x_2)\, dx_1\, dx_2}_{J_{12}}$$

$$+ \underbrace{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \varphi_1^*(x_2)\varphi_2^*(x_1) V_{\text{int}}(x_1 - x_2) \varphi_1(x_1)\varphi_2(x_2)\, dx_1\, dx_2}_{K_{12}}$$

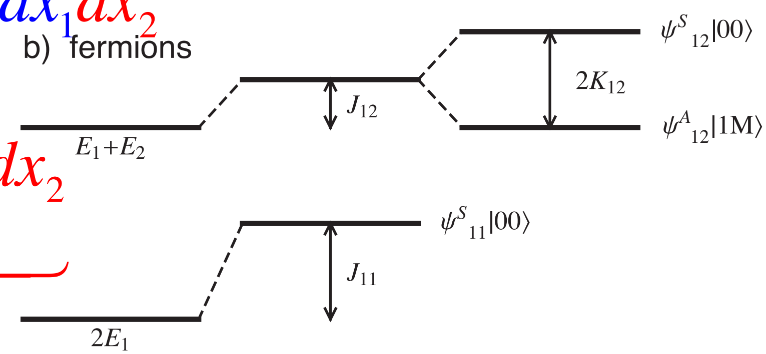
Exchange integral $K_{nm} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \varphi_n^*(x_1)\varphi_m^*(x_2) V_{\text{int}}(x_1 - x_2) \varphi_n(x_2)\varphi_m(x_1)\, dx_1\, dx_2$

Exchange - excited asymm state

$$E_{12}^{(1)} = \left\langle \psi^{(0)} \middle| V_{\text{int}} \middle| \psi^{(0)} \right\rangle$$

$$= \tfrac{1}{2}\left({}_1\langle 1|_2 \langle 2| - {}_2\langle 1|_1 \langle 2| \right) V_{\text{int}} \left(|1\rangle_1 |2\rangle_2 - |1\rangle_2 |2\rangle_1 \right)$$

$$= \frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\varphi_1^*(x_1)\varphi_2^*(x_2) - \varphi_1^*(x_2)\varphi_2^*(x_1) \right] V_{\text{int}}(x_1 - x_2) \left[\varphi_1(x_1)\varphi_2(x_2) - \varphi_1(x_2)\varphi_2(x_1) \right] dx_1 dx_2$$

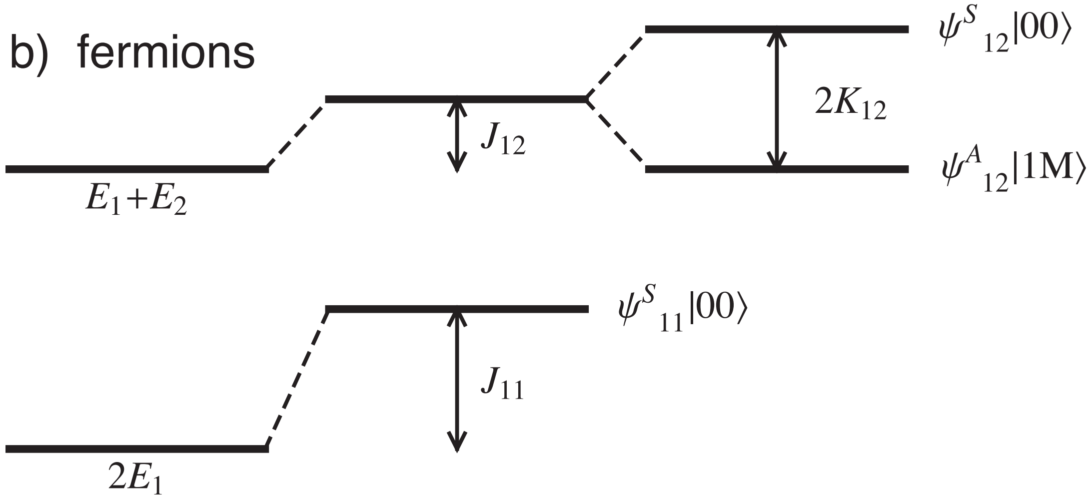


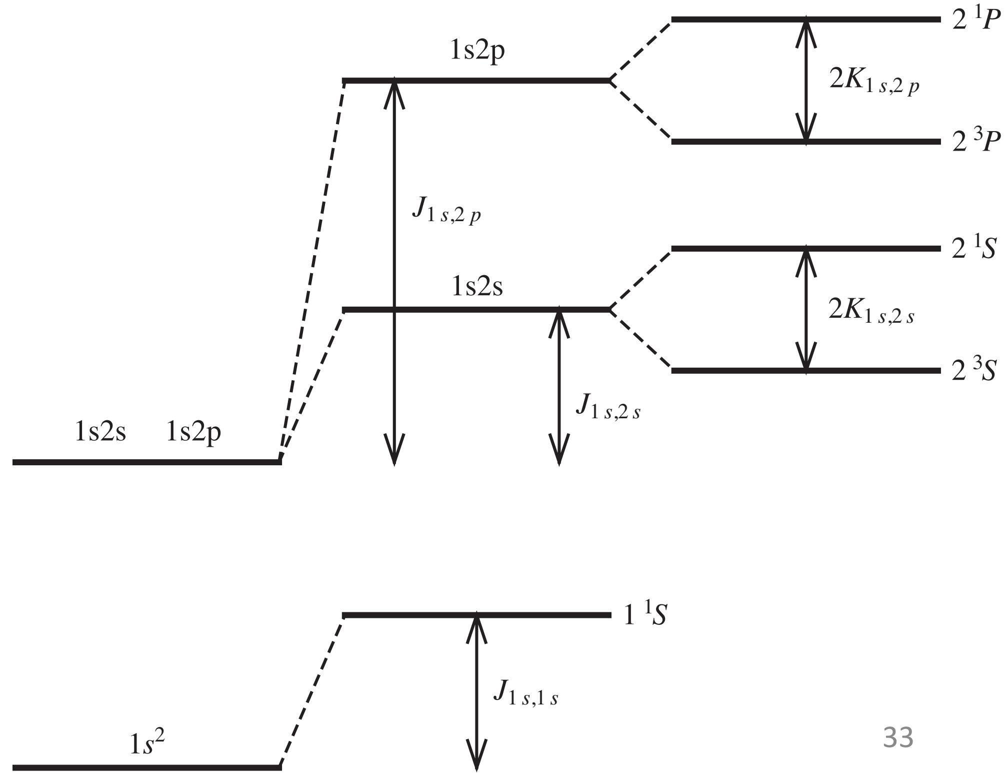
$$= \underbrace{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left|\varphi_2^*(x_2)\right|^2 \left|\varphi_1^*(x_1)\right|^2 V_{\text{int}}(x_1 - x_2)\, dx_1\, dx_2}_{J_{12}}$$

$$- \underbrace{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \varphi_1^*(x_2)\varphi_2^*(x_1) V_{\text{int}}(x_1 - x_2) \varphi_1(x_1)\varphi_2(x_2)\, dx_1\, dx_2}_{K_{12}}$$

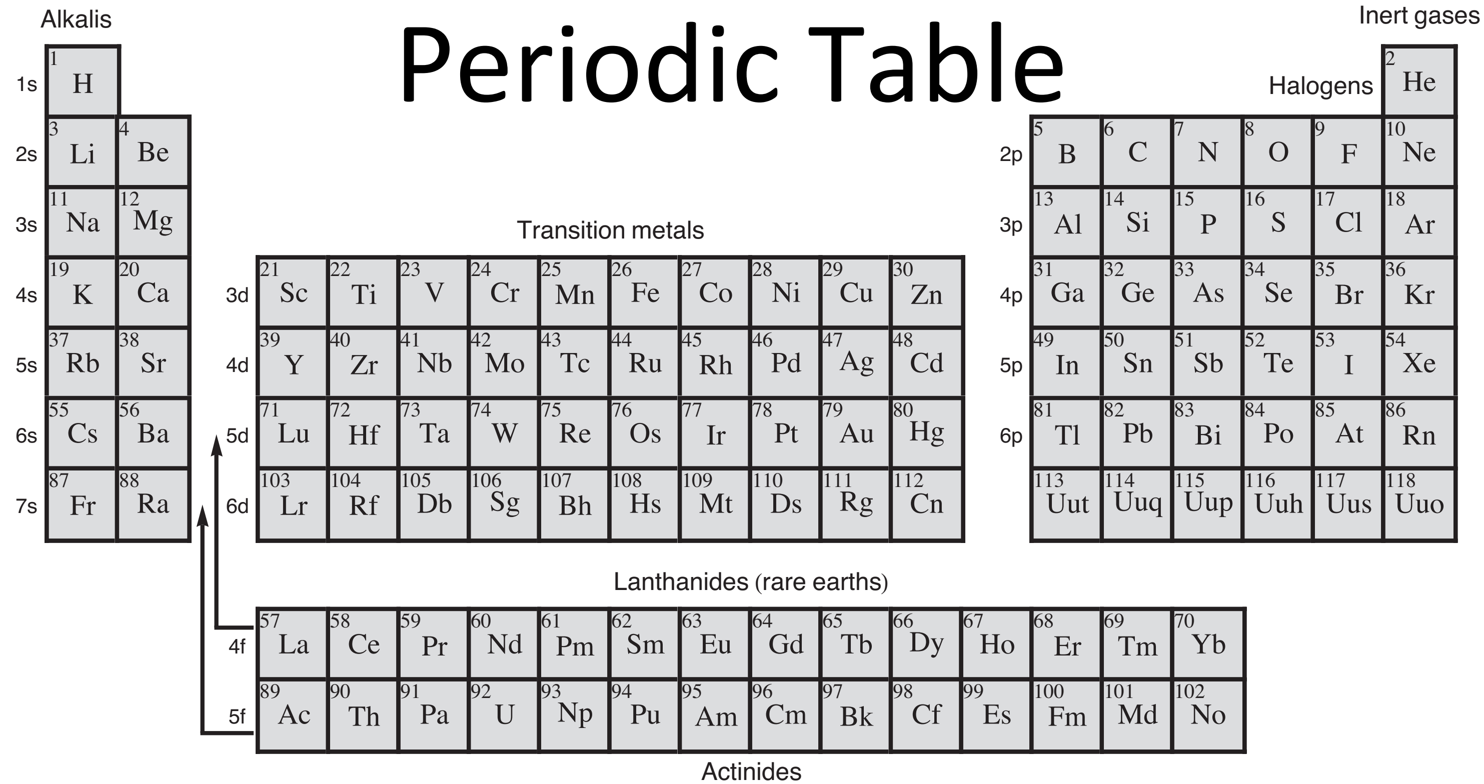
Exchange integral $K_{nm} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \varphi_n^*(x_1)\varphi_m^*(x_2) V_{\text{int}}(x_1 - x_2) \varphi_n(x_2)\varphi_m(x_1)\, dx_1\, dx_2$

Exchange – Generic & Helium



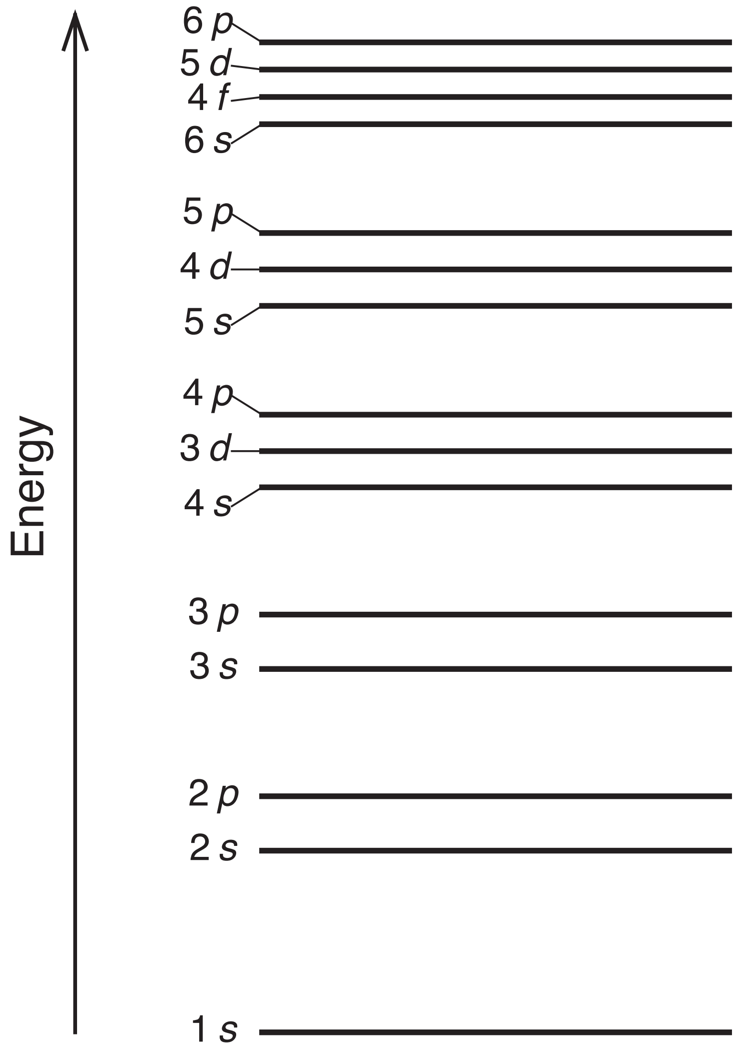


Periodic Table



shell (n)	subshell configuration	degeneracy ($2n^2$)
1	$1s^2$	2
2	$2s^2\ 2p^6$	8
3	$3s^2\ 3p^6\ 3d^{10}$	18
4	$4s^2\ 4p^6\ 4d^{10}\ 4f^{14}$	32
5	$5s^2\ 5p^6\ 5d^{10}\ 5f^{14}\ 5g^{18}$	50
6	$6s^2\ 6p^6\ 6d^{10}\ 6f^{14}\ 6g^{18}\ 6h^{22}$	72
7	$7s^2\ 7p^6\ 7d^{10}\ 7f^{14}\ 7g^{18}\ 7h^{22}\ 7i^{26}$	98

Periodic Table



Row	subshell configuration				Number of atoms
1	$1s^2$				2
2	$2s^2$			$2p^6$	8
3	$3s^2$			$3p^6$	8
4	$4s^2$		$3d^{10}$	$4p^6$	18
5	$5s^2$		$4d^{10}$	$5p^6$	18
6	$6s^2$	$4f^{14}$	$5d^{10}$	$6p^6$	32
7	$7s^2$	$5f^{14}$	$6d^{10}$	$7p^6$	32

Periodic Table

1	H	$1s^2$
2	He	$1s^2$
3	Li	$[He]\ 2s^1$
4	Be	$[He]\ 2s^2$
5	B	$[He]\ 2s^2\ 2p^1$
6	C	$[He]\ 2s^2\ 2p^2$
7	N	$[He]\ 2s^2\ 2p^3$
8	O	$[He]\ 2s^2\ 2p^4$
9	F	$[He]\ 2s^2\ 2p^5$
10	Ne	$[He]\ 2s^2\ 2p^6$
11	Na	$[Ne]\ 3s^1$
18	Ar	$[Ne]\ 3s^2 3p^6$
19	K	$[Ar]\ 4s^1$
21	Sc	$[Ar]\ 4s^2\ 3d^1$
23	V	$[Ar]\ 4s^2\ 3d^3$
24	Cr	$[Ar]\ 4s^1\ 3d^5$
25	Mn	$[Ar]\ 4s^2\ 3d^5$
28	Ni	$[Ar]\ 4s^2\ 3d^8$
29	Cu	$[Ar]\ 4s^1\ 3d^{10}$
30	Zn	$[Ar]\ 4s^2\ 3d^{10}$
36	Kr	$[Ar]\ 4s^2\ 3d^{10}\ 4p^6$
37	Rb	$[Kr]\ 5s^1$
46	Pd	$[Kr]\ 4d^{10}$
54	Xe	$[Kr]\ 5s^2\ 4d^{10}\ 5p^6$
55	Cs	$[Xe]\ 6s^1$
57	La	$[Xe]\ 6s^2\ 5d^1$
58	Ce	$[Xe]\ 6s^2\ 4f^1\ 5d^1$
59	Pr	$[Xe]\ 6s^2\ 4f^3$
86	Rn	$[Xe]\ 6s^2\ 4f^{14}\ 5d^{10}\ 6p^6$
87	Fr	$[Rn]\ 7s^1$
92	U	$[Rn]\ 7s^2\ 5f^3\ 6d^1$
94	Pt	$[Rn]\ 7s^2\ 5f^6$

OLD

Example indistinguishable, with spin (uncoupled spin basis)

1. PRODUCT wave function still OK

$$\psi_{n_a,n_b}\left(x_1,x_2,s_1,m_{s1},s_2,m_{s2}\right)$$
$$=\varphi_{n_a}\left(x_1\right)\chi_a\left(m_{s1}\right)\varphi_{n_b}\left(x_2\right)\chi_b\left(m_{s2}\right)$$

$$E=E_{n_a}+E_{n_b}$$

2. BUT neither symmetric nor antisymmetric under particle exchange if n_a and n_b are different!

$$\underbrace{\varphi_1\left(x_1\right)\begin{pmatrix}1\\0\end{pmatrix}}_{\#\ 1\text{ in ground, }\uparrow}\underbrace{\varphi_2\left(x_2\right)\begin{pmatrix}0\\1\end{pmatrix}}_{\#\ 2\text{ in 1st ex., }\downarrow}\xrightarrow{\textit{exchange}}\underbrace{\varphi_1\left(x_2\right)\begin{pmatrix}1\\0\end{pmatrix}}_{\#\ 2\text{ in gnd., }\uparrow}\underbrace{\varphi_2\left(x_1\right)\begin{pmatrix}0\\1\end{pmatrix}}_{\#\ 1\text{ in 1st ex., }\downarrow}$$

Example indistinguishable, with spin (coupled spin basis; triplet)

1. PRODUCT wave function still OK for space; take one state from spin triplet state:

$$\psi_{n_a,n_b}\left(x_1,x_2,s_1,m_{s1},s_2,m_{s2}\right)$$
$$=\varphi_{n_a}\left(x_1\right)\varphi_{n_b}\left(x_2\right)\left|10\right\rangle_c$$
$$=\varphi_{n_a}\left(x_1\right)\varphi_{n_b}\left(x_2\right)\left[\left|+-\right\rangle+\left|-+\right\rangle\right]$$

2. BUT has neither symmetry nor antisymmetry under particle exchange if n_a and n_b are different!

$$\underbrace{\varphi_1\left(x_1\right)}_{\#\ 1\text{ in ground}}\ \underbrace{\varphi_2\left(x_2\right)}_{\#\ 2\text{ in 1st ex.}}\left[\underbrace{\left|+-\right\rangle}_{\#1,\#2}+\underbrace{\left|-+\right\rangle}_{\#1,\#2}\right]\xrightarrow{exchange}\underbrace{\varphi_1\left(x_2\right)}_{\#\ 2\text{ in gnd.}}\ \underbrace{\varphi_2\left(x_1\right)}_{\#\ 1\text{ in 1st ex}}\left[\underbrace{\left|-+\right\rangle}_{\#1,\#2}+\underbrace{\left|+-\right\rangle}_{\#1,\#2}\right]$$

Example indistinguishable, with spin (coupled spin basis; triplet)

1. PRODUCT wave function still OK for space; take one state from spin triplet state:

$$\psi_{n_a,n_b}(x_1,x_2,s_1,m_{s1},s_2,m_{s2})$$
$$= \varphi_{n_a}(x_1)\varphi_{n_b}(x_2)|10\rangle_c$$
$$= \varphi_{n_a}(x_1)\varphi_{n_b}(x_2)\left[|+-\rangle+|-+\rangle\right]$$

2. BUT has neither symmetry nor antisymmetry under particle exchange if n_a and n_b are different!

$$\underbrace{\varphi_1(x_1)}_{\#\ 1\text{ in ground}}\ \underbrace{\varphi_2(x_2)}_{\#\ 2\text{ in 1st ex.}}\left[\underbrace{|+-\rangle}_{\#1,\#2}+\underbrace{|-+\rangle}_{\#1,\#2}\right]\xrightarrow{\text{exchange}}\underbrace{\varphi_1(x_2)}_{\#\ 2\text{ in gnd.}}\ \underbrace{\varphi_2(x_1)}_{\#\ 1\text{ in 1st ex}}\left[\underbrace{|-+\rangle}_{\#1,\#2}+\underbrace{|+-\rangle}_{\#1,\#2}\right]$$

Example indistinguishable, with spin (coupled spin basis; triplet)

1. But this has correct symmetry for bosons for all n_a, n_b *(check)*:

$$\psi_{na,nb}\left(x_1,x_2,s_1,m_{s1},s_2,m_{s2}\right)=$$

$$\left(\underbrace{\varphi_1\left(x_1\right)}_{\#\ 1\ \text{in ground}}\ \underbrace{\varphi_2\left(x_2\right)}_{\#\ 2\ \text{in 1st ex.}}+\underbrace{\varphi_1\left(x_2\right)}_{\#\ 2\ \text{in ground}}\ \underbrace{\varphi_2\left(x_1\right)}_{\#\ 1\ \text{in 1st ex}}\right)\left[\underbrace{\left|+-\right\rangle}_{\#1,\#2}+\underbrace{\left|-+\right\rangle}_{\#1,\#2}\right]$$

2. And this has correct antisymmetry for fermions (check). What about $n_a = n_b$?

$$\psi_{na,nb}\left(x_1,x_2,s_1,m_{s1},s_2,m_{s2}\right)=$$

$$\left(\underbrace{\varphi_1\left(x_1\right)}_{\#\ 1\ \text{in ground}}\ \underbrace{\varphi_2\left(x_2\right)}_{\#\ 2\ \text{in 1st ex.}}-\underbrace{\varphi_1\left(x_2\right)}_{\#\ 2\ \text{in ground}}\ \underbrace{\varphi_2\left(x_1\right)}_{\#\ 1\ \text{in 1st ex}}\right)\left[\underbrace{\left|+-\right\rangle}_{\#1,\#2}+\underbrace{\left|-+\right\rangle}_{\#1,\#2}\right]$$