Identical particles

Some of the most interesting and frequently-encountered aspects of quantum mechanics arise in many-body problems of identical particles. We can of course see these effects at the two-body level, but their macroscopic effects, e.g. Bose Einstein condensation (bosons) and Fermi surfaces in metals (fermions), are very dramatic, and can dominate the physics of the problem.

The issue is basically just one of counting states! (...and not overcounting).

e.g. in a state of two distinguishable particles, such as a proton (p) and an electron (e^-), clearly these are two different states

$s_1^z = \pm 1/2 \; (\cdot \hbar)$

$$|\, p(\vec{p}_1, s_1^z),\, e^-(\vec{p}_2, s_2^z) \rangle \neq |\, \vec{p}(\vec{p}_2, s_2^z),\, e^-(\vec{p}_1, s_1^z) \rangle$$

$$\text{“} |p_1 e_2^- \rangle \text{”} \neq \text{“} |p_2 e_1^- \rangle \text{”}$$

However if we consider a state of two identical particles, such as two electrons, these systems are physically equivalent and it would be double-counting to list them as separate states. To within a phase,

$$|e^-(\vec{p}_1, s_1^z)\, e^-(\vec{p}_2, s_2^z)\rangle = \underset{\pm 1}{\underline{e^{i\varphi}}}\, |e^-(\vec{p}_2, s_2^z)\, e^-(p_1, s_1^z)\rangle .$$

There are two standard ways of dealing with this danger of overcounting.

Setting up a multiparticle state space for identical particles:

I. One is to have a standard list of states, so the labels, $(\vec{p}, s^z)$ for example, tell you what order to list the particles in in the multiparticle state vector. (common in cond. mat.)
This is like "Newspeak" in 1984 ; the language is structured so that criminal statements are impossible. $|e_1^- e_2^-\rangle$ only.

II. Another approach is to symmetrize or antisymmetrize the states. In this way $|e_1^- e_2^-\rangle$ and $|e_2^- e_1^-\rangle$ are never listed separately, only

$$\underline{|e^- e^-\rangle_{[12]}} = \frac{1}{\sqrt{2}}\left\{ |e_1^- e_2^-\rangle - |e_2^- e_1^-\rangle \right\} ,$$

so double counting does not happen.

These two methods are equivalent. Note that antisymmetrizing multifermion states (2^{nd} approach) is <u>not</u> essential! (Despite what you have heard.) You simply need to avoid double counting.

Spin-Statistics Theorem

whether we I. have a restricted set of basis states, or
II. explicitly symm/antisymm the states,

we do encounter a phase in relating a state $|12\rangle$ with the exchanged state,

$$|12\rangle = \underline{\pm 1} \cdot |21\rangle$$

this phase was established by Pauli in 1940, and is specified by the "spin-statistics theorem"

The result <u>we</u> need is that it is (-1) for fermion states ($\frac{1}{2}$-integer spin)

and $(+1)$ for boson states (integer spin).

examples are : f : e^-, p, ν, μ^-, q (all $s=1/2$), Δ ($s=3/2$, composite of 3 $s=1/2$s), ^3He ($s=1/2$), $Cu^{++}(s=1/2)$, nucleus ^{17}O etc.

b : γ ($s=1$), φ ($s=0$), $h_{\mu\nu}$ ($s=2$), ^4He nucleus ($s=0$), $Ni^{++}(s=1)$, etc

The origin of the spin-statistics theorem is rather "deep".

The "particles" we encounter in nature are really excitations of a quantum field theory.

You already know conventional field theories, e.g. $\{ \vec{E}(\vec{x},t)$ and $\vec{B}(\vec{x},t) \}$.
These can be viewed as systems with coordinates

$$\{ \vec{A}(\vec{x}) \} \quad \text{(an infinite number, 3 at each point } \vec{x}\text{)}$$

and conjugate momenta,

$$\left\{ \vec{P}_A = \frac{\delta \mathcal{L}}{\delta \dot{\vec{A}}} = i\,\dot{\vec{A}}(\vec{x}) \right\}$$

electric field

when we quantize this system of coordinates and momenta, we find that $\vec{A}(\vec{x})$ becomes a field of operators, as do $\vec{E}(\vec{x})$, $\vec{B}(\vec{x})$ etc. These can be expanded in Fourier modes, e.g.

a polarization label: 2 indep choices for $\hat{\epsilon}_{k,\lambda}$.

$$\vec{A}^{\,\text{op.}}(\vec{x}) = \int \frac{d^3k}{\sqrt{(2\pi)^3\, 2\omega_k}} \left\{ a_{k\lambda} \underbrace{\hat{\epsilon}_{k\lambda} e^{i\vec{k}\cdot\vec{x}}}_{\text{plane wave}} + \underbrace{a^\dagger_{k\lambda}\, \hat{\epsilon}^*_{k\lambda}\, e^{-i\vec{k}\cdot\vec{x}}}_{\text{complex conjugate}} \right\}$$

$$\omega_k \equiv |\vec{k}|c$$

Fourier coefficient (must be an operator).

free EM field

The Hamiltonian $H = \frac{1}{2}\int d^3x \left(\vec{E}(\vec{x})^2 + \vec{B}(\vec{x})^2 \right)$ is then

$$H = \sum_\lambda \int d^3k \;\; \hbar\omega_k \left(a^\dagger_{k\lambda} a_{k\lambda} + \tfrac{1}{2} \right)$$

= an infinite number of harmonic oscillators, one for each $\vec{k}$ and λ.

The Fourier coefficients $\{a_{k\lambda}\}$ themselves have simple commutation rels. with H,

$$[H, a^\dagger_{k\lambda}] = +\hbar\omega_k\, a^\dagger_{k\lambda}$$

which tells you that $a^{\dagger}_{k\lambda}$ is a raising operator, and raises the energy of a state by $\Delta E = +\hbar\omega_{\vec{k}}$. It is interpreted as a particle creation operator, with the particle called a "photon"

$$|\vec{k},\lambda\rangle = a^{\dagger}_{\vec{k}\lambda}\,|0\rangle \qquad \text{1-photon state}$$

The creation operators commute,

$$|\vec{k}_1\lambda_1,\vec{k}_2\lambda_2\rangle = a^{\dagger}_{k_1\lambda_1}\,a^{\dagger}_{k_2\lambda_2}|0\rangle$$

"$|\gamma_1,\gamma_2\rangle$" 2-photon state

$$[a^{\dagger}_{k\lambda}, a^{\dagger}_{k'\lambda'}] = 0, \qquad ([a,a]=0)$$

which tells you that for two-photon states we have

$$|\gamma_1\gamma_2\rangle = a^{\dagger}_1 a^{\dagger}_2\,|0\rangle = |a^{\dagger}_2 a^{\dagger}_1|0\rangle = +|\gamma_2\gamma_1\rangle$$

identically the same state

and we can avoid double counting by using symmetrized two-photon states,

$$|\gamma\gamma\rangle_{12} = \frac{1}{\sqrt{2}}\left\{ |\gamma_1\gamma_2\rangle + |\gamma_2\gamma_1\rangle \right\}$$

This works for any integer-spin (bose) particle.

n.b. there <u>is</u> a nonzero commutator,

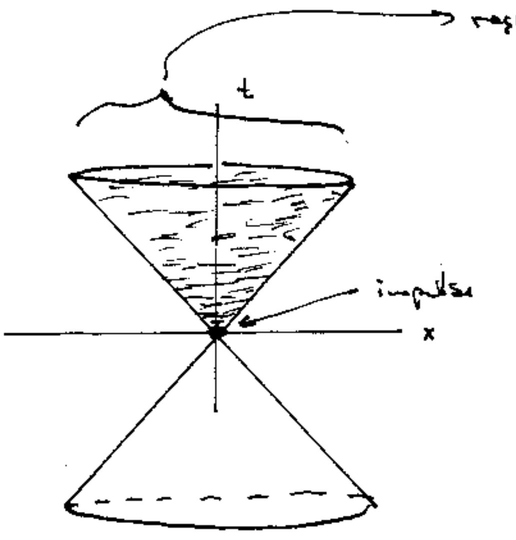
$$[a_{k\lambda}, a^{\dagger}_{k'\lambda'}] = \delta(\vec{k}-\vec{k}')\,\delta_{\lambda\lambda'} \qquad \text{continuum analog of } [a,a^{\dagger}]=1.$$

This does <u>not</u> work for fermions for the following reason:

The response to a localized disturbance in a bose quantum field theory, quantized with

$$\underbrace{[q_i, p_j]}_{\text{continuum analog}} = +i\hbar\delta_{ij}$$

fills up the forward light cone, as you might expect from causality:



(e.g. $\langle\psi|\varphi(\vec{x},t)|\psi\rangle$)

expected value of a field op.

If the response were outside the light cone, it could be used in superluminal information transfer.

For fermion quantum field theories, however, it was found that quantizing with

$$\underbrace{[q_i\,,\,p_j]}_{\text{fermi fields \& their canonical momenta}} = +i\hbar\,\delta_{ij}$$

led to a response that was nonzero only <u>outside</u> the light cone. A disaster!

It was noted by Pauli ('40) that assuming instead an <u>anti</u>commutation relation for fermi fields

$$\{q_i\,,\,p_j\} = +i\hbar\,\delta_{ij} \qquad\qquad \{A,B\} \equiv AB+BA$$

led to a response function that, as desired, only had support <u>within</u> the forward light cone. This applied to all $\frac{1}{2}$-integer spin fields and their quanta.

The corresponding particle creation operators (called $b^{\dagger}_{\underbrace{\vec{p}}_{\text{3-momentum}},\underbrace{s}_{\uparrow \text{ or } \downarrow}}$ for electrons) as a result obeyed <u>anti</u>commutation relations,

$$\{b^{\dagger}_{\vec{p},s}\,,\,b^{\dagger}_{\vec{p}',s'}\} = 0 \qquad\qquad \{b,b\}=0$$

only nonzero $\{b_{\vec{p},s}\,,\,b^{\dagger}_{\vec{p}',s'}\} = \delta(\vec{p}-\vec{p}')\,\delta_{ss'}$

n.b. still $\underbrace{[H,\,b^{\dagger}_{\vec{p},s}]}_{\text{commutator}} = +E_{\vec{p}}\,b^{\dagger}_{\vec{p},s}$

This anticommutation relation implies for a two-fermion state

$$|f_1 f_2\rangle = b_1^\dagger b_2^\dagger |0\rangle = - b_2^\dagger b_1^\dagger |0\rangle = - |f_2 f_1\rangle$$

so, if we list all states & use symmetry to eliminate identical copies, we must antisymmetrize the fermion states,

$$|ff\rangle_{12} = \frac{1}{\sqrt{2}} \left(|f_1 f_2\rangle - |f_2 f_1\rangle \right)$$

Thus, causality requires the $\left\{ \begin{matrix} \text{symm} \\ \text{antisymm} \end{matrix} \right\}$ of $\left\{ \begin{matrix} \text{Bose} \\ \text{Fermi} \end{matrix} \right\}$ particle states.

The exclusion principle follows trivially. Since Fermion creation operators for generic states i, j satisfy

$$\{ b_i^\dagger, b_j^\dagger \} = 0$$

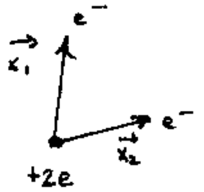
it follows that

$$b_i^{\dagger\,2} = 0$$

i.e. two fermions cannot be in the same state.

Symmetry of identical particle wavefunctions

It's intuitively satisfying to visualize multiparticle states as if they were distinguishable, e.g. to write a two-electron state in a helium atom (with $S_z = \uparrow$ for each e^-) as



$$|\psi\rangle = \iint d^3x_1\, d^3x_2\ \psi(\vec{x}_1, \vec{x}_2)\ |e^-_\uparrow(\vec{x}_1)\ e^-_\uparrow(\vec{x}_2)\rangle$$

Of course this is double counting, if we switch $\vec{x}_1$ and $\vec{x}_2$ we have a physically equivalent basis state. We must restrict our basis states so that we don't double count.

Either I. restrict $(\vec{x}_1, \vec{x}_2)$ so we never encounter the pair $(\vec{x}_2, \vec{x}_1)$ (hard), or

II. use explicitly antisymmetrized states, so $(\vec{x}_1, \vec{x}_2)$ and $(\vec{x}_2, \vec{x}_1)$ never appear separately (standard).

Using II, we still integrate over <u>all</u> $\vec{x}_1$ and $\vec{x}_2$ but combine the original and image states:

$$|\psi\rangle = \iint d^3x_1\, d^3x_2\ \psi(\vec{x}_1, \vec{x}_2) \cdot \left\{ \frac{|e^-_\uparrow(x_1)\, e^-_\uparrow(x_2)\rangle - |e^-_\uparrow(\vec{x}_2)\, e^-_\uparrow(\vec{x}_1)\rangle}{\sqrt{2}} \right\}$$

$= \begin{array}{|c|}\hline \ \\ \hline \ \\ \hline\end{array}$ spatial symm

If we divide the wavefunction $\psi(\vec{x}_1, \vec{x}_2)$ into symm and antisymm parts,

$$\psi(\vec{x}_1, \vec{x}_2) = \underbrace{\psi_S(\vec{x}_1, \vec{x}_2)}_{\frac{1}{2}\left[\psi(\vec{x}_1, \vec{x}_2) + \psi(\vec{x}_2, \vec{x}_1)\right]} + \underbrace{\psi_A(\vec{x}_1, \vec{x}_2)}_{\frac{1}{2}\left[\psi(\vec{x}_1, \vec{x}_2) - \psi(\vec{x}_2, \vec{x}_1)\right]}$$

only ψ_A survives the integral, since it's multiplied by an A quantity. Thus the state is equivalently

$$|\psi\rangle = \iint d^3x_1 d^3x_2 \;\; \psi_A(\vec{x}_1, \vec{x}_2) \left\{ \frac{|e_1^- e_2^-\rangle - |e_2^- e_1^-\rangle}{\sqrt{2}} \right\}$$

finally, since the state is multiplying an antisymmetric wavefunction, we get the same result if we use an unsymmetrized basis state, and pretend that electrons are distinguishable! :

$$|\psi\rangle = \iint d^3x_1 d^3x_2 \;\; \psi_A(\vec{x}_1, \vec{x}_2) \; \underbrace{|e_\uparrow^-(\vec{x}_1)\, e_\uparrow^-(\vec{x}_2)\rangle}_{\text{no restriction on } \vec{x}_1, \vec{x}_2.}$$

(modulo $\sqrt{2}$ factors)

Thus it suffices to antisymmetrize the multifermion wavefunction,

and to continue to use the basis states as if the fermions were distinguishable.

Careful : This approach can easily lead to misconceptions, e.g. for two ↑ electrons,

" the amplitude for electron 1 at $\vec{x}$ and electron 2 at $\vec{y}$ is
minus the amplitude for electron 1 at $\vec{y}$ and electron 2 at $\vec{x}$."

This is wrong ; there is only 1 state of an $e_\uparrow^-$ at $\vec{x}$ and an $e_\uparrow^-$ at $\vec{y}$.

bosons

Similarly, for bosons you may wish to write a two photon (or phonon) state as if they were distinguishable,

$$|\psi_{\substack{\gamma\gamma \\ \lambda_1\lambda_2 \\ = \; = \\ + \; +}}\rangle = \iint d^3k_1 d^3k_2 \; \psi(\vec{k}_1, \vec{k}_2)\, |\gamma(\vec{k}_1)\, \gamma(\vec{k}_2)\rangle .$$

To avoid double counting you may again symmetrize the state,

$$|\gamma\gamma\rangle = \left\{ \frac{|\gamma(\vec{k}_1)\gamma(\vec{k}_2)\rangle + |\gamma(\vec{k}_2)\gamma(\vec{k}_1)\rangle}{\sqrt{2}} \right\}$$

$= \square\!\square$ spatial symm

which symmetrizes the wfn,

$$\psi_s(\vec{k}_1, \vec{k}_2) = \frac{1}{2}\left[\psi(\vec{k}_1, \vec{k}_2) + \psi(\vec{k}_2, \vec{k}_1)\right]$$

with this ψ_s we may again use unsymmetrized basis states,

$$|\gamma\gamma\rangle = \iint d^3k_1\, d^3k_2\; \psi_s(\vec{k}_1, \vec{k}_2)\; |\gamma(\vec{k}_1)\gamma(\vec{k}_2)\rangle$$

which illustrates the "folklore" that one symmetrizes the boson multipartical wfn.

>1 d.o.f.

We have considered two-particle states with only one "variable" lable, such as $\vec{x}$ (S_z fixed $=\uparrow$) and $\vec{k}$ (λ fixed $= +$). Of course more generally these can vary as well. The symmetrization (bose) or antisymmetrization (fermi) of the basis vectors again leads to states that are overall symm / antisymm under exchange, but need not have these symmetries on the individual spin labels.

Thus for example for a general two electron state we have

$$|\psi\rangle = \sum_{\substack{S_1^z S_2^z \\ m_1\; m_2}} \iint d^3x_1\, d^3x_2\; \psi_{m_1 m_2}(\vec{x}_1, \vec{x}_2)\; \frac{1}{\sqrt{2}}\Big\{ |e^-(\vec{x}_1, m_1)\, e^-(\vec{x}_2, m_2)\rangle - |e^-(\vec{x}_2, m_2)\, e^-(\vec{x}_1, m_1)\rangle \Big\}$$

For the $|\uparrow\uparrow\rangle \equiv |++\rangle$ and $|--\rangle$ cases this is equivalent to having an antisymmetric spatial wfn, as discussed above. What about for the $|+-\rangle$ and $|-+\rangle$ states? Consider a two-electron state in this sector only:

$$|\psi\rangle = \iint d^3x_1\, d^3x_2 \left[\psi_{+-}(\vec{x}_1, \vec{x}_2)\, \frac{1}{\sqrt{2}} \left\{ |e^-(\vec{x}_1,+)\, e^-(\vec{x}_2,-)\rangle - |e^-(\vec{x}_2,-)\, e^-(\vec{x}_1,+)\rangle \right\} \right.$$

$$\left. + \psi_{-+}(\vec{x}_1, \vec{x}_2)\, \frac{1}{\sqrt{2}} \left\{ |e^-(\vec{x}_1,-)\, e^-(\vec{x}_2,+)\rangle - |e^-(\vec{x}_2,+)\, e^-(\vec{x}_1,-)\rangle \right\} \right]$$

We will again rewrite this as unsymmetrized two-electron states, appropriate for distinguishable particles, times wavefunctions which will therefore be appropriately symmetrized.

We write the top & bottom wfns as the sums of S and A spatial parts,

$$\psi_{+-}(\vec{x}_1, \vec{x}_2) = \psi^S_{+-}(\vec{x}_1, \vec{x}_2) + \psi^A_{+-}(\vec{x}_1, \vec{x}_2)$$

$$\text{sim} \quad \psi_{-+} = \psi^S_{-+} + \psi^A_{-+}$$

So

$$|\psi\rangle = \frac{1}{\sqrt{2}} \iint d^3x_1\, d^3x_2 \Big[\psi^S_{+-}(\vec{x}_1, \vec{x}_2)\, |e^-(\vec{x}_1,+)\, e^-(\vec{x}_2,-)\rangle - \psi^S_{+-}\, |e^-(\vec{x}_2,-)\, e^-(\vec{x}_1,+)\rangle$$

all $\psi(\ )$ arguments here are $(\vec{x}_1, \vec{x}_2)$

$$+ \psi^A_{+-}(\vec{x}_1, \vec{x}_2)\, |e^-(\vec{x}_1,+)\, e^-(\vec{x}_2,-)\rangle - \psi^A_{+-}\, |e^-(\vec{x}_2,-)\, e^-(\vec{x}_1,+)\rangle$$

$$+ \psi^S_{-+}(\vec{x}_1, \vec{x}_2)\, |e^-(\vec{x}_1,-)\, e^-(\vec{x}_2,+)\rangle - \psi^S_{-+}\, |e^-(x_2,+)\, e^-(\vec{x}_1,-)\rangle$$

$$+ \psi^A_{-+}(\vec{x}_1, \vec{x}_2)\, |e^-(\vec{x}_1,-)\, e^-(\vec{x}_2,+)\rangle - \psi^A_{-+}\, |e^-(\vec{x}_2,+)\, e^-(\vec{x}_1,-)\rangle \Big]$$

$$= \iint \frac{d^3x_1\, d^3x_2}{\sqrt{2}} \Big[|e^-(\vec{x}_1,+)\, e^-(\vec{x}_2,-)\rangle \cdot \left\{ \psi^S_{+-} - \psi^S_{-+} + \psi^A_{+-} + \psi^A_{-+} \right\}$$

$$+ |e^-(\vec{x}_1,-)\, e^-(\vec{x}_2,+)\rangle \cdot \left\{ -\psi^S_{+-} + \psi^S_{-+} + \psi^A_{+-} + \psi^A_{-+} \right\} \Big]$$

$$= \iint d^3x_1\, d^3x_2 \Big[|e^-(\vec{x}_1)\, e^-(\vec{x}_2)\rangle \cdot \frac{1}{\sqrt{2}}\big(|+-\rangle - |-+\rangle\big) \cdot \underbrace{\left\{ \psi^S_{+-} - \psi^S_{-+} \right\}}_{\equiv \psi^S(\vec{x}_1, \vec{x}_2)}$$

since $|+-\rangle$ and $|-+\rangle$ have = & opp. amps

$$+ |e^-(\vec{x}_1)\, e^-(\vec{x}_2)\rangle \cdot \frac{1}{\sqrt{2}}\big(|+-\rangle + |-+\rangle\big) \cdot \underbrace{\left\{ \psi^A_{+-} + \psi^A_{-+} \right\}}_{\equiv \psi^A(\vec{x}_1, \vec{x}_2)} \Big]$$

Since $|+-\rangle$ and $|-+\rangle$ have equal amps

$$= \iint d^3x_1\, d^3x_2 \underbrace{\underbrace{\psi^S(\vec{x}_1, \vec{x}_2)}_{S \text{ space wfn}} \cdot \underbrace{\chi^A_{m_1 m_2}}_{A \text{ spin wfn}}}_{A \text{ overall (space-spin wfn)}} |e^-(\vec{x}_1, m_1)\, e^-(\vec{x}_2, m_2)\rangle$$

$\sum_{m_1 m_2}$ implicit

$$+ \iint d^3x_1\, d^3x_2 \underbrace{\underbrace{\psi^A(\vec{x}_1, \vec{x}_2)}_{A \text{ space wfn}} \underbrace{\chi^S_{m_1, m_2}}_{S \text{ spin wfn}}}_{A \text{ overall (space-spin wfn)}} \underbrace{|e^-(\vec{x}_1, m_1)\, e^-(\vec{x}_2, m_2)\rangle}_{\text{"distinguishable particle" state vectors}}$$

Both types are legal wfns. ∴ Only the <u>total</u> wavefunction symmetry must be A for a multifermion state.

[and S for a multiboson state].

Atomic physics example?

For He, the lowest energy state is $\psi^S(\vec{x}_1, \vec{x}_2) = \psi^S(\vec{x}_2, \vec{x}_1)$.
However we must have an overall A two electron state.

This requires an A spin wfn χ^A,

$$\sum_{m_1 m_2} \chi^A_{m_1 m_2} |m_1 m_2\rangle = \frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right)$$ spin singlet.

Thus the He ground state is $1^{\overbrace{2S+1}^{\text{spin of electrons}}}L = 1^1S$. No nearby spin triplet $e^- e^-$ state.

prince. (radial) quant no.

lowest combined L

The next levels are spin triplet: 2^3S, 2^3P

spin singlet: $\underbrace{2^1S}$, $\underbrace{2^1P}$

2^1P → can have $\psi^A(\vec{x}_1, \vec{x}_2) = \psi_{SP} - \psi_{PS}$

2^1S → can have $\psi^A(\vec{x}_1, \vec{x}_2) = \psi_{2S,S} - \psi_{S,2S}$.

in order

2^3P
2^1P
2^3S
2^1S
^1S

E