Exchange symmetry

Why are bosons bosons & fermions fermions?

The basis of a field theory is the (anti) commutation relations of the operators. Consider a set of MODES $\{\phi_r(x)\}$ that are orthonormal $\int dx\, \phi_r^* \phi_s = \delta_{rs}$ & complete $\sum_r \phi_r^*(x)\phi_r(y) = \delta(\bar{x}-\bar{y})$. We'll often use the eigenfunctions of the single-particle H for this, but not necessary.

$$\{\hat{c}_r, \hat{c}_s^+\} = \delta_{rs} \quad , \quad \{\hat{c}_r, \hat{c}_s\} = \{\hat{c}_r^+, \hat{c}_s^+\} = 0$$

The occupation (or number operator) is

$$\hat{n}_s = \hat{a}_s^+ \hat{a} \qquad \text{with eigenstates } \hat{n}_s|n_s\rangle = n_s|n_s\rangle$$

What occupations are allowed?

$$\hat{a}_s^+|0\rangle = |1_s\rangle \quad \text{but} \quad a_s^+ a_s^+|0\rangle = 0$$

Since $\{a_s^+, a_s^+\} = a_s^+ a_s^+ + a_s^+ a_s^+ = 0$, so OCCUPATION CAN ONLY BE 0 or 1 for fermions. Of course, bosons don't have the same Problem:

$$\hat{b}^+|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad (\text{eg}, b_s^+ b_s^+|0\rangle = \sqrt{2}\,|2_s\rangle)$$

So <u>any</u> occupation is allowed.

Occupations & detailed balance

The equilibrium distribution is created through collisions, and maintained by it. Let's consider the implications for binary collisions,

where particles in states 1 & 2 collide, & end up in states 3 & 4.

For bosons, we can write the rate at which this happens

$$R_{1,2\to 3,4} = |M_{12\leftrightarrow 34}|^2\, n_1 n_2 (n_3+1)(n_4+1)$$

since the prior occupations of the states affect amplitudes like $\hat{b}_1 |n_1\rangle = \sqrt{n_1}\,|n_1-1\rangle$ and $b_3^\dagger |n_3\rangle = \sqrt{n_3+1}\,|n_3+1\rangle$,

& R goes like amplitude squared.

The M matrix element is otherwise equal for the reverse process, if the evolution is time-reversible. Then

$$R_{3,4\to 1,2} = |M_{34\leftrightarrow 12}|^2\, n_3 n_4 (n_1+1)(n_2+1)$$

If these rates are equal, in equilibrium, then we can constrain the equilibrium occupations $f_1 = \overline{n_1}$, etc:

$$\frac{f_1}{1+f_1}\,\frac{f_2}{1+f_2} = \frac{f_3}{1+f_3}\,\frac{f_4}{1+f_4}$$

This relation is, in fact, satisfied by Bose statistics, where

$$f(\epsilon) = \left[1 - z^{-1} e^{\beta\epsilon}\right]^{-1}$$

One can show that $f_i / 1+f_i = z e^{-\beta \epsilon_i}$, so that the balance eq becomes

$$z^2 e^{-\beta(\epsilon_1+\epsilon_2)} = z^2 e^{-\beta(\epsilon_3+\epsilon_4)}$$

This is true when the collision is elastic, ie $\epsilon_1+\epsilon_2 = \epsilon_3+\epsilon_4$. We see that Bose STIMULATION IS BUILT INTO THE DISTRIBUTION.

One can make a stronger statement: "BOSE STIMULATION IS JUST AS FUNDAMENTAL AS BOSE STATISTICS." [W. Ketterle]

The same is true for fermions. Scattering is now Pauli blocked: $a_s^\dagger |n_s\rangle = \sqrt{1-n_s}\,|n_s+1\rangle$, so

$$\Gamma_{1,2\to3,4} = |M_{12\leftrightarrow34}|^2\, n_1 n_2 (1-n_3)(1-n_4)$$

$$\Gamma_{34\to12} = |\qquad|^2\, n_3 n_4 (1-n_1)(1-n_2)$$

setting these equal, & using $f_i / 1-f_i = -z e^{-\beta\epsilon_i}$ for FD statistics, we again find that blocking is built into the distribution.

[Motivation: see slides!]

Field operators, and the many-body wave function.

If instead of mode occupation, we want to know density or amplitude of particles at a position $\vec{x}$, then we need "field" operators,

$$\hat{\psi}(x) = \sum_r \hat{c}_r \phi_r^*(x) \qquad \left(\& \ \hat{\psi}^+ = \sum_r \hat{c}_r^+ \phi_r(x) \right)$$

or the inverse transform, $\hat{c}_r = \int dx\, \phi_r(x)\, \hat{\psi}(x)$, which uses the completeness & orthogonality of the $\{\phi_r\}$.

The density is $\hat{\rho}(x) = \hat{\psi}^+(r)\hat{\psi}(r)$, & $\{\psi^+(x), \psi(x)\} = \delta(x-y)$, etc.

Let's consider the two-particle state, $\hat{c}_r^+ \hat{c}_s^+ |0\rangle = |1_r 1_s\rangle$

What is its spatial wave function?

The recipe to go from this kind of second-quantised state "back" to a wave function is

$$\underbrace{\Psi(x_1, \ldots, x_N)}_{\text{wave function}} = \frac{1}{\sqrt{N!}} \underset{\uparrow \text{ vacuum}}{\langle 0|} \underbrace{\hat{\psi}(x_1) \cdots \hat{\psi}(x_N)}_{\text{field operators}} |\Psi\rangle \ \llcorner \text{2nd-q state}$$

For our example,

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} \langle 0| \hat{\psi}(x_1) \hat{\psi}(x_2) |\Psi\rangle$$

$$= \frac{1}{\sqrt{2}} \langle 0| \left(\sum_a \hat{c}_a \phi_a(x_1) \right) \left(\sum_b \hat{c}_b \phi_b(x_2) \right) \hat{c}_r^+ \hat{c}_s^+ |0\rangle$$

This comes down to the calculation of the matrix element

$$\langle 0 | \hat{c}_a \hat{c}_b \hat{c}_r^\dagger \hat{c}_s^\dagger | 0 \rangle = \delta_{as}\delta_{br} - \delta_{ar}\delta_{bs}$$

and thus wf for Fermions in two modes

$$\boxed{\Psi(x_1 x_2) = \frac{1}{\sqrt{2}}\left(\phi_r(x_1)\phi_s(x_2) - \phi_r(x_2)\phi_s(x_1)\right)}$$

So that the 2nd quantization math takes the state $|1_r 1_s\rangle$ and "automatically" anti-symmetrize it – no need to do this by hand / Slater determinant etc.

If we had done this for bosons in two modes, we would have the same wf, except with a "+":

$$\Psi = \frac{1}{\sqrt{2}}\left(\phi_r(x_1)\phi_s(x_2) + \phi_r(x_2)\phi_s(x_1)\right)$$

But for two bosons in one mode,

$$\Psi = \phi_r(x_1)\phi_r(x_2)$$

Now, look @ experiments. We find measures of $g^{(2)}$, joint detection probability @ $x_1 = x_2$, normalized by the flux of either one.

$g^{(2)}$ is the probability of joint detection $P(x_1, x_2)$ divided by the geometric mean of $\underbrace{P(x_1) \text{ and } P(x_2)}_{\text{single-particle probability}}$.

$$P(x_1 = x_2) = |\Psi(x, x)|^2$$
$$P(x_1) = \int dx_2 \, |\Psi(x_1, x_2)|^2$$
$$P(x_2) = \int dx_1 \, |\Psi(x_1, x_2)|^2$$

$$\rightarrow \; g^{(2)} = \frac{P(x_1 = x_2)}{\sqrt{P(x_1) P(x_2)}}$$

One can show that the single-particle

$$P(x_1) = \frac{1}{2}\left(|\phi_r|^2 + |\phi_s|^2\right) = P(x_2)$$

whereas the joint probability is

$$P(x_1 = x_2) = |\phi_r|^2 |\phi_s|^2 \pm |\phi_r|^2 |\phi_s|^2$$

Let's furthermore say there is perfect mode overlap, so that $|\phi_r|^2 = |\phi_s|^2$ everywhere. Then

$$g^{(2)} = \begin{cases} 2 & \text{for bosons} \\ 0 & \text{for fermions} \end{cases}$$

For comparison, for the BEC case where all particles are in the same mode,

$$P(x_1 = x_2) = |\phi_r|^2 |\phi_s|^2$$

& $g^{(2)} = 1$. This is as observed.

Interactions & Exchange

Two-body interactions are two-body correlation detectors! So, a Bose gas in its thermal state has twice the interaction energy as a BEC at the same density. Similarly, a spin-polarised Fermi gas is non-interacting.

This can be seen by considering an interaction potential $V(r_{12})$ that depends only on $r_{12} \equiv |\vec{x}_1 - \vec{x}_2|$.

$$\langle E_{int} \rangle = \int d\vec{x}_1 \, d\vec{x}_2 \, |\Psi(\vec{x}_1, \vec{x}_2)|^2 \, V(|\vec{x}_1 - \vec{x}_2|)$$

using the wf derived previously, $\Psi = \frac{1}{\sqrt{2}}(\phi_a(x_1)\phi_b(x_2) - \phi_a(x_2)\phi_b(x_1))$ one finds

$$\langle E_{int} \rangle = \langle E_{int} \rangle_{direct} - \langle E_{int} \rangle_{exchange}$$

where $\langle E_{int} \rangle_{direct} = \int dx_1 \, dx_2 \, |\phi_a(x_1)|^2 \, |\phi_b(x_2)|^2 \, V(|x_1 - x_2|)$

$$\langle E_{int} \rangle_{exch} = \int dx_1 \, dx_2 \, \phi_a^*(x_1) \, \phi_b^*(x_1) \, \phi_a(x_2) \, \phi_b(x_2) \, V(|x_1 - x_2|)$$

If $V(r_{12}) = g\,\delta(r_{12})$, then $\langle E_{int} \rangle_{direct} = \langle E_{int} \rangle_{exchange}$, and zero interaction energy. Just like $g^{(2)}(0) = 0$!

However, for ^{161}Dy and ^{167}Er, dipolar interactions are not zero range, and $\langle E_{int}\rangle_{exch} \neq \langle E_{int}\rangle_{direct}$.

Then, spin polarized gases of fermions can interact, as do electrons with long-range Coulomb interactions. One can also use p-wave interaction resonance in alkali.

Alternately, we can extend the Hilbert space of modes to include spin, which can satisfy antisymmetry, & allow the spatial part of the wf to remain symmetric.

$$\chi_s = \frac{1}{\sqrt{2}}\left(\chi_\uparrow(1)\chi_\downarrow(2) - \chi_\downarrow(1)\chi_\uparrow(2)\right) \quad \text{spin singlet}$$

for instance, these three states

$$\Psi = \phi_a(x_1)\,\phi_a(x_2)\,\chi_s$$

$$\phi_b(x_1)\,\phi_b(x_2)\,\chi_s$$

$$\frac{1}{\sqrt{2}}\left(\phi_a(x_1)\phi_b(x_2) + \phi_b(x_1)\phi_a(x_2)\right)\chi_s$$

are all symmetric spatial wf's that satisfy anti-symmetric exchange symmetry through the χ_s. (There are three others that are triplet spin, & singlet spatially, which would be non-int'g for a contact interaction.)