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IV. Many identical particles

In the following we give an introduction to quantum many-body theory, using reduced density matrices.

IV.1 Fundamentals

The wave function of two particles is of the form $\psi(t,\alpha_1,\alpha_2)$, where α_1 and α_2 are variables such as, e.g., 3-component of spin s and position $\vec{x}$, $\alpha=(s,\vec{x})$. If the particles are identical, then $|\psi(t,\alpha_1,\alpha_2)|^2=|\psi(t,\alpha_2,\alpha_1)|^2$ must hold.

For $d=3$, relativistic QFT implies the existence of spin and the spin-statistics theorem (first shown by Pauli): particles with half-integer spin are fermions, particles with integer spins are bosons — and these are all possibilities. In the nonrelativistic limit, this means that

$$\psi(t,\alpha_2,\alpha_1)=\pm\psi(t,\alpha_1,\alpha_2) \qquad \begin{matrix} + \ldots \text{bosons} \\ - \ldots \text{fermions}\end{matrix}$$

are the only possibilities.

For $d=2$, other kinds of statistics are possible (anyons). There are interesting attempts to prove a spin-statistics theorem in the framework of nonrelativistic QM [Berry & Co].

In the following, we shall consider only Fermi- and Bose statistics. That is, the wave function of n identical particles must satisfy

$$\psi(\alpha_{\pi(1)},\ldots,\alpha_{\pi(n)})=(\pm 1)^{\pi}\,\psi(\alpha_1,\ldots,\alpha_n) \qquad \forall \pi\in S_n$$

where $(+1)^{\pi}=1$ and $(-1)^{\pi}:=\operatorname{sgn}(\pi)$ is the sign of the permutation π. (Note that α's, not just $\vec{x}$'s, need to be permuted)

Many-particle wave functions with the correct (anti)symmetrisation properties can be obtained from product wave functions by antisymmetrisation,

$$\mathbb{P}_\pm \left(\phi_1(\alpha_1) \cdot \phi_2(\alpha_2) \dots \phi_n(\alpha_n) \right)$$
$$= \frac{1}{n!} \sum_{\pi \in \sigma_n} (\pm 1)^\pi \prod_{k=1}^n \phi_k(\alpha_{\pi(k)}))$$

The prefactor $\frac{1}{n!}$ makes $\mathbb{P}_\pm$ to a projector, $\mathbb{P}_\pm^2 = \mathbb{P}_\pm$. We sometimes write $\mathbb{S}$ for $\mathbb{P}_+$ and $\mathbb{A}$ for $\mathbb{P}_-$. For $n = 2$

$$\mathbb{P}_+ (\phi_1(\alpha_1) \phi_2(\alpha_2)) = \frac{1}{2} (\phi_1(\alpha_1) \phi_2(\alpha_2) + \phi_2(\alpha_1) \phi_1(\alpha_2))$$

and

$$\mathbb{P}_- (\phi_1(\alpha_1) \phi_2(\alpha_2)) = \frac{1}{2} (\phi_1(\alpha_1) \phi_2(\alpha_2) - \phi_1(\alpha_2) \phi_2(\alpha_1))$$
$$= \begin{vmatrix} \phi_1(\alpha_1) & \phi_1(\alpha_2) \\ \phi_2(\alpha_1) & \phi_2(\alpha_2) \end{vmatrix}$$

This generalizes to arbitrary n!

$$\mathbb{P}_\pm \left(\phi_1(\alpha_1) \dots \phi_n(\alpha_n) \right) = \det{}_\pm \left((\phi_j(\alpha_k))_{j,k} \right)$$

where $\det_+$ is the permanent and $\det_-$ is the determinant of a matrix

$$\det{}_\pm M = \sum_{\pi \in \sigma_n} (\pm 1)^\pi \prod_{k=1}^n M_{k \pi(k)} .$$

For bosons, the permanent becomes maximal for $\phi_1 = \phi_2 = \dots = \phi_n$ (arithmetic-geometric inequality).

For fermions, the determinant vanishes if

$$\exists\, k \neq l : \phi_k = \phi_l$$

This is the Pauli principle: no 2 fermions can occupy the same state. Historically, these det's are called Slater determinants.

As for ordinary product ansatzes, ~~the $\det_I$ states~~ functions one can build an ONB of the n-particle ~~wave~~functions from the $\mathbb{P}_\pm (e_1(\alpha_1) \dots e_n(\alpha_n))$ if $(e_i)_{i \in I}$ are an ONB of the one-particle space:

$$\psi(\alpha_1, \dots, \alpha_n) = \sum_{i_1, \dots, i_n \in I} c_{i_1 \dots i_n} \, \mathbb{P}_\pm \left(e_{i_1}(\alpha_1) \dots e_{i_n}(\alpha_n) \right),$$

with $c_{i_1 \dots i_n} \in \mathbb{C}$.

A pure n-particle state $\rho = |\Psi\rangle\langle\Psi|$ is then given by its integral kernel

$$\rho(\alpha_1 \dots \alpha_n, \alpha_1' \dots \alpha_n') = \psi(\alpha_1, \dots, \alpha_n) \overline{\psi(\alpha_1', \dots, \alpha_n')}$$

so that $(\rho v)(\alpha_1, \dots, \alpha_n) = \int d\mu(\alpha_1') \dots d\mu(\alpha_n') \, \rho(\alpha_1, \dots, \alpha_n, \alpha_1', \dots, \alpha_n') v(\alpha_1', \dots, \alpha_n')$.

The $\int d\mu$ depends on the nature of the α's, e.g. $\int d\mu(\alpha) = \sum_s \int d\vec{x}$ for $\alpha = (s, \vec{x})$.

For many particles, working with wave functions in the Hilbert space norm is not very easy, since small errors tend to get very large if n gets large. To illustrate this, consider two bosonic product states[1)]

$$\Phi(\vec{x}_1,..,\vec{x}_n) = \phi(\vec{x}_1)\dots\phi(\vec{x}_n) \qquad \text{where } \|\phi\|^2 = \int |\phi(\vec{x})|^2 d\vec{x} = 1$$

and

$$\Psi(\vec{x}_1,..,\vec{x}_n) = \psi(\vec{x}_1)\dots\psi(\vec{x}_n) \quad \text{where } \|\psi\|^2 = 1$$

Their inner product is

$$\langle \Phi | \Psi \rangle = \int \prod_{j=1}^{n} d\vec{x}_j \, \overline{\phi}(\vec{x}_j)\, \psi(\vec{x}_j)$$
$$= \prod_{j=1}^{n} \langle \phi | \psi \rangle = \langle \phi | \psi \rangle^n$$

Because ϕ, ψ are normalized $|\langle \phi|\psi\rangle| \le \|\phi\| \cdot \|\psi\| = 1$, with "$=1$" $\iff \phi = \psi$. Thus if ϕ differs a little bit from ψ, $|\langle\phi|\psi\rangle| = q < 1$, so

$$|\langle \Phi | \Psi \rangle| \le q^n \xrightarrow[n\to\infty]{} 0$$

Thus the overlap of these states gets very small as $n \to \infty$. The conclusion is that one should in general not hope to get a good description with wave functions in the natural L^2 norm. Instead, one should use weaker norms or restrict to quantities that contain less information

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1) since all $\phi_i = \phi$, ~~[illegible]~~ Φ and Ψ are symmetric

Such quantities are, in fact, the reduced density matrices we have already introduced. The only special aspect is that the reduction from all N to some $k \ll N$ particles is particularly natural because of the symmetry.

The reduced one-particle density matrix is

$$\rho_1(\alpha,\alpha') = \int d\mu(\alpha_2) \ldots \int d\mu(\alpha_n)\, \rho(\alpha, \alpha_2, \ldots \alpha_n; \alpha', \alpha_2, \ldots \alpha_n)$$

i.e.

$$\rho_1 = \mathrm{Tr}_{2\ldots n}\, \rho$$

By symmetry, $\rho_1 = \mathrm{Tr}_{13\ldots n}\, \rho$, etc.

The reduced two-particle density matrix is

$$\rho_2(\alpha_1, \alpha_2; \alpha_1', \alpha_2') = \int d\mu(\alpha_3) \ldots \int d\mu(\alpha_n)\, \rho(\alpha_1, \alpha_2, \alpha_3, \ldots \alpha_n, \alpha_1' \alpha_2' \alpha_3 \ldots \alpha_n)$$

i.e. $\rho_2 = \mathrm{Tr}_{3\ldots n}\, \rho$, etc.

Conventions differ, and in some situations it is convenient to use $\tilde{\rho}_1 = N\rho_1$, $\tilde{\rho}_2 = \frac{N(N-1)}{2}\rho_2$ and $\tilde{\rho}_k = \binom{N}{k}\rho_k$ instead. As defined, the ρ_k are DM by our general theory.

II.2 Second quantization

A) The wave functions discussed above are really (anti) symmetrized tensor products. Let $\mathcal{H}^{(1)} = \mathcal{H}$ be some Hilbert space for the one-particle states, and $(e_\alpha)_{\alpha\in A}$ be an ONB for $\mathcal{H}$. Typical examples in applications are the following

1. momentum eigenstates for a particle in a box. Assuming that the box Λ is a cube of sidelength L in d-dimensional space[x)], these states are labelled by wavevectors $k \in \frac{2\pi}{L}\nu$, $\nu\in\mathbb{Z}^d$. The normalized vector $|k\rangle$ corresponds to the wavefunction

$$\langle x|k\rangle = L^{-d/2}\, e^{ik\cdot x} .$$

We denote $V = L^d$. If in addition, the particles have spin S, then $\alpha = (s,k)$, where $s\in\{-S,-S+1,\dots,S-1,S\}$, and

$$e_\alpha = |k\rangle\otimes|\eta_s\rangle$$

with η_s some spin-ONB on $\mathbb{C}^{2S+1}$, $\langle\eta_s|\eta_{s'}\rangle = \delta_{ss'}$;

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x) with periodic b.c., i.e. $\Lambda = \mathbb{R}^d / L\mathbb{Z}^d$.

2. Atomic or molecular orbitals, possibly also combined with spin. ≠3. states in traps.

We assume that the set A labelling the basis is countable, and we choose some enumeration $\mathbb{N} \to A$ of A, so $A = \{a_1, a_2, \dots\}$. (None of the constructions we do in the following depend on this enumeration, or on the chosen basis).[1]

B) The above considerations can be summarized as follows. The Hilbert space for N particles is

$$\mathcal{H}_\pm^{(N)} = \mathbb{P}_\pm(\mathcal{H}\otimes\dots\otimes\mathcal{H}) = \mathbb{P}_\pm\Big(\bigotimes^N \mathcal{H}\Big)$$

Defining the space for no particles as

$$\mathcal{H}_\pm^{(0)} = \mathbb{C},$$

we can form the Fock space

$$\mathcal{F}_\pm = \bigoplus_{N\geq 0} \mathcal{H}_\pm^{(N)}$$

→ C)

A vector $\Psi \in \mathcal{F}_\pm$ is a sequence of N-particle states $\psi^{(N)}$

$$\Psi = (\psi^{(0)}, \psi^{(1)}, \psi^{(2)}, \dots)$$

and the inner product on $\mathcal{F}_\pm$ is

$$\langle \Psi | \Phi \rangle = \sum_{N\geq 0} \langle \psi^{(N)} | \Phi^{(N)} \rangle_{\mathcal{H}_\pm^{(N)}}.$$

1) example: for the momentum lattice $\cong d=2$ order the k's as follows

 etc.

For any ONB $(e_\alpha)_{\alpha\in A}$ of $\mathcal{H}$, the vectors

$$|\alpha_{i_1},..,\alpha_{i_N}\rangle = \mathcal{N}^{(\pm)}_{\alpha_{i_1}..\alpha_{i_N}} \mathbb{P}_\pm(e_{\alpha_{i_1}}\otimes ... \otimes e_{\alpha_{i_N}})$$

form an ONB of $\mathcal{H}_\pm^{(N)}$, provided that, for fermions, , and for bosons, $\alpha_i \leq \alpha_j$ for $i \leq j$

$$\mathcal{N}^{(+)}_{\alpha_{i_1}..\alpha_{i_N}} = \sqrt{\frac{N!}{n_1! n_2! n_3! ...}} \quad \text{with } n_\ell = |i^{-1}(\{\ell\})|.$$

$$\mathcal{N}^{(-)}_{\alpha_{i_1}..\alpha_{i_N}} = \sqrt{N!}$$

To see this, first note that the antisymmetry implies that $\mathbb{P}_-(e_{\alpha_1}\otimes ... \otimes e_{\alpha_N}) = 0$ if $\alpha_i = \alpha_j$ for some $i \neq j$. (Pauli principle).

Assume that $i \neq j \Rightarrow \alpha_i \neq \alpha_j$. Then
$\quad\quad\quad\quad i \neq j \Rightarrow \alpha'_i \neq \alpha'_j$

$$\langle \mathbb{P}_- e_{\alpha_1}\otimes ... \otimes e_{\alpha_N} | \mathbb{P}_- e_{\alpha'_1}\otimes ... \otimes e_{\alpha'_N}\rangle$$

$$= \frac{1}{N!^2} \sum_{\sigma,\pi\in S_N} (-1)^\pi (-1)^\sigma \langle e_{\alpha_{\pi(1)}}\otimes ... \otimes e_{\alpha_{\pi(N)}} | e_{\alpha'_{\sigma(1)}}\otimes ... \otimes e_{\alpha'_{\sigma(N)}}\rangle$$

$$= \frac{1}{N!^2} \sum_{\sigma,\pi} (-1)^\pi (-1)^\sigma \prod_{k=1}^N \langle e_{\alpha_{\pi(k)}} | e_{\alpha'_{\sigma(k)}}\rangle$$

$$= \frac{1}{N!} \sum_\rho (-1)^\rho \prod_{k=1}^N \langle e_{\alpha_k} | e_{\alpha'_{\rho(k)}}\rangle \underbrace{\frac{1}{N!}\sum_\sigma 1}_{1}$$

$\pi^{-1}\circ\sigma = \rho$

$(-1)^\pi(-1)^\sigma = (-1)^\rho$

$$\underset{\substack{\uparrow \\ \text{all } \alpha\text{'s and } \alpha'\text{'s are distinct}}}{=} \frac{1}{N!} \sum_\rho (-1)^\rho \prod_{k=1}^N \delta_{\alpha_k \alpha'_{\rho(k)}} \underset{\substack{\uparrow \\ \text{ordering of } \alpha\text{'s} \Rightarrow \text{only } \rho = \mathrm{id} \text{ contributes}}}{=} \frac{1}{N!}.$$

For bosons, $(-1)^{\pi}$ gets replaced by $+1$, etc.
and

$$\langle \mathbb{P}_+ e_{\alpha_{i_1}} \otimes \dots \otimes e_{\alpha_{i_N}} | \mathbb{P}_+ e_{\alpha_{j_1}} \otimes \dots \otimes e_{\alpha_{j_N}} \rangle$$

$$= \frac{1}{N!} \sum_{\rho} \prod_{k=1}^{N} \langle e_{\alpha_{i_k}} | e_{\alpha_{j_{\rho(k)}}} \rangle$$

Suppose now that the first n_1 of the i_k's are 1 (n_1 may be zero), n_2 are 2, etc., similarly for the j_k's, with a sequence $n'_1, n'_2, \dots$ The orthonormality of the e_α and the monotonic ordering imply that $n_\ell = n'_\ell$ for all ℓ, and that ρ must leave the sets $i^{-1}(\{\ell\})$ invariant. ($|i^{-1}(\{\ell\})| = n_\ell$). It follows that

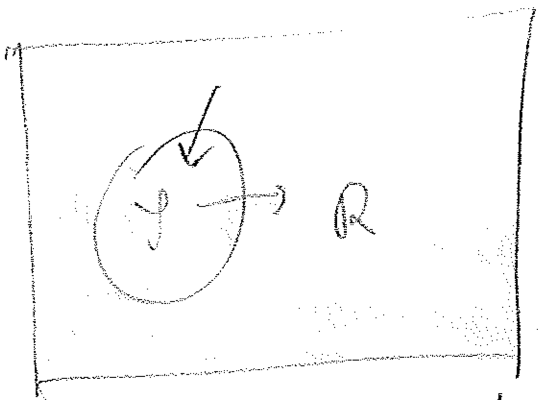
$$= \frac{n_1! \, n_2! \dots}{N!}$$

The product in the numerator contains only finitely many factors that are $\neq 1$, due to the constraint $N = \sum_k n_k$.

C) Variable particle number & Fock space

$\rightsquigarrow \otimes$

Considering the Fock space is natural if $\mathcal{H} = \mathcal{H}_S$ corresponds to a quantum system S embedded in an environment R so that S and R can exchange particles



$\mathcal{H}_S \otimes \mathcal{H}_R$

In that case, even if the dynamics on the $\mathcal{H}_S \otimes \mathcal{H}_R$ conserves the number of particles, this need not be the case on $\mathcal{H}_S$.

D) Occupation number representation

The states $|\alpha_{i_1} \dots \alpha_{i_N}\rangle$ (simpler $|i_1 \dots i_N\rangle$)
are permutation (anti)symmetric, so an efficient description is only to give the occupation numbers $n_\ell = |\{k : i_k = \ell\}|$. For instance, the 8-particle state

$$P_+ \left(e_2 \otimes e_3 \otimes e_1 \otimes e_5 \otimes e_2 \otimes e_5 \otimes e_1 \otimes e_1 \right)$$

is completely fixed by the sequence

$n_1 = 3, n_2 = 2, n_3 = 1, n_4 = 0, n_5 = 2$.

Thus the basis $|\alpha_{i_1} \dots \alpha_{i_N}\rangle$ is conveniently & efficiently described by the occupation numbers $(n_a)_{a \in A}$.
For an N-particle state, $\sum_a n_a = N$ $(n_a \geq 0)$.

For fermions, $n_a = 0$ or $n_a = 1$, by the Pauli principle

For bosons $n_a = 0, 1, 2, \dots$ can be any nonnegative integer.

As shown above, $\langle n | n' \rangle = \delta_{nn'}$

The ~~state~~ vector with no particles $\Omega = |0\rangle = |0 \dots 0\rangle$ is called the vacuum.

E) Creation and annihilation operators

Bosons. $a_\alpha |n\rangle = \begin{cases} \sqrt{n_\alpha}\, |n-\delta_\alpha\rangle & \text{if } n_\alpha \neq 0 \\ 0 & \text{otherwise} \end{cases}$

adjoint is $a^*_\alpha |n\rangle = \sqrt{n_\alpha + 1}\, |n+\delta_\alpha\rangle$

Easy calc. gives

$$[a_\alpha, a^*_\beta] = \delta_{\alpha\beta} 1 \quad , \quad [a_\alpha, a_\beta] = 0 \qquad (CCR)$$

Extend a^*_α to a linear function on $\mathcal{H}$, $f \to a^*(f)$

so that for $f = \sum \varphi_\alpha e_\alpha$, $a^*(f) = \sum \varphi_\alpha \underbrace{a^*(e_\alpha)}_{= a^*_\alpha}$.

$a(f)$ is then antilinear in f.

Exercise: Show that ~~for~~ a unitary transformation on $\mathcal{H}$ do not change the CCR.

in the commutator calculation we also see that $a^*_\alpha a_\alpha$ has the property

$$a^*_\alpha a_\alpha |n\rangle = n_\alpha \cdot |n\rangle$$

$n_\alpha = a^*_\alpha a_\alpha$ is called number operator for α.

The total number op. $\mathcal{N} = \sum_\alpha a^*_\alpha a_\alpha$

is densely defined on $\mathcal{F}$.

We have $[n_\alpha, n_\beta] = 0$ for all α, β.

Fermions:

$$a_\alpha|n\rangle = \begin{cases} \xi_\alpha(n)\sqrt{n_\alpha}\;|n-\delta_\alpha\rangle & n_\alpha=1 \\ 0 & n_\alpha=0 \end{cases}$$

$$\Rightarrow a^*_\alpha|n\rangle = \xi_\alpha(n)\sqrt{n_\alpha+1}\;|n+\delta_\alpha\rangle$$

Here $\xi_\alpha = (-1)^{\sum_{\gamma<\alpha} n_\gamma}$.

$$\{a_\alpha, a^*_\beta\} = a_\alpha a^*_\beta + a^*_\beta a_\alpha = \delta_{\alpha\beta}\mathbb{1}$$

$$\{a_\alpha, a_\beta\} = 0.$$

The Pauli principle reads $(a^*_\alpha)^2 = 0$

Again $n_\alpha = a^*_\alpha a_\alpha$ counts particles in state α, $[n_\alpha, n_\beta] = 0$, and for fermions also $n_\alpha^2 = n_\alpha$.

In terms of the creation operators,

$$|n\rangle = \frac{1}{\sqrt{n_{\alpha_1}!\,n_{\alpha_2}!\cdots}}\,(a^*_{\alpha_1})^{n_{\alpha_1}}(a^*_{\alpha_2})^{n_{\alpha_2}}\cdots|0\rangle$$

so

$$|n\rangle = \frac{1}{\sqrt{\prod_a n_a!}}\prod_a (a^*_a)^{n_a}|0\rangle$$

too many a's.