Advanced quantum mechanics

Chapter 2 – Indistinguishable particles

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Outline

1. Indistinguishable particles
   - The symmetrization postulate
   - Symmetric states in first quantization
   - Second quantization
   - Quantum statistics of composite particles
   - Gaussian quantum states and Wick's theorem

Chapter 2 – Indistinguishable particles

Several identical quantum particles cannot simply be described by a tensor product.

- The symmetrization postulate: the state must be symmetric (bosons) or antisymmetric (fermions) under exchange.
- It is a genuine additional postulate, not a consequence of indistinguishability.
- It drastically reduces the size of the Hilbert space.
- The formalism of second quantization makes it automatic.

Labels: classical versus quantum

Classical mechanics. A system of N particles is specified by

$$\big(\mathbf{r}_i(t), \mathbf{v}_i(t)\big)_{1\leq i\leq N}.$$

Labels can be attached to particles and followed continuously. Exchanging the labels of two identical particles changes no prediction.

Quantum mechanics. No observable distinguishes one identical particle from another. With

$$\hat{P}_\sigma \, |k_1\rangle \otimes \cdots \otimes |k_N\rangle = |k_{\sigma(1)}\rangle \otimes \cdots \otimes |k_{\sigma(N)}\rangle,$$

indistinguishability requires, for every observable $\hat{A}$,

$$\langle\Psi|\hat{A}|\Psi\rangle = \langle\Psi|\hat{P}_\sigma^{-1}\hat{A}\hat{P}_\sigma|\Psi\rangle \quad \Longrightarrow \quad [\hat{P}_\sigma, \hat{A}] = 0.$$

In particular the Hamiltonian is permutation invariant.

This is not enough: exchange degeneracy

The constraint $[\hat{P}_\sigma, \hat{A}] = 0$ restricts the *operators*, but says nothing about the *state*.

Two identical spin-1/2 particles in the same orbital, one up and one down. This is the most complete specification one can give, yet it is compatible with

$$|\Psi_{\alpha\beta}\rangle = \alpha\,|+\rangle \otimes |-\rangle + \beta\,|-\rangle \otimes |+\rangle, \qquad |\alpha|^2 + |\beta|^2 = 1.$$

The two product states are physically equivalent to each other:

$$\langle -,+|\hat{A}|-,+\rangle = \langle +,-|\hat{P}_{\tau_{12}}^{-1}\hat{A}\hat{P}_{\tau_{12}}|+,-\rangle = \langle +,-|\hat{A}|+,-\rangle.$$

But they are not equivalent to their superpositions. With $\hat{\mathbf{S}} = \hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2$,

$$P(S=1) = |\langle T_0|\Psi_{\alpha\beta}\rangle|^2 = \frac{|\alpha+\beta|^2}{2} = \begin{cases} 1 & \alpha = \beta = 1/\sqrt{2} \\ 0 & \alpha = -\beta = 1/\sqrt{2} \\ 1/2 & \text{product state} \end{cases}$$

One preparation, a continuum of incompatible predictions.

The symmetrization postulate

No set of commuting observables can lift this degeneracy, since *every* observable commutes with $\hat{P}_\sigma$. One cannot simply declare the two product states "the same state" either: physical equivalence does not propagate through superposition.

Symmetrization postulate [1]

The state of a system of identical particles transforms according to a one-dimensional representation of the permutation group:

$$\hat{P}_\sigma|\Psi\rangle = c(\sigma)|\Psi\rangle, \qquad |c(\sigma)| = 1.$$

This removes the ambiguity: in the family above, exactly one state survives for each sign of $c(\tau_{12})$ — the triplet $S = 1$ and the singlet $S = 0$.

Demanding a one-dimensional representation is part of the postulate. Higher-dimensional representations would describe *parastatistics*, excluded here by assumption.

Only two possibilities

(i) Composition. $\hat{P}_{\sigma\circ\sigma'} = \hat{P}_{\sigma'}\hat{P}_{\sigma}$, hence $c(\sigma\circ\sigma') = c(\sigma)c(\sigma')$.

(ii) Decomposition into transpositions. $\sigma = \tau_{i_1 j_1}\circ\cdots\circ\tau_{i_k j_k}$, so $c(\sigma) = c(\tau_{i_1 j_1})\cdots c(\tau_{i_k j_k})$.

(iii) All transpositions are equivalent. $\tau_{ij} = \rho^{-1}\circ\tau_{12}\circ\rho$ with $\rho = \tau_{1i}\circ\tau_{2j}$, hence $c(\tau_{ij}) = c(\tau_{12})$.

(iv) Exchanging twice does nothing. $\tau_{12}\circ\tau_{12} = \mathbb{1}$, hence

$$c(\tau_{12})^2 = 1 \quad \Longrightarrow \quad c(\tau_{12}) = \pm 1.$$

Step (iv) is where spatial dimension enters: it holds in 3D, where the two exchange paths can be deformed into one another. It fails in 1D and 2D.

Bosons and fermions

- Bosons: $c(\tau_{12}) = +1 \Rightarrow c(\sigma) = 1$ for all σ. Totally *symmetric* wave-function.
- Fermions: $c(\tau_{12}) = -1 \Rightarrow c(\sigma) = \varepsilon(\sigma)$, the signature. Totally *antisymmetric* wave-function.

Spin-statistics theorem [2]

In three spatial dimensions, integer spin $S = 0, 1, 2, \ldots \Rightarrow$ bosons;
half-integer spin $S = \frac{1}{2}, \frac{3}{2}, \ldots \Rightarrow$ fermions.

A proof requires relativistic quantum field theory.

Caveat. In one and two dimensions, more general exchange statistics exist: anyons, braid-group statistics [3, 4, 5]. Not considered here.

(Anti)symmetrization projectors

Single-particle space of dimension d; N distinguishable particles give dim $= d^N$.

Define

$$\hat{S} = \frac{1}{N!} \sum_{\sigma} \hat{P}_\sigma, \qquad \hat{A} = \frac{1}{N!} \sum_{\sigma} \varepsilon(\sigma) \hat{P}_\sigma.$$

These are orthogonal Hermitian projectors,

$$\hat{S}^2 = \hat{S}, \quad \hat{A}^2 = \hat{A}, \quad \hat{S}\hat{A} = \hat{A}\hat{S} = 0,$$

$$\hat{S}\hat{P}_\sigma = \hat{P}_\sigma \hat{S} = \hat{S}, \qquad \hat{A}\hat{P}_\sigma = \hat{P}_\sigma \hat{A} = \varepsilon(\sigma)\hat{A}.$$

They do not exhaust the Hilbert space

$$\hat{S} + \hat{A} \neq \mathbb{1} \qquad (N \geq 3).$$

For $N \geq 3$ there are subspaces of mixed symmetry — the parastatistics discarded by the postulate.

Fermionic states and the Pauli principle

If $|\Psi\rangle = |k_1\rangle \otimes \cdots \otimes |k_N\rangle$ contains the same state twice, then $\hat{P}_{\tau_{ij}}|\Psi\rangle = |\Psi\rangle$ while $\hat{A}\hat{P}_{\tau_{ij}} = -\hat{A}$, so

$$\hat{A}|\Psi\rangle = -\hat{A}|\Psi\rangle = 0.$$

Pauli exclusion principle: occupation numbers are 0 or 1.

For N distinct states, $\|\hat{A}|\Psi\rangle\|^2 = \langle\Psi|\hat{A}|\Psi\rangle = 1/N!$, hence

$$|k_1, \ldots, k_N\rangle = \sqrt{N!}\,\hat{A}\,|k_1\rangle \otimes \cdots \otimes |k_N\rangle,$$

whose wave-function is the Slater determinant

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \langle \mathbf{r}_1|k_1\rangle & \cdots & \langle \mathbf{r}_1|k_N\rangle \\ \vdots & \ddots & \vdots \\ \langle \mathbf{r}_N|k_1\rangle & \cdots & \langle \mathbf{r}_N|k_N\rangle \end{vmatrix}.$$

Reordering flips the sign: $|k_2, k_1, \ldots\rangle = -|k_1, k_2, \ldots\rangle$. Hence $\dim \mathcal{E}_N^{\mathrm{F}} = \binom{d}{N}$.

Bosonic states, and how small the Hilbert space becomes

Occupation numbers are arbitrary. With $\sum_i n_{k_i} = N$,

$$\left\| \hat{S}|\Psi\rangle \right\|^2 = \frac{\prod_i n_{k_i}!}{N!} \quad \Longrightarrow \quad |n_{k_1} : k_1, \ldots\rangle = \sqrt{\frac{N!}{\prod_i n_{k_i}!}}\, \hat{S}\, |k_1\rangle^{\otimes n_{k_1}} \otimes \cdots$$

No sign is attached to reordering: a bosonic state is fully specified by its occupation numbers.

$$\dim \mathcal{E}_N^{\mathrm{B}} = \binom{d+N-1}{N}, \qquad \dim \mathcal{E}_N^{\mathrm{F}} = \binom{d}{N}.$$

Example: $N = 5$ particles in $d = 10$ states

distinguishable $10^5 = 100\,000$ bosons $\binom{14}{5} = 2002$ fermions $\binom{10}{5} = 252$

Two particles: bunching and antibunching

Two identical particles in the same internal state, occupying orthogonal orbitals:

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2) + \varepsilon\, \phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_1)}{\sqrt{2}}, \qquad \varepsilon = \pm 1.$$

Fermions. Antisymmetry gives immediately

$$\psi(\mathbf{r}, \mathbf{r}) = 0$$

— the simplest manifestation of *antibunching*.

Bosons. With plane waves $\phi_i(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}_i\cdot\mathbf{r}}/\sqrt{V}$,

$$|\psi(\mathbf{r}, \mathbf{r})|^2 = \frac{2}{V^2},$$

twice the value for distinguishable particles — *bunching*.

Observed through temporal correlations in particle beams: Hanbury Brown–Twiss for light [6], antibunching for electrons [7, 8].

Two-particle interference: the Hong–Ou–Mandel effect

One particle in each input port of a 50:50 beam splitter.

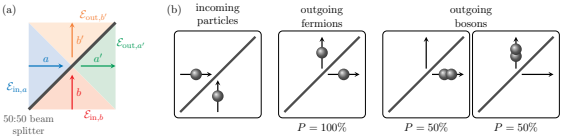
Distinguishable particles: four equally likely outcomes, each with probability $1/4$.

Indistinguishable particles: the two paths leading to a given output interfere.

The beam splitter acts on the mode functions as

$$\phi_a \to \frac{1}{\sqrt{2}}\left[\phi_a^{(0)} + \mathrm{i}\,\phi_b^{(0)}\right],$$
$$\phi_b \to \frac{1}{\sqrt{2}}\left[\phi_b^{(0)} + \mathrm{i}\,\phi_a^{(0)}\right],$$

unitarity being the only property used.



Hong–Ou–Mandel: the result

With $\psi(\mathbf{r}_1, \mathbf{r}_2) = \left[\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2) + \varepsilon\, \phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1)\right]/\sqrt{2}$, the outgoing state reads

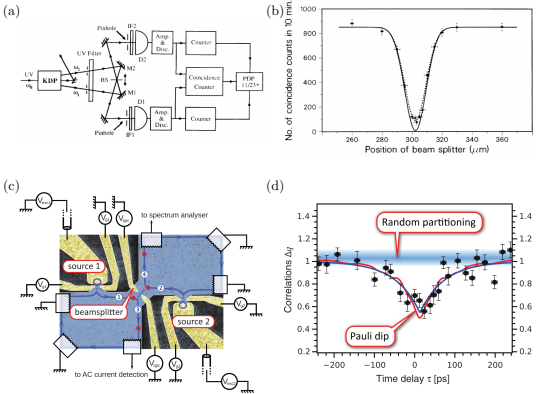
$$\psi = \frac{1}{2\sqrt{2}}\Big\{ \mathrm{i}(1+\varepsilon)\, \phi_a^{(0)}(\mathbf{r}_1)\phi_a^{(0)}(\mathbf{r}_2) + \mathrm{i}(1+\varepsilon)\, \phi_b^{(0)}(\mathbf{r}_1)\phi_b^{(0)}(\mathbf{r}_2) + (1-\varepsilon)\left[\phi_a^{(0)}(\mathbf{r}_1)\phi_b^{(0)}(\mathbf{r}_2) - \phi_a^{(0)}(\mathbf{r}_2)\phi_b^{(0)}(\mathbf{r}_1)\right]\Big\}.$$

$$P(2,0) = P(0,2) = \frac{(1+\varepsilon)^2}{8} = \begin{cases} \frac{1}{2}, & \text{bosons} \\ 0, & \text{fermions} \end{cases}$$

$$P(1,1) = \frac{(1-\varepsilon)^2}{4} = \begin{cases} 0, & \text{bosons} \\ 1, & \text{fermions} \end{cases}$$

Two identical bosons always leave together.
Two identical fermions always leave apart.

Hong–Ou–Mandel: experiments



(a,b) Original photon experiment [9]: pairs from parametric down-conversion are recombined on a beam splitter; coincidences are suppressed when the photons become indistinguishable — the *HOM dip*. (c,d) Fermionic counterpart: 1D electronic channels and a quantum point contact as beam splitter; the current noise is suppressed when the electron arrival times coincide [10].

Particles with spin, and the exchange interaction

Two identical particles of spin s, coupled basis $|S, M\rangle$ with $\hat{\mathbf{S}} = \hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2$. Under exchange the spin state acquires the phase

$$(-1)^{2s-S}.$$

For $s = 1/2$: triplet ($S = 1$) symmetric, singlet ($S = 0$) antisymmetric.

With $|\Psi\rangle = |\Psi_{\text{orb}}\rangle \otimes |\Psi_{\text{spin}}\rangle$:

- **bosons:** orbital and spin parts have the *same* exchange symmetry;
- **fermions:** they have *opposite* symmetries.

Origin of the exchange interaction (Hund's first rule)

Two electrons in two different orbitals of the same atom. The antisymmetric orbital state vanishes when the electrons coincide, lowering the Coulomb repulsion; for fermions it must be paired with a *symmetric* spin state. The triplet is pushed below the singlet:

$$-J_{\text{ex}}\, \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2, \qquad J_{\text{ex}} > 0 \ \ \text{(ferromagnetic)}.$$

Two orbitals are essential: a single orbital admits no antisymmetric orbital state.

Why we need a better formalism

For three fermions in three orbitals,

$$\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = \frac{1}{\sqrt{6}}\Big[\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\phi_3(\mathbf{r}_3) + \phi_3(\mathbf{r}_1)\phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_3) + \phi_2(\mathbf{r}_1)\phi_3(\mathbf{r}_2)\phi_1(\mathbf{r}_3) - \phi_3(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\phi_1(\mathbf{r}_3) - \phi_1(\mathbf{r}_1)\phi_3(\mathbf{r}_2)\phi_2(\mathbf{r}_3) - \phi_2(\mathbf{r}_1)\phi_1(\mathbf{r}_2)\phi_3(\mathbf{r}_3)\Big].$$

For bosons, replace all minus signs by plus signs.

Already cumbersome for $N = 3$; one must handle $N!$ terms. And the physically relevant information is not the particle labels, but the occupation numbers.

$\Longrightarrow$ second quantization, where the exchange symmetry is built into the algebra of creation and annihilation operators.

Fock space

A many-body state is specified by occupation numbers,

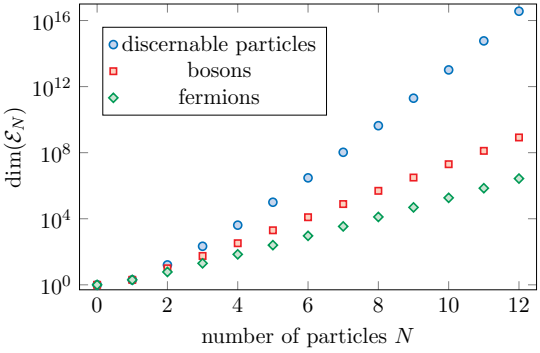
$$|n_1 : k_1, n_2 : k_2, \ldots\rangle \equiv |n_1, n_2, \ldots\rangle.$$

The Fock space allows arbitrary particle number,

$$\mathcal{E} = \mathcal{E}_0 \oplus \mathcal{E}_1 \oplus \cdots \oplus \mathcal{E}_N \oplus \cdots$$

with

$$\dim \mathcal{E}_N^{\mathrm{B}} = \binom{N+d-1}{N}, \quad \dim \mathcal{E}_N^{\mathrm{F}} = \binom{d}{N}.$$



N particles in $2N$ single-particle states. Note the logarithmic scale.

Creation and annihilation operators

The vacuum $|\varnothing\rangle \equiv |n_1 = 0, n_2 = 0, \ldots\rangle$ spans $\mathcal{E}_0$.

Definition

$$\hat{a}_k^\dagger |\psi\rangle = \sqrt{N+1}\,\hat{\Pi}\left(|k\rangle \otimes |\psi\rangle\right), \qquad \hat{\Pi} = \hat{S} \text{ (bosons)},\ \hat{A} \text{ (fermions)}.$$

The factor $\sqrt{N+1}$ gives the conventional normalization of Fock states.

The definition is *linear* in the single-particle state,

$$\hat{a}^\dagger_{\lambda_1|k_1\rangle + \lambda_2|k_2\rangle} = \lambda_1 \hat{a}^\dagger_{k_1} + \lambda_2 \hat{a}^\dagger_{k_2},$$

whereas $\hat{a}_k = (\hat{a}_k^\dagger)^\dagger$ carries a bra-like label and is therefore anti-linear,

$$\hat{a}_{\lambda_1|k_1\rangle + \lambda_2|k_2\rangle} = \lambda_1^* \hat{a}_{k_1} + \lambda_2^* \hat{a}_{k_2}.$$

Action on the Fock basis

(i) Fermions. If k is already occupied, the antisymmetrization vanishes:

$$\hat{a}^\dagger_{k_1}|k_1,\dots,k_N\rangle = 0 \qquad \Longleftrightarrow \qquad \left(\hat{a}^\dagger_k\right)^2 = 0.$$

Otherwise $\hat{a}^\dagger_k|k_1,\dots,k_N\rangle = |k,k_1,\dots,k_N\rangle$, so that

$$|k_1,\dots,k_N\rangle = \hat{a}^\dagger_{k_1}\cdots\hat{a}^\dagger_{k_N}|\emptyset\rangle.$$

The ordering fixes the sign: $\hat{a}_{k_2}|k_1,k_2\rangle = -|k_1\rangle$.

(ii) Bosons.

$$\hat{a}^\dagger_{k_i}|\dots,n_i,\dots\rangle = \sqrt{n_i+1}\,|\dots,n_i+1,\dots\rangle, \qquad \hat{a}_{k_i}|\dots,n_i,\dots\rangle = \sqrt{n_i}\,|\dots,n_i-1,\dots\rangle,$$

the factor $\sqrt{n_i+1}$ being the characteristic bosonic enhancement. Hence

$$|n_1:k_1,\dots,n_p:k_p\rangle = \frac{(\hat{a}^\dagger_{k_1})^{n_1}\cdots(\hat{a}^\dagger_{k_p})^{n_p}}{\sqrt{n_1!\cdots n_p!}}|\emptyset\rangle.$$

The algebra encodes the statistics

Bosons

$$[\hat{a}^\dagger_{k_1}, \hat{a}^\dagger_{k_2}] = 0$$

$$[\hat{a}_{k_1}, \hat{a}^\dagger_{k_2}] = \delta_{k_1 k_2}$$

$$[\hat{a}_{\phi_1}, \hat{a}^\dagger_{\phi_2}] = \langle \phi_1 | \phi_2 \rangle$$

Fermions

$$\{\hat{a}^\dagger_{k_1}, \hat{a}^\dagger_{k_2}\} = 0$$

$$\{\hat{a}_{k_1}, \hat{a}^\dagger_{k_2}\} = \delta_{k_1 k_2}$$

$$\{\hat{a}_{\phi_1}, \hat{a}^\dagger_{\phi_2}\} = \langle \phi_1 | \phi_2 \rangle$$

These relations are the central ingredient of second quantization: they encode the exchange symmetry without any sum over permutations.

Number operators. $\hat{n}_k = \hat{a}^\dagger_k \hat{a}_k$ is diagonal in the Fock basis. For fermions,

$$\hat{n}_k^2 = \hat{a}^\dagger_k (1 - \hat{a}^\dagger_k \hat{a}_k) \hat{a}_k = \hat{n}_k$$

is a projector, so $n_k \in \{0, 1\}$ — Pauli exclusion once more. The total number is $\hat{N} = \sum_k \hat{n}_k$, whose eigenspaces are the $\mathcal{E}_N$.

Field operators

Take the single-particle basis $|\mathbf{r}, \sigma\rangle = |\mathbf{r}\rangle \otimes |\sigma\rangle$ and define

$$\hat{\psi}_\sigma(\mathbf{r}) \equiv \hat{a}_{\mathbf{r},\sigma},$$

so that $\hat{\psi}^\dagger_\sigma(\mathbf{r})$ adds one particle *at the point* $\mathbf{r}$.

With $\phi_{k,\sigma}(\mathbf{r}) = \langle \mathbf{r}, \sigma | k \rangle$, completeness and the anti-linearity of $\hat{a}$ give

$$\hat{\psi}_\sigma(\mathbf{r}) = \sum_k \phi_{k,\sigma}(\mathbf{r})\, \hat{a}_k,$$

and the canonical relations become

$$[\hat{\psi}_\sigma(\mathbf{r}), \hat{\psi}^\dagger_{\sigma'}(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}')\delta_{\sigma,\sigma'} \quad \text{(bosons)}, \qquad \{\cdot, \cdot\} = \delta(\mathbf{r} - \mathbf{r}')\delta_{\sigma,\sigma'} \quad \text{(fermions)}.$$

States become compact: for a normalized orbital $\phi(\mathbf{r})$,

$$|\phi\rangle = \int \phi(\mathbf{r})\, \hat{\psi}^\dagger(\mathbf{r}) |\emptyset\rangle \, \mathrm{d}^3 r,$$

and an N-particle state follows from N field creation operators, the exchange symmetry being automatic.

One-body observables

For $\hat{B} = \sum_{i=1}^{N} \hat{b}_i$,

$$\hat{B} = \sum_{k,k'} \langle k'|\hat{b}|k\rangle\, \hat{a}^\dagger_{k'} \hat{a}_k \qquad \text{or} \qquad \hat{B} = \sum_{\sigma,\sigma'} \int \hat{\psi}^\dagger_\sigma(\mathbf{r}) \langle \mathbf{r},\sigma|\hat{b}|\mathbf{r}',\sigma'\rangle \hat{\psi}_{\sigma'}(\mathbf{r}')\, \mathrm{d}^3 r\, \mathrm{d}^3 r'.$$

Transparent reading: $\hat{a}_k$ removes a particle from mode k, $\hat{b}$ transforms it into k', $\hat{a}^\dagger_{k'}$ creates it. For $k = k'$ it reduces to $\hat{n}_k$, and summing gives $\hat{N}$.

Density. With $\hat{b} = \delta(\hat{\mathbf{r}} - \mathbf{r})$, diagonal in position,

$$\hat{\rho}(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}), \qquad \hat{N} = \int \hat{\rho}(\mathbf{r})\, \mathrm{d}^3 r.$$

Notation: $\hat{\rho}(\mathbf{r})$ and $\hat{\rho}_2(\mathbf{r},\mathbf{r}')$, with position arguments, are densities; $\hat{\rho}, \hat{\rho}_1, \hat{\rho}_2$ without arguments are density matrices.

Reduced density matrix. $\hat{\rho}_1 = N \operatorname{Tr}_{2,\dots,N} \hat{\rho}$ gives $\operatorname{Tr} \hat{\rho}_1 = N$ and $\langle \hat{B} \rangle = \operatorname{Tr}(\hat{b}\hat{\rho}_1)$.

Kinetic energy: locality of $\hat{p}^2$

In the position representation $\hat{p}^2$ acts as $-\hbar^2\Delta$, so

$$\langle \mathbf{r}|\hat{p}^2|\phi\rangle = -\hbar^2 \Delta_{\mathbf{r}}\, \phi(\mathbf{r}) = \int \langle \mathbf{r}|\hat{p}^2|\mathbf{r}'\rangle \phi(\mathbf{r}')\, \mathrm{d}^3 r',$$

which identifies the kernel

$$\langle \mathbf{r}|\hat{p}^2|\mathbf{r}'\rangle = -\hbar^2\, \Delta_{\mathbf{r}}\, \delta(\mathbf{r}-\mathbf{r}').$$

- This is a *distribution*: the Laplacian of a Dirac delta only makes sense under an integral.
- The essential point: the kernel $\propto \delta(\mathbf{r}-\mathbf{r}')$, i.e. $\hat{p}^2$ is local. This collapses the double integral into a single one.

Transferring the derivatives by two integrations by parts, $\langle \mathbf{r}|\hat{p}^2|\mathbf{r}'\rangle = -\hbar^2\delta(\mathbf{r}-\mathbf{r}')\Delta_{\mathbf{r}'}$, we obtain

$$\hat{T} = \int \hat{\psi}^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m}\Delta\right) \hat{\psi}(\mathbf{r})\, \mathrm{d}^3 r,$$

the familiar expression with the wave-function replaced by the field operator.

Two-body observables

For $\hat{C} = \sum_{i \neq j} \hat{c}_{i,j}$ — the sum running over ordered pairs, hence counting each pair twice:

$$\hat{C} = \sum_{k_1', k_2', k_1, k_2} \langle k_1', k_2' | \hat{c} | k_1, k_2 \rangle \, \hat{a}^\dagger_{k_1'} \hat{a}^\dagger_{k_2'} \hat{a}_{k_2} \hat{a}_{k_1}.$$

Note the reversed order of the two annihilation operators relative to the creation operators: this is what makes the fermionic signs come out correctly, automatically.

For a local interaction,

$$\hat{V} = \frac{1}{2} \int \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \, \mathrm{d}^3 r \, \mathrm{d}^3 r' = \frac{1}{2} \int V(\mathbf{r} - \mathbf{r}') \, \hat{\rho}_2(\mathbf{r}, \mathbf{r}') \, \mathrm{d}^3 r \, \mathrm{d}^3 r',$$

with the pair-density operator $\hat{\rho}_2(\mathbf{r}, \mathbf{r}') = \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r})$.

Normal ordering removes any spurious self-interaction, since $\hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r})$ annihilates two *distinct* particles. The factor $1/2$ compensates the double counting.

With $\hat{\rho}_2 = N(N-1) \, \mathrm{Tr}_{3,\ldots,N} \, \hat{\rho}$, one has $\langle \hat{C} \rangle = \mathrm{Tr}(\hat{c} \hat{\rho}_2)$.

Evolution of quantum fields

$$\hat{H} = \int \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\Delta + U(\mathbf{r}) \right] \hat{\psi}(\mathbf{r})\, \mathrm{d}^3 r + \frac{1}{2} \int \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r}-\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r})\, \mathrm{d}^3 r\, \mathrm{d}^3 r'.$$

In the Heisenberg picture, $\mathrm{i}\hbar\, \partial_t \hat{\psi} = [\hat{\psi}, \hat{H}]$. Writing the canonical relations compactly as $\hat{\psi}(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') + \varepsilon\, \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r})$, one obtains

$$\mathrm{i}\hbar\, \partial_t \hat{\psi}(\mathbf{r}) = \left[-\frac{\hbar^2}{2m}\Delta + U(\mathbf{r}) + \int V(\mathbf{r}-\mathbf{r}') \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}')\, \mathrm{d}^3 r' \right] \hat{\psi}(\mathbf{r}).$$

The exchange signs cancel inside the complete interaction term: the result is the same for bosons and fermions.

This looks like a Schrödinger equation, but $\hat{\psi}$ is an operator, not a wave-function. Hence the name *second quantization*.

Every term has as many creation as annihilation operators, so $[\hat{N}, \hat{H}] = 0$. Fock space is nevertheless useful — and becomes indispensable when particle number is *not* conserved (photons, Bogoliubov excitations).

Composite particles

A composite object with N_{F} fermionic constituents picks up an exchange phase $(-1)^{N_{\mathrm{F}}}$:

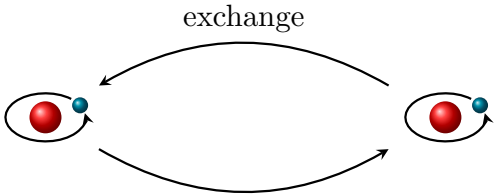
- N_{F} even $\Rightarrow$ boson
- N_{F} odd $\Rightarrow$ fermion

The two helium isotopes.

- ^{4}He: 2 p + 2 n + 2 e = 6 fermions $\Rightarrow$ boson, superfluid below 2.17 K.
- ^{3}He: one neutron less, 5 fermions $\Rightarrow$ fermion; superfluidity requires Cooper pairing, in the *millikelvin* range.

A single neutron, irrelevant to chemistry, changes the collective behaviour completely.

Likewise ^{87}Rb (124 fermions, bosonic) versus ^{40}K (59 fermions, fermionic).



Exchanging two hydrogen atoms: π from the electrons, π from the protons, total 2π — bosonic.

When does a composite particle behave as a boson?

Pairs of fermions of species $1, 2$ bound in $\phi(\mathbf{r}_1 - \mathbf{r}_2)$, with the pair creation operator

$$\hat{c}^\dagger = \int \phi(\mathbf{r}_1 - \mathbf{r}_2)\hat{\psi}_1^\dagger(\mathbf{r}_1)\hat{\psi}_2^\dagger(\mathbf{r}_2)\,\mathrm{d}^3 r_1\,\mathrm{d}^3 r_2 = \sum_{\mathbf{k}} \phi_{\mathbf{k}}\,\hat{a}_{\mathbf{k},1}^\dagger \hat{a}_{-\mathbf{k},2}^\dagger,$$

and the "coherent state of pairs" $|\Psi\rangle \propto \exp(\alpha \hat{c}^\dagger)|\varnothing\rangle$.

If the pairs were true bosons one would expect $\langle \hat{N} \rangle = |\alpha|^2$. But

$$\left(\hat{a}_{\mathbf{k},1}^\dagger \hat{a}_{-\mathbf{k},2}^\dagger\right)^2 = 0$$

(Pauli exclusion), so the exponential truncates and the state factorizes:

$$|\Psi\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}}\,\hat{a}_{\mathbf{k},1}^\dagger \hat{a}_{-\mathbf{k},2}^\dagger\right)|\varnothing\rangle, \qquad \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} = \alpha\phi_{\mathbf{k}}, \quad |u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1.$$

Hence

$$\langle \hat{N} \rangle = \sum_{\mathbf{k}} |v_{\mathbf{k}}|^2 = |\alpha|^2 \sum_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{1 + |\alpha|^2 |\phi_{\mathbf{k}}|^2}.$$

The diluteness criterion

With the normalization $\sum_{\mathbf{k}} |\phi_{\mathbf{k}}|^2 = 1$,

$$\text{bosonic behaviour} \iff \langle \hat{N} \rangle \simeq |\alpha|^2 \iff |\alpha|^2 |\phi_{\mathbf{k}}|^2 \ll 1 \quad \forall \mathbf{k}.$$

If σ is the size of the bound state, $\max_{\mathbf{k}} |\phi_{\mathbf{k}}| \simeq \sqrt{\sigma^3/V}$, and with $\rho = \langle \hat{N} \rangle / V$,

$$\text{bosonic behaviour} \iff \rho\, \sigma^3 \ll 1.$$

Interpretation. The composite particle behaves as a pointlike boson when there is, on average, much less than one constituent of the same species inside the volume σ^3 of the bound state — Pauli exclusion between *different* composites is then irrelevant.

Same criterion from the commutator. Instead of $[\hat{c}, \hat{c}^\dagger] = 1$,

$$[\hat{c}, \hat{c}^\dagger] = 1 - \sum_{\mathbf{k}} |\phi_{\mathbf{k}}|^2 \left(\hat{n}_{\mathbf{k},1} + \hat{n}_{-\mathbf{k},2} \right),$$

a correction again of order $\rho\sigma^3$. [11, 12]

The opposite limit: the BEC–BCS crossover

When the criterion fails, $|\alpha|^2|\phi_{\mathbf{k}}|^2 \gg 1$, the occupations saturate, $|v_{\mathbf{k}}|^2 \to 1$: each pair mode is filled at most once and $\langle \hat{N} \rangle$ grows far more slowly than $|\alpha|^2$. The pairs strongly overlap.

The state obtained above,

$$|\Psi\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}}\, \hat{a}^{\dagger}_{\mathbf{k},1} \hat{a}^{\dagger}_{-\mathbf{k},2} \right) |\emptyset\rangle,$$

is exactly the variational wave-function of BCS theory, the two species playing the role of the two spin states of the electron.

The two limits are the two ends of one family:

- $\rho\sigma^3 \ll 1$: small, tightly bound molecules condensing as elementary bosons;
- $\rho\sigma^3 \gg 1$: large, strongly overlapping Cooper pairs.

The continuous evolution between them is the BEC–BCS crossover.

Gaussian states

A Gaussian state has a density matrix that is the exponential of a quadratic operator,

$$\hat{\rho} = \frac{1}{\mathcal{Z}} \exp(-\hat{H}), \qquad \hat{H} = \sum_k E_k \, \hat{a}_k^\dagger \hat{a}_k$$

after a Bogoliubov transformation to the normal modes.

Examples. An ideal gas at thermal equilibrium, $\hat{\rho} = \Xi^{-1} \exp[-\beta(\hat{H} - \mu\hat{N})]$, is Gaussian because $\hat{H} - \mu\hat{N}$ is quadratic. So is any interacting system treated within a quadratic mean-field approximation.

The simplification

As for Gaussian random variables, all higher moments reduce to two-point moments.

A quadratic Hamiltonian preserves parity, so $\hat{\rho}$ commutes with the parity operator and

$$\langle \hat{b}_1 \cdots \hat{b}_{2n+1} \rangle = 0.$$

We therefore consider an even number $2n$ of operators.

The key relation, and the recursion

Since $\hat{\rho} \propto \exp(-\sum_j E_j \hat{n}_j)$ factorizes over modes, and $\hat{a}_k f(\hat{n}_k) = f(\hat{n}_k + 1)\hat{a}_k$,

$$\hat{a}_k\, \hat{\rho} = \mathrm{e}^{-E_k}\, \hat{\rho}\, \hat{a}_k, \qquad \hat{a}_k^\dagger\, \hat{\rho} = \mathrm{e}^{E_k}\, \hat{\rho}\, \hat{a}_k^\dagger.$$

Commuting an annihilation operator through $\hat{\rho}$ costs e^{-E_k}, because it lowers by one the occupation appearing in the exponent.

Using cyclicity of the trace and then moving $\hat{b}_1$ through the others with $\hat{b}_i \hat{b}_1 = -\hat{b}_1 \hat{b}_i + \{\hat{b}_i, \hat{b}_1\}$, one finds for fermions

$$\left(1 + \mathrm{e}^{E_k}\right) \langle \hat{b}_1 \cdots \hat{b}_{2n} \rangle = \mathrm{e}^{E_k} \sum_{i=2}^{2n} (-1)^i \{\hat{b}_i, \hat{b}_1\} \langle \hat{b}_2 \cdots \hat{b}_{i-1} \hat{b}_{i+1} \cdots \hat{b}_{2n} \rangle.$$

The prefactor is precisely the two-point function — e.g. $\langle \hat{a}_k^\dagger \hat{a}_k \rangle = 1/(1 + \mathrm{e}^{E_k})$, the Fermi–Dirac occupation. Hence

$$\langle \hat{b}_1 \cdots \hat{b}_{2n} \rangle = \sum_{i=2}^{2n} (-1)^i \langle \hat{b}_1 \hat{b}_i \rangle \langle \hat{b}_2 \cdots \hat{b}_{i-1} \hat{b}_{i+1} \cdots \hat{b}_{2n} \rangle.$$

Wick's theorem

Fermions

$$\langle \hat{b}_1 \cdots \hat{b}_{2n} \rangle = \sum_{\text{pairings } \sigma} \varepsilon(\sigma) \langle \hat{b}_{\sigma(1)} \hat{b}_{\sigma(2)} \rangle \cdots \langle \hat{b}_{\sigma(2n-1)} \hat{b}_{\sigma(2n)} \rangle$$

Bosons – same, without the signs

$$\langle \hat{b}_1 \cdots \hat{b}_{2n} \rangle = \sum_{\text{pairings } \sigma} \langle \hat{b}_{\sigma(1)} \hat{b}_{\sigma(2)} \rangle \cdots \langle \hat{b}_{\sigma(2n-1)} \hat{b}_{\sigma(2n)} \rangle$$

There are $(2n)!/(2^n n!)$ pairings — 3, 15, 105 for $2n = 4, 6, 8$. For four operators,

$$\langle \hat{b}_1 \hat{b}_2 \hat{b}_3 \hat{b}_4 \rangle = \langle \hat{b}_1 \hat{b}_2 \rangle \langle \hat{b}_3 \hat{b}_4 \rangle - \langle \hat{b}_1 \hat{b}_3 \rangle \langle \hat{b}_2 \hat{b}_4 \rangle + \langle \hat{b}_1 \hat{b}_4 \rangle \langle \hat{b}_2 \hat{b}_3 \rangle .$$

Do not forget the anomalous pairings

The normal modes are *quasiparticle* operators, in general combinations of creation *and* annihilation operators of the original particles. A Gaussian state therefore has non-vanishing anomalous averages $\langle \hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}} \rangle$, to be retained as possible pairings.

A simple check

The harmonic-oscillator ground state is Gaussian — the $E \to \infty$ limit of $\hat{\rho} \propto \mathrm{e}^{-E\hat{a}^\dagger\hat{a}}$. Its only non-zero second moment is

$$\langle \hat{a}\hat{a}^\dagger \rangle = 1, \qquad \langle \hat{a}\hat{a} \rangle = \langle \hat{a}^\dagger\hat{a}^\dagger \rangle = \langle \hat{a}^\dagger\hat{a} \rangle = 0.$$

With $\hat{x} = \sigma(\hat{a} + \hat{a}^\dagger)$, $\sigma^2 = \hbar/(2m\omega)$,

$$\langle \hat{x}^2 \rangle = \sigma^2 \langle (\hat{a} + \hat{a}^\dagger)^2 \rangle = \sigma^2,$$

and Wick's theorem gives immediately

$$\langle \hat{x}^4 \rangle = 3\langle \hat{x}^2 \rangle^2 = 3\sigma^4.$$

Wick's theorem reduces higher-order correlation functions to products of two-point functions. This is the tool used throughout the next chapter.

Summary – Chapter 2

- The symmetrization postulate is a genuine additional postulate, needed to remove exchange degeneracy. One-dimensional representations of $S_N \Rightarrow$ bosons or fermions only (in 3D).
- It drastically reduces the Hilbert space: $\binom{d+N-1}{N}$ or $\binom{d}{N}$ instead of d^N.
- Second quantization encodes the statistics in the algebra $[\hat{a}, \hat{a}^\dagger]_\mp = \delta$, making symmetrization automatic. One- and two-body operators take a universal form, and the field obeys an operator-valued Schrödinger equation.
- Composite particles are bosons for an even number of fermionic constituents, and behave as such provided $\rho\sigma^3 \ll 1$. The opposite limit is BCS, the two being connected by the BEC–BCS crossover.
- For Gaussian states, Wick's theorem reduces every correlation function to two-point functions — including the anomalous ones.

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