Many-body quantum mechanics

2.1. Two-particle systems with distinguishable particles

Consider a system with two particles which can be distinguished by mass and/or charge and/or spin...
and an interaction which depends only on their relative coordinates:

$$H = \frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} + V(\vec{r}_1 - \vec{r}_2)$$

(from now on the hat over operators is dropped whenever there is no problem to decide whether the studied object is an operator or not)

The wave function depends on both coordinates. For example, the probability amplitude to find particle 1 at position $\vec{r}_1$ and particle 2 at $\vec{r}_2$ is (at time t)

$$\psi(\vec{r}_1, \vec{r}_2; t) = \langle \vec{r}_1, \vec{r}_2 | \psi(t) \rangle$$

where we used the Schrödinger picture (but dropped the index S)

The two-particle Schrödinger equation is (in coordinate space)

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}_1, \vec{r}_2; t) = \left(-\frac{\hbar^2 \Delta_{r_1}}{2m_1} - \frac{\hbar^2 \Delta_{r_2}}{2m_2} + V(\vec{r}_1 - \vec{r}_2) \right) \psi(\vec{r}_1, \vec{r}_2; t)$$

$$\text{with } \Delta_{r_i} = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \quad \text{for } i = 1, 2 \; ; \; \vec{r}_i = (x_i, y_i, z_i)$$

The space spanned by $\langle \vec{r}_1, \vec{r}_2 |$ is just a product space $\langle \vec{r}_1, \vec{r}_2 | = \langle \vec{r}_1 | \langle \vec{r}_2 |$ with normalization

$$\langle \vec{r}_1, \vec{r}_2 | \vec{r}_1{}', \vec{r}_2{}' \rangle = \langle \vec{r}_1 | \vec{r}_1{}' \rangle \langle \vec{r}_2 | \vec{r}_2{}' \rangle = \delta(\vec{r}_1 - \vec{r}_1{}') \, \delta(\vec{r}_2 - \vec{r}_2{}')$$

It is appropriate to introduce center-of-mass and relative coordinates

$$\vec{R} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2}, \quad \vec{r} = \vec{r}_1 - \vec{r}_2$$

i.e. the two-particle state

$$\langle \vec{R}, \vec{r} | := \int d^3 r_1 \, d^3 r_2 \; \delta\left(\vec{R} - \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2}\right) \delta\left(\vec{r} - (\vec{r}_1 - \vec{r}_2)\right) \langle \vec{r}_1 | \langle \vec{r}_2 |$$

---

exercise: Show that the Schrödinger equation can be rewritten in the form

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{R}, \vec{r}; t) = \left(-\frac{\hbar^2 \Delta_R}{2M} - \frac{\hbar^2 \Delta_r}{2\mu} + V(\vec{r}) \right) \psi(\vec{R}, \vec{r}; t) \qquad (*)$$

with $M = m_1 + m_2$ total mass

$\mu = \frac{m_1 m_2}{M}$ reduced mass

$$\Delta_R = \frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2}, \quad \vec{R} = (X, Y, Z)$$

$$\Delta_r = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}, \quad \vec{r} = (x, y, z)$$

---

ansatz: separate off center-of-mass motion (to solve (*))

$$\psi(\vec{R}, \vec{r}; t) = \chi(\vec{R}, t) \, \varphi(\vec{r}, t)$$

with $\chi(\vec{R}, t)$ solving the <u>free</u> Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \chi(\vec{R}, t) = -\frac{\hbar^2}{2M} \Delta_R \, \chi(\vec{R}, t)$$

and $\varphi(\vec{r}, t)$ solving the effective one-body Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \varphi(\vec{r}, t) = \left(-\frac{\hbar^2}{2\mu} \Delta_r + V(\vec{r}) \right) \varphi(\vec{r}, t)$$

Of course one can also separate off the time evolution (effectively one comes in that way to the Heisenberg picture) and solve the equation for χ:

$$\chi(\vec{R},t) = e^{-iE_{cm}t/\hbar}\, e^{i\vec{P}\cdot\vec{R}/\hbar}$$

with $E_{cm} = \dfrac{P^2}{2M}$, the energy of the center-of-mass motion

$$\varphi(\vec{r},t) = e^{-iE_{rel}t/\hbar}\,\varphi(\vec{r})$$

$$E_{rel}\,\varphi(\vec{r}) = \left(-\frac{\hbar^2}{2\mu}\Delta_r + V(\vec{r})\right)\varphi(\vec{r})$$ time-independent Schrödinger equation

For the special case (which appears often in nature) that the potential depends only on the distance $r = |\vec{r}|$,

$$V = V(|\vec{r}|) = V(r),$$

(and not on the direction of $\vec{r}$) one has conservation of (orbital) angular momentum (spins are ignored here)

$$\Delta_r = \frac{1}{r}\frac{d^2}{dr^2}r - \frac{L^2}{\hbar^2 r^2}$$

$$\varphi(\vec{r}) = \frac{1}{r} f_\ell(r)\, Y_{\ell m}(\vartheta, \varphi)$$

$$L^2 Y_{\ell m}(\vartheta,\varphi) = \hbar^2 \ell(\ell+1) Y_{\ell m}(\vartheta,\varphi), \quad \ell \in \mathbb{N}_0, \; m = -\ell, -\ell+1, \dots, \ell$$

$$E_{rel} f_\ell(r) = -\frac{\hbar^2}{2\mu} f_\ell''(r) + \underbrace{\left(V(r) + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2}\right)}_{V_{eff}(r)} f_\ell(r)$$

2.2. Two-particle systems with indistinguishable particles

Consider again

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(|\vec{r}_1 - \vec{r}_2|)$$

have same masses since identical particles

The particles may be characterised by additional properties / quantum numbers q, e.g. their spin, besides their location

$\rightsquigarrow$ the two-particle wave function $\psi(\vec{r}_1, q_1; \vec{r}_2, q_2; t)$ cannot be independent of $\psi(\vec{r}_2, q_2; \vec{r}_1, q_1; t)$ since this is the same situation for the observer

In nature there are two types of particles

1. bosons: here $\psi(\vec{r}_1, q_1; \vec{r}_2, q_2; t) = +\psi(\vec{r}_2, q_2; \vec{r}_1, q_1; t)$
2. fermions: here $\psi(\vec{r}_1, q_1; \vec{r}_2, q_2; t) = -\psi(\vec{r}_2, q_2; \vec{r}_1, q_1; t)$

There are no other possibilities:

From $|\underbrace{\psi(\vec{r}_1, q_1; \vec{r}_2, q_2; t)}_{=:\psi_{12}}| = |\underbrace{\psi(\vec{r}_2, q_2; \vec{r}_1, q_1; t)}_{=:\psi_{21}}|$

one concludes $\psi_{12} = e^{i\alpha}\psi_{21}$, $\alpha \in \mathbb{R}$

but exchanging twice leads to $\psi_{12} = e^{i\alpha}\psi_{21} = e^{i\alpha}e^{i\alpha}\psi_{12}$

$\Rightarrow e^{2i\alpha} = 1 \Rightarrow \alpha = 0, \pi$

One can show under rather general conditions (relativistic local quantum field theory) that bosons have integer spin while fermions have half-integer spin, i.e. bosons: spin $0, 1, \dots$

fermions: spin $\frac{1}{2}, \frac{3}{2}, \dots$

("spin-statistics theorem" - not proven here)

One can also formulate the boson/fermion property for the quantum eigen states instead of the wave function:

$$\langle \vec{r}_1, q_1; \vec{r}_2, q_2 | = \pm \langle \vec{r}_2, q_2; \vec{r}_1, q_1 | \quad \text{for} \begin{cases} \text{bosons} \\ \text{fermions} \end{cases}$$

$\Rightarrow$ normalization:

$$\langle \vec{r}_1, q_1; \vec{r}_2, q_2 | \vec{r}_1{}', q_1'; \vec{r}_2{}', q_2' \rangle$$

$$= \delta(\vec{r}_1 - \vec{r}_1{}')\, \delta_{q_1 q_1'}\, \delta(\vec{r}_2 - \vec{r}_2{}')\, \delta_{q_2 q_2'} \pm \delta(\vec{r}_1 - \vec{r}_2{}')\, \delta_{q_1 q_2'}\, \delta(\vec{r}_2 - \vec{r}_1{}')\, \delta_{q_2 q_1'}$$

Application:

Suppose that spins (and other quantum numbers) do not play a role for the considered system, e.g. both spins point in the same direction

$\rightsquigarrow q_1 = q_2$ and we drop q_i in the following

We will see that not all solutions which we found in section 2.1 are possible now:

case 1 : two (indistinguishable) bosons:

$$\psi(\vec{r}_1, \vec{r}_2; t) = \psi(\vec{r}_2, \vec{r}_1; t)$$

$$\Rightarrow \psi(\vec{R}, \vec{r}; t) = \psi(\vec{R}, -\vec{r}; t)$$

$\Rightarrow$ no contraint for $\chi(\vec{R}, t)$, but

$$f(\vec{r}) = f(-\vec{r})$$

$$\Rightarrow Y_{\ell m}(\vartheta, \varphi) = \underbrace{Y_{\ell m}(\pi - \vartheta, \varphi + \pi)}_{= (-1)^\ell Y_{\ell m}(\vartheta, \varphi)}$$

$\Rightarrow$ only even ℓ allowed

case 2 : two (indistinguishable) fermions:

$$\psi(\vec{r}_1, r_2; t) = -\psi(\vec{r}_2, \vec{r}_1; t)$$

$$\Rightarrow f(\vec{r}) = -f(-\vec{r})$$

$\Rightarrow$ only odd ℓ allowed

general remark: two fermions cannot be in the very same state

$\rightsquigarrow$ suppose this state is characterised by one-particle quantum numbers $q, r, s, \ldots$

$\rightsquigarrow$ if fermions were in same state $\rightsquigarrow$ $|\underbrace{q, r, s, \ldots}_{\text{first particle}}; \underbrace{q, r, s, \ldots}_{\text{second particle}}\rangle$

on the other hand

$$|q, r, s, \ldots; q, r, s, \ldots\rangle = -|q, r, s, \ldots; q, r, s, \ldots\rangle$$

$$\Rightarrow |q, r, s, \ldots; q, r, s, \ldots\rangle = 0$$

$\Rightarrow$ zero probability for existence of this state

This is the Pauli principle: Two fermions cannot be in the very same state. It leads to the shell structure of the electrons in atoms and finally to chemistry.
Another consequence is the existence of white dwarfs and neutron stars.

2.3. Many-particle systems and the particle-number representation

a) Creation and annihilation operators

Consider a system with n indistinguishable particles (fermions or bosons). Spins (and other quantum numbers) are neglected concentrating only on spatial coordinates. Also the time variable is not written down explicitly.

The n-body coordinate eigen states $|\vec{r}_1, \dots, \vec{r}_n\rangle$ satisfy

$$|\vec{r}_1, \dots, \vec{r}_a, \dots, \vec{r}_b, \dots, \vec{r}_n\rangle = \pm |\vec{r}_1, \dots, \vec{r}_b, \dots, \vec{r}_a, \dots, \vec{r}_n\rangle$$

where here and in the following the upper sign refers to bosons, the lower to fermions.

Already the normalisation condition for these states is complicated:

Example: $n = 3$

$$\langle \vec{r}_1, \vec{r}_2, \vec{r}_3 | \vec{r}_1{}', \vec{r}_2{}', \vec{r}_3{}' \rangle =$$
$$= \delta(\vec{r}_1 - \vec{r}_1{}')\,\delta(\vec{r}_2 - \vec{r}_2{}')\,\delta(\vec{r}_3 - \vec{r}_3{}') \pm \delta(\vec{r}_1 - \vec{r}_2{}')\,\delta(\vec{r}_2 - \vec{r}_1{}')\,\delta(\vec{r}_3 - \vec{r}_3{}')$$
$$\pm \delta(\vec{r}_1 - \vec{r}_3{}')\,\delta(\vec{r}_2 - \vec{r}_2{}')\,\delta(\vec{r}_3 - \vec{r}_1{}') \pm \delta(\vec{r}_1 - \vec{r}_1{}')\,\delta(\vec{r}_2 - \vec{r}_3{}')\,\delta(\vec{r}_3 - \vec{r}_2{}')$$
$$+ \delta(\vec{r}_1 - \vec{r}_2{}')\,\delta(\vec{r}_2 - \vec{r}_3{}')\,\delta(\vec{r}_3 - \vec{r}_1{}') + \delta(\vec{r}_1 - \vec{r}_3{}')\,\delta(\vec{r}_2 - \vec{r}_1{}')\,\delta(\vec{r}_3 - \vec{r}_2{}')$$

for n particles $n!$ terms ($n!$ permutations)!

If already the normalization is complicated, the necessary calculations, e.g., for the time evolution, will not be simpler.

$\rightsquigarrow$ In the following a new technical formalism will be developed. It will be simpler in the end. It is important to stress that no new physical concepts are needed, it is still quantum mechanics.

First we enlarge our concept and consider instead of

a Hilbert space of one particle with vectors $|\vec{r}\rangle$

OR

a Hilbert space of two particles, $|\vec{r}_1, \vec{r}_2\rangle$,

OR

a Hilbert space of three particles, $|\vec{r}_1, \vec{r}_2, \vec{r}_3\rangle$,

OR

⋮

all at once the "Fock space" consisting of

a Hilbert space of one particle, $|\vec{r}\rangle$

AND

a Hilbert space of two particles, $|\vec{r}_1, \vec{r}_2\rangle$

AND

⋮

AND

THE VACUUM consisting of a vector with NO PARTICLE, $|0\rangle$

For non-relativistic quantum mechanics we do that because it leads to a formalism which is technically simpler. For relativistic systems we need to do that, because particles can be created or annihilated, i.e. the particle number can change.

The scalar product is defined in the Fock space as follows:

$$\langle 0|0\rangle = 1, \quad \langle 0|\vec{r}\rangle = 0, \quad \langle 0|\vec{r}_1, \vec{r}_2\rangle = 0, \ldots$$

$$\langle \vec{r}|0\rangle = 0, \quad \langle \vec{r}|\vec{r}\,'\rangle = \delta(\vec{r}-\vec{r}\,'), \quad \langle \vec{r}|\vec{r}_1, \vec{r}_2\rangle = 0, \ldots$$

$$\vdots$$

in general $\langle \vec{r}_1, \ldots, \vec{r}_m | \vec{r}_1{}', \ldots, \vec{r}_n{}' \rangle = \delta_{nm} \underbrace{\langle \vec{r}_1, \ldots, \vec{r}_m | \vec{r}_1{}', \ldots, \vec{r}_m{}' \rangle}_{\text{this part is still complicated}}$

Introduce a "creation operator"

$$\psi^+(\vec{r}) = \sum_{n=0}^{\infty} \frac{1}{n!} \int d^3r_1' \cdots d^3r_n' \underbrace{|\vec{r}, \vec{r}_1{}', \ldots, \vec{r}_n{}'\rangle}_{n+1 \text{ particles}} \underbrace{\langle \vec{r}_1{}', \ldots, \vec{r}_n{}'|}_{n \text{ particles}}$$

Note: this definition is also complicated, but in the end we will have found simple rules how to calculate with $\psi^+(\vec{r})$. Then we do not need the definition any more.

Why $\varphi^+(\vec{r})$ is called creation operator:

$$\varphi^+(\vec{r})|0\rangle = \sum_{n=0}^{\infty} \frac{1}{n!}\int d^3r_1' \dots d^3r_n' \, |\vec{r}, \vec{r}_1', \dots, \vec{r}_n'\rangle \underbrace{\langle \vec{r}_1', \dots, \vec{r}_n'|0\rangle}_{=\delta_{n0}}$$

$$= |\vec{r}\rangle$$

$$\varphi^+(\vec{r})|\vec{r}_1\rangle = \int d^3r_1' \, |\vec{r}, \vec{r}_1'\rangle \underbrace{\langle \vec{r}_1'|\vec{r}_1\rangle}_{\delta(\vec{r}_1' - \vec{r}_1)} = |\vec{r}, \vec{r}_1\rangle$$

$$\varphi^+(\vec{r})|\vec{r}_1, \vec{r}_2\rangle = \frac{1}{2!}\int d^3r_1' \, d^3r_2' \, |\vec{r}, \vec{r}_1', \vec{r}_2'\rangle \langle \vec{r}_1', \vec{r}_2'|\vec{r}_1, \vec{r}_2\rangle$$

$$= \frac{1}{2}\int d^3r_1' \, d^3r_2' \, |\vec{r}, \vec{r}_1', \vec{r}_2'\rangle \left(\delta(\vec{r}_1' - \vec{r}_1)\delta(\vec{r}_2' - \vec{r}_2) \pm \delta(\vec{r}_1' - \vec{r}_2)\delta(\vec{r}_2' - \vec{r}_1)\right)$$

$$= \frac{1}{2}\left(|\vec{r}, \vec{r}_1, \vec{r}_2\rangle \pm \underbrace{|\vec{r}, \vec{r}_2, \vec{r}_1\rangle}_{=\pm|\vec{r}, \vec{r}_1, \vec{r}_2\rangle}\right)$$

$$= |\vec{r}, \vec{r}_1, \vec{r}_2\rangle$$

in general: $\varphi^+(\vec{r})|\vec{r}_1, \dots, \vec{r}_n\rangle = |\vec{r}, \vec{r}_1, \dots, \vec{r}_n\rangle$

$\rightsquigarrow$ "creates" additional state at $\vec{r}$

$\Rightarrow$ all states can be built out of the no-particle state:

$$|\vec{r}\rangle = \varphi^+(\vec{r})|0\rangle$$

$$|\vec{r}_1, \vec{r}_2\rangle = \varphi^+(\vec{r}_1)\varphi^+(\vec{r}_2)|0\rangle$$

$$\vdots$$

$$|\vec{r}_1, \dots, \vec{r}_n\rangle = \varphi^+(\vec{r}_1)\dots\varphi^+(\vec{r}_n)|0\rangle$$

As we will see, the adjoint of ρ^+ annihilates particles,

$$\rho(\vec{r}) = (\rho^+(\vec{r}))^+ = \sum_{n=0}^{\infty} \frac{1}{n!} \int d^3r_1' \cdots d^3r_n' \, |\vec{r}_1' \ldots \vec{r}_n'\rangle\langle \vec{r}, \vec{r}_1', \ldots, \vec{r}_n'|$$

But first of all one can use it to create n-particle bra's:

$$\langle \vec{r}| = (|\vec{r}\rangle)^+ = (\rho^+(\vec{r})|0\rangle)^+ = \langle 0|\rho(\vec{r})$$

$$\rightsquigarrow \langle \vec{r}_1, \ldots, \vec{r}_n| = \langle 0|\rho(\vec{r}_n) \ldots \rho(\vec{r}_1)$$

note the ordering!

Why ρ is an annihilation operator (when acting to the right):

Since there is no bra $\langle 0|$ in the definition of $\rho(\vec{r})$ (sum starts with $\langle \vec{r}|$)

$$\rightsquigarrow \rho(\vec{r})|0\rangle = 0$$

$$\rho(\vec{r})|\vec{r}_1\rangle = |0\rangle\langle \vec{r}|\vec{r}_1\rangle = \delta(\vec{r}-\vec{r}_1)|0\rangle$$ (only non-zero if there was a particle at $\vec{r}$)

$$\rho(\vec{r})|\vec{r}_1, \vec{r}_2\rangle = \int d^3r_1' \, |\vec{r}_1'\rangle\langle \vec{r}, \vec{r}_1'|\vec{r}_1, \vec{r}_2\rangle$$

$$= \int d^3r_1' \, |\vec{r}_1'\rangle \left(\delta(\vec{r}-\vec{r}_1)\delta(\vec{r}_1'-\vec{r}_2) \pm \delta(\vec{r}-\vec{r}_2)\delta(\vec{r}_1'-\vec{r}_1)\right)$$

$$= |\vec{r}_2\rangle\,\delta(\vec{r}-\vec{r}_1) \pm |\vec{r}_1\rangle\,\delta(\vec{r}-\vec{r}_2)$$

in general:

$$\rho(\vec{r})|\vec{r}_1, \ldots, \vec{r}_n\rangle = \sum_{a=1}^{n} (\pm 1)^{a+1} \delta(\vec{r}-\vec{r}_a) \underbrace{|\vec{r}_1, \ldots, \vec{r}_{a-1}, \vec{r}_{a+1}, \ldots, \vec{r}_n\rangle}_{n-1 \text{ particles}}$$

Note: This is again a complicated - at least lengthy - formula. We will not need it in the end, but for intermediate steps.

Consider now

$$\rho^+(\vec{r})\,\rho^+(\vec{r}\,')\,|\vec{r}_1,\dots,\vec{r}_n\rangle = |\vec{r},\vec{r}\,',\vec{r}_1,\dots,\vec{r}_n\rangle$$
$$= \pm\,|\vec{r}\,',\vec{r},\vec{r}_1,\dots,\vec{r}_n\rangle = \pm\,\rho(\vec{r}\,')\,\rho(\vec{r})\,|\vec{r}_1,\dots,\vec{r}_n\rangle$$

$$\Rightarrow \left(\rho^+(\vec{r})\,\rho^+(\vec{r}\,') - (\pm 1)\,\rho(\vec{r}\,')\,\rho(\vec{r})\right)|\vec{r}_1,\dots,\vec{r}_n\rangle = 0$$

since all $|\vec{r}_1,\dots,\vec{r}_n\rangle$ form a complete set of states for the Fock space

$$\rightsquigarrow \quad [\rho^+(\vec{r}),\rho^+(\vec{r}\,')]_{\mp} = 0 \qquad (*)$$

where we have introduced

the commutator $[A,B]_- = AB - BA = [A,B]$
and
the anti-commutator $[A,B]_+ = AB + BA = \{A,B\}$

Note that the commutator appears for bosons and the anti-commutator for fermions

Taking the adjoint of the rather simple equation $(*)$ yields

$$[\rho(\vec{r}),\rho(\vec{r}\,')]_{\mp} = 0$$

Finally we are heading for the (anti-) commutator of ρ and ρ^+:

$$\rho(\vec{r})\,\rho^+(\vec{r}\,')\,|\vec{r}_1,\dots,\vec{r}_n\rangle = \rho(\vec{r})\,|\vec{r}\,',\vec{r}_1,\dots,\vec{r}_n\rangle$$
$$= \delta(\vec{r}-\vec{r}\,')\,|\vec{r}_1,\dots,\vec{r}_n\rangle + \sum_{a=2}^{n+1}(\pm 1)^{a+1}\,\delta(\vec{r}-\vec{r}_{a-1})\,|\vec{r}\,',\vec{r}_1,\dots,\vec{r}_{a-2},\vec{r}_a,\dots,\vec{r}_n\rangle$$
$$= \delta(\vec{r}-\vec{r}\,')\,|\vec{r}_1,\dots,\vec{r}_n\rangle \pm \sum_{b=1}^{n}(\pm 1)^{b+1}\,\delta(\vec{r}-\vec{r}_b)\,|\vec{r}\,',\vec{r}_1,\dots,\vec{r}_{b-1},\vec{r}_{b+1},\dots,\vec{r}_n\rangle$$

$b = a-1$

$$\rho^+(\vec{r}\,')\,\rho(\vec{r})\,|\vec{r}_1,\dots,\vec{r}_n\rangle$$

$$= \rho^+(\vec{r}\,')\sum_{a=1}^{n}(\pm 1)^{a+1}\,\delta(\vec{r}-\vec{r}_a)\,|\vec{r}_1,\dots,\vec{r}_{a-1},\vec{r}_{a+1},\dots,\vec{r}_n\rangle$$

$$= \sum_{a=1}^{n}(\pm 1)^{a+1}\,\delta(\vec{r}-\vec{r}_a)\,|\vec{r}\,',\vec{r}_1,\dots,\vec{r}_{a-1},\vec{r}_{a+1},\dots,\vec{r}_n\rangle$$

$$\Rightarrow \rho(\vec{r})\,\rho^+(\vec{r}\,')\,|\vec{r}_1,\dots,\vec{r}_n\rangle = \delta(\vec{r}-\vec{r}\,')\,|\vec{r}_1,\dots,\vec{r}_n\rangle$$

$$\pm\, \rho^+(\vec{r}\,')\,\rho(\vec{r})\,|\vec{r}_1,\dots,\vec{r}_n\rangle$$

$$\Rightarrow \left[\rho(\vec{r}),\,\rho^+(\vec{r}\,')\right]_{\mp} = \delta(\vec{r}-\vec{r}\,')$$

Summary of the formulae one needs for actual calculations

$$\langle 0|0\rangle = 1$$

$$|\vec{r}_1,\dots,\vec{r}_n\rangle = \rho^+(\vec{r}_1)\cdots\rho^+(\vec{r}_n)\,|0\rangle \quad \text{(and adjoint)}$$

$$\rho(\vec{r})\,|0\rangle = 0 \quad , \quad \langle 0|\,\rho^+(\vec{r}) = 0$$

$$\left[\rho(\vec{r}),\,\rho(\vec{r}\,')\right]_{\mp} = 0 = \left[\rho^+(\vec{r}),\,\rho^+(\vec{r}\,')\right]_{\mp}$$

$$\left[\rho(\vec{r}),\,\rho^+(\vec{r}\,')\right]_{\mp} = \delta(\vec{r}-\vec{r}\,')$$

Note: None of the other formulae are needed any more. In particular one does not need the definition of $\rho^+(\vec{r})$. All complicated relations can be derived from the simple rules given above.

General strategy for calculations:

Move annihilators to the right and/or creators to the left using the (anti-) commutation relations

Example: Want to know

$\psi(\vec r)\,|\vec r_1, \vec r_2\rangle$:

$$
\begin{aligned}
\psi(\vec r)\,|\vec r_1, \vec r_2\rangle &= \psi(\vec r)\,\psi^+(\vec r_1)\,\psi^+(\vec r_2)\,|0\rangle \\
&= \left([\psi(\vec r), \psi^+(\vec r_1)]_\mp \pm \psi^+(\vec r_1)\,\psi(\vec r) \right) \psi^+(\vec r_2)\,|0\rangle \\
&= \delta(\vec r - \vec r_1)\,\psi^+(\vec r_2)\,|0\rangle \pm \psi^+(\vec r_1)\,\psi(\vec r)\,\psi^+(\vec r_2)\,|0\rangle \\
&= \delta(\vec r - \vec r_1)\,|\vec r_2\rangle \pm \psi^+(\vec r_1) \left([\psi(\vec r), \psi^+(\vec r_2)]_\mp \pm \psi^+(\vec r_2)\,\psi(\vec r) \right) |0\rangle \\
&= \delta(\vec r - \vec r_1)\,|\vec r_2\rangle \pm \psi^+(\vec r_1)\,\delta(\vec r - \vec r_2)\,|0\rangle + \psi^+(\vec r_1)\,\psi^+(\vec r_2)\,\underbrace{\psi(\vec r)\,|0\rangle}_{=0} \\
&= \delta(\vec r - \vec r_1)\,|\vec r_2\rangle \pm \delta(\vec r - \vec r_2)\,|\vec r_1\rangle
\end{aligned}
$$

Calculations might be long, but rules are simple.

b) Observables

In the following we will see that all observables of an n-body system can be formulated as operators in Fock space in terms of the annihilation and creation operators.

Consider first the Hermitian operator

$$\varrho(\vec{r}) = \psi^{+}(\vec{r})\,\psi(\vec{r})$$

$$\leadsto \quad \varrho(\vec{r})|0\rangle = 0$$

Calculate

$$[\varrho(\vec{r}), \psi^{+}(\vec{r}\,')] = \psi^{+}(\vec{r})\,[\psi(\vec{r}), \psi^{+}(\vec{r}\,')]_{\mp} \pm \underbrace{[\psi^{+}(\vec{r}), \psi^{+}(\vec{r}\,')]_{\mp}}_{=0}\,\psi(\vec{r})$$

$$[AB, C] = A[B,C]_{\mp} \pm [A,C]_{\mp} B$$

$$= \psi^{+}(\vec{r})\,\delta(\vec{r}-\vec{r}\,')$$

$$\Rightarrow \quad [\varrho(\vec{r}), \psi(\vec{r}\,')] = [\psi^{+}(\vec{r}\,'), \varrho(\vec{r})]^{+} = \left(-\psi^{+}(\vec{r})\,\delta(\vec{r}-\vec{r}\,')\right)^{+}$$

$$= -\psi(\vec{r})\,\delta(\vec{r}-\vec{r}\,')$$

Note that we look at the commutator here both for fermions and bosons. The deeper reason is that the product of two fermion operators is of boson type, hence the commutator is the appropriate object to look at.

Action of $\varrho(\vec{r})$ on n-body states:

$$\varrho(\vec{r})|\vec{r}_1, \dots, \vec{r}_n\rangle = \varrho(\vec{r})\,\psi^{+}(\vec{r}_1)\cdots\psi^{+}(\vec{r}_n)|0\rangle$$

$$= [\varrho(\vec{r}), \psi^{+}(\vec{r}_1)\cdots\psi^{+}(\vec{r}_n)]|0\rangle$$

$\varrho(\vec{r})|0\rangle = 0$

$$= [\varrho(\vec{r}), \psi^{+}(\vec{r}_1)]\,\psi^{+}(\vec{r}_2)\cdots\psi^{+}(\vec{r}_n)|0\rangle$$

$$+ \psi^{+}(\vec{r}_1)\,[\varrho(\vec{r}), \psi^{+}(\vec{r}_2)]\,\psi^{+}(\vec{r}_3)\cdots\psi^{+}(\vec{r}_n)|0\rangle$$

$$+ \dots$$

$[A, BC\cdots] = [A,B]C\cdots + B[A,C]\cdots + BC[A,\cdots]\cdots + \cdots$

$$\Rightarrow \rho(\vec{r})\,|\vec{r}_1,\ldots,\vec{r}_n\rangle = \sum_{a=1}^{n} \delta(\vec{r}-\vec{r}_a)\,|\vec{r}_1,\ldots,\vec{r}_n\rangle$$

$\rightsquigarrow$ $\rho(\vec{r})$ is the particle-density operator

The volume integral

$$N = \int d^3r\, \rho(\vec{r})$$

is the particle-number operator:

$$N|\vec{r}_1,\ldots,\vec{r}_n\rangle = n\,|\vec{r}_1,\ldots,\vec{r}_n\rangle$$

Next we define

$$\vec{P} := \int d^3r\, \psi^\dagger(\vec{r})\, \frac{\hbar}{i}\vec{\nabla}\psi(\vec{r})$$

and claim that this is the Fock-space operator of total momentum.

What do we have to do, to prove that?

We know the coordinate-space representation of a one-body momentum $\vec{p}$:

$$\langle\vec{r}|\vec{p}|\vec{r}'\rangle = i\hbar\,\vec{\nabla}_{r'}\overbrace{\delta(\vec{r}'-\vec{r})}^{\langle\vec{r}|\vec{r}'\rangle} \quad\text{or}\quad \vec{p}|\vec{r}'\rangle = i\hbar\vec{\nabla}_{r'}|\vec{r}'\rangle$$

The total momentum is the sum of the single-particle momenta

$\rightsquigarrow$ have to show

1. $\vec{P}$ is Hermitian

2. $\vec{P}|\vec{r}_1,\ldots,\vec{r}_n\rangle = i\hbar\sum_{a=1}^{n}\vec{\nabla}_{r_a}|\vec{r}_1,\ldots,\vec{r}_n\rangle$

① $$\vec{P}^{+} = \int d^3r \, \frac{\hbar}{-i} \left(\vec{\nabla}\psi^{+}(\vec{r})\right) \psi(\vec{r})$$

$$\underset{\substack{\uparrow \\ \text{integration by} \\ \text{parts}}}{=} \int d^3r \, \frac{\hbar}{i} \psi^{+}(\vec{r}) \, \vec{\nabla} \psi(\vec{r}) = \vec{P}$$

② $$\vec{P} |\vec{r}_1, \dots, \vec{r}_n\rangle = \vec{P} \psi^{+}(\vec{r}_1) \cdots \psi^{+}(\vec{r}_n) |0\rangle$$

$$= [\vec{P}, \psi^{+}(\vec{r}_1)] \psi^{+}(\vec{r}_2) \cdots \psi^{+}(\vec{r}_n) |0\rangle$$

$$+ \psi^{+}(\vec{r}_1) [\vec{P}, \psi^{+}(\vec{r}_2)] \cdots + \cdots$$

$$+ \psi^{+}(\vec{r}_1) \cdots \psi^{+}(\vec{r}_n) \vec{P} |0\rangle$$

calculate first

$$[\vec{P}, \psi^{+}(\vec{r}_j)] = \int d^3r \, \frac{\hbar}{i} [\psi^{+}(\vec{r}) \vec{\nabla}_r \psi(\vec{r}), \psi^{+}(\vec{r}_j)]$$

$$= \int d^3r \, \frac{\hbar}{i} \psi^{+}(\vec{r}) \, \vec{\nabla}_r \delta(\vec{r} - \vec{r}_j) = i\hbar \vec{\nabla}_{r_j} \psi^{+}(\vec{r}_j)$$

$$[AB, C] = A[B,C]_{\mp} \pm [A,C]_{\mp} B$$

in addition $\vec{P}|0\rangle = 0$ (vacuum has no momentum)

$$\psi(\vec{r})|0\rangle = 0 \Rightarrow \nabla_r \psi(\vec{r})|0\rangle = 0$$

$$\Rightarrow \vec{P} |\vec{r}_1, \dots, \vec{r}_n\rangle = i\hbar \vec{\nabla}_{r_1} |\vec{r}_1, \dots, \vec{r}_n\rangle + i\hbar \vec{\nabla}_{r_2} |\vec{r}_1, \dots, \vec{r}_n\rangle + \cdots$$

as claimed

Next we want to construct a Fock-space Hamiltonian.

Suppose first that the n-body system has no interactions among the constituents, but only an external potential V_1 acting on the n particles

$$\rightsquigarrow H = \int d^3r \, \psi^+(\vec{r}) \left(-\frac{\hbar^2 \Delta_r}{2m} + V_1(\vec{r}) \right) \psi(\vec{r})$$

In exactly the same way as for $\vec{P}$ one can show:

→ H is Hermitian

→ $H|0\rangle = 0$, i.e. the vacuum has no energy

→ $$\left[H, \psi^+(\vec{r}_j) \right] = \left(-\frac{\hbar^2 \Delta_{r_j}}{2m} + V_1(\vec{r}_j) \right) \psi^+(\vec{r}_j)$$

or equivalently

$$\left[\psi(\vec{r}_j), H \right] = \left(-\frac{\hbar^2 \Delta_{r_j}}{2m} + V_1(\vec{r}_j) \right) \psi(\vec{r}_j)$$

→ and finally

$$\langle \vec{r}_1, \dots, \vec{r}_n | H | \underset{\substack{\text{any state}\\\text{vector}}}{\psi} \rangle = \underbrace{\left[\sum_{j=1}^{n} \left(-\frac{\hbar^2 \Delta_{r_j}}{2m} + V_1(\vec{r}_j) \right) \right]}_{\substack{n\text{-body Hamiltonian}\\\text{(in coordinate-space}\\\text{representation)}}} \underbrace{\langle \vec{r}_1, \dots, \vec{r}_n | \psi \rangle}_{\substack{n\text{-body}\\\text{wave function}}}$$

as it should be.

Note that the structure of the potential energy is

$$\int d^3r \, \psi^+(\vec{r}) \, V_1(\vec{r}) \, \psi(\vec{r}) = \int d^3r \, V_1(\vec{r}) \, \varrho(\vec{r})$$

with the density operator $\varrho(\vec{r})$.

$\rightsquigarrow$ interpretation: $\varrho(\vec{r})$ tells where the particles are and $V_1(\vec{r})$ is the potential energy at this location.

Finally we construct H for a system with two-body interactions $V_2(\vec{r}_1, \vec{r}_2) = V_2(\vec{r}_2, \vec{r}_1)$

$$H = \int d^3r\, \psi^+(\vec{r}) \left(-\frac{\hbar^2 \Delta_r}{2m} + V_1(\vec{r}) \right) \psi(\vec{r})$$
$$+ \frac{1}{2} \int d^3r\, d^3r'\, \psi^+(\vec{r})\, \psi^+(\vec{r}')\, V_2(\vec{r}, \vec{r}')\, \psi(\vec{r}')\, \psi(\vec{r})$$

Notes:

→ The factor $\frac{1}{2}$ is introduced to avoid that the same interaction is counted twice ($V_2(\vec{r}, \vec{r}')$ and $V_2(\vec{r}', \vec{r})$)

→ The ordering of the ψ and ψ^+ is chosen such that

a) the vacuum is annihilated, i.e. has zero energy

b) H is Hermitian

→ Apart from ordering one has the structure

$$\psi^+(\vec{r})\, \psi(\vec{r})\, V_2(\vec{r}, \vec{r}')\, \psi^+(\vec{r}')\, \psi(\vec{r}')$$
$$= \rho(\vec{r})\, V_2(\vec{r}, \vec{r}')\, \rho(\vec{r}')$$

which is intuitive

To show that H is indeed the Hamiltonian we calculate as before

$$\langle \vec{r}_1, \dots, \vec{r}_n | H | \psi \rangle$$

We can restrict ourselves to the V_2 term:

$$\rightsquigarrow \langle \vec{r}_1, \dots, \vec{r}_n |\, \psi^+(\vec{r})\, \psi^+(\vec{r}')\, \psi(\vec{r}')\, \psi(\vec{r})$$
$$= \langle 0 |\, \psi(\vec{r}_n) \cdots \psi(\vec{r}_1) \underbrace{\psi^+(\vec{r})\, \psi^+(\vec{r}')\, \psi(\vec{r}')\, \psi(\vec{r})}_{=:D}$$
$$= \langle 0 | \left[\psi(\vec{r}_n), D \right] \psi(\vec{r}_{n-1}) \cdots \psi(\vec{r}_1) + \langle 0 |\, \psi(\vec{r}_n) \left[\psi(\vec{r}_{n-1}), D \right] \cdots + \dots$$

$$[\psi(\vec r_j), D] = [\psi(\vec r_j), \psi^+(\vec r)\,\psi^+(\vec r')\,\psi(\vec r')\,\psi(\vec r)]$$

$$= [\psi(\vec r_j), \psi^+(\vec r)\,\psi^+(\vec r')]\,\psi(\vec r')\,\psi(\vec r)$$

$$+ \psi^+(\vec r)\,\psi^+(\vec r')\,[\psi(\vec r_j), \psi(\vec r')\,\psi(\vec r)]$$

$$= \left(\pm\psi^+(\vec r)\,\delta(\vec r_j - \vec r') + \delta(\vec r_j - \vec r)\,\psi^+(\vec r')\right)\psi(\vec r')\,\psi(\vec r)$$

$$[AB, C] = A[B,C]_\mp \pm [A,C]_\mp B$$

$$\Rightarrow [C, AB] = -A[B,C]_\mp \mp [A,C]_\mp B$$

$$= \pm A[C,B]_\mp + [C,A]_\mp B$$

$$= \pm\,\psi^+(\vec r)\,\psi(\vec r_j)\,\psi(\vec r)\,\delta(\vec r_j - \vec r') + \psi^+(\vec r')\,\psi(\vec r')\,\psi(\vec r_j)\,\delta(\vec r_j - \vec r)$$

$$= \varrho(\vec r)\,\psi(\vec r_j)\,\delta(\vec r_j - \vec r') + \varrho(\vec r')\,\psi(\vec r_j)\,\delta(\vec r_j - \vec r)$$

$$\psi(\vec r_j)\,\varrho(\vec r) = \pm\,\psi(\vec r)\,\psi(\vec r_j)$$

$$\Rightarrow \langle 0|\,\psi(\vec r_n)\cdots[\psi(\vec r_j), D]\,\psi(\vec r_{j-1})\cdots\psi(\vec r_1)$$

$$= \langle \vec r_n \cdots \vec r_{j+1}|\left(\varrho(\vec r)\,\delta(\vec r_j - \vec r') + \varrho(\vec r')\,\delta(\vec r_j - \vec r)\right)\psi(\vec r_j)\cdots\psi(\vec r_1)$$

$$= \langle \vec r_n \cdots \vec r_1|\sum_{k=j+1}^{n}\left(\delta(\vec r - \vec r_k)\,\delta(\vec r' - \vec r_j) + \delta(\vec r' - \vec r_k)\,\delta(\vec r - \vec r_j)\right)$$

page 17

$$\Rightarrow \langle \vec r_1, \dots, \vec r_n|\,\psi^+(r)\,\psi^+(\vec r')\,\psi(\vec r')\,\psi(\vec r)$$

$$= \sum_{j=1}^{n}\sum_{k=j+1}^{n}\left(\delta(\vec r - \vec r_k)\,\delta(\vec r' - \vec r_j) + \delta(\vec r' - \vec r_k)\,\delta(\vec r - \vec r_j)\right)\langle \vec r_1, \dots, \vec r_n|$$

$$\Rightarrow \langle \vec{r}_1, \ldots, \vec{r}_N | \frac{1}{2} \int d^3r\, d^3r'\, \rho^+(\vec{r})\, \rho^+(\vec{r}')\, V_2(\vec{r}, \vec{r}')\, \rho(\vec{r}')\, \rho(\vec{r})\, | \psi \rangle$$

$$= \underbrace{\sum_{j=1}^{n} \sum_{k=j+1}^{n}}_{\sum_{\substack{j,k \\ k>j}}} \underbrace{\frac{1}{2} \left(V_2(\vec{r}_k, \vec{r}_j) + V_2(\vec{r}_j, \vec{r}_k) \right)}_{= V_2(\vec{r}_j, \vec{r}_k)} \langle \vec{r}_1, \ldots, \vec{r}_n | \psi \rangle$$

$\rightsquigarrow$ sum of all potential energies (without double counting) as it should be

c) time evolution

So far we have not displayed the time dependence.
In the Heisenberg picture we have (cf. page 22)

$$-i\hbar \frac{d}{dt} | \vec{r}_1, \ldots, \vec{r}_n ; t \rangle = H | \vec{r}_1, \ldots, \vec{r}_n ; t \rangle$$

since $H|0\rangle = 0$ we have $\frac{d}{dt}|0;t\rangle = 0$,

i.e. the vacuum state is time independent and we can just write $|0\rangle$

$\Rightarrow$ rules for calculation:

$$\langle 0 | 0 \rangle = 1$$

$$| \vec{r}_1, \ldots, \vec{r}_n ; t \rangle = \rho^+(\vec{r}_1, t)\, \rho^+(\vec{r}_2, t) \cdots \rho^+(\vec{r}_n, t)\, |0\rangle$$

$$\rho(\vec{r}, t) |0\rangle = 0$$

$$[\rho(\vec{r}, t), \rho(\vec{r}', t)]_{\mp} = 0 = [\rho^+(\vec{r}, t), \rho^+(\vec{r}', t)]_{\mp}$$

$$[\rho(\vec{r}, t), \rho^+(\vec{r}', t)]_{\mp} = \delta(\vec{r} - \vec{r}')$$

note: same time argument

For operators the time evolution is given by

$$\hbar i \frac{d}{dt} O(t) = [O(t), H(t)]$$

important example:

take $H = \int d^3r' \, \psi^+(\vec{r}', t)\left(-\frac{\hbar^2 \Delta}{2m} + V_1(\vec{r}')\right) \psi(\vec{r}', t)$

and study time differential equation for annihilation operator $\psi(\vec{r}, t)$

we already know (page 19)

$$[H(t), \psi^+(\vec{r}, t)] = \left(-\frac{\hbar^2 \Delta}{2m} + V_1(\vec{r})\right) \psi^+(\vec{r}, t)$$

$$\Rightarrow [\psi(\vec{r}, t), H(t)] = \left(-\frac{\hbar^2 \Delta}{2m} + V_1(\vec{r})\right) \psi(\vec{r}, t)$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left(-\frac{\hbar^2 \Delta}{2m} + V_1(\vec{r})\right) \psi(\vec{r}, t) \qquad (*)$$

This looks like the Schrödinger equation, but it is NOT !!!

The object which appears in the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left(-\frac{\hbar^2 \Delta}{2m} + V_1(\vec{r})\right) \psi(\vec{r}, t)$$

is the number-valued (coordinate-space) wave function for a single-particle system.

The object which appears in $(*)$ is an operator in Fock space (for a system of particles which only interact with an external potential).

Later we will learn about relativistic generalizations of $(*)$. Historically they were <u>misinterpreted</u> as generalizations of the Schrödinger equation.