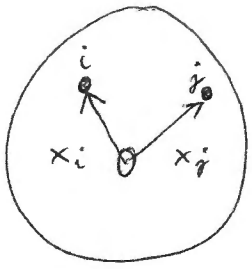
2) Identical particles

Gordon Baym, QM, ch. 18

Elementary particles (e^-, p, n, ...) are <u>identical</u>. In classical physics, the identity of particles leads only to fairly trivial modifications (same mass, charge, etc.), but <u>in QM</u> it has <u>profound consequences</u>, as we will show.



For identical particles, the many-body Hamiltonian must be invariant under the exchange of any two particle coordinates x_i and x_j, i.e.

<u>Suggestion: check Hatom</u>

$$\boxed{H(\dots, x_i, \dots, x_j, \dots) = H(\dots, x_j, \dots, x_i, \dots)} \quad (1)$$

We define the exchange operator for the particle coordinates

$$\boxed{P_{ij} =: \quad x_i \leftrightarrow x_j} \quad (2)$$

and consider the foll. expression

$$\left.\begin{aligned} P_{ij}\, H(\dots, x_i, \dots, x_j, \dots)\, \psi(\dots, x_i, \dots, x_j, \dots) &\overset{\text{def}}{=} \\ = H(\dots, x_j, \dots, x_i, \dots)\, \psi(\dots, x_j, \dots, x_i, \dots) & \\ \| \text{eq.(1)} \qquad\qquad \| \text{eq.(2)} & \\ = H(\dots, x_i, \dots, x_j, \dots)\, P_{ij}\, \psi(\dots, x_i, \dots, x_j, \dots) & \end{aligned}\right\} \quad (3)$$

From eq. (3) we conclude

$$P_{ij} H \psi - H P_{ij} \psi = 0 \quad \Rightarrow \quad \boxed{[P_{ij}, H] = 0} \quad (4)$$

Eq. (4) states that it is possible to construct simultaneous eigenfunctions of the operators P_{ij} and H, i.e.

$$\left.\begin{aligned} P_{ij}\,\psi_{p,E} &= p\,\psi_{p,E} \\ H\,\psi_{p,E} &= E\,\psi_{p,E} \end{aligned}\right\} \quad (5)$$

Theorem: The eigenvalues of P_{ij} are $p = \pm 1$

Proof: $\psi = P_{ij}^2\,\psi = p^2\,\psi \Rightarrow p^2 = 1 \Rightarrow p = \pm 1$
($P_{ij}^2 = 1$)

Definition: boson ($p = +1$ & totally sym. WF)

In the case $p = +1$, we have from (5)

$$P_{ij}\,\psi_{p=+1,E}(\ldots, x_i, \ldots, x_j, \ldots) \overset{\text{def}}{=} \psi_{p=+1,E}(\ldots, x_j, \ldots, x_i, \ldots)$$
$$= (+1)\cdot\psi_{p=+1,E}(\ldots x_i \ldots, x_j, \ldots) \quad (6)$$

i.e. the many-body WF is totally sym. under exchange $x_i \leftrightarrow x_j$.

Def: fermion ($p = -1$ & totally antisym. WF)

In the case $p = -1$, we have from (5)

$$P_{ij}\,\psi_{p=-1,E}(\ldots, x_i, \ldots, x_j, \ldots) \overset{\text{def}}{=} \psi_{p=-1,E}(\ldots, x_j, \ldots, x_i, \ldots)$$
$$= (-1)\cdot\psi_{p=-1,E}(\ldots, x_i, \ldots, x_j, \ldots) \quad (7)$$

i.e. the many-body WF is totally antisymmetric under the $x_i \leftrightarrow x_j$ exchange.

Note: Eq. (5) shows that there exist solutions with definite $p=+1$ or $p=-1$, but the most general solution could be a superposition of the form

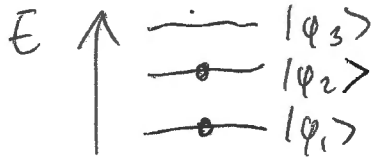
$$\psi = a\,\psi_{p=+1} + b\,\psi_{p=-1}\,.$$

However, by comparison of many-body quantum theory with experiment one finds:

> The quantum many-body WF is always either totally symmetric (bosons) or totally anti-symmetric (fermions)

Simple illustrations: bosonic / fermionic few-particle systems (2-3 particles)

a) 2 bosons in s.p. states $|\varphi_1\rangle, |\varphi_2\rangle$

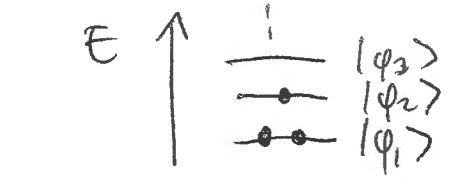


The WF

$$\psi_S(x_1,x_2) = \frac{1}{\sqrt{2}}\left(\varphi_1(x_1)\varphi_2(x_2) + \varphi_1(x_2)\varphi_2(x_1)\right)$$

is obviously symmetric under the interchange $P_{12}: x_1 \leftrightarrow x_2$.

b) 3 bosons



2 bosons in state $|\varphi_1\rangle$,

1 boson in state $|\varphi_2\rangle$.

This situation is described by the state vector

$$\psi(x_1,x_2,x_3) = \mathcal{N}\ \varphi_1(x_1)\,\varphi_1(x_2)\,\varphi_2(x_3)$$

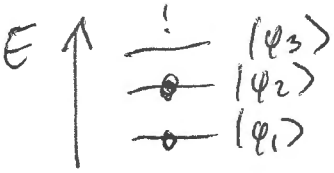
Using a cyclic permutation of the coordinates

$$(x_1,x_2,x_3) \to (x_2,x_3,x_1) \to (x_3,x_1,x_2)$$

we can generate the totally symmetric WF (see Fetter/Walecka p. 9)

$$\psi_S(x_1,x_2,x_3) = \frac{1}{\sqrt{3}}\Big(\varphi_1(x_1)\,\varphi_1(x_2)\,\varphi_2(x_3) + \varphi_1(x_2)\,\varphi_1(x_3)\,\varphi_2(x_1) + \varphi_1(x_3)\,\varphi_1(x_1)\,\varphi_2(x_2)\Big).$$

c) 2 fermions in s.p. states $|\varphi_1\rangle, |\varphi_2\rangle$



The following WF is obviously anti-sym. under the coordinate interchange

$$P_{12}: x_1 \Leftrightarrow x_2:$$

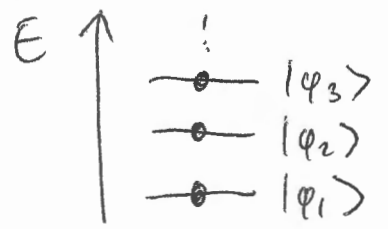
$$\boxed{\psi_a(x_1,x_2) = \frac{1}{\sqrt{2}}\Big(\varphi_1(x_1)\,\varphi_2(x_2) - \varphi_1(x_2)\,\varphi_2(x_1)\Big)}$$

Proof: $P_{12}\,\psi_a(x_1,x_2) \overset{\text{def}}{=} \psi_a(x_2,x_1) = \frac{1}{\sqrt{2}}\Big(\varphi_1(x_2)\,\varphi_2(x_1) - \varphi_1(x_1)\,\varphi_2(x_2)\Big) = -\psi_a(x_1,x_2).$

Note that we can write $\psi_a(x_1,x_2)$ in form of a "Slater determinant":

$$\boxed{\psi_a(x_1,x_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \varphi_1(x_1) & \varphi_1(x_2) \\ \varphi_2(x_1) & \varphi_2(x_2) \end{vmatrix}}$$

d) 3 fermions



The Slater determinant

$$\psi_a(x_1,x_2,x_3) = \frac{1}{\sqrt{3!}} \begin{vmatrix} \varphi_1(x_1) & \varphi_1(x_2) & \varphi_1(x_3) \\ \varphi_2(x_1) & \varphi_2(x_2) & \varphi_2(x_3) \\ \varphi_3(x_1) & \varphi_3(x_2) & \varphi_3(x_3) \end{vmatrix}$$

has the desired properties: for example, if we apply $P_{ij}: x_i \leftrightarrow x_j$, we interchange 2 columns of the determinant, and the determinant changes its sign! Note: Pauli exclusion principle is also included: if $\varphi_i = \varphi_j$ 2 determinat vanishes (2 identical rows).

Spin-statistic theorem (W. Pauli, 1940)

a) particles with spins $S = 0, 1, 2, \ldots$ are bosons, i.e. WF is totally symmetric ($p=+1$).

examples: photon ($S=1$), $W^{\pm}/Z^0$ ($S=1$), gluons ($S=1$), graviton ($S=2$), pion ($S=0$), ...

b) particles with spins $S = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$ are fermions, i.e. WF is totally anti-symmetric ($p=-1$).

examples: all leptons, in particular electron ($S=\frac{1}{2}$)
all quarks ($S=\frac{1}{2}$)
all baryons ($S=\frac{1}{2}, \frac{3}{2}, \ldots$), in particular proton and neutron ($S=\frac{1}{2}$).

Note: a formal proof of this theorem requires quantum field theory (see e.g. Itzykson & Zuber, QFT, p. 149).

Non-interacting systems (one-body Hamiltonians): total energy and many-body WF in coord. space

a) non-interacting (free) Fermi gas, e.g. electron gas

Ref: Fetter & Walecka, p. 21

The Hamiltonian of the system is simply the sum of all kinetic energy operators

$$H = T = \sum_{i=1}^{N} T_i = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla_i^2 \right) \overset{def}{=} \sum_{i=1}^{N} h^{(1)}(\vec{r}_i)$$

$\Rightarrow$ H is a one-body operator.

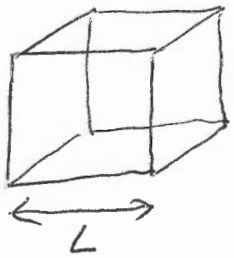
The s.p. problem can easily be solved analytically:

The eigenfunctions of $h^{(1)}(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2$ are, of course, plane wave states with def. momentum $\vec{p} = \hbar\vec{k}$:

$$-\frac{\hbar^2}{2m}\nabla^2 \varphi_{\vec{k}}(\vec{r}) = E_{\vec{k}}\, \varphi_{\vec{k}}(\vec{r})$$

with

$$\varphi_{\vec{k}}(\vec{r}) = \frac{1}{L^{3/2}} e^{i\vec{k}\cdot\vec{r}}$$



Using periodic boundary conditions in a box of length L in (x,y,z) yields the discrete momenta / wave numbers

$$\vec{k} = (k_x, k_y, k_z) = \frac{2\pi}{L}(n_x, n_y, n_z)$$

with $n_i = 0, \pm 1, \pm 2, \ldots$

$\Rightarrow$ $\boxed{E_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}}$

The Hamiltonian in this simple case is spin-indep., but the s.p. WF contains the spin-info via a spinor:

free Fermi gas eigenfunctions

$$h^{(1)}(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2$$

$$h^{(1)}(\vec{r})\,\varphi_{\vec{k},s_z}(\vec{r}) = E_{\vec{k}}\,\varphi_{\vec{k},s_z}(\vec{r})$$

$$\varphi_{\vec{k},s_z}(\vec{r}) = \underbrace{\frac{1}{L^{3/2}} e^{i\vec{k}\cdot\vec{r}}}_{\text{space}}\ \underbrace{\chi^{s=\frac{1}{2}}_{s_z}}_{\text{spinor}}$$

with the $s=\frac{1}{2}$ spinors

$$\chi^{s=\frac{1}{2}}_{s_z=+\frac{1}{2}} = \begin{pmatrix}1\\0\end{pmatrix}, \qquad \chi^{s=\frac{1}{2}}_{s_z=-\frac{1}{2}} = \begin{pmatrix}0\\1\end{pmatrix}.$$

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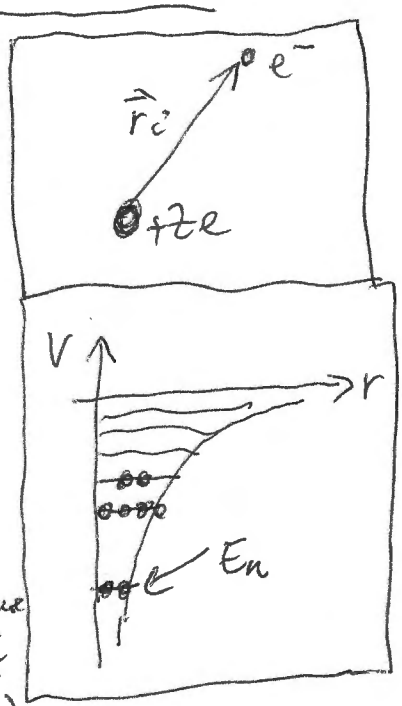
b) N-electron atom (without e^-e^- interaction)

$$H = \sum_{i=1}^{N} \underbrace{\left(-\frac{\hbar^2}{2m_e}\nabla_i^2 - \frac{Ze^2}{|\vec{r}_i|}\right)}_{= h^{(1)}(\vec{r}_i)}$$



The s.p. problem has the solution

$$h^{(1)}(\vec{r})\,\varphi_{n,l,m_e,s_z}(\vec{r}) = E_n\,\varphi_{n,l,m_e,s_z}(\vec{r})$$

with $E_n = -(m_e c^2)\frac{1}{2}\left(\frac{Z\alpha}{n}\right)^2$ fine structure constant α

and (in "product basis" = uncoupled repr.)

$$\varphi_{n,l,m_e,s_z}(r,\theta,\varphi) = R_{nl}(r)\,Y_{lm_e}(\theta,\varphi)\,\chi^{s=\frac{1}{2}}_{s_z}.$$

If we couple orbital ang. mom. (l, m_l) and spin $(s=\frac{1}{2}, s_z)$ to good total ang. momentum (j, m_j), we can write

$$\varphi_{n,l,j,m_j}(r,\theta,\varphi) = R_{nl}(r) \sum_{m_l, s_z} \underbrace{\left(l\,\tfrac{1}{2}\,j \,|\, m_l\, s_z\, m_j\right)}_{\text{Clebsch-Gordan}} Y_{l m_l}(\theta,\varphi) \times \chi^{s=\frac{1}{2}}_{s_z}$$

The radial WF's $R_{nl}(r)$ are obtained from the 1-D differential equation for the external potential $V(r) = \frac{-Ze^2}{r}$.

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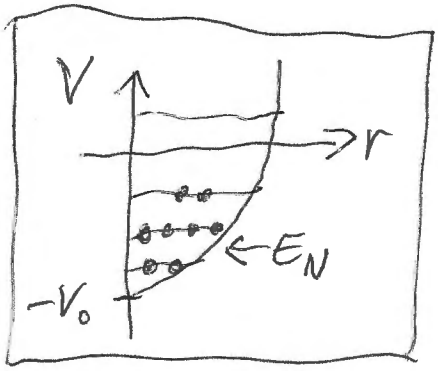
c) Nuclear shell model (3-D harmonic oscillator)

$$H = \sum_{i=1}^{N} \underbrace{\left(-\frac{\hbar^2}{2m_N}\nabla_i^2 + \frac{1}{2}m_N\omega^2 \vec{r}_i^{\,2}\right)}_{= h^{(1)}(\vec{r}_i)}$$



The s.p. solution has the same structure as in the atomic case, but with the energies of 3-D oscillator

$$E_N = -V_0 + \hbar\omega\left(N + \frac{3}{2}\right) \text{ with } \begin{cases} N = 2(n-1)+l \\ n = 1, 2, 3, \ldots \\ l = 0, 1, 2, \ldots \end{cases}$$

The WF's look the same, except that we have different radial functions $f_{nl}(r)$, which have to be determined from 1-D differential equation for the 3-D oscillator potential $V(r) = \frac{1}{2}m_N\omega^2 r^2$.

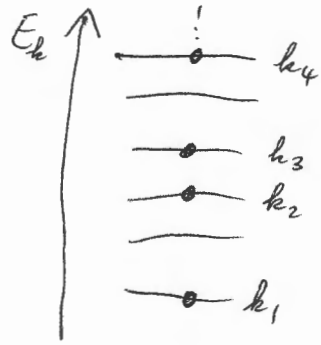
Based on these 3 examples, we now give a general solution for the one-body Hamiltonian problem:

Theorem: Given is a many-body quantum system described by a one-body Hamiltonian

$$H^{(1)} = \sum_{i=1}^{N} h^{(1)}(x_i).$$

Suppose, the single-particle problem has been solved, i.e. we have

$$h^{(1)}(x)\,\varphi_k(x) = E_k\,\varphi_k(x).$$



In this case, the total energy of the system is given by

$$E = \sum_{i=1}^{N} E_{k_i}$$

where $(k_1, k_2, \ldots, k_N)$ are the occupied s.p. states.

The many-body WF, i.e. soln of Schrödinger eq.

$$H^{(1)}\,\psi(x_1, x_2, \ldots, x_N) = E\,\psi(x_1, x_2, \ldots, x_N)$$

has the foll. structure:

a) for distinguishable particles

$$\psi(x_1, x_2, \ldots, x_N) = \varphi_{k_1}(x_1)\,\varphi_{k_2}(x_2) \cdots \varphi_{k_N}(x_N)$$

i.e. product of s.p. WF's

b) for fermions / bosons

$$\psi(x_1, x_2, \ldots, x_N) = \hat{A}\,[\varphi_{k_1}(x_1)\,\varphi_{k_2}(x_2) \cdots \varphi_{k_N}(x_N)]$$

($\hat{A}$: ↓ antisym. (particle exchange); ↑ symmetriser)

i.e. (anti-) sym. product of s.p. WF's

We now prove the theorem for case a). The proof for b) is similar, but involves more writing:

Proof: $H^{(1)}\psi(x_1,x_2,\dots,x_N) = \sum_{i=1}^{N} h^{(1)}(x_i)\,[\varphi_{k_1}(x_1)\cdots\varphi_{k_i}(x_i)\cdots$

$$\cdots\varphi_{k_N}(x_N)] = \sum_{i=1}^{N}[\varphi_{k_1}\cdots\varphi_{k_{i-1}}\varphi_{k_{i+1}}\cdots\varphi_{k_N}]\,\underbrace{h^{(1)}(x_i)\varphi_{k_i}(x_i)}_{=E_{k_i}\varphi_{k_i}(x_i)}$$

$$= \sum_{i=1}^{N} E_{k_i}\underbrace{[\varphi_{k_1}\cdots\varphi_{k_N}]}_{=\psi(x_1,\dots,x_N)} = \underbrace{\left(\sum_{i=1}^{N}E_{k_i}\right)}_{=E}\psi(x_1,\dots,x_N).$$

q.e.d.

Let's now write down the antisym. WF for fermions. It has the structure

$$\psi(x_1,\dots,x_N) = \frac{1}{\sqrt{N!}}\sum_{\nu}\overbrace{(-1)^{\nu}\hat{P}_{\nu}}^{=\hat{A}=\text{antisym. op.}}[\varphi_{k_1}(x_1)\varphi_{k_2}(x_2)\cdots\varphi_{k_N}(x_N)]$$

where the permutation operator $\hat{P}_\nu$ carries out an arbitrary permutation of the indices $(1,2,\dots,N)$. The sign $(-1)^\nu$ is $(+1)$ for even permutations and (-1) for odd permutations. From the theory of determinants one infers that the above many-body WF can be written in form of a "Slater determinant"

$$\psi(x_1,\dots,x_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \varphi_{k_1}(x_1) & \varphi_{k_1}(x_2) & \cdots & \varphi_{k_1}(x_N) \\ \varphi_{k_2}(x_1) & \varphi_{k_2}(x_2) & \cdots & \varphi_{k_2}(x_N) \\ \vdots & \vdots & & \vdots \\ \varphi_{k_N}(x_1) & \varphi_{k_N}(x_2) & \cdots & \varphi_{k_N}(x_N) \end{vmatrix}$$

↑ for fermions

From the theory of determinants we know:

a) det changes sign, if any two columns (say, i and j) are interchanged. For Slater det., this corresponds to the antisymmetry under coord. exch. operation $\hat{P}_{ij}$: $x_i \leftrightarrow x_j$.

b) det. changes sign also, if any two rows are interchanged. As a special case of this, if any two rows are equal, det = 0. For Slater det., the row index characterizes the s.p. quantum states, say φ_i and φ_j. $\Rightarrow$

> We have proven the Pauli principle for one-body Hamiltonians: if any two occupied s.p. states φ_i and φ_j have the same quantum numbers, the many-body WF vanishes, i.e. it cannot be normalized $\Rightarrow$ ψ does not exist.

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3. "Second quantization" / occupation # representation

From now on, we will discuss only interacting fermions (think of $s = \frac{1}{2}$ electrons in atoms, molecules, condensed matter). As we said, the Slater det. consists of s.p. WF's

$$\varphi_i(x) = \langle x | i \rangle$$

and the Pauli principle tells us that the only allowed particles numbers are

$$\text{or} \begin{cases} n_i = 1 & \text{(occupied)} \\ n_i = 0 & \text{(unoccupied).} \end{cases}$$

To avoid confusion, we clarify that the kets $|i\rangle \equiv |\varphi_i\rangle$

are a shorthand notation for <u>all</u> s.p. quantum numbers.

<u>Examples:</u>

- <u>N-electron atom</u>: using the "product basis" representation we have

$$|i\rangle \equiv |\varphi_i\rangle = |n, \ell, m_\ell; s=\tfrac{1}{2}, m_s\rangle$$

with the s.p. WF's:

$$\varphi_i(x) = \langle x|i\rangle = \varphi_{n\ell m_\ell;\, s=\frac{1}{2}, m_s}(\vec{r}, s_z) =$$

$$= R_{n\ell}(r)\, Y_{\ell, m_\ell}(\theta,\varphi)\, \chi^{s=1/2}_{m_s} \quad \leftarrow \text{spinor}, \begin{pmatrix}1\\0\end{pmatrix} \text{or} \begin{pmatrix}0\\1\end{pmatrix}$$

- <u>Electrons in a metal</u> (momentum $\vec{p} = \hbar\vec{k}$):

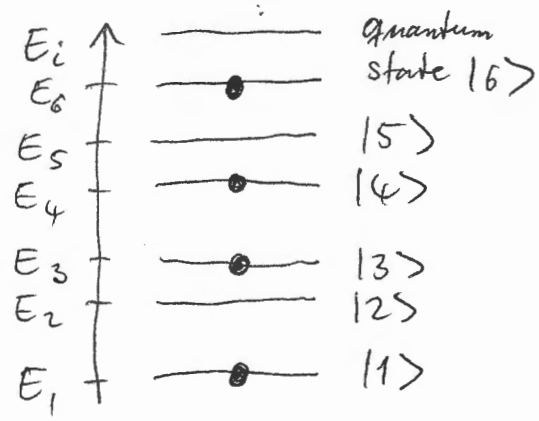
$|i\rangle \equiv |\varphi_i\rangle = |\vec{k}\rangle \otimes |s=\tfrac{1}{2}, m_s\rangle$ with s.p. WF's:

$$\varphi_i(x) = \langle x|i\rangle = \underbrace{L^{-3/2} e^{i\vec{k}\cdot\vec{r}}}_{\text{space}} \underbrace{\chi^{s=\frac{1}{2}}_{m_s}}_{\text{spinor}}$$

Let us now consider a <u>model system</u> with s.p. energies

$$E_1 < E_2 < E_3 < \ldots < E_N < E_{N+1} \ldots$$

Suppose now (see figure) that the levels # 1, 3, 4 and 6 are filled with identical fermions, and all other s.p. levels are unfilled.



The corresponding Slater determinant has the structure:

$$\Psi_{n_1=1,n_2=0,n_3=1,n_4=1,n_5=0,n_6=1,n_{\geq 7}=0}(x_1,x_2,x_3,x_4) =$$

$$= \frac{1}{\sqrt{4!}} \begin{vmatrix} \varphi_1(x_1) & \varphi_1(x_2) & \varphi_1(x_3) & \varphi_1(x_4) \\ \varphi_3(x_1) & \varphi_3(x_2) & \varphi_3(x_3) & \varphi_3(x_4) \\ \varphi_4(x_1) & \varphi_4(x_2) & \varphi_4(x_3) & \varphi_4(x_4) \\ \varphi_6(x_1) & \varphi_6(x_2) & \varphi_6(x_3) & \varphi_6(x_4) \end{vmatrix}$$

Clearly, this complicated structure in coordinate space is a reflection of the fact that all 4 fermions are identical and we can't really say which fermion is in what quantum state. We may say that the inefficiency of the coord.-space repr. lies in the fact that we first label the particles and then effectively "unlabel" them via imposing the exchange antisymmetry! There must be a more efficient representation.

Occupation # representation

Ref: Fetter & Walecka, ch. 1

A little bit of thought reveals that all we need to specify for identical fermions is

a) the s.p. states $|i\rangle \equiv |\varphi_i\rangle$ and their occupation number n_i (0 or 1) and $N = \sum_i n_i$

b) we must satisfy the Pauli principle for fermions.

This suggests that one should work in occ. number space

and introduce fermion creation and annihilation operators $(\hat{c}_i^+, \hat{c}_i)$ for the quantum states $|i\rangle \equiv |\varphi_i\rangle$.

$\Rightarrow$ Slater det. in occupation # space

$$|\phi\rangle = \hat{c}_1^+ \hat{c}_3^+ \hat{c}_4^+ \hat{c}_6^+ |0\rangle$$

- $|\phi\rangle$: many-particle state vector
- $\hat{c}_1^+ \hat{c}_3^+ \hat{c}_4^+ \hat{c}_6^+$: fermion creation operators
- $|0\rangle$: vacuum

This appears to make sense (compare to fig. on p. 12). But how do we take care of the Pauli principle? First recall the commutation relations, introduced by Paul Dirac, for the 1-D harmonic oscillator (spin zero $\Rightarrow$ bosons):

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \quad \text{(def. of commutator)}$$

$$[\hat{a}, \hat{a}^+] = \hat{a}\hat{a}^+ - \hat{a}^+\hat{a} = 1.$$

In 1928, Jordan and Wigner showed that the Pauli principle for fermions can be incorporated by requiring anti-commutation relations for the $\hat{c}_i$ and $\hat{c}_j^+$:

define anticommutator $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$

with the requirements

$$\{\hat{c}_i, \hat{c}_j\} = 0, \quad \{\hat{c}_i^+, \hat{c}_j^+\} = 0, \quad \{\hat{c}_i, \hat{c}_j^+\} = \delta_{ij} \qquad (*)$$

Again, let us clarify the shorthand notation with an

example, using an N-electron atom:

$$\{\hat{c}_i, \hat{c}_j^+\} = 0 \iff \{\hat{c}_{n\ell m_\ell m_s}, \hat{c}^+_{n'\ell' m_\ell' m_s'}\} = 0$$

Consequences of anticommutation relations (*):

① Pauli principle is contained, because for $j = i$

$$0 = \{\hat{c}_i^+, \hat{c}_i^+\} \overset{\text{def}}{=} c_i^+ c_i^+ + c_i^+ c_i^+ = 2\, c_i^+ c_i^+ \Rightarrow c_i^+ c_i^+ = 0$$

$$\Rightarrow \boxed{\hat{c}_i^+ \hat{c}_i^+ |0\rangle = 0}$$ ↝ no 2 fermions in same quantum state $|i\rangle \equiv |\varphi_i\rangle$.

② The number of fermions n_i in a given quantum state $|i\rangle$ is either zero or one (note: unrestricted for bosons)

Proof: We define the fermion number operator in state $|i\rangle$:

$$\boxed{\hat{n}_i = \hat{c}_i^+ \hat{c}_i}$$ (same as for bosons!)

and constant eigenstates $\hat{n}_i |n_i\rangle = n_i |n_i\rangle$.

$\hat{n}_i = \hat{c}_i^+ \hat{c}_i =$ anticom. rel. $= 1 - \hat{c}_i \hat{c}_i^+$, take square of this eq.

$$\boxed{\hat{n}_i^2} = (\hat{c}_i^+ \hat{c}_i)^2 = (1 - \hat{c}_i \hat{c}_i^+)^2 = 1 - 2\hat{c}_i \hat{c}_i^+ + \hat{c}_i (\hat{c}_i^+ \hat{c}_i) \hat{c}_i^+ =$$

$$= 1 - 2\hat{c}_i \hat{c}_i^+ + \hat{c}_i (1 - \hat{c}_i \hat{c}_i^+) \hat{c}_i^+ = 1 - 2\hat{c}_i \hat{c}_i^+ + \hat{c}_i \hat{c}_i^+ -$$

$$- \hat{c}_i^2 (\hat{c}_i^+)^2 = 1 - \hat{c}_i \hat{c}_i^+ = \text{see above} = \hat{c}_i^+ \hat{c}_i = \boxed{\hat{n}_i}$$

($\hat{c}_i^2 = 0$, $(\hat{c}_i^+)^2 = 0$)

$$\Rightarrow \hat{n}_i^2 = \hat{n}_i \quad \text{or} \quad \hat{n}_i^2 - \hat{n}_i = 0 \Rightarrow \hat{n}_i (\hat{n}_i - 1) = 0$$

Apply this to $\hat{n}_i$-eigenstates

$$\hat{n}_i (\hat{n}_i - 1) |n_i\rangle = 0 \Rightarrow \underbrace{n_i (n_i - 1)}_{\text{eigenvalues}} |n_i\rangle = 0 \Rightarrow \boxed{n_i = 0 \text{ or } 1}$$ q.e.d.

Furthermore, from the anticom. relations of $\hat{c}_i, \hat{c}_j^+$ and the properties of the fermion number operators $\hat{n}_i$ one can prove:

(3) $\boxed{\hat{c}_i |0\rangle = 0} \Rightarrow \hat{c}_i^+ \hat{c}_i |0\rangle = 0 \Rightarrow \hat{n}_i |0\rangle = 0$

i.e. $|0\rangle$ is the fermion vacuum state (no real particles).

(4) Properties of the $\boxed{\text{one-particle state } |n_i = 1\rangle = \hat{c}_i^+ |0\rangle}$:

$\Rightarrow \hat{c}_i |n_i = 1\rangle = \hat{c}_i \hat{c}_i^+ |0\rangle = (1 - \hat{c}_i^+ \hat{c}_i)|0\rangle = |0\rangle$

$\Rightarrow \hat{c}_i^+ |n_i = 1\rangle = (\hat{c}_i^+)^2 |0\rangle = \text{Pauli!} = 0$ (state does not exist!)

($(\hat{c}_i^+)^2 |0\rangle = 0$)

(5) One can show that for arbitrary s.p. states $|i\rangle$ and $|j\rangle$

$$[\hat{n}_i, \hat{n}_j] = 0$$

$\Rightarrow$ we can construct simultaneous eigenstates of all number operators:

$$|n_1, n_2, \ldots n_j, \ldots, n_\infty\rangle \overset{\text{def}}{=} |n_1\rangle |n_2\rangle \cdots |n_j\rangle \cdots |n_\infty\rangle$$

with the property

$$\hat{n}_j |n_1, n_2, \ldots, n_j, \ldots, n_\infty\rangle = n_j |n_1, n_2, \ldots, n_\infty\rangle$$

Using the one-particle states $|n_i\rangle = \hat{c}_i^+ |0\rangle$, we can express the many-particle state vectors in the form ($N = \sum_{i=1}^{\infty} n_i$ fermions):

$$\boxed{|\Phi\rangle = |n_1, n_2, \ldots, n_\infty\rangle = (\hat{c}_1^+)^{n_1} (\hat{c}_2^+)^{n_2} \cdots (\hat{c}_\infty^+)^{n_\infty} |0\rangle}$$

with $n_i = 0$ or 1

In summary, the creation/annihilation operators in occupation number space obey anticommutation relations which incorporate the Pauli principle ($n_i = 0$ or $n_i = 1$).

In what follows, we will show that this representation in "Fock space" is far more efficient than the coordinate-space representation, because it avoids "labeling" of identical particles by product WF and then the effective "unlabeling" via anti-symmetry operator, because the particles are, after all identical.

In Fock space, all one needs to specify is a given set of single particle states $|\varphi_i\rangle$ with WFs $\varphi_i(x) = \langle x|\varphi_i\rangle$ and the associated occupation numbers $n_i = 0$ or $n_i = 1$.

Relation between occupation # space and coordinate space

References: 1) Bohr & Mottelson, Nuclear Structure, vol. 1, p. 272 - 278

2) Blaizot & Ripka, ch. 1

1. Single-particle basis

One introduces s.p. basis states $|i\rangle \equiv |\varphi_i\rangle$ which are assumed to be

- orthonormal : $\langle \varphi_i | \varphi_j \rangle = \delta_{ij}$
- complete : $\sum_{i=1}^{\infty} |\varphi_i\rangle\langle\varphi_i| = 1$

This is usually accomplished by using the eigenstates of a s.p. Hamiltonian

$$h_{s.p.}(x)\, \varphi_i(x) = E_i\, \varphi_i(x)$$

where

$$\varphi_i(x) = \langle x | \varphi_i \rangle \equiv \langle x | i \rangle$$

The quantity x is a shorthand notation for all coordinates, e.g.

$$x = (\vec{r}\ ;\ s=\tfrac{1}{2}, s_z\ ;\ t=\tfrac{1}{2}, t_z)$$

position; spin; isospin [for some elem. particles]

2. Creation/annih. operators for quantum states $|i\rangle$

We have already introduced creation/annih. operators for s.p. quantum states $|i\rangle$, such as

$$\hat{c}_i,\ \hat{c}_i^{+} \xrightarrow[\text{atom}]{} \hat{c}_{n\ell m_\ell m_s},\ \hat{c}^{+}_{n\ell m_\ell m_s}.$$

If we introduce creation/annih. operators (in a generic way, without referring to any repr.)

$$\hat{c},\ \hat{c}^+$$

then we can re-interpret the $\hat{c}_i,\ \hat{c}_i^+$ as projections of $\hat{c},\hat{c}^+$ onto the s.p. basis states, i.e.

$$\boxed{\hat{c}_i \overset{\text{def}}{=} \langle i|\hat{c}\rangle \quad \text{and} \quad \hat{c}_i^+ = \langle i|\hat{c}^+\rangle}$$

s.p. state in occ. # repr: $|i\rangle = \hat{c}_i^+|0\rangle$

N-particle state (fermions): $|k_1, k_2, \ldots, k_N\rangle_a = \hat{c}_{k_1}^+ \hat{c}_{k_2}^+ \cdots \hat{c}_{k_N}^+ |0\rangle$ (antisymm.)

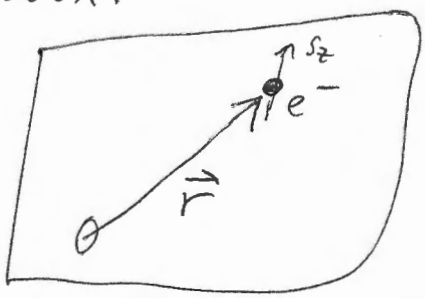
3. Quantum field operators ≡ creation/annih. operators in coord. space

We define the operators

$$\boxed{\hat{c}^+(x) \overset{\text{def}}{=} \langle x|\hat{c}^+\rangle} \quad \text{and} \quad \boxed{\hat{c}(x) = \langle x|\hat{c}\rangle}$$

which create/annih. particles at coord. x.

Important example:



For an electron, we have

$$\hat{c}^+(x) \to \hat{c}^+(\vec{r}; s=\tfrac{1}{2}, s_z)$$

which creates an electron at position $\vec{r}$ with spin proj. s_z

Similarly, the operator

$$\hat{c}(x) \to \hat{c}(\vec{r}; s=\tfrac{1}{2}, s_z)$$

destroys an electron at position $\vec{r}$ with spin proj. s_z.

one particle at x_1 : $|x_1\rangle = \hat{c}^+(x_1)|0\rangle$

N-particle state (x-repr.) : $|x_1, x_2, \dots, x_N\rangle = \hat{c}^+(x_1)\hat{c}^+(x_2)\dots\hat{c}^+(x_N)|0\rangle$

Important: relation between $\hat{c}^+(x), \hat{c}(x)$ and $\hat{c}_i^+, \hat{c}_i$

This relation can be obtained by inserting the completeness relation ($\sum_{i=1}^{\infty} |i\rangle\langle i| = 1$):

$$\hat{c}(x) = \langle x|\hat{c}\rangle = \sum_{i=1}^{\infty} \langle x|i\rangle\langle i|\hat{c}\rangle = \sum_{i=1}^{\infty} \varphi_i(x)\,\hat{c}_i \quad , \text{ i.e.}$$

$$\boxed{\hat{c}(x) = \sum_{i=1}^{\infty} \hat{c}_i\, \varphi_i(x)}$$

$\hat{c}(x)$: field annih.-op. ; $\hat{c}_i$: annihilation op. for state $|i\rangle$; $\varphi_i(x)$: s.p. WF's (basis)

By taking the adjoint, we find

$$\boxed{\hat{c}^+(x) = \sum_{i=1}^{\infty} \hat{c}_i^+\, \varphi_i^+(x)}$$

$\hat{c}^+(x)$: field creation op. ; $\hat{c}_i^+$: creation op. for state $|i\rangle$; $\varphi_i^+(x)$: s.p. WF's (basis)

Example: field creation operator for Fermi gas of $s=\frac{1}{2}$ electrons, with momenta $\vec{p} = \hbar\vec{k}$:

$$\hat{c}^+(\vec{r}, s_z) = \underbrace{\sum_{\text{all } \vec{k}}}_{\text{s.p. quantum numbers}} \underbrace{\sum_{s_z = \pm\frac{1}{2}}}_{\text{s.p. quantum numbers}} \hat{c}^+_{\vec{k}, s_z} \underbrace{L^{-3/2} e^{-i\vec{k}\cdot\vec{r}}}_{\text{space}} \underbrace{\chi^{+}_{s=\frac{1}{2}}_{s_z}}_{\text{spin}}$$

Note: $\chi^+ = (\chi_1^*, \chi_2^*)$ denotes row vector in spin space.

$\chi = \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix}$ = column vector. See Shankar, ch. 14.

Relation between Slater determinant and quantum field operators

Ref: Bohr & Mottelson, Nucl. Structure, vol. 1, p. 272–278

The Slater determinant for N particles

$$\phi_{k_1, k_2, \ldots, k_N}(x_1, x_2, \ldots, x_N)_a$$ ← anti-sym.

may be written in the form

$$\phi_{\ldots} = \langle x_1, \ldots, x_N | k_1, k_2, \ldots, k_N \rangle_a$$

Use result from p. 20; for the "ket" vector:

$$|x_1, \ldots, x_N\rangle = \hat{c}^+(x_1)\, \hat{c}^+(x_2) \ldots \hat{c}^+(x_N)|0\rangle$$

This implies that the "bra" vector is

$$\langle x_1, \ldots, x_N| = |x_1, \ldots, x_N\rangle^+ =$$

$$= \langle 0|\, \hat{c}(x_N)\, \hat{c}(x_{N-1}) \ldots \hat{c}(x_2)\hat{c}(x_1)$$

↓

Slater determinant

$$\phi_{k_1, k_2, \ldots, k_N}(x_1, x_2, \ldots, x_N)_a =$$

$$= \langle 0 | \underbrace{\hat{c}(x_N) \ldots \hat{c}(x_1)}_{\text{quantum field annih. ops}} | \underbrace{k_1, \ldots, k_N}_{\text{occupied s.p. states}} \rangle_a$$

One-body operator in 1st and 2nd quantization

1st quantization: in coordinate space

2nd quantization: occupation number space

a) 1st quantization

For simplicity, we consider 2 particles (fermions).

Slater determinant: $\psi(x_1,x_2) = \frac{1}{\sqrt{2}}\left[\varphi_1(x_1)\varphi_2(x_2) - \varphi_1(x_2)\varphi_2(x_1)\right]$

One-body operator: $T^{(1)} = \sum_{i=1}^{2} t(x_i) = t(x_1) + t(x_2)$

Basic idea of procedure:

Consider the expectation value of one-body operator in the many-particle state $\psi(x_1,x_2)$:

$$\langle \psi | T^{(1)} | \psi \rangle . \qquad (1)$$

This exp. value represents a number (in general complex).

In coordinate space, one obtains

$$\langle \psi | T^{(1)} | \psi \rangle = \int dx_1 \int dx_2 \, \psi^*(x_1,x_2) \left[\sum_{i=1}^{2} t(x_i)\right] \psi(x_1,x_2) . \qquad (2)$$

On the other hand, we can represent the matrix element using creation operators for $|\psi\rangle$, i.e.

$$|\psi\rangle = |n_1=1, n_2=1\rangle = \hat{a}_1^{c\,+} \hat{a}_2^{c\,+} |0\rangle . \qquad (3)$$

In both cases, we must get the same answer for (1).

This determines the structure of $\hat{T}^{(1)}$ in occup.-# representation!

Evaluate (2) in coord. space:

$$\langle\psi|T^{(1)}|\psi\rangle = \frac{1}{2}\int dx_1 \int dx_2 \left[\varphi_1^*(x_1)\varphi_2^*(x_2) - \varphi_1^*(x_2)\varphi_2^*(x_1)\right]$$
$$\left[t(x_1)+t(x_2)\right]\left[\varphi_1(x_1)\varphi_2(x_2) - \varphi_1(x_2)\varphi_2(x_1)\right]$$

$$= \frac{1}{2}\int dx_1 \int dx_2 \left[\varphi_1^*(x_1)\varphi_2^*(x_2) - \varphi_1^*(x_2)\varphi_2^*(x_1)\right]$$
$$\left[t(x_1)\varphi_1(x_1)\varphi_2(x_2) - \varphi_1(x_2)t(x_1)\varphi_2(x_1) + \varphi_1(x_1)t(x_2)\varphi_2(x_2) - t(x_2)\varphi_1(x_2)\varphi_2(x_1)\right] =$$

$$= \frac{1}{2}\Bigg[\underbrace{\int dx_2\, \varphi_2^*(x_2)\varphi_2(x_2)}_{=\langle\varphi_2|\varphi_2\rangle = 1} \underbrace{\int dx_1\, \varphi_1^*(x_1)\, t(x_1)\varphi_1(x_1)}_{=\langle\varphi_1|t|\varphi_1\rangle}$$
$$- \underbrace{\int dx_2\, \varphi_1^*(x_2)\varphi_2(x_2)}_{=\langle\varphi_1|\varphi_2\rangle = 0} \underbrace{\int dx_1\, \varphi_2^*(x_1)\, t(x_1)\varphi_1(x_1)}_{=\langle\varphi_2|t|\varphi_1\rangle}$$
$$- \underbrace{\int dx_2\, \varphi_2^*(x_2)\varphi_1(x_2)}_{=\langle\varphi_2|\varphi_1\rangle = 0} \underbrace{\int dx_1\, \varphi_1^*(x_1)\, t(x_1)\varphi_2(x_1)}_{=\langle\varphi_1|t|\varphi_2\rangle}$$
$$+ \underbrace{\int dx_2\, \varphi_1^*(x_2)\varphi_1(x_2)}_{=\langle\varphi_1|\varphi_1\rangle = 1} \underbrace{\int dx_1\, \varphi_2^*(x_1)\, t(x_1)\varphi_2(x_1)}_{=\langle\varphi_2|t|\varphi_2\rangle}$$
$$+ \underbrace{\int dx_1\, \varphi_1^*(x_1)\varphi_1(x_1)}_{=\langle\varphi_1|\varphi_1\rangle = 1} \underbrace{\int dx_2\, \varphi_2^*(x_2)\, t(x_2)\varphi_2(x_2)}_{=\langle\varphi_2|t|\varphi_2\rangle}$$
$$- \underbrace{\int dx_1\, \varphi_2^*(x_1)\varphi_1(x_1)}_{=\langle\varphi_2|\varphi_1\rangle = 0} \underbrace{\int dx_2\, \varphi_1^*(x_2)\, t(x_2)\varphi_2(x_2)}_{=\langle\varphi_1|t|\varphi_2\rangle}$$
$$- \underbrace{\int dx_1\, \varphi_1^*(x_1)\varphi_2(x_1)}_{=\langle\varphi_1|\varphi_2\rangle = 0} \underbrace{\int dx_2\, \varphi_2^*(x_2)\, t(x_2)\varphi_1(x_2)}_{=\langle\varphi_2|t|\varphi_1\rangle}$$

$$+ \underbrace{\int dx_1\, \varphi_2^*(x_1)\varphi_2(x_1)}_{=\langle\varphi_2|\varphi_2\rangle=1} \underbrace{\int dx_2\, \varphi_1^*(x_2)\, t(x_2)\, \varphi_1(x_2)}_{=\langle\varphi_1|t|\varphi_1\rangle} \Big]$$

Adding up all non-zero terms, we obtain

$$\langle\psi|T^{(1)}|\psi\rangle = \frac{1}{2}\left[\langle\varphi_1|t|\varphi_1\rangle + \langle\varphi_2|t|\varphi_2\rangle + \langle\varphi_2|t|\varphi_2\rangle + \langle\varphi_1|t|\varphi_1\rangle\right]$$

$$\Rightarrow \langle\psi|T^{(1)}|\psi\rangle = \langle\varphi_1|t|\varphi_1\rangle + \langle\varphi_2|t|\varphi_2\rangle = \sum_{i=1}^{2}\langle\varphi_i|t|\varphi_i\rangle \qquad (4a)$$

What was done here for 2 particles, can be generalized to N particles. In this case we have the Slater determinant

$$\psi(x_1,\ldots,x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(x_1) & \cdots & \varphi_1(x_N) \\ \vdots & & \vdots \\ \varphi_N(x_1) & \cdots & \varphi_N(x_N) \end{vmatrix}$$

and the one-body operator is

$$T^{(1)} = \sum_{i=1}^{N} t(x_i).$$

The result is the same as above, except that one has to add up N s.p. matrix elements, rather than just 2:

Summary: "1st quantization" (coordinate space)

many-body WF = Slater determinant $\psi(x_1,\ldots,x_N)$.

one-body operator: $T^{(1)} = \sum_{i=1}^{N} t(x_i)$ (4b)

exp. value $\langle\psi|T^{(1)}|\psi\rangle = \sum_{i=1}^{N}\langle\varphi_i|t|\varphi_i\rangle$

b) 2nd quantization (= occupation # space)

The state vector for N fermions is given by

$$|\psi\rangle = \hat{c}_1^+ \dots \hat{c}_N^+ |0\rangle \quad \rightarrow \quad \langle\psi| = \langle 0| \hat{c}_N \dots \hat{c}_1$$

Hence, the exp. value in occup. # space becomes

$$\langle\psi| \hat{T}^{(1)} |\psi\rangle = \langle 0| \underbrace{\hat{c}_N \dots \hat{c}_1}\ \hat{T}^{(1)}\ \underbrace{c_1^+ \dots c_N^+} |0\rangle \qquad (5)$$

Main question: what is the operator $\hat{T}^{(1)}$ in 2nd quantization?

Note that (5) must produce the same answer as (4). From that we conclude that $\hat{T}^{(1)}$ must contain s.p. matrix elements of the form $\langle\varphi_i|t|\varphi_j\rangle$. Secondly, since $\hat{T}^{(1)}$ is an operator in occup. # space, it might contain creation/annihilation operators $\hat{c}_i^+, \hat{c}_j$. The operator

$$\hat{T}^{(1)} \stackrel{\text{def}}{=} \sum_{i,j=1}^{\infty} \langle\varphi_i|t|\varphi_j\rangle \hat{c}_i^+ \hat{c}_j \qquad (6)$$

satisfies the above criteria. We show now that using (6), we get the same answer for many-body matrix element $\langle\psi|\hat{T}^{(1)}|\psi\rangle$ as in coord. space, as we must:

$$\left.\begin{aligned} \langle\psi|\hat{T}^{(1)}|\psi\rangle &\overset{(6)}{=} \langle\psi| \sum_{i,j=1}^{\infty} \langle\varphi_i|t|\varphi_j\rangle \hat{c}_i^+ \hat{c}_j |\psi\rangle = \\ &= \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \langle\varphi_i|t|\varphi_j\rangle \langle\psi|\hat{c}_i^+ \hat{c}_j|\psi\rangle \end{aligned}\right\} (7)$$

Consider the matrix element $\langle\psi|\hat{c}_i^+\hat{c}_j|\psi\rangle$: We start from the N-particle state $|\psi\rangle = \hat{c}_1^+ \ldots \hat{c}_N^+|0\rangle$, destroy and create 2 particles, and then we return to the same state $\langle\psi|$. This is only possible if we create and destroy fermions with the same quantum numbers: $i = j$. Therefore

$$\langle\psi|\hat{c}_i^+\hat{c}_j|\psi\rangle = \delta_{ij}\langle\psi|\hat{c}_i^+\hat{c}_i|\psi\rangle. \quad (8)$$

Insert (8) into (7):

$$\langle\psi|\hat{T}^{(1)}|\psi\rangle = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\langle\varphi_i|t|\varphi_j\rangle\delta_{ij}\langle\psi|\hat{c}_i^+\hat{c}_i|\psi\rangle$$

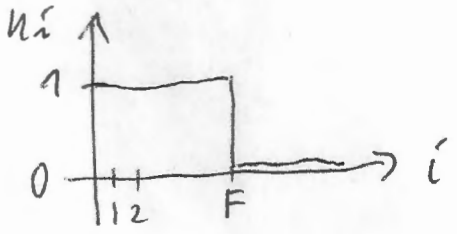
$$= \sum_{i=1}^{\infty}\langle\varphi_i|t|\varphi_i\rangle\langle\psi|\hat{c}_i^+\hat{c}_i|\psi\rangle \quad (9)$$

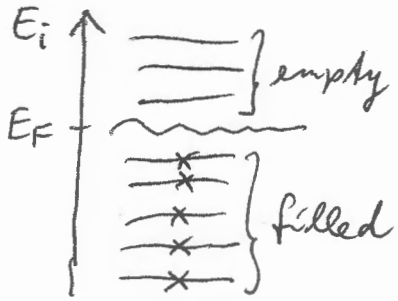
But the underlined quantity is the number of particles in state $|i\rangle$:

$$\langle\psi|\hat{c}_i^+\hat{c}_i|\psi\rangle = \langle\psi|\hat{n}_i|\psi\rangle = n_i$$

and $n_i = 1$ below Fermi level and $n_i = 0$ above Fermi level F.

$$\searrow \quad n_i = \langle\psi|\hat{n}_i|\psi\rangle = \theta(i - F) \quad (10)$$





Insert (10) into (9):

$$\langle\psi|\hat{T}^{(1)}|\psi\rangle = \sum_{i=1}^{\infty} \langle\varphi_i|t|\varphi_i\rangle \underbrace{\theta(i-F)}_{=n_i} = \sum_{i=1}^{F=N} \langle\varphi_i|t|\varphi_i\rangle \qquad (11)$$

which indeed the same result as in coordinate space (4b).

Summary: "2nd quantization" (occupation # space)

many-body state $= |\psi\rangle = \hat{c}_1^+ \dots \hat{c}_N^+ |0\rangle$

→ one-body operator: $\hat{T}^{(1)} = \sum_{i,j=1}^{\infty} \langle\varphi_i|t|\varphi_j\rangle \hat{c}_i^+ \hat{c}_j$

exp. value $\langle\psi|\hat{T}^{(1)}|\psi\rangle = \sum_{i=1}^{N} \langle\varphi_i|t|\varphi_i\rangle$ (12a)

see Fetter/Walecka, eq. (1.60)

Alternative formulation in terms of field operators $\hat{c}(x), c^+(x)$:

Theorem: (see Fetter/Walecka eq. (2.4))

$$\hat{T}^{(1)} = \int dx\, \hat{c}^+(x)\, t(x)\, \hat{c}(x) \qquad (12b)$$

($\hat{c}^+(x)$: field operator; $t(x)$: s.p. operator; $\hat{c}(x)$: field operator)

Proof: expand field ops in s.p. basis

$$\hat{T}^{(1)} = \int dx \underbrace{\left[\sum_{k=1}^{\infty} \hat{c}_k^+ \varphi_k^+(x)\right]}_{=\hat{c}^+(x)} t(x) \underbrace{\left[\sum_{\ell=1}^{\infty} \hat{c}_\ell \varphi_\ell(x)\right]}_{=\hat{c}(x)}$$

$$= \sum_{k,\ell=1}^{\infty} \underbrace{\left[\int dx\, \varphi_k^+(x)\, t(x)\, \varphi_\ell(x)\right]}_{=\langle\varphi_k|t|\varphi_\ell\rangle} \hat{c}_k^+ \hat{c}_\ell$$

$$\Rightarrow \hat{T}^{(1)} = \sum_{k,\ell=1}^{\infty} \langle\varphi_k|t|\varphi_\ell\rangle \hat{c}_k^+ \hat{c}_\ell \,. \quad \text{q.e.d.}$$

Two-body operators

a) coordinate representation

$$V^{(2)} = \frac{1}{2} \sum_{\substack{i,j=1 \\ (i \neq j)}}^{N} v^{(2)}(x_i, x_j) \qquad (13a)$$

b) occupation numbers representation

For $T^{(1)}$, we found a s.p. matrix element $\langle \varphi_i | t | \varphi_j \rangle$ and one creation/annih. op. pair $\hat{c}_i^+, \hat{c}_j$. Alternatively, one field creation ($\hat{c}^+(x)$) and destruction operator ($\hat{c}(x)$).

Not surprisingly, a lengthy calculation shows that

(13b)

$$\hat{V}^{(2)} = \frac{1}{2} \sum_{i,j,k,l=1}^{\infty} \langle ij | v^{(2)} | kl \rangle \, \hat{c}_i^+ \hat{c}_j^+ \hat{c}_l \hat{c}_k$$

note sequence!

with the two-body matrix element

$$\langle ij | v^{(2)} | kl \rangle = \int dx \int dx' \, \varphi_i^*(x) \, \varphi_j^*(x') \, v^{(2)}(x,x') \, \varphi_k(x) \varphi_l(x')$$

see Fetter/Walecka, eq. (1.60).

Alternative formulation in terms of field operators:

$$\hat{V}^{(2)} = \frac{1}{2} \int dx \int dx' \, \hat{c}^+(x) \, \hat{c}^+(x') \, v^{(2)}(x,x') \, \hat{c}(x') \, \hat{c}(x), \qquad (13c)$$

see Fetter/Walecka, eq. (2.4).

Three-body operators (only in nuclear theory!)

a) coord. representation

$$V^{(3)} = \frac{1}{6} \sum_{\substack{i,j,k=1 \\ (i \neq j \neq k)}}^{N} v^{(3)}(x_i, x_j, x_k) \qquad (14a)$$

b) occupation number representation

$$\hat{V}^{(3)} = \frac{1}{6} \sum_{i,j,k,l,m,n=1}^{\infty} \langle ijk | v^{(3)} | lmn \rangle \hat{c}_i^+ \hat{c}_j^+ \hat{c}_k^+ \hat{c}_n \hat{c}_m \hat{c}_l$$

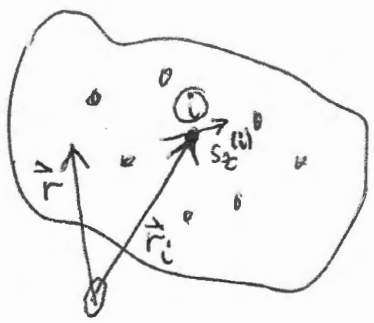
note sequence!

or in terms of field operators

$$\hat{V}^{(3)} = \frac{1}{6} \int dx \int dx' \int dx'' \, \hat{c}^+(x) \hat{c}^+(x') \hat{c}^+(x'') v^{(3)}(x, x', x'') \times \hat{c}(x'') \hat{c}(x') \hat{c}(x)$$

Illustrative example: one-body operators in occupation # space

Example 1: density operator for $s = \frac{1}{2}$ fermions



The density operator for N point particles ($s = \frac{1}{2}$ fermions) is a one-body operator:

$$\rho(\vec{r}, s_z) = \sum_{i=1}^{N} \delta(\vec{r} - \vec{r}_i) \delta_{s_z, s_z^{(i)}}$$

Using the expression on p. 27, we find

the density operator in occup.-# space

quantum field operators

$$\hat{\rho} = \int dx\, \hat{c}^+(x)\, \rho(x)\, \hat{c}(x) \rightarrow \int d^3r \underbrace{\sum_{s_z=\pm\frac{1}{2}}}_{=\int dx} \hat{c}^+(\vec{r}, s_z)\, \rho(\vec{r}, s_z)\, \hat{c}(\vec{r}, s_z)$$

↑ s.p. density

Inserting from above

$$\rho(\vec{r}, s_z) = \delta(\vec{r} - \vec{r}')\, \delta_{s_z, s_z'} \rightarrow$$

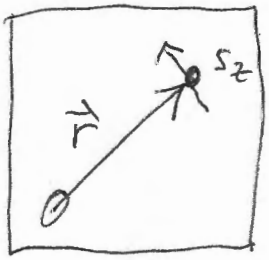
$$\hat{\rho} = \int d^3r \sum_{s_z} \hat{c}^+(\vec{r}, s_z)\, \delta(\vec{r} - \vec{r}')\, \delta_{s_z, s_z'}\, \hat{c}(\vec{r}, s_z) =$$

$$\hat{\rho}(\vec{r}', s_z') = \hat{c}^+(\vec{r}', s_z')\, \hat{c}(\vec{r}', s_z') \quad ; \text{ now we can leave out the primes:}$$

density operator (for $s = \frac{1}{2}$):

$$\hat{\rho}(\vec{r}, s_z) = \hat{c}^+(\vec{r}, s_z)\, \hat{c}(\vec{r}, s_z)$$

← field operators



Physical interpretation: (Gordon Baym, QM) the operator $\hat{\rho}$ "examines" the density at position $\vec{r}$ (for given spin projection $s_z = \pm\frac{1}{2}$) by first "destroying" the particle, via $\hat{c}(\vec{r}, s_z)$, and then "putting it back" again ($\hat{c}^+(\vec{r}, s_z)$)!

Alternative representation (expand field ops in basis φ_i):

$$\hat{\rho}(\vec{r}, s_z) = \left[\sum_{j=1}^{\infty} \hat{c}_j^+\, \varphi_j^+(\vec{r}, s_z)\right]\left[\sum_{i=1}^{\infty} \hat{c}_i\, \varphi_i(\vec{r}, s_z)\right]$$

$$\rightarrow \quad \hat{\rho}(\vec{r}, s_z) = \sum_{i,j=1}^{\infty} \left(\varphi_j^+(\vec{r}, s_z)\, \varphi_i(\vec{r}, s_z)\right) \hat{c}_j^+\, \hat{c}_i$$

Note that $\hat{\rho}$ is just an operator. To calculate an observable, say the ground state density, we need the

> state vector for the ground state $|\Phi_{g.s.}\rangle$

$$\rho_{g.s.}(\vec{r}, s_z) = \langle \Phi_{g.s.} | \hat{\rho}(\vec{r}, s_z) | \Phi_{g.s.} \rangle =$$

$$= \sum_{i,j=1}^{\infty} \varphi_j^+(\vec{r}, s_z)\, \varphi_i(\vec{r}, s_z) \underbrace{\langle \Phi_{g.s.} | \hat{c}_j^+ \hat{c}_i | \Phi_{g.s.} \rangle}_{\stackrel{\text{def}}{=} \rho_{ij}}$$

Summary: expression for g.s. density ($s = \frac{1}{2}$)

$$\rho_{g.s.}(\vec{r}, s_z) = \sum_{i,j=1}^{\infty} \varphi_j^+(\vec{r}, s_z)\, \varphi_i(\vec{r}, s_z)\, \rho_{ij}$$

(s.p. basis WF's)

with $\rho_{ij} \stackrel{\text{def}}{=} \langle \Phi_{g.s.} | \hat{c}_j^+ \hat{c}_i | \Phi_{g.s.} \rangle$

(density parameters)

Note: if we have a model for the exact ground state of the system, then we can calculate the density parameters ρ_{ij}. In the next chapter, ch. 3, we will do this for the non-interacting ground state $|\Phi_0\rangle$.

$$|\Phi_{g.s.}\rangle \longrightarrow |\Phi_0\rangle.$$

The determination of the exact g.s. is a very difficult task; may use Green's function (= propagator) techniques (see later in our course).

Example 2: linear momentum operator ($s=\frac{1}{2}$)

The total linear momentum operator is a one-body operator:

$$\vec{P} = \sum_{k=1}^{N} (-i\hbar\nabla_k) \qquad \text{(coordinate repr.)}$$

Using expression on p. 27, we find in occup # repr:

$$\hat{\vec{P}} = \sum_{m,n=1}^{\infty} \langle m|-i\hbar\nabla|n\rangle \hat{c}_m^+ \hat{c}_n .$$

This is all one can say for an arbitrary s.p. basis $|n\rangle \equiv |\varphi_n\rangle$. with s.p. matrix elements

$$\langle m|-i\hbar\nabla|n\rangle = \int dx\, \varphi_m^+(x)\,[-i\hbar\nabla]\,\varphi_n(x).$$

Let us now choose the eigenfunctions for a free Fermi gas (p. 7):

$$\varphi_n(x) \to \varphi_{\vec{k},s_z}(\vec{r}) = L^{-3/2} e^{i\vec{k}\cdot\vec{r}} \chi_{s_z}^{s=\frac{1}{2}}$$

which yields

$$\hat{\vec{P}} = \sum_{\vec{k}',s_z'} \sum_{\vec{k},s_z} \langle \vec{k}',s_z'|-i\hbar\nabla|\vec{k},s_z\rangle \hat{c}^+_{\vec{k}',s_z'} \hat{c}_{\vec{k},s_z}$$

Because the mom. operator $(-i\hbar\nabla)$ does not affect spin space we get

$$\langle \vec{k}',s_z'|-i\hbar\nabla|\vec{k},s_z\rangle = \underbrace{\langle s_z'|s_z\rangle}_{=\delta_{s_z',s_z}} \underbrace{\langle \vec{k}'|-i\hbar\nabla|\vec{k}\rangle}_{=\hbar\vec{k}\langle\vec{k}'|\vec{k}\rangle,\ \langle\vec{k}'|\vec{k}\rangle = \delta_{\vec{k}',\vec{k}}}$$

resulting in

$$\boxed{\hat{\vec{P}} = \sum_{\text{all } \vec{k},\, s_z=\pm\frac{1}{2}} \hbar\vec{k}\, \hat{c}^+_{\vec{k},s_z} \hat{c}_{\vec{k},s_z} = \text{number operator } \hat{n}_{\vec{k},s_z}}$$

Again, to calculate an observable, we take e.g. g.s. expectation value:

Summary: expression for total linear g.s. momentum ($s=\frac{1}{2}$)

$$\vec{P}_{g.s.} = \sum_{\text{all } \vec{k}} \sum_{S_z=\pm\frac{1}{2}} \hbar\vec{k} \langle \phi_{g.s.} | \hat{c}^{+}_{\vec{k},S_z} \hat{c}_{\vec{k},S_z} | \phi_{g.s.} \rangle$$

$= \hat{n}_{\vec{k},S_z}$ (number op.)

Again, once we have a model g.s., we can calculate the expectation value above (e.g. for free Fermi gas).

Example 3: total angular momentum operator

see homework!
