IDENTICAL PARTICLES

This is a uniquely quantum concept - in classical physics if we have the equation of motion for any particular particle we always know exactly where it is & we are not likely to confuse it with any other particle even if it "looks" the same.

Let's consider how quantum mechanics might differ by considering the case of just two particles.
We'll describe the state of a particle that we'll call #1 by the ket $|\alpha\rangle$,
where α contains information about quantum #s of a complete set of observables.
The state of the other particle, #2, is described by the ket $|\alpha'\rangle$.

Hence the state of the pair of particles can be described by the product ket $\underset{\#1}{|\alpha\rangle}\underset{\#2}{|\alpha'\rangle}$.

Note that an independent (actually orthogonal) ket is $\underset{\#1}{|\alpha'\rangle}\underset{\#2}{|\alpha\rangle}$.

Suppose we make a set of commuting measurements on the system (both #1 & #2) - since the particles are indistinguishable, each of the states

$$|\alpha\rangle|\alpha'\rangle \quad \& \quad |\alpha'\rangle|\alpha\rangle$$

will give the same results. Hence all kets of the form

$$c_1|\alpha\rangle|\alpha'\rangle + c_2|\alpha'\rangle|\alpha\rangle$$

will have the same set of eigenvalues. These states are considered to be "exchange degenerate".

We can define a permutation operator P_{12}, which has the following property

$$P_{12}|\alpha\rangle|\alpha'\rangle = |\alpha'\rangle|\alpha\rangle \qquad \text{Obviously } P_{12} = P_{21} \quad \& \quad P_{12}^2 = 1 \qquad (P_{12}^{-1}\ P_{12})$$

Certain operators in quantum systems act on only one particle & carry a label indicating as such, e.g. in $\vec{S}_1\cdot\vec{S}_2$, $\vec{S}_1$ acts on particle 1 & $\vec{S}_2$ on particle 2.

generally
$$A_1|a\rangle|a'\rangle = a|a\rangle|a'\rangle$$
$$A_2|a\rangle|a'\rangle = a'|a\rangle|a'\rangle$$

then
$$\left.\begin{aligned} P_{12}A_1|a\rangle|a'\rangle &= P_{12}A_1P_{12}\,P_{12}|a\rangle|a'\rangle = P_{12}A_1P_{12}\,|a'\rangle|a\rangle \\ &= P_{12}\,a|a\rangle|a'\rangle = a|a'\rangle|a\rangle = A_2|a'\rangle|a\rangle \end{aligned}\right\} \underline{P_{12}A_1P_{12} = A_2}$$

so the permutation operator acts on operators by changing their particle label.

A Hamiltonian for two particles must appear symmetrically, e.g.

$$H = \frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} + V(|\vec{x}_1 - \vec{x}_2|) + V(\vec{x}_1) + V(\vec{x}_2)$$

then $P_{12} H P_{12} = H \quad \Rightarrow \quad [H, P_{12}] = 0$ & the eigenstates of P_{12} are stationary.

Since $P_{12}^2 = 1 \Rightarrow$ the eigenvalues of P_{12} must be ± 1. This corresponds to symmetric & antisymmetric states.

$$|\alpha\alpha'\rangle_S = \frac{1}{\sqrt{2}}\left(|\alpha\rangle|\alpha'\rangle + |\alpha'\rangle|\alpha\rangle\right) \quad : \quad P_{12}|\alpha\alpha'\rangle_S = +|\alpha\alpha'\rangle_S$$

$$|\alpha\alpha'\rangle_A = \frac{1}{\sqrt{2}}\left(|\alpha\rangle|\alpha'\rangle - |\alpha'\rangle|\alpha\rangle\right) \quad : \quad P_{12}|\alpha\alpha'\rangle_A = -|\alpha\alpha'\rangle_A$$

Notice what happens if we have three identical particles - naively we have 6 possible exchange degenerate states:

$$|\alpha\rangle|\alpha'\rangle|\alpha''\rangle,\ |\alpha'\rangle|\alpha\rangle|\alpha''\rangle,\ |\alpha'\rangle|\alpha''\rangle|\alpha\rangle,\ |\alpha\rangle|\alpha''\rangle|\alpha'\rangle,\ |\alpha''\rangle|\alpha\rangle|\alpha'\rangle,\ |\alpha''\rangle|\alpha'\rangle|\alpha\rangle$$

but if we insist on states that are totally symmetric or antisymmetric we have only 2:

$$|\alpha\alpha'\alpha''\rangle_S = \frac{1}{\sqrt{6}}\Big(|\alpha\rangle|\alpha'\rangle|\alpha''\rangle + |\alpha\rangle|\alpha''\rangle|\alpha'\rangle + |\alpha'\rangle|\alpha\rangle|\alpha''\rangle + |\alpha'\rangle|\alpha''\rangle|\alpha\rangle + |\alpha''\rangle|\alpha\rangle|\alpha'\rangle + |\alpha''\rangle|\alpha'\rangle|\alpha\rangle\Big)$$

$$|\alpha\alpha'\alpha''\rangle_A = \frac{1}{\sqrt{6}}\Big(|\alpha\rangle|\alpha'\rangle|\alpha''\rangle - |\alpha\rangle|\alpha''\rangle|\alpha'\rangle - |\alpha'\rangle|\alpha\rangle|\alpha''\rangle + |\alpha'\rangle|\alpha''\rangle|\alpha\rangle + |\alpha''\rangle|\alpha\rangle|\alpha'\rangle - |\alpha''\rangle|\alpha'\rangle|\alpha\rangle\Big)$$

Particles described by the first type of state satisfy "Bose-Einstein statistics" & are usually called "Bosons" $\quad P_{ij}\,|N \text{ identical bosons}\rangle = +\,|N \text{ identical bosons}\rangle$

Particles described by the second type of state satisfy "Fermi-Dirac statistics" & are usually called "Fermions" $\quad P_{ij}\,|N \text{ identical fermions}\rangle = -\,|N \text{ identical fermions}\rangle$

It turns out to be the case that all particles of half-integer spin are fermions, and all particles of integer spin are bosons. This just has to be accepted within non-relativistic quantum mechanics, but can be proven within the relativistic quantum field theory.

If we accept this we immediately come to the Pauli exclusion principle for fermions, which states that "no two fermions may occupy the same quantum state". This is obvious if a two fermion state must be

$$|\alpha\alpha'\rangle_A = \frac{1}{\sqrt{2}}\left(|\alpha\rangle|\alpha'\rangle - |\alpha'\rangle|\alpha\rangle\right)$$

if $\alpha = \alpha'$, $|\alpha\alpha\rangle_A = 0$.

The Pauli exclusion principle explains why all the electrons in atoms don't just drop into the ground state, this gives rise to the wide variety of properties of the chemical elements.

$\boxed{\text{A system of two electrons}}$

Consider a two-electron system in a state $|\alpha\rangle$ - we can express this in the position-spin basis, with wavefunction

$$\psi_\alpha(\vec{x}_1, \vec{x}_2) = \sum_{m_{s1}, m_{s2}} C_{m_{s1}, m_{s2}} \langle \vec{x}_1, \tfrac{1}{2}, m_{s1}; \vec{x}_2, \tfrac{1}{2}, m_{s2} | \alpha\rangle$$

Notice that the spin-coupled basis states have definite symmetry under exchange $1 \leftrightarrow 2$

$$|S=0, M_S=0\rangle = \frac{1}{\sqrt{2}}\left(|\tfrac{1}{2}+\tfrac{1}{2}; \tfrac{1}{2}-\tfrac{1}{2}\rangle - |\tfrac{1}{2}-\tfrac{1}{2}, \tfrac{1}{2}+\tfrac{1}{2}\rangle\right) \rightsquigarrow \frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{-+}) \quad \text{"singlet" antisymmetric}$$

$$\left.\begin{cases} |S=1, M_S=+1\rangle = |\tfrac{1}{2}\tfrac{1}{2}, \tfrac{1}{2}\tfrac{1}{2}\rangle & \chi_{++} \\ |S=1, M_S=0\rangle = \frac{1}{\sqrt{2}}\left(|\tfrac{1}{2}+\tfrac{1}{2}, \tfrac{1}{2}-\tfrac{1}{2}\rangle + |\tfrac{1}{2}-\tfrac{1}{2}; \tfrac{1}{2}+\tfrac{1}{2}\rangle\right) & \rightsquigarrow \frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{-+}) \\ |S=1, M_S=-1\rangle = |\tfrac{1}{2}-\tfrac{1}{2}; \tfrac{1}{2}-\tfrac{1}{2}\rangle & \chi_{--} \end{cases}\right\} \quad \text{"triplet" symmetric}$$

We can express the wavefunction as $\psi = \phi(\vec{x}_1, \vec{x}_2)\,\chi$.

Recall that for Fermi-Dirac statistics, $P_{12}|\alpha\rangle = -|\alpha\rangle$
& from the definition $P_{12}|\vec{x}_1 \tfrac{1}{2} m_{s1}; \vec{x}_2 \tfrac{1}{2} m_{s2}\rangle = |\vec{x}_2 \tfrac{1}{2} m_{s2}; \vec{x}_1 \tfrac{1}{2} m_{s1}\rangle$

& thus $\langle \vec{x}_1 \tfrac{1}{2} m_{s1}; \vec{x}_2 \tfrac{1}{2} m_{s2}|\alpha\rangle = -\langle \vec{x}_2 \tfrac{1}{2} m_{s2}; \vec{x}_1 \tfrac{1}{2} m_{s1}|\alpha\rangle$

hence the wavefunction ψ must be antisymmetric under the joint exchange $\begin{matrix}\vec{x}_1 \leftrightarrow \vec{x}_2 \\ m_{s1} \leftrightarrow m_{s2}\end{matrix}$

Thus if the system is in the singlet state (spin antisymmetric) the space wavefunction must be symmetric $\phi(\vec{x}_1, \vec{x}_2) = \phi(\vec{x}_2, \vec{x}_1)$

If the system is in the triplet state (spin symmetric) the space wavefunction must be antisymmetric $\phi(\vec{x}_1, \vec{x}_2) = -\phi(\vec{x}_2, \vec{x}_1)$

The probability to find electron #1 in a volume $d^3\vec{x}_1$ around $\vec{x}_1$ and electron #2 in a volume $d^3\vec{x}_2$ around $\vec{x}_2$ is

$$P(\vec{x}_1, \vec{x}_2) = |\phi(\vec{x}_1, \vec{x}_2)|^2 \, d^3\vec{x}_1 \, d^3\vec{x}_2$$

Suppose the Hamiltonian for the two-electron system includes no interaction between the electrons: $H = \vec{p}_1^{\,2}/2m + \vec{p}_2^{\,2}/2m + V(\vec{x}_1) + V(\vec{x}_2)$

clearly this is separable such that the wavefunction $\phi(\vec{x}_1, \vec{x}_2) = \varphi_A(\vec{x}\ \ \varphi_B(\vec{x}_2)$.

But we have already determined that the space wavefunction must be definite symmetry - a basis of wavefunctions allowed by Fermi-Dirac statistics is

$$\psi_{\substack{S=0\\ M_S=0};AB}(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{-+}) \cdot \frac{1}{\sqrt{2}}\left(\varphi_A(\vec{x}_1)\varphi_B(\vec{x}_2) + \varphi_B(\vec{x}_1)\varphi_A(\vec{x}_2)\right)$$

$$\psi_{\substack{S=1\\ M_S};AB}(\vec{x}_1, \vec{x}_2) = \begin{Bmatrix} \chi_{++} \\ \frac{1}{\sqrt{2}}(\chi_{+-} + \chi_{-+}) \\ \chi_{--} \end{Bmatrix} \cdot \frac{1}{\sqrt{2}}\left(\varphi_A(\vec{x}_1)\varphi_B(\vec{x}_2) - \varphi_B(\vec{x}_1)\varphi_A(\vec{x}_1)\right)$$

then the probability

$$P_{S=\{^0_1\},AB}(\vec{x}_1, \vec{x}_2) = \frac{1}{2}\Big[|\varphi_A(\vec{x}_1)|^2|\varphi_B(\vec{x}_2)|^2 + |\varphi_B(\vec{x}_1)|^2|\varphi_A(\vec{x}_2)|^2$$
$$\underbrace{\pm 2 \cdot \mathrm{Re}\left\{ \varphi_A(\vec{x}_1)\varphi_B^*(\vec{x}_1)\varphi_A^*(\vec{x}_2)\varphi_B(\vec{x}_2) \right\}}_{\text{"exchange density"}} \Big] d^3\vec{x}_1 d^3\vec{x}_2$$

Consider the spin-triplet state & the electrons in the same orbital state, $A=B$

then $P_{S=1,AA}(\vec{x}_1, \vec{x}_2) \propto |\varphi_A(\vec{x}_1)|^2|\varphi_A(\vec{x}_2)|^2 - \mathrm{Re}\{|\varphi_A(x_1)|^2|\varphi_A(\vec{x}_2)|^2\} = \underline{\underline{0}}$

so as we enforced, two identical electrons be in exactly the same quantum state

Now consider the spin-triplet state with the electrons occupying different orbital states, $A \neq B$. Suppose we wish to know the probability that the electrons will be located at the same position $(\vec{x}_1 = \vec{x}_2)$, this is

$$P_{\substack{S=1 \\ AB}}(\vec{x},\vec{x}) \propto \tfrac{1}{2}\left[2|\varphi_A(\vec{x})|^2|\varphi_B(\vec{x})|^2 - 2\,\mathrm{Re}\left\{|\varphi_A(\vec{x})|^2|\varphi_B(\vec{x})|^2\right\}\right] = 0$$

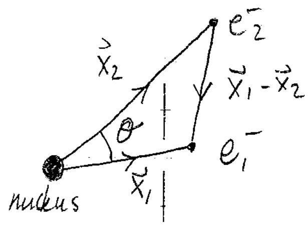
So in the spin-triplet state the electrons tend not to be found together.

In the singlet state however, $P_{\substack{S=0 \\ AB}}(\vec{x},\vec{x}) \propto 2|\varphi_A(\vec{x})|^2|\varphi_B(\vec{x})|^2$,

which is twice as large as one would naively expect for non-interacting particles, so in the spin-singlet state the electrons like to be found together.

This spin-dependent effect has a striking impact on the spectrum of the helium atom. Consider the Hamiltonian for two electrons bound to an infinitely heavy nucleus:

$$H = \vec{p}_1^{\,2}/2m + \vec{p}_2^{\,2}/2m - 2e^2/r_1 - 2e^2/r_2 + e^2/|\vec{x}_1 - \vec{x}_2|$$



as a basis we'll use the products of the non-interacting Hamiltonian eigenstates

$$\left(\vec{p}_1^{\,2}/2m - 2e^2/r_1\right)\psi_{nlm}(\vec{x}_1) = E\,\psi_{nlm}(\vec{x}_1)$$
$$\left(\vec{p}_2^{\,2}/2m - 2e^2/r_2\right)\psi_{nlm}(\vec{x}_2) = E\,\psi_{nlm}(\vec{x}_2).$$

Consider the ground state - the state of lowest energy in this basis is $\psi_{000}(\vec{x}_1)\psi_{000}(\vec{x}_2)$,

which is clearly symmetric under $\vec{x}_1 \leftrightarrow \vec{x}_2$, thus to satisfy Fermi-Dirac statistics, the spin wavefunction must be the antisymmetric singlet.

$$\psi_{000}(\vec{x}_1)\psi_{000}(\vec{x}_2)\frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{-+}).$$

We have already considered how to use this state as the trial function for a variational solution including the spin-independent interaction $e^2/|\vec{x}_1 - \vec{x}_2|$.

Let's consider what happens to the excited state constructions when e^2/r_{12} is included.

Consider the excitation in which only one electron is excited:

$$\psi_{000}(\vec{x}_1)\,\psi_{n\ell m}(\vec{x}_2)$$

but we know now that this must be $\begin{pmatrix}\text{symmetrised}\\ \text{antisymmetrised}\end{pmatrix}$ for a $\begin{pmatrix}\text{singlet}\\ \text{triplet}\end{pmatrix}$ state

$$\frac{1}{\sqrt{2}}\Big(\psi_{000}(\vec{x}_1)\,\psi_{n\ell m}(\vec{x}_2) \pm \psi_{n\ell m}(\vec{x}_1)\,\psi_{000}(\vec{x}_2)\Big)$$

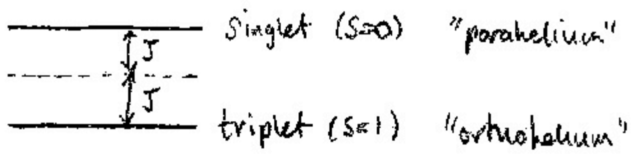
then the expectation values of the interaction potential can be expressed

$$\left\langle \frac{e^2}{r_{12}} \right\rangle = I \pm J \qquad \begin{pmatrix}\text{singlet}\\ \text{triplet}\end{pmatrix}$$

$$I \equiv \int d^3\vec{x}_1\, d^3\vec{x}_2\; |\psi_{000}(\vec{x}_1)|^2\, |\psi_{n\ell m}(\vec{x}_2)|^2 \cdot \frac{e^2}{r_{12}} \qquad \text{"direct integral"}$$

$$J \equiv \int d^3\vec{x}_1\, d^3\vec{x}_2\; \psi_{000}(\vec{x}_1)\, \psi_{n\ell m}(\vec{x}_2)\, \frac{e^2}{r_{12}}\, \psi^*_{000}(\vec{x}_2)\, \psi^*_{n\ell m}(\vec{x}_1) \qquad \text{"exchange integral"}$$

both $I \geq 0$ & $J \geq 0$ $\Rightarrow$ the spin-singlet is always at higher energy



The origin of the splitting is obvious from our previous observation that triplet states have small probability for the electrons getting close (where their interaction energy is large & positive), while the singlet states have large probability to be close together.

Note well: the Hamiltonian was completely SPIN-INDEPENDENT, but the identity of the particles gave rise to an apparent spin-dependent interaction.

EXCITED STATES OF HELIUM $\quad H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$

variational calculation – hydrogenic basis states with effective charges

$$\psi_{1P,m_\ell}(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}\left(\psi_S(\vec{r}_1)\psi_{P,m_\ell}(\vec{r}_2) + \psi_{P,m_\ell}(\vec{r}_1)\psi_S(\vec{r}_2)\right)\chi_{S=0} \quad \text{spin-singlet}$$

$$\psi_{3P,m_\ell m_s}(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}\left(\psi_S(\vec{r}_1)\psi_{P,m_\ell}(\vec{r}_2) - \psi_{P,m_\ell}(\vec{r}_1)\psi_S(\vec{r}_2)\right)\chi_{S=1,m_s} \quad \text{spin-triplet}$$

$$\psi_S(\vec{r}) = Y_0^0(\theta,\phi)\, 2\left(\frac{Z_S}{a_B}\right)^{3/2} e^{-Z_S r/a_B}$$

$$\psi_{P,m_\ell}(\vec{r}) = Y_1^{m_\ell}(\theta,\phi)\,\frac{1}{\sqrt{3}}\left(\frac{Z_P}{2a_B}\right)^{3/2}\frac{Z_P}{a_B}\, r\, e^{-Z_P r/2a_B}$$

P electron tends to be far out in r while S electron closer in, S shields P but not vice versa? $\Big\} \Rightarrow$ $Z_P \simeq 1$, $Z_S \simeq 2$?

$\binom{\text{singlet}}{\text{triplet}}$ $\langle H\rangle_{\pm} = \langle H_1 + H_2\rangle + I \pm J$

"direct" $I = \int d^3\vec{r}_1 d^3\vec{r}_2\, \frac{e^2}{r_{12}}\, |\psi_S(\vec{r}_1)|^2\, |\psi_P(\vec{r}_2)|^2$

electrostatic repulsion between charge densities $-e|\psi_S(\vec{r}_1)|^2$ & $-e|\psi_P(\vec{r}_2)|^2$

"exchange" $J = \int d^3\vec{r}_1 d^3\vec{r}_2\, \frac{e^2}{r_{12}}\, \psi_S^*(\vec{r}_1)\psi_P^*(\vec{r}_2)\psi_S(\vec{r}_2)\psi_P(\vec{r}_1)$

only present for identical particles.

we can evaluate the integrals to compute

$\langle H\rangle(Z_S, Z_P)$ then the variational best estimate follows

from $\quad 0 = \frac{\partial\langle H\rangle}{\partial Z_S} = \frac{\partial\langle H\rangle}{\partial Z_P}$

[? why don't we just get the ground state energy here?]

	Z_S	Z_P	$\lvert E^{thy}/R_H$	$\lvert E^{expt}/R_H$
→ 3P	1.99	1.09	.262	.266
1P	2.003	0.97	.245	.248

many particle states of identical particles - operator construction

A useful mathematical technique to describe many-particle states involves defining creation & annihilation operators for particles in a certain single particle state. In this section we will work out how to do this in a general manner consistent with the unitarity of quantum mechanics.

Suppose that a single particle is in a quantum state described by a set of quantum numbers which we label by α_i

$$\left(\text{e.g. } \alpha = \{n l m\} \quad \alpha_1 = 000,\ \alpha_2 = 100 \ldots \right)$$

Suppose that more than one identical particle is in the system having quantum numbers α_i - we call this the "occupation" of the state α_i & is described by the integer, $n_i \geq 0$.

Fock state : $|n_1, n_2 \ldots\rangle$ $\Rightarrow$ n_1 particles in state α_1
n_2 particles in state α_2
$\vdots$

simplest fock state - the "vacuum" state $|0\rangle \equiv |0,0\ldots\rangle$

So far we've mostly dealt with <u>single particle states</u> like

$|1,0,0\ldots\rangle \equiv |\alpha_1\rangle$ (ground state)
$|0,1,0\ldots\rangle \equiv |\alpha_2\rangle$ (1st excited state)
$\vdots$ $\vdots$

We can define creation & annihilation operators which have the following action

$$a_i^\dagger |n_1, n_2 \ldots n_i \ldots\rangle \propto |n_1, n_2 \ldots n_i + 1 \ldots\rangle$$

$$a_i |n_1, n_2 \ldots n_i \ldots\rangle \propto |n_1, n_2 \ldots n_i - 1 \ldots\rangle$$

for the single particle **states** $|\alpha_i\rangle \equiv |0,0,\ldots n_i = 1 \ldots\rangle = a_i^\dagger |0\rangle$

& obviously $a_i|0\rangle = 0$, $a_i |0,0\ldots, n_j = 1 \ldots\rangle = \delta_{ij} |0\rangle$

We know for single particle states that we can transform between bases using unitary transformations, generically these transformations take the form

$$|\alpha_i\rangle = \sum_q |\beta_q\rangle \underbrace{\langle \beta_q|\alpha_i\rangle}_{\text{unitary matrix}}$$

Consider the change of basis describing the single particle states - the new basis has single-particle Fock states

$$|0,0\ldots \tilde{n}_q = 1 \ldots\rangle \equiv |\beta_q\rangle$$

$\tilde{n}_q$ = occupation of state β_q.

we can define new basis creation/annihilation operators, $b_q^\dagger, b_q$

$$b_q^\dagger |\tilde{n}_1, \tilde{n}_2 \ldots \tilde{n}_q \ldots\rangle \propto |\tilde{n}_1, \tilde{n}_2 \ldots \tilde{n}_q + 1 \ldots\rangle$$

now

$$\left.\begin{aligned} |\alpha_i\rangle &= a_i^\dagger |0\rangle \\ \sum_q |\beta_q\rangle\langle\beta_q|\alpha_i\rangle &= \sum_q b_q^\dagger |0\rangle \langle \beta_q|\alpha_i\rangle \end{aligned}\right\} \Rightarrow \boxed{a_i^\dagger = \sum_q b_q^\dagger \langle \beta_q|\alpha_i\rangle}$$

$$\& \quad \boxed{a_i = \sum_q b_q \langle \alpha_i|\beta_q\rangle}$$

now let's consider what this imposition of unitary symmetry does when we look at many-particle states

e.g. the state $a_i^\dagger a_j^\dagger|\psi\rangle$ can only differ from the state $a_j^\dagger a_i^\dagger|\psi\rangle$ by a normalisation $\Rightarrow (a_i^\dagger a_j^\dagger - \lambda a_j^\dagger a_i^\dagger)|\psi\rangle = 0$ for any state $|\psi\rangle$.

now consider how this looks in the β basis

$$0 = (a_i^\dagger a_j^\dagger - \lambda a_j^\dagger a_i^\dagger)|\psi\rangle = \sum_{qr} \langle\beta_q|\alpha_i\rangle\langle\beta_r|\alpha_j\rangle \left(b_q^\dagger b_r^\dagger - \lambda b_r^\dagger b_q^\dagger\right)|\psi\rangle$$

in order for this to hold for all states $|\psi\rangle$ and all transformations $\alpha \to \beta$, we must have $b_q^\dagger b_r^\dagger - \lambda b_r^\dagger b_q^\dagger = 0$

& since q, r are dummy variables in the sum, also $b_r^\dagger b_q^\dagger - \lambda b_q^\dagger b_r^\dagger = 0$

$\Rightarrow \lambda^2 = 1 \quad \Rightarrow \underline{\lambda = \pm 1}$ hence either $a_i^\dagger a_j^\dagger - a_j^\dagger a_i^\dagger = 0 = [a_i^\dagger, a_j^\dagger]$

or $a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = 0 = \{a_i^\dagger, a_j^\dagger\}$

the creation operators either commute $([a_i^\dagger, a_j^\dagger] = 0)$ or anticommute $(\{a_i^\dagger, a_j^\dagger\} = 0)$

$\Rightarrow [a_i, a_j] = 0 \qquad \Rightarrow \{a_i, a_j\} = 0$

Now consider $a_i a_j^\dagger |\psi\rangle \propto a_j^\dagger a_i |\psi\rangle \Rightarrow (a_i a_j^\dagger - \mu a_j^\dagger a_i)|\psi\rangle = 0.$ $\underline{\underline{i \neq j}}$

perform a basis transformation (for $i \neq j$)

$$0 = (a_i a_j^\dagger - \mu a_j^\dagger a_i)|\psi\rangle = \sum_{qr} \langle \alpha_i | \beta_q \rangle \langle \beta_r | \alpha_j \rangle (b_q b_r^\dagger - \mu b_r^\dagger b_q)|\psi\rangle$$

recall that the basis transformation is unitary so $\sum_q \langle \alpha_i | \beta_q \rangle \langle \beta_q | \alpha_j \rangle = \delta_{ij}$

$$\Rightarrow 0 = \sum_q \langle \alpha_i | \beta_q \rangle \langle \beta_q | \alpha_j \rangle (b_q b_q^\dagger - \mu b_q^\dagger b_q)|\psi\rangle + \sum_{q \neq r} \langle \alpha_i | \beta_q \rangle \langle \beta_r | \alpha_j \rangle (b_q b_r^\dagger - \mu b_r^\dagger b_q)|\psi\rangle$$

to have the second sum zero for all states $|\psi\rangle$ and all $\alpha \to \beta$ transformations we require $\underline{b_q b_r^\dagger - \mu b_r^\dagger b_q = 0 \quad r \neq q}$ & $\underline{a_i a_j^\dagger - \mu a_j^\dagger a_i = 0}$ $i \neq j$

the first sum will be zero if $b_q b_q^\dagger - \mu b_q^\dagger b_q = c$ where c is independent of q since then

$$0 = c \sum_q \langle \alpha_i | \beta_q \rangle \langle \beta_q | \alpha_j \rangle = c\delta_{ij} = 0 \quad \text{for } i \neq j$$

hence $a_i a_i^\dagger - \mu a_i^\dagger a_i = \sum_{qr} \langle \alpha_i | \beta_q \rangle \langle \beta_r | \alpha_i \rangle (b_q b_r^\dagger - \mu b_r^\dagger b_q) = \sum_q \langle \alpha_i | \beta_q \rangle \langle \beta_q | \alpha_i \rangle (b_q b_q^\dagger - \mu b_q^\dagger b_q)$

(i not summed)

$$= c\delta_{ii} = c \qquad \boxed{a_i a_i^\dagger - \mu a_i^\dagger a_i = c}$$

consider $c|0\rangle = (a_i a_i^\dagger - \mu a_i^\dagger a_i)|0\rangle = a_i a_i^\dagger |0\rangle = |0\rangle \Rightarrow \underline{c = 1}$ $\boxed{a_i a_i^\dagger - \mu a_i^\dagger a_i = 1}$

We can define an occupation number operator, N_i which counts the number of particles having the quantum numbers α_i.
The total number of particles with any quantum numbers, $N = \sum_i N_i$.
This shouldn't change if we use a different single particle basis $\alpha \to \beta$

$$N = \sum_i N_i \to N = \sum_q \tilde{N}_q$$

The operator that does the trick is $N_i = a_i^\dagger a_i$

$$\left(\begin{aligned} \sum_i N_i &= \sum_i a_i^\dagger a_i = \sum_i \sum_{qr} \langle \beta_q | \alpha_i \rangle \langle \alpha_i | \beta_r \rangle b_q^\dagger b_r \\ &= \sum_{qr} \delta_{qr} b_q^\dagger b_r = \sum_q b_q^\dagger b_q = \sum_q \tilde{N}_q \end{aligned} \right)$$

It is easy to show that $[N_i, a_k] = [N_i, a_k^\dagger] = 0$ $(i \neq k)$

consider $N_i a_i |\dots n_i \dots\rangle = N_i k_i |\dots n_i - 1 \dots\rangle = k_i (n_i - 1) |\dots n_i - 1 \dots\rangle$

& $a_i N_i |\dots n_i \dots\rangle = n_i a_i |\dots n_i \dots\rangle = k_i n_i \cdot |\dots n_i - 1 \dots\rangle$

$\Rightarrow [N_i, a_i] |\dots n_i \dots\rangle = -k_i |\dots n_i - 1 \dots\rangle = -a_i |\dots n_i \dots\rangle$

$$\Rightarrow \underline{[N_i, a_i] = -a_i} \qquad \& \qquad \underline{[N_i, a_i^\dagger] = +a_i^\dagger}$$

now if $a_i a_j^\dagger - \mu a_j^\dagger a_i = 0$ & $[N_i, a_k] = 0$

$$\begin{aligned} 0 = N_i a_k - a_k N_i &= a_i^\dagger a_i a_k - a_k a_i^\dagger a_i = a_i^\dagger a_i a_k - \mu a_i^\dagger a_k a_i \\ &= a_i^\dagger a_i a_k - \mu a_i^\dagger a_i a_k (\pm) = (1 \mp \mu) a_i^\dagger a_i a_k = (1 \mp \mu) N_i a_k \end{aligned}$$

$\Rightarrow$ in order to be always zero we must have $\mu = \pm 1$ & thus we have the two possible forms of quantum statistics :

<u>Bose-Einstein</u>	<u>Fermi-Dirac</u>
$[a_i^\dagger, a_j^\dagger] = [a_i, a_j] = 0$	$\{a_i^\dagger, a_j^\dagger\} = \{a_i, a_j\} = 0$
$[a_i, a_j^\dagger] = \delta_{ij}$	$\{a_i, a_j^\dagger\} = \delta_{ij}$

NB $\{a_i^\dagger, a_i^\dagger\} = 2a_i^\dagger a_i^\dagger = 0$ $\Rightarrow$ can never put two fermions in the same quantum state $\rightarrow$ "Pauli exclusion principle"

BOSONS: $\boxed{\hbar = 1}$

a many boson state (spin-0) $|\{N_{\vec p}\}\rangle = \prod_{\vec p} \frac{1}{\sqrt{N_{\vec p}!}} (a^{+}_{\vec p})^{N_{\vec p}} |0\rangle$ (A)

↑ occupation numbers

$$\hat N_{\vec q} |\{N_{\vec p}\}\rangle = \prod_{\vec p \neq \vec q} \frac{1}{\sqrt{N_{\vec p}!}} (a^{+}_{\vec p})^{N_{\vec p}} \frac{1}{\sqrt{N_{\vec q}!}} \hat N_{\vec q} (a^{+}_{\vec q})^{N_{\vec q}} |0\rangle$$

$$[\hat N_{\vec q}, a^{+}_{\vec q}] = a^{+}_{\vec q} \Rightarrow [\hat N_{\vec q}, (a^{+}_{\vec q})^2] = a^{+}_{\vec q} [\hat N_{\vec q}, a^{+}_{\vec q}] + [\hat N_{\vec q}, a^{+}_{\vec q}] a^{+}_{\vec q} = 2(a^{+}_{\vec q})^2$$

$$\cdots \Rightarrow [N_{\vec q}, (a^{+}_{\vec q})^n] = n(a^{+}_{\vec q})^n$$

$$\hat N_{\vec q} |\{N_{\vec p}\}\rangle = \prod_{\vec p \neq \vec q} \frac{1}{\sqrt{N_{\vec p}!}} (a^{+}_{\vec p})^{N_{\vec p}} \cdot \frac{1}{\sqrt{N_{\vec q}!}} \left(N_{\vec q} (a^{+}_{\vec q})^{N_{\vec q}} + (a^{+}_{\vec q})^{N_{\vec q}} \hat N_{\vec q} \right) |0\rangle \qquad \hat N_{\vec q} |0\rangle = 0$$

$$\boxed{\hat N_{\vec q} |\{N_{\vec p}\}\rangle = N_{\vec q} |\{N_{\vec p}\}\rangle}$$

this state is symmetric under the exchange of any two bosons since the a^{+} commute,

e.g. $|\vec p_1 \vec p_2\rangle \equiv a^{+}_{\vec p_1} a^{+}_{\vec p_2} |0\rangle = +a^{+}_{\vec p_2} a^{+}_{\vec p_1} |0\rangle = +|\vec p_2 \vec p_1\rangle$

---

observables can be constructed from the $a_{\vec p}$ & $a^{+}_{\vec p}$ - in the case of particle number conserving operators we'll have an equal number of a & a^{+},

e.g. the total momentum of the many-boson system

$$\vec P = \sum_{\vec p} \vec p\, a^{+}_{\vec p} a_{\vec p} = \sum_{\vec p} \vec p\, \hat N_{\vec p}$$

---

clearly our many-boson state (A) is an eigenstate of this operator $\vec P |\{N_{\vec p}\}\rangle = \sum_{\vec p} \vec p N_{\vec p} |\{N_{\vec p}\}\rangle$

∴ it is easy to show that the action of $a^{+}_{\vec q}$ is to increase the momentum of a state by $\vec q$:

$$\vec P a^{+}_{\vec q} = \sum_{\vec p} \vec p \hat N_{\vec p} a^{+}_{\vec q} = \left(\sum_{\vec p \neq \vec q} \vec p \hat N_{\vec p} + \vec q \hat N_{\vec q} \right) a^{+}_{\vec q} = a^{+}_{\vec q} \sum_{\vec p \neq \vec q} \vec p \hat N_{\vec p} + \vec q \left(a^{+}_{\vec q} + a^{+}_{\vec q} \hat N_{\vec q} \right)$$

$$= a^{+}_{\vec q} \left(\sum_{\vec p \neq \vec q} \vec p \hat N_{\vec p} + \vec q (\hat N_{\vec q} + 1) \right)$$ such that $\vec P a^{+}_{\vec q} |\{N_{\vec p}\}\rangle = \left(\sum_{\vec p \neq \vec q} \vec p N_{\vec p} + \vec q (N_{\vec q} + 1) \right) a^{+}_{\vec q} |\{N_{\vec p}\}\rangle$

& similarly $a_{\vec q}$ reduces the momentum by $\vec q$.

for a set of non-interacting spin-0 bosons then, we'd write the Hamiltonian

as
$$H = \sum_{\vec{p}} \frac{|\vec{p}|^2}{2m} a^\dagger_{\vec{p}} a_{\vec{p}} = \sum_{\vec{p}} \frac{|\vec{p}|^2}{2m} \hat{N}_{\vec{p}} .$$

But recall that in quantum mechanics, all bases are equivalent provided they can be related by a unitary transform, so there's nothing special about the momentum basis.
E.g. let's consider the position-space basis, where we can define a set of operators

$$\underline{\hat{\psi}(\vec{x}) \equiv \frac{1}{\sqrt{V}} \sum_{\vec{p}} e^{i\vec{p}\cdot\vec{x}} a_{\vec{p}}} \quad \& \text{ therefore } \quad \hat{\psi}^\dagger(\vec{x}) \equiv \frac{1}{\sqrt{V}} \sum_{\vec{p}} e^{-i\vec{p}\cdot\vec{x}} a^\dagger_{\vec{p}}$$

which can be named <u>Bose</u> <u>field</u> operators. (Remember the finite spatial volume renders the momenta discrete. $\vec{p} = \frac{2\pi}{L}\vec{n}$)

Since $\frac{1}{V}\int_V d^3\vec{x}\, e^{-i(\vec{p}-\vec{p}')\cdot\vec{x}} = \delta_{\vec{p},\vec{p}'}$ we have inverse relations

$$\underline{a_{\vec{p}} = \frac{1}{\sqrt{V}} \int d^3\vec{x}\, e^{-i\vec{p}\cdot\vec{x}} \hat{\psi}(\vec{x})} \quad , \quad a^\dagger_{\vec{p}} = \frac{1}{\sqrt{V}} \int d^3\vec{x}\, e^{i\vec{p}\cdot\vec{x}} \hat{\psi}^\dagger(\vec{x})$$

in a finite volume, the plane waves with discrete $\vec{p}$ are complete: $\frac{1}{V}\sum_{\vec{p}} e^{i(\vec{x}-\vec{x}')\cdot\vec{p}} = \delta(\vec{x}-\vec{x}')$

let's consider $[\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{x}')] = \frac{1}{V}\sum_{\vec{p}\vec{q}} e^{i\vec{p}\cdot\vec{x}} e^{-i\vec{q}\cdot\vec{x}'} \underbrace{[a_{\vec{p}}, a^\dagger_{\vec{q}}]}_{\delta_{\vec{p}\vec{q}}} = \frac{1}{V}\sum_{\vec{p}} e^{i(\vec{x}-\vec{x}')\cdot\vec{p}} = \delta(\vec{x}-\vec{x}')$

$$\longrightarrow \boxed{\begin{gathered} [\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{x}')] = \delta(\vec{x}-\vec{x}') \\ [\hat{\psi}(\vec{x}), \hat{\psi}(\vec{x}')] = [\hat{\psi}^\dagger(\vec{x}), \hat{\psi}^\dagger(\vec{x}')] = 0 \end{gathered}}$$

BOSON FIELD COMMUTATION RELATIONS

notice that while the "number of particles with a given momentum" operator, $\hat{N}_{\vec{p}}$ is not simple in position space,

$$\hat{N}_{\vec{p}} = a^\dagger_{\vec{p}} a_{\vec{p}} = \frac{1}{V}\int d^3\vec{x}\, d^3\vec{x}'\, e^{i\vec{p}\cdot(\vec{x}-\vec{x}')} \hat{\psi}^\dagger(\vec{x})\hat{\psi}(\vec{x}')$$

the <u>total</u> number of particles operator, $\hat{N} = \sum_{\vec{p}} \hat{N}_{\vec{p}}$, is simple

$$\boxed{\hat{N} = \int d^3\vec{x}\, \hat{\psi}^\dagger(\vec{x})\hat{\psi}(\vec{x})}$$

it is easy to show that $[\hat{\psi}(\vec{x}), \hat{N}] = \hat{\psi}(\vec{x})$ & $[\hat{\psi}^\dagger(\vec{x}), \hat{N}] = -\hat{\psi}^\dagger(\vec{x})$

so $\hat{\psi}^\dagger(\vec{x})$ increases the number of particles by one : $\hat{N}|N\rangle = N|N\rangle$

$$\hat{N}\left(\hat{\psi}^\dagger(\vec{x})|N\rangle\right) = \hat{\psi}^\dagger(\vec{x})(\hat{N}+1)|N\rangle = (N+1)\left(\hat{\psi}^\dagger(\vec{x})|N\rangle\right)$$

& $\hat{\psi}(\vec{x})$ decreases the number by one.

given that $\hat{N} = \int d^3\vec{x}\, \hat{\psi}^\dagger(\vec{x})\hat{\psi}(\vec{x})$, it looks like $\hat{\psi}^\dagger(\vec{x})\hat{\psi}(\vec{x})$ is the number density operator in position space, which would suggest that $|\vec{x}\rangle \equiv \hat{\psi}^\dagger(\vec{x})|0\rangle$ is "one particle at posn $\vec{x}$"

this supposition seems reasonable since the one-particle momentum eigenstate $|\vec{p}\rangle = a_{\vec{p}}^\dagger|0\rangle$

and it combine as expected:
$$\langle\vec{x}|\vec{p}\rangle = \langle 0|\hat{\psi}(\vec{x})a_{\vec{p}}^\dagger|0\rangle$$
$$= \frac{1}{\sqrt{V}}\int_V d^3\vec{x}'\, \langle 0|\hat{\psi}(\vec{x})\, e^{+i\vec{p}\cdot\vec{x}'}\, \hat{\psi}^\dagger(\vec{x}')|0\rangle$$
$$= \frac{1}{\sqrt{V}}\int_V d^3\vec{x}'\, e^{i\vec{p}\cdot\vec{x}'}\, \langle 0|\left(\delta(\vec{x}-\vec{x}') + \hat{\psi}^\dagger(\vec{x}')\hat{\psi}(\vec{x})\right)|0\rangle$$
$$= \frac{1}{\sqrt{V}}\langle 0|0\rangle \int d^3\vec{x}'\, e^{i\vec{p}\cdot\vec{x}'}\,\delta(\vec{x}-\vec{x}') = \frac{1}{\sqrt{V}}e^{i\vec{p}\cdot\vec{x}}$$

also $\langle\vec{x}|\vec{x}'\rangle = \langle 0|\hat{\psi}(\vec{x})\hat{\psi}^\dagger(\vec{x}')|0\rangle = \delta(\vec{x}-\vec{x}')$ as expected.

consider the operator $\hat{N}_{\Delta V} \equiv \int_{\Delta V} d^3\vec{x}\, \hat{\psi}^\dagger(\vec{x})\hat{\psi}(\vec{x})$ which we suspect counts the number of particles in the volume ΔV :

$$\hat{N}_{\Delta V}\left(\hat{\psi}^\dagger(\vec{y})|0\rangle\right) = \int_{\Delta V} d^3\vec{x}\, \hat{\psi}^\dagger(\vec{x})\hat{\psi}(\vec{x})\, \hat{\psi}^\dagger(\vec{y})|0\rangle$$
$$= \begin{cases} 0 \text{ if } \vec{y} \text{ is not in the volume } \Delta V \\ \int_{\Delta V} d^3\vec{x}\, \hat{\psi}^\dagger(\vec{x})\left(\delta(\vec{x}-\vec{y}) + \hat{\psi}^\dagger(\vec{y})\hat{\psi}(\vec{x})\right)|0\rangle = \hat{\psi}^\dagger(\vec{y})|0\rangle \text{ if } \vec{y} \text{ is in the volume } \Delta V \end{cases}$$

so as expected $\hat{\psi}^\dagger(\vec{y})|0\rangle$ describes <u>one</u> particle at $\vec{y}$ since we can make ΔV so small it contains <u>only</u> the point $\vec{y}$.

an N-particle state can thus be constructed as $\prod_{i=1}^{N} \hat{\varphi}^\dagger(\vec{y}_i)|0\rangle$, and we can try

to relate our many-particle states to a conventional many-particle wavefunction, $\varphi_a(\vec{y}_1 \ldots \vec{y}_N)$:

consider the ket $|\varphi_a\rangle \equiv \frac{1}{\sqrt{N!}} \int d^3\vec{x}_1 \cdots d^3\vec{x}_N \; \varphi_a(\vec{x}_1 \ldots \vec{x}_N) \; \hat{\varphi}^\dagger(\vec{x}_1) \cdots \hat{\varphi}^\dagger(\vec{x}_N)|0\rangle$

completely symmetric function

then

$$\langle \varphi_b | \varphi_a \rangle = \frac{1}{N!} \int d^3\vec{x}_1 \ldots d^3\vec{x}_N \, d^3\vec{y}_1 \cdots d^3\vec{y}_N \; \varphi_b^*(\vec{y}_1 \cdots \vec{y}_N)\varphi_a(\vec{x}_1 \cdots \vec{x}_N)$$
$$\cdot \langle 0 | \hat{\varphi}(\vec{y}_N) \ldots \hat{\varphi}(\vec{y}_1) \, \hat{\varphi}^\dagger(\vec{x}_1) \ldots \hat{\varphi}^\dagger(\vec{x}_N) | 0 \rangle$$

but if φ_a, φ_b are ordinary wavefunctions we'd want

$$\langle \varphi_b | \varphi_a \rangle = \int d^3\vec{x}_1 \ldots d^3\vec{x}_N \; \varphi_b^*(\vec{x}_1 \ldots \vec{x}_N)\varphi_a(\vec{x}_1 \ldots \vec{x}_N)$$

so we need to evaluate $\langle 0 | \hat{\varphi}(\vec{y}_N) \ldots \hat{\varphi}(\vec{y}_1) \, \hat{\varphi}^\dagger(\vec{x}_1) \ldots \hat{\varphi}^\dagger(\vec{x}_N) | 0 \rangle$ which can be done by pushing the $\hat{\varphi}$ to the right until they act on the vacuum. It is illustrative to consider simple cases: e.g. 1 particle state $\langle 0 | \hat{\varphi}(\vec{y}_1)\hat{\varphi}^\dagger(\vec{x}_1)|0\rangle = \delta(\vec{y}_1 - \vec{x}_1)$

e.g. 2 particle state $\langle 0 | \hat{\varphi}(\vec{y}_2)\hat{\varphi}(\vec{y}_1)\hat{\varphi}^\dagger(\vec{x}_1)\hat{\varphi}^\dagger(\vec{x}_2)|0\rangle$

$$= \langle 0 | \hat{\varphi}(\vec{y}_2) \left(\hat{\varphi}^\dagger(\vec{x}_1)\hat{\varphi}(\vec{y}_1) + \delta(\vec{x}_1 - \vec{y}_1) \right) \hat{\varphi}^\dagger(\vec{x}_2) | 0 \rangle$$
$$= \delta(\vec{x}_1 - \vec{y}_1)\delta(\vec{x}_2 - \vec{y}_2) + \langle 0 | \hat{\varphi}(\vec{y}_2) \hat{\varphi}^\dagger(\vec{x}_1) \hat{\varphi}(\vec{y}_1) \hat{\varphi}^\dagger(\vec{x}_2) | 0 \rangle$$
$$= \delta(\vec{x}_1 - \vec{y}_1)\delta(\vec{x}_2 - \vec{y}_2) + \langle 0 | \hat{\varphi}(\vec{y}_2) \hat{\varphi}^\dagger(\vec{x}_1) \delta(\vec{y}_1 - \vec{x}_2) | 0 \rangle$$
$$= \delta(\vec{x}_1 - \vec{y}_1)\delta(\vec{x}_2 - \vec{y}_2) + \delta(\vec{y}_2 - \vec{x}_1)\delta(\vec{y}_1 - \vec{x}_2)$$

in general $\langle 0 | \hat{\varphi}(\vec{y}_N) \ldots \hat{\varphi}(\vec{y}_1) \, \hat{\varphi}^\dagger(\vec{x}_1) \ldots \hat{\varphi}^\dagger(\vec{x}_N) | 0 \rangle$

$$= \sum_{\mathbb{P}} \delta(\vec{y}_1 - \vec{x}_1) \ldots \delta(\vec{y}_N - \vec{x}_N)$$ where $\sum_{\mathbb{P}}$ sums over all $N!$ permutations of the N vectors $\{\vec{x}_1 \ldots \vec{x}_N\}$

$$\Rightarrow \langle \varphi_b | \varphi_a \rangle = \frac{1}{N!} \int d^3\vec{x}_1 \ldots d^3\vec{x}_N \, d^3\vec{y}_1 \ldots d^3\vec{y}_N \; \varphi_b^*(\vec{y}_1 \ldots \vec{y}_N)\varphi_a(\vec{x}_1 \ldots \vec{x}_N) \sum_{\mathbb{P}} \delta(\vec{y}_1 - \vec{x}_1) \ldots \delta(\vec{y}_N - \vec{x}_N)$$
$$= \frac{1}{N!} \int d^3\vec{x}_1 \ldots d^3\vec{x}_N \; \varphi_a(\vec{x}_1 \ldots \vec{x}_N) \sum_{\mathbb{P}} \varphi_b^*(\vec{x}_1 \ldots \vec{x}_N) \xrightarrow[\varphi\,\mathrm{sym}]{} \frac{N!}{N!} \int d^3\vec{x}_1 \ldots d^3\vec{x}_N \; \varphi_a(\vec{x}_1 \ldots \vec{x}_N)\varphi_b^*(\vec{x}_1 \ldots \vec{x}_N)$$

as demanded.

then correctly normalised N-particle position eigenkets are

$$|\vec{x}_1 \dots \vec{x}_N; N\rangle \equiv \frac{1}{\sqrt{N!}} \hat{\psi}^\dagger(\vec{x}_1) \dots \hat{\psi}^\dagger(\vec{x}_N)|0\rangle$$

& co-ordinate space wavefunctions are $\varphi_a(\vec{x}_1 \dots \vec{x}_N) = \langle \vec{x}_1 \dots \vec{x}_N; N | \varphi_a \rangle$

$$\hat{\psi}^\dagger(\vec{y})\,|\vec{x}_1 \dots \vec{x}_N; N\rangle = \frac{1}{\sqrt{N!}} \hat{\psi}^\dagger(\vec{y}) \hat{\psi}^\dagger(\vec{x}_1) \dots \hat{\psi}^\dagger(\vec{x}_N)|0\rangle$$

$$= \sqrt{N+1} \cdot \frac{1}{\sqrt{(N+1)!}} \hat{\psi}^\dagger(\vec{y}) \hat{\psi}^\dagger(\vec{x}_1) \dots \hat{\psi}^\dagger(\vec{x}_N)|0\rangle$$

$$\underline{\hat{\psi}^\dagger(\vec{y})|\vec{x}_1 \dots \vec{x}_N; N\rangle = \sqrt{N+1}\, |\vec{y}, \vec{x}_1 \dots \vec{x}_N; N+1\rangle}$$

$\hat{\psi}(\vec{y})\,|\vec{x}_1 \dots \vec{x}_N; N\rangle = 0$ if none of the $\vec{x}_i$ are equal to $\vec{y}$

$\neq 0$ otherwise where the commutator with the $\vec{x}_i = \vec{y}$ will give a $\delta(\vec{x}_i - \vec{y})$

$$= \frac{1}{\sqrt{N}} \sum_{s=1}^{N} \delta(\vec{x}_s - \vec{y})\,|\vec{x}_1 \dots \vec{x}_{s-1}\ \vec{x}_{s+1} \dots \vec{x}_N; N-1\rangle$$

eliminated the $\vec{x}_s$

$$\hat{\psi}^\dagger(\vec{y})\hat{\psi}(\vec{y}')\,|\vec{x}_1 \dots \vec{x}_N; N\rangle = \sum_{s=1}^{N} \delta(\vec{x}_s - \vec{y}')\,|\vec{x}_1 \dots \vec{x}_{s-1}\ \vec{y}\ \vec{x}_{s+1} \dots \vec{x}_N; N\rangle$$

replaced $\vec{x}_s$ with $\vec{y}$ (if there was an $\vec{x}_s$ equal to $\vec{y}'$)

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consider an operator that is a symmetric sum of one-particle observables (e.g. the linear momentum or angular momentum)

then in "wavefunction" quantum mechanics we'd have $\hat{F} = \sum_{i=1}^{N} \hat{f}_i$ where $\hat{f}_i$ acts only on the co-ordinates of particle i (e.g. $\hat{f}_2 = \hat{1}_1 \otimes \hat{f}_2 \otimes \hat{1}_3 \cdots \hat{1}_N$)

Symmetrised posn eigenket $|\vec{x}_1 \dots \vec{x}_N\rangle_S = \frac{1}{\sqrt{N!}} \sum_{P} |x_1\rangle_1 \dots |x_N\rangle_N$ ($|\vec{x}\rangle_i$ is a posn eigenket for particle i)

$$\hat{F}|\vec{x}_1 \dots \vec{x}_N\rangle_S = \frac{1}{\sqrt{N!}} \sum_{P} \underbrace{\int d^3\vec{y}\ |\vec{y}\rangle_1\, {}_1\langle \vec{y}|}_{\text{complete set of particle \#1 posn eigenkets}} \hat{f}_1 |\vec{x}_1\rangle_1\ |x_2\rangle_2 \cdots |x_N\rangle_N$$

$$+ \frac{1}{\sqrt{N!}} \sum_{P} \int d^3\vec{y}\ |\vec{y}\rangle_2\, {}_2\langle \vec{y}| f_2 |\vec{x}_2\rangle_2\ |\vec{x}_1\rangle_1 |\vec{x}_3\rangle_3 \dots |\vec{x}_N\rangle_N$$

$$+ \dots$$

but ${}_i\langle \vec{y}|\hat{f}_i|\vec{x}\rangle_i$ are the same for all i since the particles are identical,

call them $\langle \vec{y}|\hat{f}|\vec{x}\rangle$ & thus

$$\hat{F}\,|\vec{x}_1 \ldots \vec{x}_N\rangle_S = \int d^3\vec{y} \sum_{s=1}^{N} |\vec{x}_1 \ldots \vec{x}_{s-1}\,\vec{y}\,\vec{x}_{s+1} \ldots \vec{x}_N\rangle\,\langle \vec{y}|\hat{f}|\vec{x}_s\rangle$$

but we already found that

$$\hat{\psi}^{\dagger}(\vec{y})\,\hat{\psi}(\vec{y}\,')\,|\vec{x}_1 \ldots \vec{x}_N; N\rangle = \sum_{s=1}^{N} \delta(\vec{x}_s - \vec{y}\,')\,|\vec{x}_1 \ldots \vec{x}_{s-1}\,\vec{y}\,\vec{x}_{s+1} \ldots x_N; N\rangle$$

so $\int d^3\vec{y}\,d^3\vec{y}\,'\,\hat{\psi}^{\dagger}(\vec{y})\,\langle \vec{y}|\hat{f}|\vec{y}\,'\rangle\,\hat{\psi}(\vec{y}\,')\,|\vec{x}_1 \ldots \vec{x}_N; N\rangle$

$$= \int d^3\vec{y} \sum_{s=1}^{N} |\vec{x}_1 \ldots \vec{x}_{s-1}\,\vec{y}\,\vec{x}_{s+1} \ldots \vec{x}_N\rangle\,\langle \vec{y}|\hat{f}|\vec{x}_s\rangle = \hat{F}\,|\vec{x}_1 \ldots \vec{x}_N; N\rangle$$

&
$$\boxed{\hat{F} = \int d^3\vec{x}\,d^3\vec{x}\,'\,\hat{\psi}^{\dagger}(\vec{x}\,')\,\langle \vec{x}\,'|\hat{f}|\vec{x}\rangle\,\hat{\psi}(\vec{x})}$$

additive single particle operator

annihilate particle at $\vec{x}$

create a particle at $\vec{x}\,'$

amplitude for the process.

similarly we can show the following representation for symmetric sums of <u>two-body</u> operators $\left(\hat{G} = \sum_{i>j} \hat{g}_{ij} = \frac{1}{2}\sum_{i\neq j} \hat{g}_{ij}\right)$

for two-particle (<u>unsymmetrized</u>) matrix elements $\langle \vec{x}_1\,\vec{x}_2|\hat{g}|\vec{x}_1\,'\vec{x}_2\,'\rangle$ the operator is

$$\boxed{\hat{G} = \frac{1}{2}\int d^3\vec{x}_1\,d^3\vec{x}_2\,d^3\vec{x}_1\,'\,d^3\vec{x}_2\,'\;\hat{\psi}^{\dagger}(\vec{x}_1)\,\hat{\psi}^{\dagger}(\vec{x}_2)\,\langle \vec{x}_1\,\vec{x}_2|\hat{g}|\vec{x}_1\,'\vec{x}_2\,'\rangle\,\hat{\psi}(\vec{x}_2\,')\,\hat{\psi}(\vec{x}_1\,')}$$

examples: * total momentum in position space:

$$\text{since } -i\vec{\nabla}_{\vec{x}}\hat{\psi}(\vec{x}) = -i\vec{\nabla}_{\vec{x}}\frac{1}{\sqrt{V}}\sum_{\vec{p}} e^{i\vec{p}\cdot\vec{x}}a_{\vec{p}} = \frac{1}{\sqrt{V}}\sum_{\vec{p}}\vec{p}\,e^{i\vec{p}\cdot\vec{x}}a_{\vec{p}}$$

we have
$$\vec{P} = \int d^3\vec{x}\,\hat{\psi}^\dagger(\vec{x})\left(-i\vec{\nabla}_{\vec{x}}\right)\hat{\psi}(\vec{x})$$

$$\left[\begin{aligned} &= \frac{1}{V}\sum_{\vec{p}\vec{q}}\int d^3\vec{x}\,e^{i\vec{p}\cdot\vec{x}}e^{-i\vec{q}\cdot\vec{x}}\,\vec{p}\,a^\dagger_{\vec{q}}a_{\vec{p}} \\ &= \sum_{pq}\delta_{pq}\,\vec{p}\,a^\dagger_{\vec{q}}a_{\vec{p}} = \sum_{\vec{p}}\vec{p}\,a^\dagger_{\vec{p}}a_{\vec{p}} \checkmark \end{aligned} \right]$$

$$\langle\vec{x}'|\hat{p}|\vec{x}\rangle = \delta(\vec{x}'-\vec{x})\left(-i\vec{\nabla}_{\vec{x}}\right)$$

& the kinetic energy
$$K = -\frac{1}{2m}\int d^3\vec{x}\;\hat{\psi}^\dagger(\vec{x})\,\vec{\nabla}^2_{\vec{x}}\,\psi(\vec{x})$$

* coulomb energy between two particles of electric charge e:

$$\langle\vec{x}_1\vec{x}_2|\hat{g}|\vec{x}_1'\vec{x}_2'\rangle = \frac{e^2}{|\vec{x}_1-\vec{x}_2|}\,\delta(\vec{x}_1-\vec{x}_1')\,\delta(\vec{x}_2-\vec{x}_2') \qquad \text{(a local potential)}$$

$$\Rightarrow V_c = \frac{1}{2}e^2\int d^3\vec{x}_1\,d^3\vec{x}_2\,\frac{1}{|\vec{x}_1-\vec{x}_2|}\,\hat{\psi}^\dagger(\vec{x}_1)\,\hat{\psi}^\dagger(\vec{x}_2)\cdot\psi(\vec{x}_2)\,\psi(\vec{x}_1)$$

So we've formulated our many-particle quantum mechanics in two representations, position & momentum space. But remember there are an infinite number of other choices:

let $\{u_\nu(\vec{x})\}$ be any complete, orthonormal set of <u>one-particle</u> wavefunctions

& define
$$\hat{b}_\nu = \int d^3\vec{x}\,u^*_\nu(\vec{x})\,\hat{\psi}(\vec{x}) \quad\rightarrow\quad \hat{b}^\dagger_\nu = \int d^3x\,u_\nu(\vec{x})\,\hat{\psi}^\dagger(\vec{x})$$

then
$$[\hat{b}_\nu,\hat{b}^\dagger_{\nu'}] = \int d^3\vec{x}\,d^3\vec{x}'\,u^*_\nu(\vec{x})\,u_{\nu'}(\vec{x}')\,\underbrace{[\hat{\psi}(\vec{x}),\hat{\psi}^\dagger(\vec{x}')]}_{\delta(\vec{x}-\vec{x}')} = \int d^3x\,u^*_\nu(\vec{x})\,u_{\nu'}(\vec{x}) = \delta_{\nu\nu'}$$

$$\boxed{\begin{aligned}&[\hat{b}_\nu,\hat{b}^\dagger_{\nu'}] = \delta_{\nu\nu'}\\ &[\hat{b}_\nu,\hat{b}_{\nu'}] = [\hat{b}^\dagger_\nu,\hat{b}^\dagger_{\nu'}] = 0\end{aligned}}$$

$$\& \quad \hat{F} = \sum_{\nu\nu'}\hat{b}^\dagger_\nu\,\langle\nu|\hat{f}|\nu'\rangle\,\hat{b}_{\nu'}$$

$$\hat{G} = \frac{1}{2}\sum_{\substack{\nu_1\nu_2\\ \nu_1'\nu_2'}}\hat{b}^\dagger_{\nu_1}\hat{b}^\dagger_{\nu_2}\,\langle\nu_1\nu_2|\hat{g}|\nu_1'\nu_2'\rangle\,\hat{b}_{\nu_2'}\,\hat{b}_{\nu_1'}$$

FERMIONS:

here the occupation of any single-particle state can be only 0 or 1 - the "exclusion principle".

we already know that $\{a_\nu^\dagger, a_{\nu'}\} = \delta_{\nu\nu'}$ & $\{a_\nu, a_{\nu'}\} = 0$

& the number operator $\hat{N}_\nu = a_\nu^\dagger a_\nu$ has eigenvalues of zero & 1.

$$[a_\nu, \hat{N}_{\nu'}] = a_\nu \delta_{\nu\nu'} \quad ; \quad [a_\nu^\dagger, \hat{N}_{\nu'}] = -a_\nu^\dagger \delta_{\nu\nu'}$$

a many fermion state is $|\{N_\nu\}\rangle = \prod_\nu (a_\nu^\dagger)^{N_\nu} |0\rangle$ where $N_\nu = 0$ or 1

& where we require an ordering prescription for the $a_{\nu_1}^\dagger a_{\nu_2}^\dagger \cdots$

define posn space field operators:

$$\hat{\psi}_s(\vec{x}) = \sum_\nu a_\nu \langle \nu | \vec{x} s \rangle \quad , \quad \hat{\psi}_s^\dagger(\vec{x}) = \sum_\nu a_\nu^\dagger \langle \vec{x} s | \nu \rangle \quad \text{(for spin projection, } s\text{)}$$

then $\{\hat{\psi}_s(\vec{x}), \hat{\psi}_{s'}^\dagger(\vec{x}')\} = \delta_{ss'} \delta(\vec{x}-\vec{x}')$; $\{\hat{\psi}_s(\vec{x}), \hat{\psi}_{s'}(\vec{x}')\} = 0$

& $\langle 0 | \hat{\psi}_{s_N'}(\vec{x}_N') \cdots \hat{\psi}_{s_1'}(\vec{x}_1') \hat{\psi}_{s_1}^\dagger(\vec{x}_1) \cdots \hat{\psi}_{s_N}^\dagger(\vec{x}_N) | 0 \rangle$

$$= \sum_{\mathbb{P}} \epsilon_{\mathbb{P}} \prod_{i=1}^N \delta_{s_i s_i'} \delta(\vec{x}_i - \vec{x}_i')$$

signature of permutation (-1 for each swap)

permutations of $\{\vec{x}_1 \ldots \vec{x}_N\}$

for an N-particle antisymmetric wavefunction $\varphi_a(\vec{x}_1 s_1 \ldots \vec{x}_N s_N)$, the many-particle ket is

$$|\varphi_a\rangle = \frac{1}{\sqrt{N!}} \int d^3\vec{x}_1 \cdots d^3\vec{x}_N \sum_{s_1 \ldots s_N} \varphi_a(\vec{x}_1 s_1 \cdots \vec{x}_N s_N) \hat{\psi}_{s_1}^\dagger(\vec{x}_1) \cdots \hat{\psi}_{s_N}^\dagger(\vec{x}_N) |0\rangle$$

operators are as in the Bose case:

$$\hat{F} = \sum_{ss'} \int d^3\vec{x}\, d^3\vec{x}'\, \hat{\psi}_{s'}^\dagger(\vec{x}') \langle \vec{x}' s' | \hat{f} | \vec{x} s \rangle \hat{\psi}_s(\vec{x})$$

$$\hat{G} = \frac{1}{2} \sum_{s_1 s_2 s_1' s_2'} \int d^3\vec{x}_1 d^3\vec{x}_2 d^3\vec{x}_1' d^3\vec{x}_2'\, \hat{\psi}_{s_1}^\dagger(\vec{x}_1) \hat{\psi}_{s_2}^\dagger(\vec{x}_2) \langle \vec{x}_1 s_1 \vec{x}_2 s_2 | \hat{g} | \vec{x}_1' s_1' \vec{x}_2' s_2' \rangle \hat{\psi}_{s_2'}(\vec{x}_2') \hat{\psi}_{s_1'}(\vec{x}_1')$$

CLOSED FERMION SHELLS HAVE ANG. MOM ZERO

$$\vec{J} = \sum_j \sum_{mm'} a^\dagger_{jm'} a_{jm} \langle jm' | \vec{J} | jm \rangle$$

$$|\text{closed}\rangle = \prod_{m=-j}^{j} a^\dagger_{jm} |0\rangle = a^\dagger_{jj} a^\dagger_{jj-1} \ldots a^\dagger_{j-j+1} a^\dagger_{j-j} |0\rangle$$

$$\vec{J}|\text{closed}\rangle = \sum_J \sum_{MM'} \langle JM' | \vec{J} | JM \rangle a^\dagger_{JM'} a_{JM} \; a^\dagger_{jj} a^\dagger_{j,j-1} \ldots a^\dagger_{j,-j+1} a^\dagger_{j-j} |0\rangle$$

$$= \sum_J \sum_{MM'} \langle JM' | \vec{J} | JM \rangle a^\dagger_{JM'} \Big(\delta_{Jj} \delta_{Mj} a^\dagger_{j,j-1} \ldots |0\rangle$$
$$- \delta_{Jj} \delta_{M,j-1} a^\dagger_{jj} a^\dagger_{jj-2} \ldots |0\rangle$$
$$+ \delta_{Jj} \delta_{M,j-2} a^\dagger_{jj} a^\dagger_{jj-1} a^\dagger_{jj-3} \ldots |0\rangle$$
$$- \ldots$$
$$+ \delta_{Jj} \delta_{M,-j} a^\dagger_{jj} a^\dagger_{jj-1} \ldots a^\dagger_{j,-j+1} |0\rangle \Big)$$

$$\langle JM' | \vec{J} | JM \rangle = \tfrac{1}{2}(\hat{x} + i\hat{y}) \langle JM' | J_- | JM \rangle = \tfrac{1}{2}(\hat{x}+i\hat{y}) \hbar \sqrt{J(J+1) + M(M-1)}\; \delta_{M',M-1}$$
$$+ \tfrac{1}{2}(\hat{x} - i\hat{y}) \langle JM' | J_+ | JM \rangle \qquad + \tfrac{1}{2}(\hat{x} \mp i\hat{y}) \hbar \sqrt{J(J+1) + M(M+1)}\; \delta_{M',M+1}$$
$$+ \hat{z} \langle JM' | J_z | JM \rangle \qquad + \hat{z} \hbar M \delta_{M'M}$$

$$\vec{J}|\text{closed}\rangle = \sum_{M'} \langle jM' | \vec{J} | j,j \rangle a^\dagger_{jM'} a^\dagger_{j,j-1} \ldots |0\rangle$$
$$- \sum_{M'} \langle jM' | \vec{J} | j,j-1 \rangle a^\dagger_{jM'} a^\dagger_{jj} a^\dagger_{jj-2} \ldots |0\rangle$$
$$+ \sum_{M'} \langle jM' | \vec{J} | j,j-2 \rangle a^\dagger_{jM'} a^\dagger_{jj} \ldots |0\rangle$$
$$\vdots$$
$$+ \sum_{M'} \langle jM' | \vec{J} | j,-j \rangle a^\dagger_{jM'} a^\dagger_{jj} \ldots a^\dagger_{j,-j+1} |0\rangle$$

the raising & lowering action produces a duplicate $a^\dagger_{jm}$ so for fermions this would give zero - only the $\hat{z}$ terms survive

$$= \hat{z}\hbar \Big(j|\text{closed}\rangle + (j-1)|\text{closed}\rangle + (j-2)|\text{closed}\rangle + \ldots - j|\text{closed}\rangle \Big)$$

$$= \underline{\underline{0}}$$

Suppose a single m value is missing, can make this state as

$|m\text{-hole}\rangle \propto a_{jm}\,|\text{closed}\rangle$ (up to a normalisation)

$$\hat{J}_z\left(a_{jm}|\text{closed}\rangle\right)$$

$$= a_{jm}\left(\hat{J}_z - \hbar m\right)|\text{closed}\rangle$$

$$= -\hbar m\left(a_{jm}|\text{closed}\rangle\right)$$

$$\left[J_z, a_{jm}\right] = \sum_J \sum_{MM'} \left[a^\dagger_{JM'} a_{JM}\, \hbar M \delta_{M'M}, a_{jm}\right]$$

$$= \sum_J \sum_{M} \hbar M \left[a^\dagger_{JM} a_{JM}, a_{jm}\right]$$

$$= \sum_J \sum_M \hbar M\, \delta_{Jj}\left(-a_{jm}\delta_{Mm}\right)$$

$$= -\hbar m\, a_{jm}$$

~~to be conventionally normalis~~

$$\left[a_{jm}, a^\dagger_{jm'}\right] = \delta_{mm'}$$

$$a_{jm}\; a^\dagger_{jj}\; a^\dagger_{j,j-1} \cdots a^\dagger_{j-j}\,|0\rangle$$

	sign	$(-1)^{m-j}$
$m=j$	$+1$	$+1$
$m=j-1$	-1	-1
$m=j-2$	$+1$	$+1$

$\Rightarrow$ conventional sign requires $(-1)^{j-m}$

DYNAMICS

we'll use the Heisenberg picture in which operators time evolve,

e.g. $\hat{\Psi}(\underset{\sim}{x}t) = e^{iHt}\,\hat{\Psi}(\underset{\sim}{x})\,e^{-iHt}$ where $\underset{\sim}{x} = (\vec{x}, s)$ if the particles have spin

N.B this unitary transformation does not change the field (anti) commutators

$$\text{e.g. } \left\{\hat{\Psi}^{\dagger}(\underset{\sim}{x}t), \hat{\Psi}(\underset{\sim}{x}'t)\right\} = \hat{\Psi}^{\dagger}(\underset{\sim}{x}t)\hat{\Psi}(\underset{\sim}{x}'t) + \hat{\Psi}(\underset{\sim}{x}'t)\hat{\Psi}^{\dagger}(\underset{\sim}{x}t)$$

$$= e^{iHt}\hat{\Psi}^{\dagger}(\underset{\sim}{x})e^{-iHt}e^{iHt}\hat{\Psi}(\underset{\sim}{x}')e^{-iHt}$$

$$+ e^{iHt}\hat{\Psi}(\underset{\sim}{x}')e^{-iHt}e^{iHt}\hat{\Psi}^{\dagger}(\underset{\sim}{x})e^{-iHt}$$

$$= e^{iHt}\left\{\hat{\Psi}^{\dagger}(\underset{\sim}{x}), \hat{\Psi}(\underset{\sim}{x}')\right\}e^{-iHt} = \delta(\underset{\sim}{x}-\underset{\sim}{x}') \quad \left(= \delta(\vec{x}-\vec{x}')\delta_{ss'}\right)$$

dynamics follow from the time-derivative

$$i\frac{d}{dt}\hat{\Psi}(\underset{\sim}{x},t) = i\left(iH\,e^{iHt}\hat{\Psi}(\underset{\sim}{x})e^{-iHt} + e^{iHt}\hat{\Psi}(\underset{\sim}{x})e^{-iHt}(-iH)\right)$$

$$\boxed{i\dot{\hat{\Psi}}(\underset{\sim}{x},t) = \left[\hat{\Psi}(\underset{\sim}{x}t), H\right]}$$ equation of motion for the field $\hat{\Psi}$

suppose H has the form $H = K + U + V$

$$V = \frac{1}{2}\int d\underset{\sim}{x}_1 d\underset{\sim}{x}_2 d\underset{\sim}{x}_1' d\underset{\sim}{x}_2'\, \hat{\Psi}^{\dagger}(\underset{\sim}{x}_1)\hat{\Psi}^{\dagger}(\underset{\sim}{x}_2)\langle \underset{\sim}{x}_1\underset{\sim}{x}_2|V|\underset{\sim}{x}_1'\underset{\sim}{x}_2'\rangle\hat{\Psi}(\underset{\sim}{x}_2')\hat{\Psi}(\underset{\sim}{x}_1')$$

two-body interactions

$$K = -\frac{1}{2m}\int d\underset{\sim}{x}\, \hat{\Psi}^{\dagger}(\underset{\sim}{x})\nabla^2\hat{\Psi}(\underset{\sim}{x})$$

kinetic energy

$$U = \int d\underset{\sim}{x}d\underset{\sim}{x}'\, \hat{\Psi}^{\dagger}(\underset{\sim}{x})\langle\underset{\sim}{x}|u|\underset{\sim}{x}'\rangle\hat{\Psi}(\underset{\sim}{x}')$$

one body potential - interaction with a static <u>external</u> field

$$[A, BC] = \{A,B\}C - B\{A,C\}$$

$$[\hat{\Psi}(\underset{\sim}{y}), K] = -\frac{1}{2m}\int d\underset{\sim}{x}\,[\hat{\Psi}(\underset{\sim}{y}), \hat{\Psi}^{\dagger}(\underset{\sim}{x})\nabla_x^2\hat{\Psi}(\underset{\sim}{x})] = -\frac{1}{2m}\int d\underset{\sim}{x}\left(\{\hat{\Psi}(\underset{\sim}{y}),\hat{\Psi}^{\dagger}(\underset{\sim}{x})\}\nabla^2\hat{\Psi}(\underset{\sim}{x}) - \hat{\Psi}^{\dagger}_{(\underset{\sim}{x})}\nabla_x^2\{\hat{\Psi}(\underset{\sim}{y}),\hat{\Psi}(\underset{\sim}{x})\}\right)$$

$$\underline{[\hat{\Psi}(\underset{\sim}{y}), K] = -\frac{1}{2m}\nabla^2\hat{\Psi}(\underset{\sim}{y})}$$

similarly $\underline{[\hat{\Psi}(\underset{\sim}{y}), U] = \int d\underset{\sim}{x}'\,\langle\underset{\sim}{y}|u|\underset{\sim}{x}'\rangle\hat{\Psi}(\underset{\sim}{x}')}$

$$\hat{\varphi}(y)\,V = \hat{\varphi}(y)\tfrac{1}{2}\int d\underset{\sim}{x}_1 d\underset{\sim}{x}_2 d\underset{\sim}{x}_1' d\underset{\sim}{x}_2'\ \hat{\varphi}^\dagger(\underset{\sim}{x}_1)\hat{\varphi}^\dagger(\underset{\sim}{x}_2)\,\hat{\varphi}(\underset{\sim}{x}_2')\hat{\varphi}(\underset{\sim}{x}_1')\ \langle \underset{\sim}{x}_1\underset{\sim}{x}_2|v|\underset{\sim}{x}_1'\underset{\sim}{x}_2'\rangle$$

push $\hat{\varphi}(y)$ through the other field ops

$$= \tfrac{1}{2}\int d\underset{\sim}{x}_1 d\underset{\sim}{x}_2 d\underset{\sim}{x}_1' d\underset{\sim}{x}_2'\ \langle \underset{\sim}{x}_1\underset{\sim}{x}_2|v|\underset{\sim}{x}_1'\underset{\sim}{x}_2'\rangle \Big(\delta(\underset{\sim}{y}-\underset{\sim}{x}_1)\,\hat{\varphi}^\dagger(\underset{\sim}{x}_2)\hat{\varphi}(\underset{\sim}{x}_2')\hat{\varphi}(\underset{\sim}{x}_1')$$
$$\pm\ \delta(\underset{\sim}{y}-\underset{\sim}{x}_2)\,\hat{\varphi}^\dagger(\underset{\sim}{x}_1)\hat{\varphi}(\underset{\sim}{x}_2')\hat{\varphi}(\underset{\sim}{x}_1') \qquad \left(\pm\ \begin{matrix}\text{boson}\\ \text{fermion}\end{matrix}\right)$$
$$+\ \hat{\varphi}^\dagger(\underset{\sim}{x}_1)\hat{\varphi}^\dagger(\underset{\sim}{x}_2)\hat{\varphi}(\underset{\sim}{x}_2')\,\hat{\varphi}(\underset{\sim}{x}_1')\,\hat{\varphi}(\underset{\sim}{y})\Big)$$

$$\Rightarrow\ [\hat{\varphi}(y), V] = \tfrac{1}{2}\int d\underset{\sim}{x}\, d\underset{\sim}{x}_1' d\underset{\sim}{x}_2' \Big(\langle \underset{\sim}{y}\,\underset{\sim}{x}|v|\underset{\sim}{x}_1'\underset{\sim}{x}_2'\rangle\, \hat{\varphi}^\dagger(\underset{\sim}{x})\hat{\varphi}(\underset{\sim}{x}_2')\hat{\varphi}(\underset{\sim}{x}_1')$$
$$\pm\ \langle \underset{\sim}{x}\,\underset{\sim}{y}|v|\underset{\sim}{x}_1'\underset{\sim}{x}_2'\rangle\, \hat{\varphi}^\dagger(\underset{\sim}{x})\hat{\varphi}(\underset{\sim}{x}_2')\hat{\varphi}(\underset{\sim}{x}_1')\Big)$$

NB we can absorb the $\pm$ signs by (anti) commuting $\hat{\varphi}(\underset{\sim}{x}_2')\hat{\varphi}(\underset{\sim}{x}_1')$

$$= \tfrac{1}{2}\int d\underset{\sim}{x}\, d\underset{\sim}{x}_1' d\underset{\sim}{x}_2'\ \hat{\varphi}^\dagger(\underset{\sim}{x})\Big(\langle \underset{\sim}{y}\,\underset{\sim}{x}|v|\underset{\sim}{x}_1'\underset{\sim}{x}_2'\rangle\, \hat{\varphi}(\underset{\sim}{x}_2')\hat{\varphi}(\underset{\sim}{x}_1')$$
$$+\ \langle \underset{\sim}{x}\,\underset{\sim}{y}|v|\underset{\sim}{x}_1'\underset{\sim}{x}_2'\rangle\, \hat{\varphi}(\underset{\sim}{x}_1')\hat{\varphi}(\underset{\sim}{x}_2')$$

swapping dummy vars $\underset{\sim}{x}_1' \leftrightarrow \underset{\sim}{x}_2'$ in the second term

$$= \tfrac{1}{2}\int d\underset{\sim}{x}\, d\underset{\sim}{x}_1' d\underset{\sim}{x}_2'\ \hat{\varphi}^\dagger(\underset{\sim}{x})\Big(\langle \underset{\sim}{y}\,\underset{\sim}{x}|v|\underset{\sim}{x}_1'\underset{\sim}{x}_2'\rangle\, \hat{\varphi}(\underset{\sim}{x}_2')\hat{\varphi}(\underset{\sim}{x}_1')$$
$$+\ \langle \underset{\sim}{x}\,\underset{\sim}{y}|v|\underset{\sim}{x}_2'\underset{\sim}{x}_1'\rangle\, \hat{\varphi}(\underset{\sim}{x}_2')\hat{\varphi}(\underset{\sim}{x}_1')\Big)$$

$$= \tfrac{1}{2}\int d\underset{\sim}{x}\, d\underset{\sim}{x}_1' d\underset{\sim}{x}_2'\ \hat{\varphi}^\dagger(\underset{\sim}{x})\hat{\varphi}(\underset{\sim}{x}_2')\hat{\varphi}(\underset{\sim}{x}_1')\Big(\langle \underset{\sim}{y}\,\underset{\sim}{x}|v|\underset{\sim}{x}_1'\underset{\sim}{x}_2'\rangle + \langle \underset{\sim}{x}\,\underset{\sim}{y}|v|\underset{\sim}{x}_2'\underset{\sim}{x}_1'\rangle\Big)$$

but it is clear from the form of the interaction that if we exchange $\underset{\sim}{x} \leftrightarrow \underset{\sim}{y}$ and $\underset{\sim}{x}_1' \leftrightarrow \underset{\sim}{x}_2'$

there is no change $\Rightarrow \langle \underset{\sim}{x}\,\underset{\sim}{y}|v|\underset{\sim}{x}_2'\underset{\sim}{x}_1'\rangle = \langle \underset{\sim}{y}\,\underset{\sim}{x}|v|\underset{\sim}{x}_1'\underset{\sim}{x}_2'\rangle$

$$\&\ [\hat{\varphi}(y), V] = \int d\underset{\sim}{x}\, d\underset{\sim}{x}_1' d\underset{\sim}{x}_2'\ \hat{\varphi}^\dagger(\underset{\sim}{x})\hat{\varphi}(\underset{\sim}{x}_2')\hat{\varphi}(\underset{\sim}{x}_1')\,\langle \underset{\sim}{y}\,\underset{\sim}{x}|v|\underset{\sim}{x}_1'\underset{\sim}{x}_2'\rangle$$

$$\Rightarrow \; i\dot{\hat{\Psi}}(\underset{\sim}{x},t) = -\frac{1}{2m}\nabla^2\hat{\Psi}(\underset{\sim}{x},t) + \int d\underset{\sim}{x}' \langle \underset{\sim}{x}|u|\underset{\sim}{x}'\rangle \hat{\Psi}(\underset{\sim}{x}',t)$$

$$+ \int d\underset{\sim}{x}' d\underset{\sim}{x}_1' d\underset{\sim}{x}_2' \; \hat{\Psi}^{\dagger}(\underset{\sim}{x}'t) \langle \underset{\sim}{x}\,\underset{\sim}{x}'|v|\underset{\sim}{x}_1'\underset{\sim}{x}_2'\rangle \hat{\Psi}(\underset{\sim}{x}_1't)\,\hat{\Psi}(\underset{\sim}{x}_2't)$$

for spin-independent local potentials $\langle \underset{\sim}{x}|u|\underset{\sim}{x}'\rangle = \delta(\underset{\sim}{x}-\underset{\sim}{x}')\,U(\vec{x})$

$$\langle \underset{\sim}{x}_1\underset{\sim}{x}_2|v|\underset{\sim}{x}_1'\underset{\sim}{x}_2'\rangle = \delta(\underset{\sim}{x}_1-\underset{\sim}{x}_1')\,\delta(\underset{\sim}{x}_2-\underset{\sim}{x}_2')\,V(\vec{x}_1-\vec{x}_2)$$

$$\& \quad i\dot{\hat{\Psi}}(\underset{\sim}{x},t) = -\frac{1}{2m}\nabla^2\hat{\Psi}(\underset{\sim}{x}t) + U(\vec{x})\hat{\Psi}(\underset{\sim}{x}t) + V_{\text{eff}}(\vec{x}t)\hat{\Psi}(\underset{\sim}{x}t)$$

$$\left[V_{\text{eff}}(\vec{x}t) = \int d^3\vec{x}'\, V(\vec{x}-\vec{x}')\,\hat{N}(\vec{x}'t) \qquad \hat{N}(\vec{x}'t) = \sum_s \hat{\Psi}_s^{\dagger}(\vec{x}'t)\hat{\Psi}_s(\vec{x}'t) \right]$$

which looks like the Schrödinger eq^n except that the Veff term makes it <u>non-linear</u> in $\hat{\Psi}$.

- Solving such equations is, in general, rather difficult.
- approximation schemes such as "Hartree-Fock" form the basis of atomic physics calculations.

DEGENERATE ELECTRON GAS

(for more details see Fetter & Walecka "Quantum Theory of many-particle systems")

$$H_{\text{electrons}} = \sum_{i=1}^{N} \frac{1}{2m} p_i^2 + \frac{1}{2} e^2 \sum_{i \neq j}^{N} \frac{e^{-\mu |\vec{r}_i - \vec{r}_j|}}{|\vec{r}_i - \vec{r}_j|}$$

$$H_{\text{pos. bkg.}} = \frac{1}{2} e^2 \int d^3\vec{x}\, d^3\vec{x}'\; n_+(\vec{x}) n_+(\vec{x}') \frac{e^{-\mu|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}$$

$$H_{e^-;\,\text{pos. bkg.}} = -e^2 \sum_{i=1}^{N} \int d^3\vec{x}\; n_+(\vec{x}) \frac{e^{-\mu|\vec{x}-\vec{r}_i|}}{|\vec{x}-\vec{r}_i|}$$

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uniform +ve backgrd $n_+(\vec{x}) = N/V$

$$H_{\text{pos. bkg.}} = \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 \int d^3\vec{x}\, d^3\vec{x}'\; \frac{e^{-\mu|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} = \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 \int d^3\vec{X}\, d^3\vec{Y}\; \frac{e^{-\mu|\vec{X}|}}{|\vec{X}|} = \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 V \int d^3\vec{x}\; e^{-\mu|\vec{x}|}/|\vec{x}|$$

$$= \frac{1}{2} e^2 \frac{N^2}{V} \cdot 4\pi \int X^2 dX\, e^{-\mu X}/X = \frac{1}{2} e^2 \frac{N^2}{V} 4\pi \int_0 dX\; X e^{-\mu X} \rightarrow \underline{\frac{1}{2} e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}}$$

divergent as $\mu \to 0$ since all +ve charges interact over all distances

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$$H_{e^-,\,\text{pos. bkg.}} = -e^2 \sum_{i=1}^{N} \int d^3\vec{x}\; \frac{N}{V} \frac{e^{-\mu|\vec{x}-\vec{r}_i|}}{|\vec{x}-\vec{r}_i|}$$

$\vec{z} = \vec{x} - \vec{r}_i$ for each i

$$= -e^2 \frac{N}{V} \left(\sum_{i=1}^{N} 1\right) \int d^3\vec{z}\; e^{-\mu z}/z = \underline{-e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}}$$

$$\boxed{H_{\text{pos. bkg}} + H_{e^-\,\text{pos. bkg}} = -\frac{1}{2} e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}}$$

$$H_{electrons} = \sum_{\substack{\vec{k}_1\vec{k}_2 \\ \lambda_1\lambda_2}} \langle \vec{k}_1\lambda_1 | \hat{T} | \vec{k}_2\lambda_2 \rangle a^\dagger_{\vec{k}_1\lambda_1} a_{\vec{k}_2\lambda_2} + \frac{1}{2} \sum_{\substack{\vec{k}_1\cdots\vec{k}_4 \\ \lambda_1\cdots\lambda_4}} \langle \vec{k}_1\lambda_1 \vec{k}_2\lambda_2 | \hat{V} | \vec{k}_3\lambda_3 \vec{k}_4\lambda_4 \rangle a^\dagger_1 a^\dagger_2 a_4 a_3$$

$$\langle \vec{k}_1\lambda_1 | \hat{T} | \vec{k}_2\lambda_2 \rangle = \frac{1}{2m} \langle \vec{k}_1\lambda_1 | \hat{p}^2 | \vec{k}_2\lambda_2 \rangle = \frac{\hbar^2 k_2^2}{2m} \delta_{\vec{k}_1\vec{k}_2} \delta_{\lambda_1\lambda_2}$$

$$\langle \vec{k}_1\lambda_1 \vec{k}_2\lambda_2 | \hat{V} | \vec{k}_3\lambda_3 \vec{k}_4\lambda_4 \rangle = e^2 \int d^3\vec{x}_1 d^3\vec{x}_2 \, \psi^*_{\vec{k}_1\lambda_1}(\vec{x}_1) \psi^*_{\vec{k}_2\lambda_2}(\vec{x}_2) \frac{e^{-\mu|\vec{x}_1-\vec{x}_2|}}{|\vec{x}_1-\vec{x}_2|} \psi_{\vec{k}_3\lambda_3}(\vec{x}_1) \psi_{\vec{k}_4\lambda_4}(\vec{x}_2)$$

$$\left(= \int d^3\vec{x}_1 d^3\vec{x}_2 d^3\vec{y}_1 d^3\vec{y}_2 \langle \vec{k}_1\lambda_1 \vec{k}_2\lambda_2 | \vec{x}_1\vec{x}_2 \rangle \underbrace{\langle \vec{x}_1\vec{x}_2 | \hat{V} | \vec{y}_1\vec{y}_2 \rangle}_{\substack{\text{potential is local} \\ = V(\vec{x}_1,\vec{x}_2)\delta(\vec{x}_1-\vec{y}_1)\delta(\vec{x}_2-\vec{y}_2)}} \langle \vec{y}_1\vec{y}_2 | \vec{k}_3\lambda_3 \vec{k}_4\lambda_4 \rangle \right)$$

$$= e^2 \delta_{\lambda_1\lambda_3}\delta_{\lambda_2\lambda_4} \int d^3\vec{x}_1 d^3\vec{x}_2 \frac{e^{-i\vec{k}_1\cdot\vec{x}_1}}{\sqrt{V}} \frac{e^{-i\vec{k}_2\cdot\vec{x}_2}}{\sqrt{V}} \frac{e^{-\mu|\vec{x}_1-\vec{x}_2|}}{|\vec{x}_1-\vec{x}_2|} \frac{e^{i\vec{k}_3\cdot\vec{x}_1}}{\sqrt{V}} \frac{e^{i\vec{k}_4\cdot\vec{x}_2}}{\sqrt{V}}$$

$$[\vec{y} = \vec{x}_1 - \vec{x}_2]$$

$$= \frac{e^2}{V^2} \delta_{\lambda_1\lambda_3}\delta_{\lambda_2\lambda_4} \int d^3\vec{y} \int d^3\vec{x}_2 \frac{e^{-\mu y}}{y} e^{i(\vec{k}_3-\vec{k}_1)\cdot\vec{y}} e^{i\vec{x}_2\cdot(\vec{k}_3+\vec{k}_4-\vec{k}_1-\vec{k}_2)}$$

$$= \frac{e^2}{V^2} \delta_{\lambda_1\lambda_3}\delta_{\lambda_2\lambda_4} V \delta_{\vec{k}_3+\vec{k}_4,\vec{k}_1+\vec{k}_2} \underbrace{\int d^3\vec{y}\, e^{i(\vec{k}_3-\vec{k}_1)\cdot\vec{y}} e^{-\mu y}/y}_{= 4\pi/(|\vec{k}_3-\vec{k}_1|^2+\mu^2)}$$

$$H_{electrons} = \sum_{\vec{k}\lambda} \frac{\hbar^2\vec{k}^2}{2m} a^\dagger_{\vec{k}\lambda} a_{\vec{k}\lambda} + \frac{e^2}{2V} \sum_{\substack{\vec{k}_1\cdots\vec{k}_4 \\ \lambda\bar{\lambda}}} \delta_{\vec{k}_3+\vec{k}_4,\vec{k}_1+\vec{k}_2} \frac{4\pi}{|\vec{k}_3-\vec{k}_1|^2+\mu^2} a^\dagger_{\vec{k}_1\lambda} a^\dagger_{\vec{k}_2\bar{\lambda}} a_{\vec{k}_4\bar{\lambda}} a_{\vec{k}_3\lambda}$$

$$H = -\frac{1}{2} e^2 \frac{N^2}{V} \cdot \frac{4\pi}{\mu^2}_{\textcircled{A}} + \sum_{\vec{k}\lambda} \frac{\hbar^2|\vec{k}|^2}{2m} a^\dagger_{\vec{k}\lambda} a_{\vec{k}\lambda} + \underbrace{\frac{e^2}{2V} \sum_{\substack{\vec{k}_1 \dots \vec{k}_4 \\ \lambda\bar{\lambda}}} \delta_{\vec{k}_1+\vec{k}_2, \vec{k}_3+\vec{k}_4} \frac{4\pi}{|\vec{k}_1-\vec{k}_3|^2+\mu^2} a^\dagger_{\vec{k}_1\lambda} a^\dagger_{\vec{k}_2\bar{\lambda}} a_{\vec{k}_4\bar{\lambda}} a_{\vec{k}_3\lambda}}$$

$$\boxed{\left.\begin{aligned} \vec{k}_1 &= \vec{k}+\vec{q} \\ \vec{k}_2 &= \vec{p}-\vec{q} \\ \vec{k}_3 &= \vec{k} \\ \vec{k}_4 &= \vec{p} \end{aligned}\right\} \left.\begin{aligned} \vec{k}_1+\vec{k}_2 &= \vec{k}+\vec{p} \\ \vec{k}_3+\vec{k}_4 &= \vec{k}+\vec{p} \end{aligned}\right\} \checkmark \qquad \vec{k}_1-\vec{k}_3 = \vec{q}}$$

$$\frac{e^2}{2V} \sum_{\substack{\vec{k}\vec{p}\vec{q} \\ \lambda\bar{\lambda}}} \frac{4\pi}{q^2+\mu^2} a^\dagger_{\vec{k}+\vec{q},\lambda} a^\dagger_{\vec{p}-\vec{q},\bar{\lambda}} a_{\vec{p}\bar{\lambda}} a_{\vec{k}\lambda}$$

separate into $\vec{q}=\vec{0}$ & $\vec{q}\neq\vec{0}$ pieces

$$= \frac{e^2}{2V} \sum_{\substack{\vec{k}\vec{p} \\ \vec{q}\neq 0 \\ \lambda\bar{\lambda}}} \frac{4\pi}{q^2+\mu^2} a^\dagger_{\vec{k}+\vec{q},\lambda} a^\dagger_{\vec{p}-\vec{q},\bar{\lambda}} a_{\vec{p}\bar{\lambda}} a_{\vec{k}\lambda}$$

$$+ \frac{e^2}{2V} \sum_{\substack{\vec{k}\vec{p} \\ \lambda\bar{\lambda}}} \frac{4\pi}{\mu^2} a^\dagger_{\vec{k},\lambda} a^\dagger_{\vec{p},\bar{\lambda}} a_{\vec{p}\bar{\lambda}} a_{\vec{k}\lambda}$$

$\vec{q}=\vec{0}$ piece $\rightarrow$

$$\frac{e^2}{2V} \frac{4\pi}{\mu^2} \sum_{\substack{\vec{k}\vec{p} \\ \lambda\bar{\lambda}}} \left(a^\dagger_{\vec{k}\lambda} a_{\vec{k}\lambda} a^\dagger_{\vec{p}\bar{\lambda}} a_{\vec{p}\bar{\lambda}} - \underset{\times a^\dagger_{\vec{k}\lambda} a_{\vec{k}\lambda}}{\delta_{\vec{k}\vec{p}} \delta_{\lambda\bar{\lambda}}} \right)$$

using anticommutators

$$= \frac{e^2}{2V} \frac{4\pi}{\mu^2} \left(\sum_{\vec{k}\lambda} a^\dagger_{\vec{k}\lambda} a_{\vec{k}\lambda} \sum_{\vec{p}\bar{\lambda}} a^\dagger_{\vec{p}\bar{\lambda}} a_{\vec{p}\bar{\lambda}} - \sum_{\vec{k}\lambda} a^\dagger_{\vec{k}\lambda} a_{\vec{k}\lambda} \right)$$

$$= \frac{e^2}{2V} \frac{4\pi}{\mu^2} \left(\hat{N}^2 - \hat{N} \right)$$

for a fixed # of particles N $\rightarrow$ $\frac{e^2}{2V} \frac{4\pi}{\mu^2} (N^2 - N)$

first term cancels the piece $\textcircled{A}$ in the Hamiltonian

second term $-\frac{e^2}{2V} N \frac{4\pi}{\mu^2}$ = an energy $-2\pi e^2 / V\mu^2$ per particle

if $L \to \infty$ & $\mu \to 0$ but with $1/\mu < L$ always (range within the volume)

then $V\mu^2 = L^3/(1/\mu)^2 \to \infty$ & this energy tends to zero.

$$\Rightarrow H = \lim_{\substack{N\to\infty \\ V\to\infty \\ n=\frac{N}{V}\text{ const}}} \left(\sum_{\vec{k}\lambda} \frac{\hbar^2|\vec{k}|^2}{2m} a^\dagger_{\vec{k}\lambda} a_{\vec{k}\lambda} + \frac{e^2}{2V} \sum_{\substack{\vec{k}\vec{p} \\ \vec{q}\neq 0}} \sum_{\lambda\bar{\lambda}} \frac{4\pi}{q^2} a^\dagger_{\vec{k}+\vec{q},\lambda} a^\dagger_{\vec{p}-\vec{q},\bar{\lambda}} a_{\vec{p}\bar{\lambda}} a_{\vec{k}\lambda} \right)$$

assign a volume to each particle $\frac{4}{3}\pi r_0^3 = V/N$ $\Rightarrow r_0 \simeq$ inter-particle distance

the potential has a length scale : Bohr radius, $a_0 = \hbar^2/me^2$

ratio between the two, $\rho = r_0/a_0$ $\Rightarrow \rho \to 0$ is a high density electron gas.

define dimless vars : $\tilde{V} = r_0^{-3} V$, $\tilde{k} = r_0 \vec{k}$, $\tilde{p} = r_0 \vec{p}$, $\tilde{q} = r_0 \vec{q}$

&

$$H = \frac{e^2}{a_0\rho^2}\Bigg(\underbrace{\sum_{\tilde{k}\lambda} \tfrac{1}{2}\tilde{k}^2 a^\dagger_{\tilde{k}\lambda} a_{\tilde{k}\lambda}}_{O(\rho^0)} + \underbrace{\frac{\rho}{2\tilde{V}} \sum_{\substack{\tilde{k}\tilde{p}\\ \tilde{q}\neq 0}} \sum_{\lambda\bar{\lambda}} \frac{4\pi}{\tilde{q}^2} a^\dagger_{\tilde{k}+\tilde{q},\lambda} a^\dagger_{\tilde{p}-\tilde{q},\bar{\lambda}} a_{\tilde{p}\bar{\lambda}} a_{\tilde{k}\lambda}}_{O(\rho^1)} \Bigg)$$

$\Rightarrow$ in the high density limit the second term is a perturbation to the first.

$$H_0 = \sum_{\vec{k}\lambda} \frac{\hbar^2 k^2}{2m} a^\dagger_{\vec{k}\lambda} a_{\vec{k}\lambda}$$

ground state is the free Fermi gas — all states occupied up to the Fermi surface ($p_F = \hbar k_F$)

e.g. in one dimension

$$|F\rangle = \dots a^\dagger_{-2\downarrow} a^\dagger_{-2\uparrow} a^\dagger_{+2\downarrow} a^\dagger_{+2\uparrow} a^\dagger_{-1\downarrow} a^\dagger_{-1\uparrow} a^\dagger_{+1\downarrow} a^\dagger_{+1,\uparrow} |0\rangle \qquad \left(k = \tfrac{2\pi}{L} n\right) \to \left(a^\dagger_{n,\lambda}\right)$$

in infinite volume sums $\to$ integrals

e.g. in one dim $\displaystyle \sum_k f(\vec{k}) = \sum_n f(\tfrac{2\pi}{L} n) \xrightarrow[L\to\infty]{} \int dn\, f(\tfrac{2\pi}{L} n) = \frac{L}{2\pi}\int dk\, f(k)$

& in 3-d $\displaystyle \sum_{\vec{k}} f(\vec{k}) \longrightarrow \frac{V}{(2\pi)^3}\int d^3\vec{k}\, f(\vec{k})$

consider the total number of electrons $\displaystyle N = \langle F|\hat{N}|F\rangle = \sum_{\vec{k}\lambda} \langle F|\underbrace{\hat{N}_{\vec{k}\lambda}}_{a^\dagger_{\vec{k}\lambda} a_{\vec{k}\lambda}}|F\rangle = \sum_{\vec{k}\lambda} \theta(k_F - k)$

ie zero if $k > k_F$
& one if $k < k_F$

$$\Rightarrow N = \frac{V}{(2\pi)^3}\sum_\lambda \int d^3\vec{k}\, \theta(k_F - k) = \frac{V}{(2\pi)^3}\cdot \underset{(\uparrow\downarrow)}{2}\cdot 4\pi \int_0^\infty k^2 dk\, \theta(k_F - k)$$

$$= \frac{V}{8\pi^3} 8\pi \int_0^{k_F} dk\, k^2 = \frac{V}{3\pi^2} k_F^3 \qquad \Rightarrow k_F = \left(3\pi^2 \frac{N}{V}\right)^{1/3} = \left(3\pi^2 \cdot \frac{3}{4\pi r_0^3}\right)^{1/3}$$

$$\underline{k_F = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_0}} \simeq 1.9/r_0$$

$$E^{(0)} \equiv \langle F|H_0|F\rangle = \frac{\hbar^2}{2m}\sum_{\vec{k}\lambda} k^2 \langle F|\hat{N}_{\vec{k}\lambda}|F\rangle = \frac{\hbar^2}{2m}\sum_{\vec{k}\lambda} k^2\,\theta(k_F-k)$$

$$\to \frac{\hbar^2}{2m}\frac{V}{(2\pi)^3}\sum_\lambda \int d^3\vec{k}\; k^2\,\theta(k_F-k) = \frac{\hbar^2}{2m}\frac{V}{(2\pi)^3}\cdot 2\cdot 4\pi\int_0^{k_F} dk\, k^4$$

$$= \frac{\hbar^2 V}{m}\frac{8\pi}{16\pi^3}\cdot\frac{1}{5}k_F^5 = \frac{\hbar^2 V}{m}\frac{1}{10\pi^2}k_F^5$$

$$= \frac{\hbar^2}{m} N\frac{4}{3}\pi r_0^3\frac{1}{10\pi^2}\left(\frac{9\pi}{4}\right)^{5/3} \frac{1}{r_0^5}$$

$$= e^2 a_0 N/r_0^2\cdot\frac{3}{10}\left(\frac{9\pi}{4}\right)^{2/3} = \frac{e^2}{a_0}N\cdot\frac{1}{\rho^2}\cdot\frac{3}{10}\left(\frac{9\pi}{4}\right)^{2/3} \simeq \frac{e^2}{2a_0}N\cdot\frac{2.2}{\rho^2}$$

first order perturbation theory

$$E^{(1)} \equiv \langle F|H_1|F\rangle = \frac{e^2}{2V}\sum_{\substack{\vec{k}\vec{p}\\ \vec{q}\neq 0}}\sum_{\lambda\bar\lambda}\frac{4\pi}{q^2}\langle F|\underbrace{a^\dagger_{\vec{k}+\vec{q},\lambda}\, a^\dagger_{\vec{p}-\vec{q},\bar\lambda}}_{\substack{\text{non-zero only if}\\ |\vec{k}+\vec{q}|<k_F\\ |\vec{p}-\vec{q}|<k_F}}\;\underbrace{a_{\vec{p}\bar\lambda}\, a_{\vec{k}\lambda}}_{\text{non-zero only if } \vec{p},\vec{k}<k_F}|F\rangle$$

non-zero only if $\underbrace{\vec{k}+\vec{q}=\vec{k},\ \&\ \vec{p}-\vec{q}=\vec{p}}_{\substack{\text{not allowed}\\ \text{since } \vec{q}\neq 0}}$ or if $\underbrace{\vec{k}+\vec{q}=\vec{p}\ \&\ \vec{p}-\vec{q}=\vec{k}}_{\text{only possibility}}$ $\&\ \bar\lambda=\lambda$

$$\Rightarrow \langle F|a^\dagger_{\vec{k}+\vec{q},\lambda}a^\dagger_{\vec{p}-\vec{q},\bar\lambda}a_{\vec{p}\bar\lambda}a_{\vec{k}\lambda}|F\rangle = \delta_{\vec{k}+\vec{q},\vec{p}}\,\delta_{\lambda,\bar\lambda}\langle F|a^\dagger_{\vec{k}+\vec{q}\lambda}a^\dagger_{\vec{k}\lambda}a_{\vec{k}+\vec{q}\lambda}a_{\vec{k}\lambda}|F\rangle$$

$$= -\delta_{\vec{k}+\vec{q},\vec{p}}\,\delta_{\lambda\bar\lambda}\langle F|\hat{N}_{\vec{k}+\vec{q},\lambda}\hat{N}_{\vec{k},\lambda}|F\rangle$$

$$= -\delta_{\vec{k}+\vec{q},\vec{p}}\,\delta_{\lambda\bar\lambda}\,\theta(k_F-|\vec{k}+\vec{q}|)\,\theta(k_F-k)$$

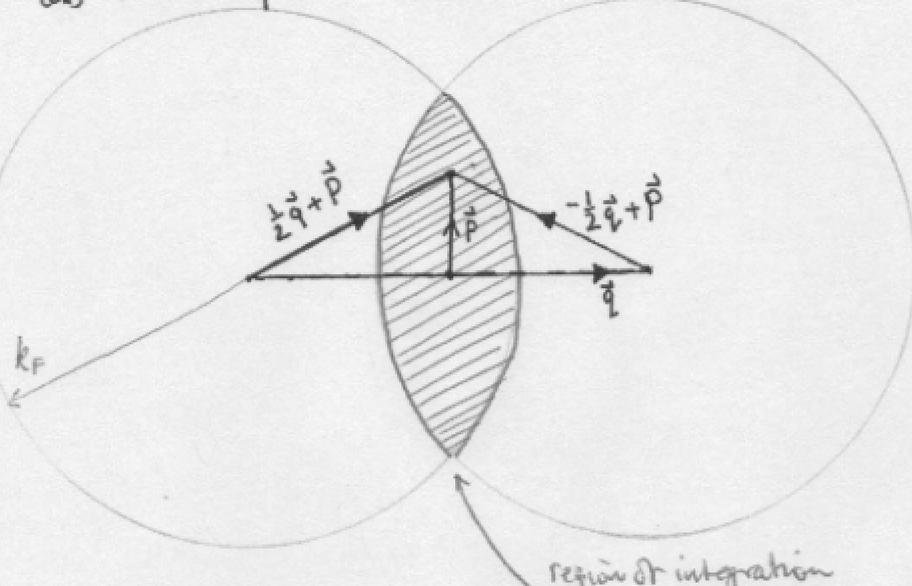
$$\Rightarrow E^{(1)} = -\frac{e^2}{2V}\sum_\lambda\sum_{\vec{k}\vec{q}}\frac{4\pi}{q^2}\theta(k_F-|\vec{k}+\vec{q}|)\theta(k_F-k)$$

$$= -\frac{e^2}{2V}\cdot 2\cdot\left(\frac{V}{(2\pi)^3}\right)^2 4\pi\int d^3\vec{k}\,d^3\vec{q}\;\theta(k_F-|\vec{k}+\vec{q}|)\theta(k_F-k)\frac{1}{q^2}$$

$$E^{(1)} = -e^2 V \frac{4\pi}{(2\pi)^6} \int d^3\vec{k}\, d^3\vec{q}\; \theta(k_F - |\vec{k}+\vec{q}|)\, \theta(k_F - k)\, \frac{1}{q^2}$$

change vars $\vec{P} = \vec{k} + \tfrac{1}{2}\vec{q}$

$$= -e^2 V \frac{4\pi}{(2\pi)^6} \int d^3\vec{q} \int d^3\vec{p}\, \frac{1}{q^2}\, \theta(k_F - |\vec{p} + \tfrac{1}{2}\vec{q}|)\, \theta(k_F - |\vec{p} - \tfrac{1}{2}\vec{q}|)$$



$$= -e^2 V \frac{4\pi}{(2\pi)^6} \int d^3\vec{q}\, \frac{1}{q^2} \cdot I(\vec{q}) \qquad I(\vec{q}) = \int d^3\vec{p}\; \theta(k_F - |\vec{p} + \tfrac{1}{2}\vec{q}|)\, \theta(k_F - |\vec{p} - \tfrac{1}{2}\vec{q}|)$$

$$= k_F^3 \int d^3\vec{\gamma}\; \theta(1 - |\vec{\gamma} + \vec{\eta}|)\, \theta(1 - |\vec{\gamma} - \vec{\eta}|) \qquad \left(\vec{\gamma} = \frac{1}{2k_F}\vec{p}\right) \left(\vec{\eta} = \frac{1}{2k_F}\vec{q}\right)$$

$$= \frac{4\pi}{3} k_F^3 \left(1 - \tfrac{3}{2}\eta + \tfrac{1}{2}\eta^3\right) \theta(1-\eta) \qquad [\text{geometry}]$$

$$= -e^2 V \frac{4\pi}{(2\pi)^6} \frac{4\pi}{3} k_F^3 \cdot 4\pi\, 2k_F \int_0^1 d\eta\, \eta^2 \frac{1}{\eta^2} \left(1 - \tfrac{3}{2}\eta + \tfrac{1}{2}\eta^3\right)$$

$$= -e^2 V \frac{(4\pi)^3}{(2\pi)^6} \frac{2}{3} k_F^4 \frac{3}{8} = -e^2 V k_F^4 \cdot \frac{1}{4\pi^3} = -e^2 N \cdot \frac{4}{3}\pi r_0^3 \frac{1}{4\pi^3} \left(\frac{9\pi}{4}\right)^{4/3} \frac{1}{r_0^4}$$

$$= -e^2 N \frac{1}{r_0} \frac{4\pi}{3} \frac{1}{4\pi^3} \frac{9\pi}{4} \left(\frac{9\pi}{4}\right)^{1/3} = \frac{-e^2}{2a_0} N \frac{1}{\rho} \cdot \frac{3}{2\pi} \left(\frac{9\pi}{4}\right)^{1/3} \simeq -\frac{e^2}{2a_0} N \cdot \frac{0.92}{\rho}$$

$$\Rightarrow \boxed{E/N \xrightarrow[\rho \to 0]{} \frac{e^2}{2a_0} \left[+ \frac{2.2}{\rho^2} - \frac{0.92}{\rho} + \ldots \right]}$$