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Second Quantization

A quantum approach to the Solid State — Philip L. Taylor (197
" " " " Condensed Matter Physics — Philip L. Taylor + Olle Heinonen (2002)

+ Lectures on Quantum Mechanics, G. Baym (1969)

1. Single Electron

$$H \psi(r) = \mathcal{E} \psi(r) \qquad H = \frac{p^2}{2m} + V(r)$$

need to find eigenfunctions & eigenenergies

$$\underbrace{u_\alpha(r) \qquad \mathcal{E}_\alpha}$$

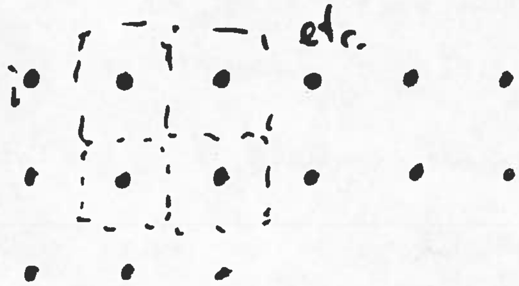
$$H u_\alpha(r) = \mathcal{E}_\alpha u_\alpha(r)$$

quantum #'s, α

orthonormal set $\Rightarrow$

$$\int dr \, u_\alpha^*(r) \, u_{\alpha'}(r) = 0 \text{ for } \alpha \neq \alpha'$$
$$= 1 \text{ for } \alpha = \alpha'$$

Think of discretizing r into cells



$\int dr \rightarrow$

$\Delta \sum_i u_\alpha^*(r_i) \, u_{\alpha'}(r_i)$

volume of each cell — i^{th} cell.

$$u_{\alpha'}(r) \rightarrow \begin{pmatrix} u_{\alpha'}(r_1) \\ u_{\alpha'}(r_2) \\ \vdots \end{pmatrix}$$

$|\alpha\rangle$

$$u_\alpha^*(r) \rightarrow \left(u_\alpha^*(r_1), u_\alpha^*(r_2), u_\alpha^*(r_3) \ldots \right)$$

$\langle \alpha |$

$\langle \alpha | \alpha' \rangle = \delta_{\alpha\alpha'}$ Dirac notation.

eg plane waves : $u_\alpha(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}_\alpha \cdot \vec{r}}$ in a box with volume V

periodic b.c.'s $\Rightarrow$ $k_\alpha = \frac{2\pi}{L}(m_x, m_y, m_z)$

m_x, m_y, m_z are integers

$L^3 \equiv V$

u_α's form a complete basis

$$\phi(\vec{r}) = \sum_\alpha c_\alpha u_\alpha(\vec{r})$$

$\int d\vec{r}\, u^*_{\alpha'}(\vec{r})$ both sides $\Rightarrow$ $c_{\alpha'} = \int d\vec{r}\, u^*_{\alpha'}(\vec{r})\,\phi(\vec{r})$

$= \langle \alpha' | \phi \rangle$

$$|\phi\rangle = \underbrace{\sum_\alpha |\alpha\rangle\langle\alpha|}_{=\hat{1}}\phi\rangle$$

$(\ )(\ ) =$ number. $\quad (\ )(\ ) =$ operator

Same for $\int u^*_\alpha(\vec{r})\, V(\vec{r})\, u_{\alpha'}(\vec{r})\, d\vec{r} \rightarrow \Delta\Omega \sum_i u^*_\alpha(\vec{r}_i)\, V(\vec{r}_i)\, u_{\alpha'}(\vec{r}_i)$

$V(\vec{r}_i)$ is a diagonal matrix $\begin{pmatrix} V(\vec{r}_1) & 0 & 0 \\ 0 & V(\vec{r}_2) & 0 \\ 0 & 0 & V(\vec{r}_3) \ldots \end{pmatrix}$

$$\langle \alpha | V | \alpha' \rangle$$

so $V(\vec{r}) = \sum_{\alpha'} |\alpha'\rangle \underbrace{\langle\alpha'|\, V \sum_{\alpha''} |\alpha''\rangle}\langle\alpha''|$

$$= \sum_{\alpha'\alpha''} \underbrace{\langle\alpha'|V|\alpha''\rangle}_{\substack{\text{a number} \\ \text{(matrix element)}}} \underbrace{|\alpha'\rangle\langle\alpha''|}_{\text{an operator}}$$

operator $|\alpha'\rangle\langle\alpha''|$ ⇐ would get zero unless we operated on $|\alpha''\rangle$

And then we get the state $|\alpha'\rangle$

we interpret $|\alpha'\rangle\langle\alpha''|$ as removing an electron from the state described by the wave function $u_{\alpha''}(\vec{r})$ and putting it into the state described by $u_{\alpha'}(\vec{r})$

i.e. operator $\boxed{\text{annihilates}}$ an electron in the state $|\alpha''\rangle$ and $\boxed{\text{creates}}$ one in the state $|\alpha'\rangle$

introduce "stepping stone" : vacuum $|0\rangle$

$$\langle 0|0\rangle = 1$$
$$\langle \alpha|0\rangle = 0 \quad \text{for all } \alpha$$

then, $|\alpha'\rangle\langle\alpha''| = \underbrace{|\alpha'\rangle\langle 0|}_{c^{\dagger}_{\alpha'}}\underbrace{|0\rangle\langle\alpha''|}_{c_{\alpha''}}$

$c^{\dagger}_{\alpha'}$ creation operator

$c_{\alpha''}$ → annihilation operator

annihilates any electron that it finds in the state $|\alpha''\rangle$

so $|\alpha'\rangle\langle\alpha''| = \hat{c}^{\dagger}_{\alpha'}\hat{c}_{\alpha''}$

$$\therefore \quad V(r) = \sum_{\alpha',\alpha''} \langle\alpha'|V|\alpha''\rangle\, \hat{c}^{\dagger}_{\alpha'}\hat{c}_{\alpha''}$$

also $$\frac{p^2}{2m} = \frac{1}{2m}\sum_{\alpha',\alpha''}\langle\alpha'|p^2|\alpha''\rangle\, \hat{c}^{\dagger}_{\alpha'}\hat{c}_{\alpha''}$$

2 occupation number representation

N identical free particles.

$$\mathcal{H} = \sum_i \mathcal{H}_i \longrightarrow \Phi' = u_1(\vec{r}_1)\, u_2(\vec{r}_2) \ldots u_N(\vec{r}_N)$$

<u>But</u>, identical particles!

Fermions:

$$\Phi = \frac{1}{\sqrt{N!}} \begin{array}{cl} \left| \begin{array}{cccc} u_1(\vec{r}_1) & u_1(\vec{r}_2), & \ldots & u_1(\vec{r}_N) \\ u_2(\vec{r}_1) & u_2(\vec{r}_2) & \ldots & u_2(\vec{r}_N) \\ \vdots & & & \\ u_N(\vec{r}_1) & u_N(\vec{r}_2) & \ldots & u_N(\vec{r}_N) \end{array} \right| & \begin{array}{l} \leftarrow \text{state } \alpha = 1 \\ \leftarrow \text{state } \alpha = 2 \\ \vdots \\ \\ \end{array} \\ \begin{array}{ccc} \uparrow & \uparrow & \\ \text{particle 1} & \text{particle 2} & \ldots \end{array} & \end{array}$$

Slater determinant.

N! terms!

big pain!

Φ form a complete set.

$$\Psi = \sum_{\alpha_1, \alpha_2, \ldots \alpha_N} c_{\alpha_1 \ldots \alpha_N}\, \Phi(\alpha_1, \ldots \alpha_N)$$

each term here has N! terms!

better to use occupation # representation

we know: (a) there are N particles

(b) all coordinates come into wavefn. on an equal footing

(c) ϕ is antisymmetrized.

why not just specify states that are occupied.

e.g. $$\phi_{\alpha\beta}(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} u_\alpha(r_1) & u_\alpha(r_2) \\ u_\beta(r_1) & u_\beta(r_2) \end{vmatrix}$$

is specified by $n_\alpha = n_\beta = 1$, all other $n_{\alpha'} = 0$

$|1,1,0,0,0\ldots\rangle \Rightarrow n_\alpha = 1,\ n_\beta = 1,\ n_\gamma = 0,\ n_\delta = 0 \ldots$

$\phi \to |\{n_\mu\}\rangle$

set of occupation numbers

for ϕ's with same # $\int \phi_\mu^* \phi_{\mu'}\, dr_1\, dr_2 \ldots dr_N = 0$

also true for different occupation #'s.

$\langle\{n_\mu\}|\{n_{\mu'}\}\rangle = \delta_{\mu,\mu'}$ orthonormal

$\sum_{\{n_\mu\}} |\{n_\mu\}\rangle\langle\{n_\mu\}| = 1$ complete set.

now write

$$V = \sum_{\{n_\mu\}\{n_{\mu'}\}} |\{n_\mu\}\rangle \underbrace{\langle\{n_\mu\}|V|\{n_{\mu'}\}\rangle}_{V_{\mu\mu'}} \langle\{n_{\mu'}\}|$$

$$V = \sum_{\{n_\mu\}\{n_{\mu'}\}} V_{\mu\mu'}\, \underbrace{|\{n_\mu\}\rangle\langle\{n_{\mu'}\}|} \quad *$$

$|\{n_\mu\}\rangle\langle\{n_{\mu'}\}|$ ← many-particle operators.

$|n_1\, n_2 \dots\rangle\langle n_1'\, n_2' \dots|$ for fermions, $n_i = 0$ or 1

potentially many changes

for fermions, <u>order</u> matters (recall determinants

simplest case: just 1 change.

$|n_1\, n_2 \dots n_p = 0, \dots\rangle\langle n_1\, n_2 \dots n_p = 1, \dots|$ acts on wave fn. that has p^{th} one-particle state occupied & gives state with p^{th} state empty.

$$\sum_{\substack{\{n_i\} \\ i \neq p}} |n_1 \dots n_p = 0 \dots\rangle\langle n_1 \dots n_p = 1 \dots|$$

acts on <u>any</u> wave function for which <u>$n_p = 1$</u>

define a number: $N_p = \sum_{j=1}^{p-1} n_j$

& now define $\boxed{\text{annihilation operator}}$: (fermions)

$$c_p = \sum_{\substack{\{n_i\} \\ i \neq p}} (-1)^{N_p} |\dots n_1 \dots n_p = 0 \dots\rangle\langle \dots n_i \dots n_p = 1, \dots|$$

clear that if $n_p = 0$ in a particular state,

$$c_p |\ldots n_i \ldots n_p = 0, \ldots\rangle = 0$$

but if p^{th} state is occupied, one term in summation will not be orthogonal +

$$c_p | n_1, n_2 \ldots n_p = 1, \ldots\rangle = (-1)^{N_p} | n_1, \ldots n_2, \ldots n_p = 0, \ldots\rangle$$

easy to see $c_p^2 = 0$

similar for creation operator:

$$c_p^\dagger = \sum_{\substack{\{n_i\} \\ i \neq p}} (-1)^{N_p} |\ldots n_p = 1, \ldots\rangle\langle \ldots n_p = 0 \ldots |$$

then
$$c_p^\dagger |\ldots n_p = 0 \ldots\rangle = (-1)^{N_p} |\ldots n_p = 1 \ldots\rangle$$
$$c_p^\dagger |\ldots n_p = 1 \ldots\rangle = 0$$

any more complicated form of $|\{n_\mu\}\rangle\langle\{n_\mu'\}|$ can be expressed as a product of the c's

e.g. $\displaystyle\sum_{\substack{\{n_i\} \\ i \neq p \\ i \neq q}} |\ldots n_p = 0, n_q = 0, \ldots\rangle\langle \ldots n_p = 1, n_q = 1, \ldots |$ 2 changes

$$= \sum |\ldots n_p = 0, n_q = 0, \ldots\rangle\langle \ldots n_p = 0, n_q = 1, \ldots | |\ldots n_p = 0, n_q = 1, \ldots\rangle\langle \ldots n_p = 1, n_q = 1, \ldots |$$

OR
$$= \sum |\ldots n_p = 0, n_q = 0 \ldots\rangle\langle \ldots n_p = 1, n_q = 0, \ldots | |\ldots n_p = 1, n_q = 0, \ldots\rangle\langle \ldots n_p = 1, n_q = 1, \ldots |$$

$(-1)^{N_q} c_q (-1)^{N_p} c_p$ (1

N_q is different than N_q'

$(-1)^{N_p} c_p (-1)^{N_q} c_q$ (2

c_p destroys the particle in the p^{th} state, so the value of N_q depends on whether we evaluate it <u>before</u> or <u>after</u> operating with c_p (assume $q>p$)

$$\Rightarrow (-1)^{N_q} c_p = c_p (-1)^{N_q+1}$$

does not include the 'p' (it has been annihilated)

includes the 'p'

N_p does not depend on n_q $(q>p)$

$$\therefore (-1)^{N_q} c_q (-1)^{N_p} c_p = (-1)^{N_p} c_p (-1)^{N_q+1} c_q$$

same N_q

$$\Rightarrow c_q c_p = -c_p c_q$$

$$\therefore c_q c_p + c_p c_q = 0 \qquad p \neq q.$$

also $\{c_p^\dagger, c_q^\dagger\} = \{c_p^\dagger, c_q\} = 0$ for $p \neq q$.

can show $\{c_p^\dagger, c_p\} = 1$

so:
$$\boxed{\begin{gathered}\{c_p^\dagger, c_q^\dagger\} = \{c_p, c_q\} = 0 \\ \{c_p, c_q^\dagger\} = \delta_{p,q}\end{gathered}}$$

now we can write any operator in terms of annihilation + creation operators.

Single particle operator

$$\sum_{i=1}^{N} V(\vec{r}_i)$$

recall we had $\quad V = \sum_{\{n_\mu\},\{n_{\mu'}\}} |\{n_\mu\}\rangle \underbrace{\langle\{n_\mu\}|V|\{n_{\mu'}\}\rangle}_{V_{\mu\mu'}} \langle\{n_{\mu'}\}|$

$$V_{\mu\mu'} = \int \phi^*(\alpha_1,\dots\alpha_N)\, V(r_i)\, \phi(\alpha_1',\dots\alpha_N')\, d\vec{r}_1 \dots d\vec{r}_N$$

only ones that do not vanish are those in which just one of the α_i's is different from α_i

$$\text{only} \quad \int u_i^*(\vec{r})\, V(\vec{r})\, u_{i'}(\vec{r})\, d\vec{r} \neq 0.$$

in occupation number representation,

$$V_{ii'} = \langle n_1 \dots n_{\alpha_i} = 1, n_{\alpha_i'} = 0, \dots | V | n_1 \dots n_{\alpha_i} = 0, n_{i'} = 1, \dots \rangle$$

so $\displaystyle V = \sum_{\substack{\alpha_i,\alpha_i' \\ \{n_j\}\, j \neq \alpha_i, \alpha_i'}} V_{ii'} |\dots n_{\alpha_i} = 1, n_{\alpha_i'} = 0, \dots\rangle\langle \dots n_{\alpha_i} = 0, n_{\alpha_i'} = 1, \dots|$

$$= \sum_{\alpha_i,\alpha_i'} V_{ii'} C^+_{\alpha_i} C_{\alpha_i'}$$

(think of k-space : $\alpha \to k$) $\quad -\frac{\hbar^2}{2m}\nabla^2 \quad u_k(r) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$

then $T_{kk'} = \frac{1}{V}\int e^{-i\vec{k}\cdot\vec{r}} H_0 e^{i\vec{k}'\cdot\vec{r}} d^3r$

and $V_{kk'} = \frac{1}{V}\int e^{-i\vec{k}\cdot\vec{r}} V(r) e^{i\vec{k}'\cdot\vec{r}} d^3r = \frac{1}{V}\int e^{-i(k-k')r} V(r)$

$$\Rightarrow \mathcal{H} =$$

$$\mathcal{H} = \sum_{kk'} T_{kk'} c_k^\dagger c_{k'} + \sum_{kk'} V_{kk'} c_k^\dagger c_{k'}$$

but $T_{kk'} = \frac{\hbar^2 k^2}{2m} \delta_{kk'}$

$$\mathcal{H} = \sum_k \underset{T_{kk}}{\overset{|||}{\varepsilon_k}} c_k^\dagger c_k + \sum_{kk'} V_{kk'} c_k^\dagger c_{k'}$$

a potential cannot remove a particle from a state without putting it back in some other state.

particle-particle interactions

$$\langle \{n_\mu\} | V | \{n_{\mu'}\} \rangle = \frac{1}{2} \sum_{i \neq j} \int \Phi^*(\alpha_1 \ldots \alpha_N)\, V(r_i - r_j)\, \Phi(\alpha_1' \ldots \alpha_N')\, d^3r_1 \ldots d^3r_N$$

determinants are sums of products of functions u_α

$$\int u_a^*(r_1) u_b^*(r_2) \ldots u_z^*(r_N)\, V(r_i - r_j)\, u_{a'}(r_1) u_{b'}(r_2) \ldots u_z(r_N)\, d^3r_1 \ldots d^3r_N$$

$$\int u_a^*(r_1) u_{a'}(r_1)\, dr_1 \int u_b^*(r_2) u_{b'}(r_2)\, dr_2 \;\ldots \text{etc.}$$

get $\quad V_{\alpha\beta\gamma\delta} = \int u_\alpha^*(r_i) u_\beta^*(r_j) V(r_i - r_j) u_\gamma(r_j) u_\delta(r_i)\, d^3r_i\, d^3r_j \qquad (3)$

these require $a = a'$, $b = b'$ etc.

$\therefore$ V can only alter occupation of the states $\alpha, \beta, \gamma, \delta$ (2 body term

$$\therefore V = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} V_{\alpha\beta\gamma\delta}\, c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta \qquad (4)$$

need to have correct ordering (take V=1)

$c_p^\dagger c_q^\dagger|0\rangle$ differs (by a minus sign) from $c_q^\dagger c_p^\dagger|0\rangle$

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same minus sign that was in the Slater determinant also shows up in "minus sign problem" in some kinds of Monte Carlo.

Then we rewrote Hamiltonians

$$H = \sum_\alpha \varepsilon_\alpha c_\alpha^\dagger c_\alpha + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta}\, c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta$$

kinetic energy

1-body potential

$$\varepsilon_\alpha = \int d^3r\, u_\alpha^*(r)\left\{-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right\}u_\alpha(r)$$ one-body term.

$$V_{\alpha\beta\gamma\delta} \equiv \int d^3r_1 \int d^3r_2\, u_\alpha^*(r_1)\, u_\beta^*(r_2)\, V(r_1-r_2)\, u_\gamma(r_2)\, u_\delta(r_1)$$ 2-body term

2-body potential.

basis states (e.g. plane waves: $\frac{1}{\sqrt{V}}e^{ik_\alpha\cdot r}$)

note: with bosons, we obtain similar results:

commutation relation $\rightarrow [a_i, a_j^\dagger] = \delta_{ij} = a_i a_j^\dagger - a_j^\dagger a_i$

$[a_i, a_j] = 0 = [a_i^\dagger, a_j^\dagger] \Rightarrow a_i^\dagger a_j^\dagger = a_j^\dagger a_i^\dagger$

order does NOT matter

Back to fermions:

some useful quantities:

$$G_s(\vec{r}-\vec{r}') = \langle \Phi_0 | \hat{\psi}_s^{+}(\vec{r})\, \hat{\psi}_s(r') | \Phi_0 \rangle$$

ground state for a gas of free electrons.

creation operator for an electron with spin 's' at position r

annihilation operator for an electron with spin 's' at position r'

amplitude for removing a particle at $\vec{r}'$ with spin 's' from the ground state & ~~by~~ replacing with a particle with spin s at point $\vec{r}$.

For free electron gas, a complete set of states are plane waves.

$$\therefore \quad \hat{\psi}_s(r) = \frac{1}{\sqrt{V}} \sum_p e^{i\vec{p}\cdot\vec{r}}\, \hat{a}_{ps}$$

$$\hat{\psi}_s^{+}(r) = \frac{1}{\sqrt{V}} \sum_p e^{-i\vec{p}\cdot\vec{r}}\, \hat{a}_{ps}^{+}$$

so, density operator is, for example,

$$\hat{\rho}(r) = \sum_s \hat{\psi}_s^{+}(r)\hat{\psi}_s(r) = \sum_s \frac{1}{V} \sum_{pp'} e^{i(p-p')r}\, \hat{a}_{ps}^{+}\, \hat{a}_{p's}$$

expectation value:

$$\langle \hat{\rho}(r) \rangle \equiv \langle \Phi_0 | \hat{\rho}(r) | \Phi_0 \rangle = \sum_s \sum_{pp'} \frac{1}{V} e^{i(p-p')r} \langle \Phi_0 | \hat{a}_{ps}^{+}\, \hat{a}_{p's} | \Phi_0 \rangle$$

where

$$|\Phi_0\rangle = \prod_{\substack{p \\ E_p < E_F}} \hat{a}_{p\uparrow}^{+}\hat{a}_{p\downarrow}^{+} |0\rangle \quad \text{is the Fermi sea.}$$

note that with 2 spin species, it doesn't really matter about the ordering of p'

need $\langle \phi_0 | a^\dagger_{ps} a_{p's} | \phi_0 \rangle$

$a_{p's} \prod_k a^\dagger_{k\uparrow} a^\dagger_{k\downarrow} |0\rangle$

p' should be ~~absent~~ present

after acting with $a_{p's}$ it is gone.

so $a^\dagger_{ps}$ better put it back. $\Rightarrow a^\dagger_{ps} a_{p's} \to \delta_{pp'} n_{ps}$

where $n_{ps} \equiv a^\dagger_{ps} a_{ps}$ is the number operator.

note: $a_{ps} \; \underbrace{a^\dagger_{k_1\uparrow} a^\dagger_{k_1\downarrow}}\,\underbrace{a^\dagger_{k_2\uparrow} a^\dagger_{k_2\downarrow}} \cdots \underbrace{a^\dagger_{p\uparrow} a^\dagger_{p\downarrow}} \cdots a^\dagger_{k_N\uparrow} a^\dagger_{k_N\downarrow} |0\rangle$

commute through each pair always get $(-1)^2 = 1$

$a_{ps}\, a^\dagger_{p\uparrow} a^\dagger_{p\downarrow} a^\dagger_{k_1\uparrow} a^\dagger_{k_1\downarrow} \cdots |0\rangle$

if $s = \uparrow$ get $a_{p\uparrow} a^\dagger_{p\uparrow} \equiv 1 - a^\dagger_{p\uparrow} a_{p\uparrow}$

But $(1 - a^\dagger_{p\uparrow} a_{p\uparrow}) a^\dagger_{p\downarrow} a^\dagger_{k_1\uparrow} a^\dagger_{k_1\downarrow} a^\dagger_{k_2\uparrow} a^\dagger_{k_2\downarrow} \cdots |0\rangle$

$= (1)\, a^\dagger_{p\downarrow} a^\dagger_{k_1\uparrow} a^\dagger_{k_1\downarrow} a^\dagger_{k_2\uparrow} a^\dagger_{k_2\downarrow} \cdots |0\rangle$

since $a^\dagger_{p\uparrow} a_{p\uparrow}$ can be commuted through and gives zero.

$$\therefore\ a^\dagger_{p\uparrow} a_{p\uparrow} |\Phi_0\rangle = a^\dagger_{p\uparrow} a^\dagger_{p\downarrow} \underbrace{a^\dagger_{k_1\uparrow} a^\dagger_{k_1\downarrow} a^\dagger_{k_2\uparrow} a^\dagger_{k_2\downarrow} \cdots a^\dagger_{k_N\uparrow} a^\dagger_{k_N\downarrow}}_{\text{missing } p} |0\rangle$$

now, $a^\dagger_{p\uparrow} a^\dagger_{p\downarrow}$ can be commuted through to its proper place

Then what remains once again is $|\Phi_0\rangle$

i.e. $a^\dagger_{p\uparrow} a_{p\uparrow} |\Phi_0\rangle = |\Phi_0\rangle$ if $\varepsilon_p < \varepsilon_F$ (i.e. $p < p_F$)

same thing if $s = \downarrow$

$$\therefore \langle \rho(r) \rangle = \sum_s \sum_{pp'} \frac{1}{V} e^{i(p-p')\cdot r} \langle \Phi_0 | a^\dagger_{ps} a_{p's} | \Phi_0 \rangle$$

$$= \sum_s \sum_{pp'} \frac{1}{V} e^{i(p-p')r} \delta_{pp'} \, 1 \, \Theta(p_F - p)$$

$$= \underset{\substack{\uparrow \\ \text{spin}}}{2} \frac{1}{V} \sum_p \Theta(p_F - p)$$

But $N = \sum_{ps} \langle \Phi_0 | \underbrace{a^\dagger_{ps} a_{ps}}_{n_{ps}} | \Phi_0 \rangle$

$$= 2 \sum_p \Theta(p_F - p)$$

so $\langle \rho(r) \rangle = \dfrac{N}{V} = n$, where n = uniform density.

so $\langle \rho(r) \rangle$ is a constant.

Back to $G_s(\vec{r}-\vec{r}\,') = \frac{1}{V}\sum_{pp'} e^{-i\vec{p}\cdot\vec{r}} e^{+i\vec{p}\,'\cdot\vec{r}\,'} \underbrace{\langle \phi_0 | a^{+}_{ps} a_{p's} | \phi_0 \rangle}_{n_{ps}\,\delta_{pp'}}$

$$= \frac{1}{V}\sum_{p} e^{-i\vec{p}(\vec{r}-\vec{r}\,')} n_{ps}$$

$$\frac{1}{V}\sum_{p} \to \int \frac{d^3p}{(2\pi)^3} e^{-i\vec{p}(\vec{r}-\vec{r}\,')} n_{ps}$$

$n_{ps} = \begin{cases} 1 & \text{for } p < p_F \\ 0 & \text{for } p > p_F \end{cases}$

$$G_s(\vec{r}-\vec{r}\,') = \frac{1}{(2\pi)^3}\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_0^{\infty} dp\, p^2 e^{-ip|\vec{r}-\vec{r}\,'|\cos\theta}\,\theta(p_F - p)$$

$\mu = \cos\theta$

$$= \frac{1}{(2\pi)^2}\int_0^{p_F} dp\, p^2 \int_{-1}^{1} d\mu\, e^{-ip|\vec{r}-\vec{r}\,'|\mu}$$

$$= \frac{1}{(2\pi)^2}\int_0^{p_F} dp\, p^2 \frac{1}{-ip|\vec{r}-\vec{r}\,'|} e^{-ip|\vec{r}-\vec{r}\,'|\mu}\Big|_{-1}^{1}$$

$$= \frac{1}{2\pi^2}\frac{1}{|\vec{r}-\vec{r}\,'|}\int_0^{p_F} dp\, p \sin p|\vec{r}-\vec{r}\,'|$$

let $x = |\vec{r}-\vec{r}\,'|$

$$= \frac{1}{2\pi^2}\frac{1}{x}\int_0^{p_F} dp\, p \sin px$$

$$= \frac{1}{2\pi^2}\frac{1}{x}\left(-\frac{\partial}{\partial x}\right)\int_0^{p_F} dp \cos px$$

$$= \frac{1}{2\pi^2}\frac{1}{x}\,\frac{-\partial}{\partial x}\left(\frac{\sin p_F x}{x}\right)$$

$$= -\frac{1}{2\pi^2}\frac{1}{x}\left\{\frac{p_F \cos p_F x}{x} - \frac{1}{x^2}\sin p_F x\right\}$$

let $u \equiv p_F x = p_F|\vec{r}-\vec{r}\,'|$

$$= \frac{1}{2\pi^2} p_F^3 \frac{1}{u^3}\left\{\sin u - u\cos u\right\}$$

$$n = \frac{N}{V} = \frac{2}{V}\sum_{p} \Theta(p_F - p)$$

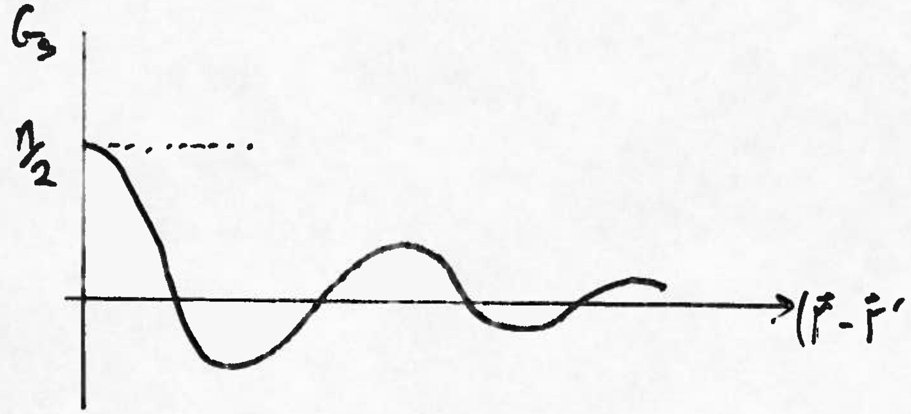
$$= 2\int \frac{d^3p}{(2\pi)^3}\, \Theta(p_F - p)$$

$$= 2 \cdot \frac{1}{(2\pi)^3} \cdot 4\pi \int_0^{p_F} dp\, p^2$$

$$= \frac{1}{\pi^2}\frac{p_F^3}{3}$$

$$\therefore \boxed{p_F^3 = 3\pi^2 n}$$

$$\therefore G_3(\vec{r}-\vec{r}') = \frac{3n}{2}\left\{\frac{\sin u - u\cos u}{u^3}\right\} \qquad \text{where } u = p_F|\vec{r}-\vec{r}'|$$



Pair correlation functions

- 2 particles, no interactions with one another

Does one particle care where the other one is?

Ans: yes!

probability that one particle is at $\underline{r}$ and the other is at $\underline{r}'$:

$$\langle \Phi_0 | \underbrace{\hat{\psi}^{\dagger}_{s'}(\vec{r}') \hat{\psi}_{s'}(\vec{r}')}_{\substack{\text{one particle} \\ \text{spin } s'}} \underbrace{\hat{\psi}^{\dagger}_{s}(\vec{r}) \hat{\psi}_{s}(\vec{r})}_{\substack{\text{other particle} \\ \text{spin } s}} | \Phi_0 \rangle$$

Customary to use

$$\langle \Phi_0 | \hat{\psi}^{\dagger}_{s}(\vec{r}) \hat{\psi}^{\dagger}_{s'}(\vec{r}') \hat{\psi}_{s'}(\vec{r}') \hat{\psi}_{s}(\vec{r}) | \Phi_0 \rangle \equiv \left(\frac{n}{2}\right)^2 g_{ss'}(\vec{r}-\vec{r}')$$

use

$$\left.\begin{aligned} \hat{\psi}^{\dagger}_{s}(\vec{r}) &\equiv \frac{1}{\sqrt{V}} \sum_{p} e^{-i\vec{p}\cdot\vec{r}} \hat{a}^{\dagger}_{ps} \\ \hat{\psi}_{s}(\vec{r}) &\equiv \frac{1}{\sqrt{V}} \sum_{p} e^{i\vec{p}\cdot\vec{r}} \hat{a}_{ps} \end{aligned}\right\} \text{as before}$$

$$\left(\frac{n}{2}\right)^2 g_{ss'}(\vec{r}-\vec{r}') = \frac{1}{V^2} \sum_{\substack{pp' \\ kk'}} e^{-i(\vec{p}-\vec{p}')\cdot\vec{r}'} e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}} \langle \Phi_0 | \hat{a}^{\dagger}_{ks} \hat{a}^{\dagger}_{ps'} \hat{a}_{p's'} a_{k's} | \Phi_0 \rangle$$

<u>Fermions</u>: $|\phi_0\rangle$ = Fermi sea.

remove k's + p's'

we have to put them back!

2 possibilities: (a) <u>$s' \neq s$</u>

then $a^\dagger_{ps'}$ has to put back what $a_{p's'}$ removed.

$$\Rightarrow p = p'$$

p' has to be part of $|\phi_0\rangle$ (otherwise we get zero.)

so

$$a^\dagger_{ps'} a_{p's'} = \delta_{pp'} a^\dagger_{ps'} a_{ps'}$$

this can go through a_k's

Now what about

$$a^\dagger_{ps'} a_{ps'} |\phi_0\rangle \qquad \{a^\dagger_{ps'}, a_{ps'}\} = 1$$

$$= \left(1 - a_{ps'} a^\dagger_{ps'}\right) |\phi_0\rangle$$

0 because $|\phi_0\rangle$ contains $a^\dagger_{ps'}$ and $a^\dagger_{ps'} a^\dagger_{ps'} = 0$

so $$a^\dagger_{ps'} a_{ps'} |\phi_0\rangle = \theta(p_F - p) |\phi_0\rangle$$

then have

$$a^\dagger_{ks} a_{k's} |\phi_0\rangle \rightsquigarrow \text{same thing.}$$

so we get:

$$\left(\frac{n}{2}\right)^2 g_{ss'}(\vec{r} - \vec{r}') = \frac{1}{V^2} \sum_{\substack{pp' \\ kk'}} e^{-i(p-p')r'} e^{-i(k-k')r} \theta(p_F - p) \delta_{pp'} \ldots$$

$$= \frac{1}{V^2} \sum_{p,k} \theta(p_F - p)\, \theta(p_F - k)$$

$$= \left[\frac{1}{V} \sum_{p} \theta(p_F - p)\right]^2$$

did this on p. 17 — get $\frac{n}{2}$

$$= \left(\frac{n}{2}\right)^2$$

$\therefore \quad g_{ss'} = 1 \quad \text{if } s \neq s'$

(b) $s = s'$?

$$\left(\frac{n}{2}\right)^2 g_{ss}(r - r') = \frac{1}{V^2} \sum_{\substack{pp' \\ kk'}} e^{-i(p-p')r} e^{-i(k-k')r'} \langle \Phi_0 | a^\dagger_{ks} a^\dagger_{ps} a_{p's} a_{k's} | \Phi_0 \rangle$$

now, same as before: $|\Phi_0\rangle$ must contain both k's and p's $\neq k$'s.
these must be put back; so either

2 possibilities $\begin{cases} p = p' \quad \text{and} \quad k = k' \\ \text{or} \\ k = p' \quad \text{and} \quad p = k' \end{cases}$

if $p = p'$ and $k = k'$, same as before.

if $k = p'$ and $p = k'$, $\quad a^\dagger_{ks} \underbrace{a^\dagger_{ps}\, a_{p's}} a_{k's}$

[remember $p \neq h'$ $\quad = a^\dagger_{ks} \underbrace{a_{p's}\, a^\dagger_{ps}} a_{k's} (-1)$
$\therefore$ $p \neq k$]
$k \neq k'$
$p \neq p'$

because $a^\dagger_{ps} a_{p's} = - a_{p's} a^\dagger_{p}$

$$\text{so}\quad \left(\frac{n}{2}\right)^2 g_{ss}(r-r') = \frac{1}{V^2}\sum_{\substack{pp'\\kk'}} e^{-i(p-p')r'} e^{-i(k-k')r'} \Big\{ \delta_{pp'}\delta_{kk'} \overbrace{\langle \Phi_0 | n_{ks}\, n_{ps} | \Phi_0 \rangle}^{\Theta(p_F-p)\,\Theta(p_F-k)}$$

$$+ \delta_{kp'}\delta_{pk'} \underbrace{\langle \Phi_0 | n_{ks}\, n_{ps} | \Phi_0 \rangle}_{\Theta(p_F-k)\,\Theta(p_F-p)} (-1) \Big\}$$

$$= \left(\frac{n}{2}\right)^2 - \frac{1}{V^2}\sum_{pk} e^{-i(p-k)r} e^{-i(k-p)r'}\,\Theta(p_F-k)\,\Theta(p_F-p)$$

$$= \left(\frac{n}{2}\right)^2 - \frac{1}{V^2}\sum_{k,k'} e^{+i(k-k')(r-r')}\,\Theta(p_F-k)\,\Theta(p_F-k')$$

$$= \left(\frac{n}{2}\right)^2 - \underbrace{\left[\frac{1}{V}\sum_{k} e^{ik\cdot(\bar{r}-\bar{r}')}\,\Theta(p_F-k)\right]}_{G_s^*(\bar{r}-\bar{r}')} \underbrace{\left[\frac{1}{V}\sum_{k'} e^{-ik'\cdot(\bar{r}-\bar{r}')}\,\Theta(p_F-k')\right]}_{G_s(\bar{r}-\bar{r}')}$$

see p. 16.

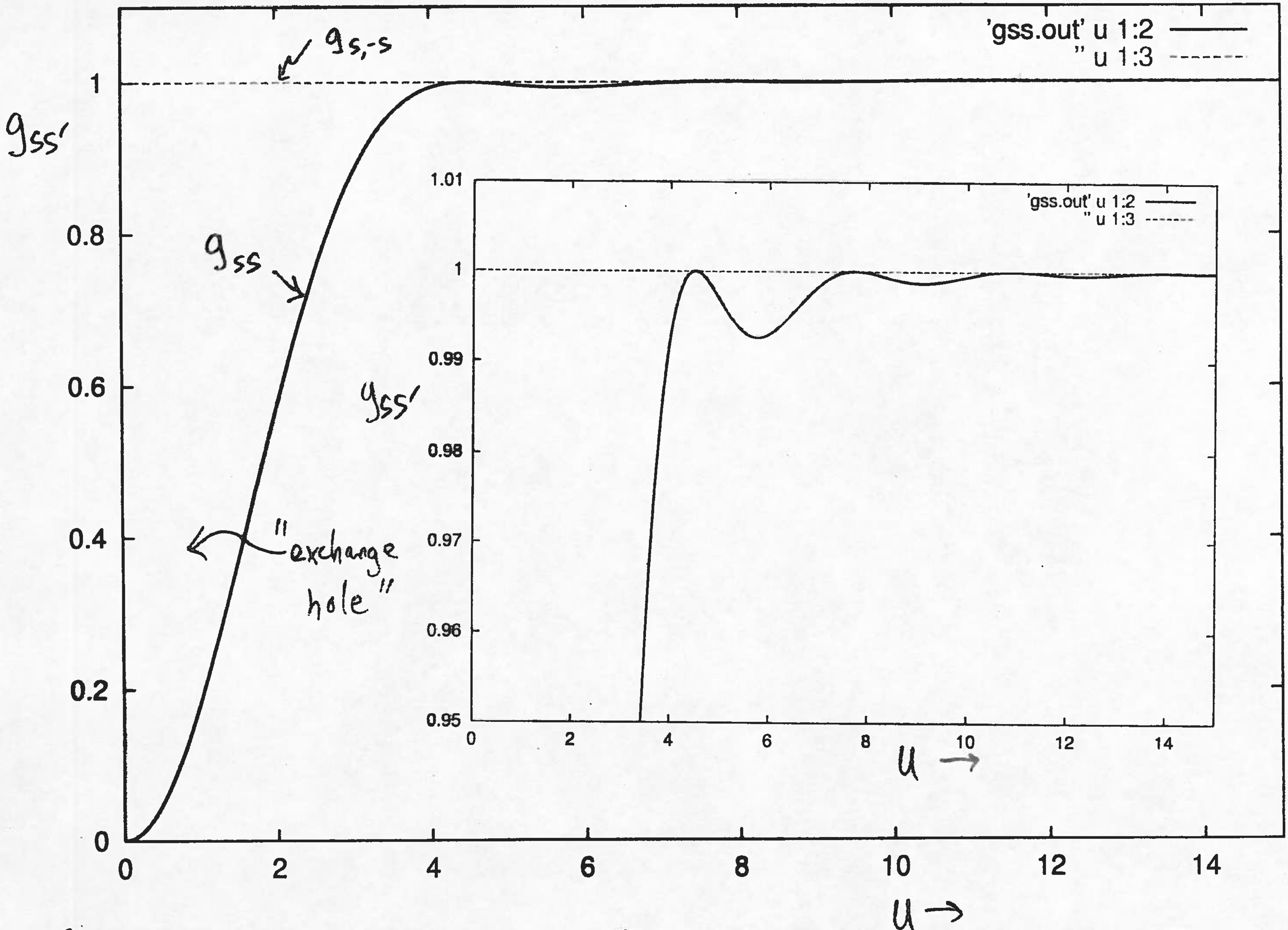
$$= \left(\frac{n}{2}\right)^2 - \left|G_s(\bar{r}-\bar{r}')\right|^2$$

$$= \left(\frac{n}{2}\right)^2 \left[1 - 9\left[\frac{\sin u - u\cos u}{u^3}\right]^2\right]$$

$$\therefore\quad g_{ss}(r-r') = 1 - \frac{9}{u^6}\left[\sin u - u\cos u\right]^2 \qquad u = p_F|\bar{r}-\bar{r}'|$$

just the Pauli exclusion principle causes large correlations in the motion of fermions with the same spin.

looks like a repulsion.



'gss.out' u 1:2
'' u 1:3
g s,-s
g ss'
g ss
"exchange hole"
u →