Ch. 3: Non-interacting ground state and particle-hole transformation

In ch. 2, p. 9, we proved a theorem for one-body Hamiltonians

$$H^{(1)} = \sum_{i=1}^{N} h^{(1)}(x_i), \quad \text{[coordinate repr.]} \qquad \underline{(1)}$$

We showed that if the single-particle wave functions $\varphi_i(x)$ and single-particle energies E_i are known, i.e. the problem

$$\boxed{h^{(1)}(x)\, \varphi_i(x) = E_i \varphi_i(x)} \qquad \underline{(2)}$$

has been solved, then the total energy of the system is given by

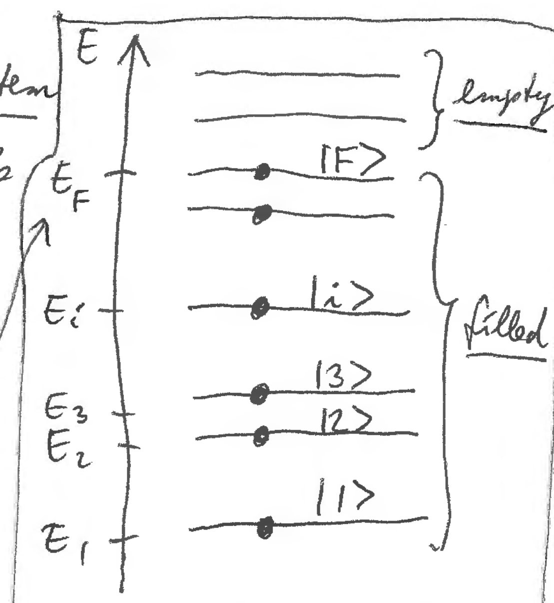
$$E = \sum_i E_i \,(\text{occupied}) \qquad \underline{(3a)}$$

and, for fermions, the many-body WF is a Slater determinant of the occupied s.p. WF's.

Clearly, the minimum energy of the system (= g.s. energy) is obtained by ordering the s.p. levels according to their energy

$$\boxed{E_1 \le E_2 \le E_3 \le \ldots \le E_F} \qquad \underline{(3b)}$$

"Fermi energy"



the non-interacting g.s.

(taking into account degenerate states) and filling the lowest N levels, up to the Fermi level $|F\rangle$:

$$\boxed{E_{g.s.} \equiv E_0 = \sum_{i=1}^{F} E_i} \qquad \underline{(3c)}$$

and the corresponding state vector is

$$\boxed{|\phi_{g.s.}\rangle \equiv |\phi_0\rangle = \left(\hat{c}_1^+ \hat{c}_2^+ \dots \hat{c}_F^+\right)|0\rangle}. \quad (3d)$$

We emphasize that (3c) and (3d) represent the "non-interacting ground state". Any 2-body interaction will scatter some particles into unoccupied state above E_F and create holes below E_F ("particle-hole excitation"). We will see this particularly clearly in the BCS-theory section later!

Particle-hole transformation, "quasi-particles"

Ref: Fetter & Walecka, p. 70-71

We start with an illustrative example: consider the quantum field operators for a free Fermi gas

$$\left.\begin{aligned} \hat{c}^+(\underbrace{\vec{r},\lambda}_{=x}) &\equiv \hat{c}_\lambda^+(\vec{r}) = \sum_{\vec{k}=1}^{\infty} \hat{c}_{\vec{k}\lambda}^+ \, \varphi_{\vec{k}\lambda}^+(\vec{r}) \\ \hat{c}(\underbrace{\vec{r},\lambda}_{=x}) &\equiv \hat{c}_\lambda(\vec{r}) = \sum_{\vec{k}=1}^{\infty} \hat{c}_{\vec{k}\lambda} \, \varphi_{\vec{k}\lambda}(\vec{r}) \end{aligned}\right\} \quad \text{where } \boxed{\lambda \equiv s_z = \uparrow, \downarrow}$$

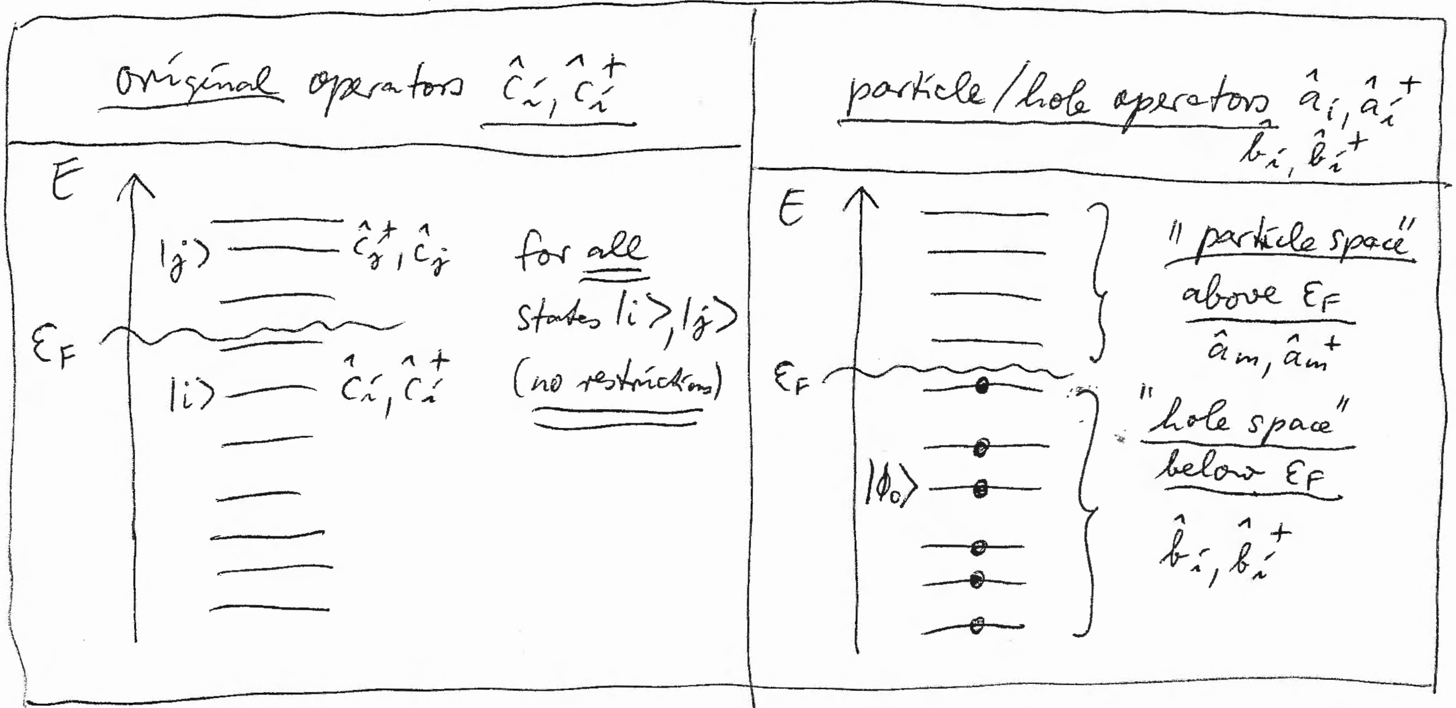
where the s.p. WF's $\varphi_{\vec{k}\lambda}(\vec{r})$ are given in ch. 2, p. 7.

Now we introduce new operators for "particle" and "hole" states which are defined with respect to the Fermi surface:

$$\hat{c}_{\vec{k}\lambda} \stackrel{def}{=} \begin{cases} \hat{a}_{\vec{k}\lambda}, & \text{for } |\vec{k}| = k > k_F \quad \text{"particles"} \\ \hat{b}_{-\vec{k}\lambda}^+, & \text{for } |\vec{k}| = k \leq k_F \quad \text{"holes"} \end{cases}$$

Taking the adjoint, we obtain

$$\hat{c}^{+}_{\vec{k}\lambda} = \begin{cases} \hat{a}^{+}_{\vec{k}\lambda}\,, & \text{for } |\vec{k}| = k > k_F \quad \text{"particle creation"} \\ \hat{b}_{-\vec{k}\lambda}\,, & \text{for } |\vec{k}| = k \le k_F \quad \text{"hole destruction"} \end{cases}$$



Generalization of p–h transf. for arbitrary s.p. states $|i\rangle$

$$\left.\begin{aligned} \hat{c}_i &= \hat{a}_i\,\theta(\varepsilon_i - \varepsilon_F) + \hat{b}^{+}_{-i}\,S_i\,\theta(\varepsilon_F - \varepsilon_i) \\ c_i^{+} &= \hat{a}_i^{+}\,\theta(\varepsilon_i - \varepsilon_F) + \hat{b}_{-i}\,S_i\,\theta(\varepsilon_F - \varepsilon_i) \end{aligned}\right\}$$

see Fetter Walecka p. 506

where S_i = phase factor; for Fermi gas $S_i = +1$.

From the original anticomm. relations for $\hat{c}_i, \hat{c}_j^+$

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

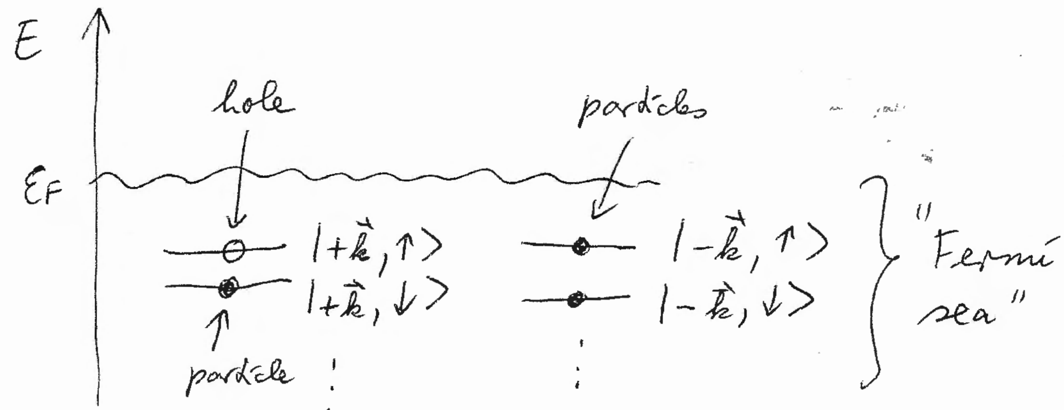
one derives

$$\left.\begin{aligned} &\{\hat{a}_i, \hat{a}_j^+\} = \delta_{ij}\,, \quad \{\hat{b}_i, \hat{b}_j^+\} = \delta_{ij} \\ &\text{all other anticomm} = 0 \end{aligned}\right\}$$

Since p-h transf. leaves anticommutators unchanged, it is a canonical transf. [compare to Shankar, p. 95].

$$\boxed{\text{Comments on quantum numbers of hole state } (\hat{b}^+_{-i} / \hat{b}^+_{-\vec{k}\lambda})}$$

Consider free Fermi gas as example. The 4 s.p. states $|\pm\vec{k}, \uparrow\downarrow\rangle$ are energetically degenerate:



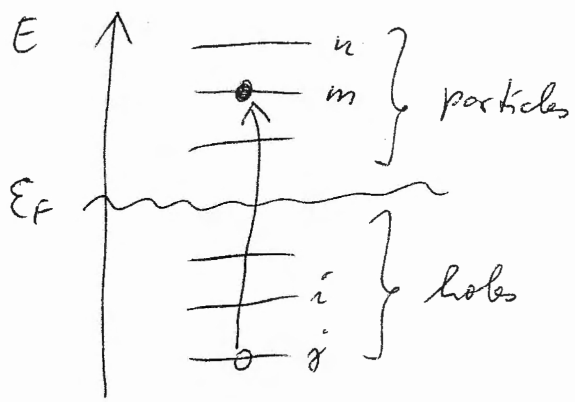
From above figure, we infer that the destruction of a particle in the filled "Fermi sea" $(\hat{c}_{\vec{k},\lambda})$ is equivalent to creating a hole $(\hat{b}^+)$. Note that after we destroy the particle in the state $|+\vec{k},\lambda\rangle$, the N-particle system is left with an occupied state $|-i\rangle = |-\vec{k},\lambda\rangle$.

Fetter & Walecka, p. 70: "The absence of a particle with momentum $+\vec{k}$ from the filled Fermi sea implies that the system possesses a momentum $-\vec{k}$." Hence, the proper quantum numbers of the hole state in the Fermi sea are

$$\hat{b}^+_{-\vec{k}\lambda}.$$

Excited states of the N-body system: (multiple) particle-hole excitations

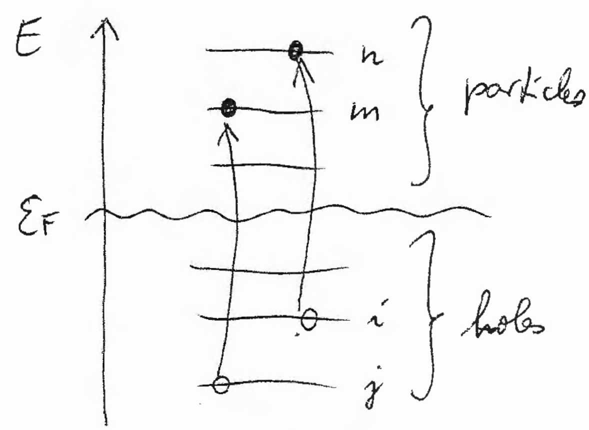
"1 particle – 1 hole" (1p-1h)



state vector of excited state

$$|\phi_{mj}\rangle = \hat{a}_m^+ \hat{b}_j^+ \underset{\text{g.s.}}{|\phi_0\rangle}$$

"2 particle – 2 hole" (2p-2h)

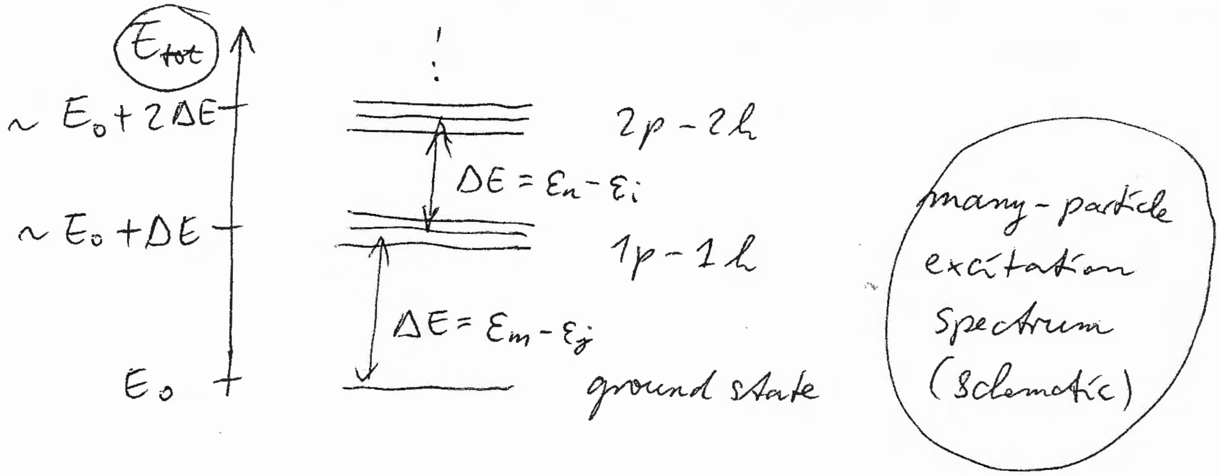


state vector of excited state

$$|\phi_{mnji}\rangle =$$
$$= \hat{a}_m^+ \hat{a}_n^+ \hat{b}_j^+ \hat{b}_i^+ |\phi_0\rangle$$

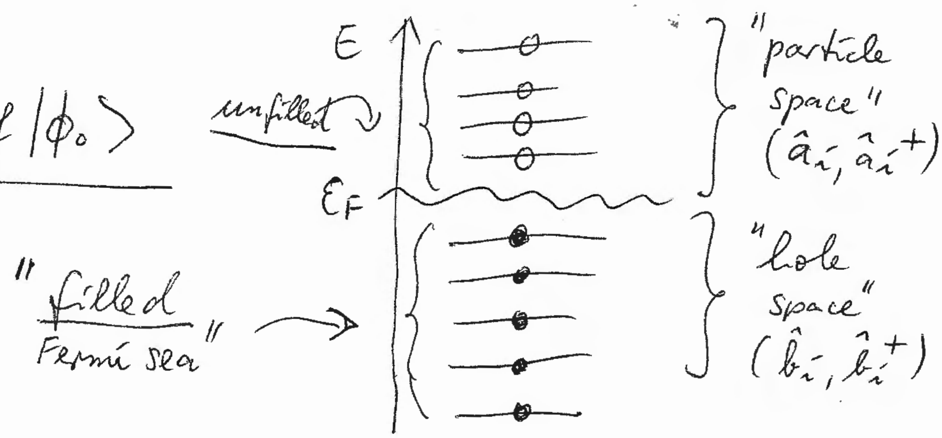
etc. for n-particle – n hole excitations!

The (schematic) spectrum of excited states of the many-particle system looks like this:



$$\boxed{\text{Nonint. ground state } |\phi_0\rangle \equiv \text{p–h vacuum} \rightarrow \text{important for practical calculations}}$$

Structure of $|\phi_0\rangle$



From the figure, we observe:

(1) $\boxed{\hat{a}_i |\phi_0\rangle = 0}$ because in the particle space (where the $\hat{a}_i$ are defined), there are no particles, hence, we cannot destroy any particles! The statement $\hat{a}_i |\phi_0\rangle = 0$ means that this state cannot be normalized and does not exist!

(2) $\boxed{\hat{b}_i |\phi_0\rangle = 0}$ because in the hole space (where the $\hat{b}_i$ are defined), there are no holes, hence we cannot destroy any holes!

Important conclusion:

The non-interacting g.s. $|\phi_0\rangle$ behaves like a vacuum state with respect to the particle and hole operators, i.e.

$$\boxed{\hat{a}_i |\phi_0\rangle = 0 \quad \text{and} \quad \hat{b}_i |\phi_0\rangle = 0}$$

First application of p-h transformation:
density parameters $\rho_{\beta\alpha} = \langle\phi_0| \hat{c}_\alpha^+ \hat{c}_\beta |\phi_0\rangle$

In chapter 2, p. 31 we derived an expression for the ground-state density of a many-body system. In the special case of the non-int. g.s. one obtains the density parameters

$$\boxed{\rho_{\beta\alpha}^{(0)} \stackrel{def}{=} \langle \phi_{g.s.} | \hat{c}_\alpha^+ \hat{c}_\beta | \phi_{g.s.}\rangle \rightarrow \langle \phi_0 | \hat{c}_\alpha^+ \hat{c}_\beta | \phi_0 \rangle}.$$

We evaluate now $\rho_{\beta\alpha}$, using the p-h transformation. We have actually evaluated $\rho_{\beta\alpha}$ earlier using "physical" arguments (see ch. 2, p. 26), but the following derivation is more rigorous and will later on be generalized in the famous BCS theory.

$$\rho_{\beta\alpha}^{(0)} \stackrel{def}{=} \langle \phi_0 | \hat{c}_\alpha^+ \hat{c}_\beta | \phi_0 \rangle = \text{insert p-h transf} =$$

$$= \langle \phi_0 | \left[\theta(\varepsilon_\alpha - \varepsilon_F) a_\alpha^+ + \theta(\varepsilon_F - \varepsilon_\alpha) S_\alpha \hat{b}_{-\alpha} \right] \cdot \left[\theta(\varepsilon_\beta - \varepsilon_F) \hat{a}_\beta + \right.$$
$$\left. + \theta(\varepsilon_F - \varepsilon_\beta) S_\beta \hat{b}_{-\beta}^+ \right] | \phi_0 \rangle =$$

$$= \theta(\varepsilon_\alpha - \varepsilon_F)\, \theta(\varepsilon_\beta - \varepsilon_F) \langle \phi_0 | \hat{a}_\alpha^+ \hat{a}_\beta | \phi_0 \rangle + \quad ①$$
$$+ \theta(\varepsilon_F - \varepsilon_\alpha)\, \theta(\varepsilon_\beta - \varepsilon_F) S_\alpha \langle \phi_0 | \hat{b}_{-\alpha} \hat{a}_\beta | \phi_0 \rangle + \quad ②$$

$$\left.\begin{aligned} &+ \theta(\varepsilon_\alpha - \varepsilon_F)\,\theta(\varepsilon_F - \varepsilon_\beta)\, S_\beta \langle \phi_0 | \hat{a}_\alpha^+ \hat{b}_{-\beta}^+ | \phi_0 \rangle + \\ &+ \theta(\varepsilon_F - \varepsilon_\alpha)\,\theta(\varepsilon_F - \varepsilon_\beta)\, S_\alpha S_\beta \langle \phi_0 | \hat{b}_{-\alpha} \hat{b}_{-\beta}^+ | \phi_0 \rangle . \end{aligned}\right\} \begin{matrix} ③ \\ ④ \end{matrix}$$

- The first two terms vanish because $\hat{a}_\beta |\phi_0\rangle = 0$.
- The 3^{rd} term vanishes because $\langle \phi_0 | \hat{a}_\alpha^+ = (|\phi_0\rangle)^+ \hat{a}_\alpha^+ = \big(\underbrace{\hat{a}_\alpha |\phi_0\rangle}_{=0}\big)^+$.
- For the 4^{th} term, we use the anticommutation relation

$$\{ \hat{b}_{-\alpha}, \hat{b}_{-\beta}^+ \} = \delta_{-\alpha,-\beta} \equiv \delta_{\alpha\beta} \quad \Downarrow$$

$$\boxed{\hat{b}_{-\alpha} \hat{b}_{-\beta}^+ = \delta_{\alpha\beta} - \hat{b}_{-\beta}^+ \hat{b}_{-\alpha}}$$

which leads to

$$\rho_{\beta\alpha}^{(0)} = 4^{th} \text{ term only} = \theta(\varepsilon_F - \varepsilon_\alpha)\,\theta(\varepsilon_F - \varepsilon_\beta)\, S_\alpha S_\beta \cdot$$

$$\cdot \langle \phi_0 | \underline{\underline{\delta_{\alpha\beta}}} - \hat{b}_{-\beta}^+ \underbrace{\hat{b}_{-\alpha} | \phi_0 \rangle}_{=0} \qquad \text{Use } \delta_{\alpha\beta} \text{ properties:}$$

$$\rho_{\beta\alpha}^{(0)} = \underbrace{\theta^2(\varepsilon_F - \varepsilon_\alpha)}_{=\theta(\varepsilon_F - \varepsilon_\alpha)} \underbrace{S_\alpha^2}_{=+1} \delta_{\alpha\beta} = \theta(\varepsilon_F - \varepsilon_\alpha)\, \delta_{\alpha\beta}$$

Summary: density parameters in non-interacting g.s. $\|\phi_0\rangle$
$\rho_{\beta\alpha}^{(0)} \overset{def}{=} \langle \phi_0 \| \hat{c}_\alpha^+ \hat{c}_\beta \| \phi_0 \rangle = \theta(\varepsilon_F - \varepsilon_\alpha)\, \delta_{\alpha\beta}$

Example 1: density in non-int. g.s. $|\phi_0\rangle$

From ch. 2, p. 31, we get, using $|\phi_{g.s.}\rangle \to |\phi_0\rangle$:

$$\rho^{(0)}(\underbrace{\vec{r}, s_z}_{=x}) = \sum_{i,j=1}^{\infty} \varphi_j^+(\vec{r}, s_z)\, \varphi_i(\vec{r}, s_z)\, \rho_{ij}^{(0)}$$

↑ s.p. WF's ↑ density parameters

$$\rho^{(0)}(\vec{r}, s_z) = \sum_{i,j=1}^{\infty} \varphi_j^{+}(\vec{r}, s_z)\, \varphi_i(r, s_z)\, \underline{\theta(\varepsilon_F - \varepsilon_i)}\, \underline{\delta_{ij}}$$

$$\boxed{\rho^{(0)}(\vec{r}, s_z) = \sum_{i=1}^{F} \underbrace{\varphi_i^{+}(\vec{r}, s_z)\, \varphi_i(\vec{r}, s_z)}_{\equiv \rho_i(\vec{r}, s_z)}}$$

Interpretation: for non-int. system, the density is obtained by adding up the probability densities for all occupied levels $i = 1, 2, \dots, i_F$.

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a) apply to free Fermi gas

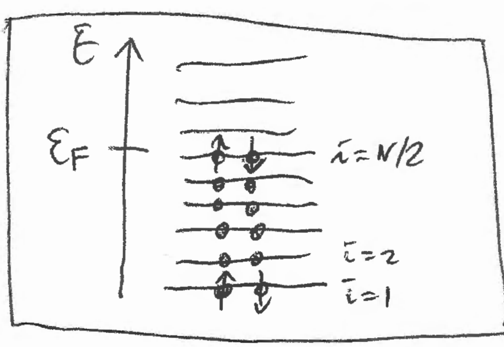
Use s.p. WF's from ch. 2, p. 7

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

$$\curvearrowright \; \underline{\rho_i(\vec{r}, s_z)} = \varphi_i^{+} \varphi_i = \frac{1}{L^3} \underbrace{e^{-i\vec{k}\cdot\vec{r}} e^{+i\vec{k}\cdot\vec{r}}}_{=1} \underbrace{\chi_{s_z}^{+} \chi_{s_z}}_{=1} = \underline{\frac{1}{L^3}}$$

$$\Rightarrow \rho^{(0)}(\vec{r}, s_z) = \sum_{i=1}^{F} \rho_i = \sum_{i=1}^{F} \left(\frac{1}{L^3}\right) = \frac{1}{L^3} \underbrace{\sum_{i=1}^{F}}_{=\frac{N}{2}} = \frac{1}{2} \frac{N}{L^3}$$

because



because of spin-up/down degeneracy (see fig.)

Hence: for free Fermi gas:

$$\underset{\text{g.s. density}}{\rho^{(0)}(\vec{r}, s_z)} = \frac{1}{2} \rho_0 ; \quad \text{with} \quad \boxed{\underset{\text{total density}}{\rho_0 = N/L^3}}$$

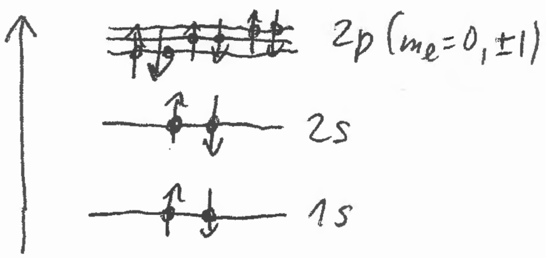
We obtain the obvious result that in a <u>free Fermi gas</u> the density is <u>homogeneous</u> (i.e. independent of $\vec{r}$), and the g.s. density for a given spin projection ($s_z = \uparrow$ or $\downarrow$) is one half of the total density ρ_0.

<u>b) apply to N-electron atom (without $e^- e^-$ int.)</u>

s.p. WF's: $\varphi_i(\vec{r}, s_z) = R_{nl}(r)\, Y_{l,m_l}(\theta,\varphi)\, \chi^{s=\frac{1}{2}}_{s_z}$

<u>s.p. probability density</u>: $\underline{\rho_i(r,\theta,\varphi) = R^2_{nl}(r)\, |Y_{l,m_l}(\theta,\varphi)|^2}\, \underbrace{\chi^+\chi}_{=1}$

$\Rightarrow$ indep. of s_z $\Rightarrow$ degeneracy of 2 for every level (n, l, m_l).



<u>atomic g.s. density $\rho^{(0)}(r,\theta,\varphi)$</u>
add up prob. densities $\rho_i(r,\theta,\varphi)$ for all filled orbitals!

<u>Example 2: total energy of free Fermi gas</u>

In <u>coord. repr.</u>, H is the sum of N kinetic energy operators

$$H = T = \sum_{i=1}^{N} t_i = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\nabla_i^2$$

In <u>occup. # repr.</u>, this one-body operator becomes

$$\hat{H} = \hat{T} = \sum_{k,l=1}^{\infty} \langle k | -\frac{\hbar^2}{2m}\nabla^2 | l \rangle\, \hat{c}_k^+ \hat{c}_l$$

Using the free Fermi gas s.p. eigenstates as basis

$$|l\rangle = |\vec{k}, s_z\rangle$$

we obtain

$$\hat{H} = \sum_{\vec{k}', s_z'} \sum_{\vec{k}, s_z} \langle \vec{k}', s_z' | -\frac{\hbar^2}{2m}\nabla^2 | \vec{k}, s_z \rangle \, \hat{c}^{+}_{\vec{k}' s_z'} \, \hat{c}_{\vec{k} s_z}$$

The s.p. matrix element is spin-indep. and diagonal (compare to notes ~~[illegible]~~ ch. 2 p. 32 for $\hat{\vec{p}}$):

$$\langle \vec{k}', s_z' | -\frac{\hbar^2}{2m}\nabla^2 | \vec{k}, s_z \rangle = \underbrace{\langle s_z' | s_z \rangle}_{\delta_{s_z' s_z}} \underbrace{\langle \vec{k}' | -\frac{\hbar^2}{2m}\nabla^2 | \vec{k} \rangle}_{\frac{\hbar^2 \vec{k}^2}{2m}\delta_{\vec{k}'\vec{k}}}$$

resulting in

$$\boxed{\hat{H} = \sum_{\vec{k}, s_z} \frac{\hbar^2 \vec{k}^2}{2m} \underbrace{\hat{c}^{+}_{\vec{k}, s_z} \hat{c}_{\vec{k}, s_z}}_{= \hat{n}_{\vec{k}, s_z} \leftarrow \text{number operator}}}$$

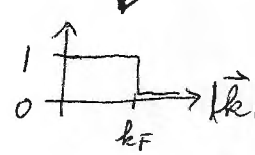
Hamiltonian for free Fermi gas

The total g.s. energy is

$$E_{tot} = \langle \phi_0 | \hat{H} | \phi_0 \rangle = \langle \phi_0 | \sum_{\vec{k}, s_z}^{\infty} \frac{\hbar^2 \vec{k}^2}{2m} \hat{n}_{\vec{k}, s_z} | \phi_0 \rangle$$

The number operator has the same effect as in the calculation of the density on p. 8:

$$\hat{n}_{\vec{k}, s_z} | \phi_0 \rangle = \underbrace{2}_{\text{spin-deg.}} \cdot \, \hat{n}_{\vec{k}} | \phi_0 \rangle = 2 \cdot \Theta(k_F - |\vec{k}|) | \phi_0 \rangle$$

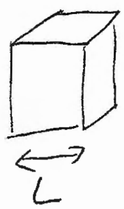


resulting in

$$E_{tot} = 2 \cdot \langle \phi_0 | \sum_{\vec{k}}^{\infty} \frac{\hbar^2 \vec{k}^2}{2m} \Theta(k_F - |\vec{k}|) | \phi_0 \rangle =$$

$$= 2 \cdot \sum_{\vec{k}}^{k_F} \frac{\hbar^2 \vec{k}^2}{2m} \underbrace{\langle \phi_0 | \phi_0 \rangle}_{=1} \Rightarrow \boxed{E_{tot} = 2 \sum_{\vec{k}}^{k_F} \frac{\hbar^2 \vec{k}^2}{2m}}$$

We have used s.p. WFs in a cubic box of length L.



Taking the large-L limit (which is appropriate for a gas with large # particles) one has to make the replacement (see Fetter & Walecka, p. 26):

$$\boxed{\frac{1}{L^3}\sum_{\vec{k}} f(\vec{k}) \rightarrow \frac{1}{(2\pi)^3}\int d^3k\, f(\vec{k})}$$

Apply this to E_{tot} with $f(\vec{k}) = \frac{\hbar^2\vec{k}^2}{2m}$

$$E_{tot} = 2\sum_{\vec{k}}^{k_F}\frac{\hbar^2\vec{k}^2}{2m} \longrightarrow 2\cdot\frac{L^3}{8\pi^3}\int d^3k\,\frac{\hbar^2 k^2}{2m} =$$

$$= 2\cdot\frac{L^3}{8\pi^3}\underbrace{\int d\Omega_k}_{4\pi}\int_0^{k_F} k^2 dk\left(\frac{\hbar^2k^2}{2m}\right) = \frac{L^3}{\pi^2}\int_0^{k_F}\frac{\hbar^2}{2m}k^4 dk$$

$$\boxed{E_{tot} = \frac{L^3}{\pi^2}\,\frac{\hbar^2}{2m}\,\frac{k_F^5}{5}} \quad (1)$$

There is an important relation between Fermi momentum, $\hbar k_F = p_F$ and density $\rho_0 = N/L^3$. We start from

$$N = \underset{\nearrow \text{ spin deg.}}{2}\cdot\sum_{\vec{k}}\theta(k_F - |\vec{k}|).$$

Using, like above, the large L-limit with $f(\vec{k}) = \theta(k_F - |\vec{k}|)$, one finds easily the result

$$N = \frac{L^3}{\pi^2}\frac{k_F^3}{3} \Rightarrow \boxed{k_F = \left(3\pi^2\frac{N}{L^3}\right)^{1/3} = \left(3\pi^2\rho_0\right)^{1/3}}$$

(2)

Inserting (2) into (1) we obtain

$$E_{tot} \overset{(1)}{=} \left(\frac{L^3}{\pi^2} \frac{\hbar^2}{2m} \frac{k_F^2}{5} \right) \cdot \underbrace{k_F^3}_{\overset{(2)}{=} \left(3\pi^2 \frac{N}{L^3}\right)} = \left(\frac{\cancel{L^3}}{\cancel{\pi^2}} \frac{\hbar^2}{2m} \frac{k_F^2}{5} \right) \left(3\cancel{\pi^2} \frac{N}{\cancel{L^3}} \right)$$

$$\Rightarrow E_{tot} = N \cdot \left(\frac{3}{5} \frac{\hbar^2 k_F^2}{2m} \right) \Rightarrow \underline{\frac{E_{tot}}{N} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m}}$$

Summary: total energy per particle for free Fermi gas

Define: Fermi momentum $\boxed{p_F = \hbar k_F}$

$\boxed{k_F = (3\pi^2 \rho_0)^{1/3}}$ ← Fermi momentum depends on density

Fermi energy $\boxed{\varepsilon_F = \frac{p_F^2}{2m}}$

$$\boxed{\frac{E_{tot}}{N} = \frac{3}{5} \varepsilon_F}$$