- this is the closed set of eq.-s
  - they have to be solved simultaneously
- self-consistent iteration.

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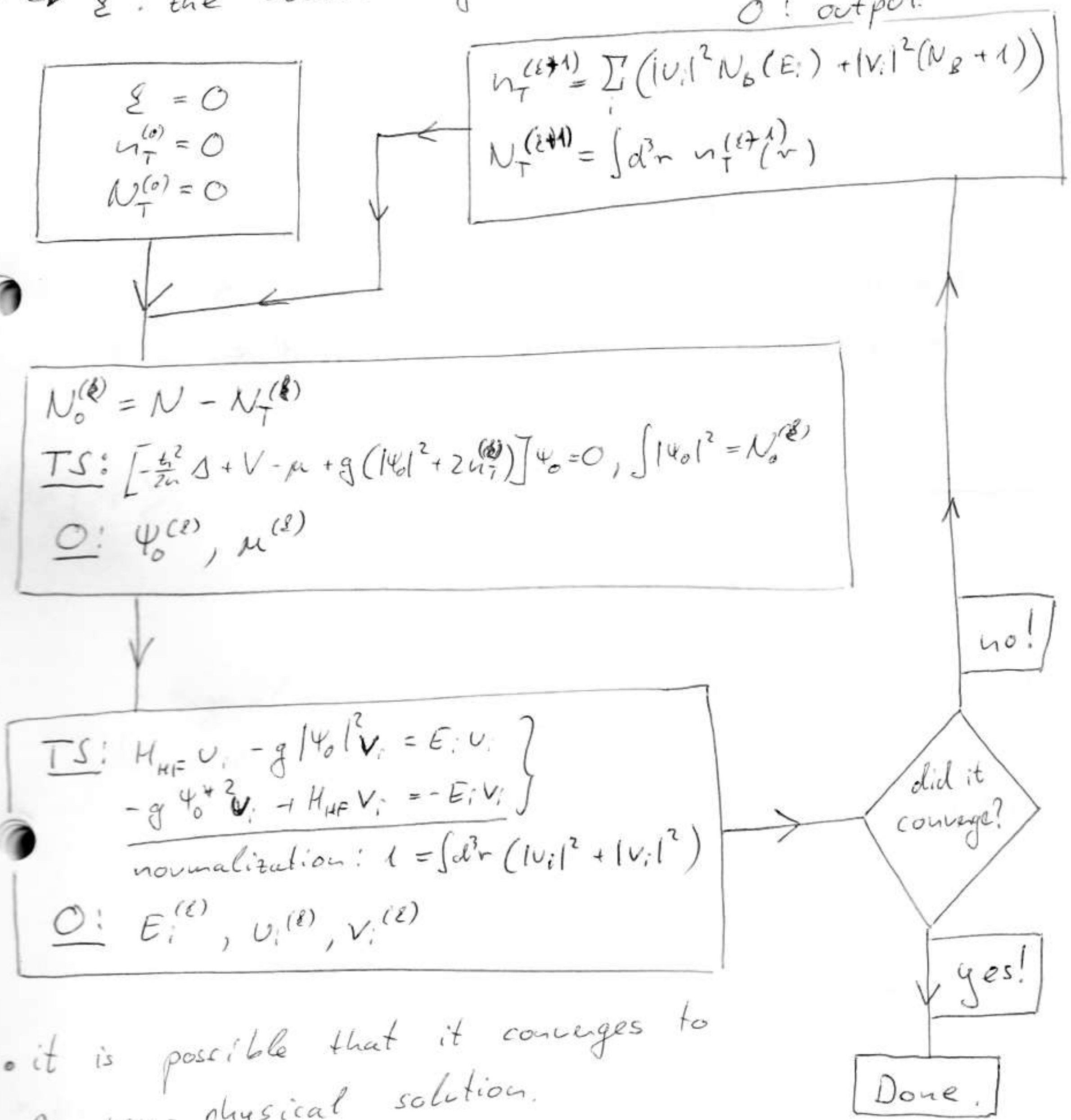
↝ ℓ : the number of iterations ; TS : to be solved
O : output.



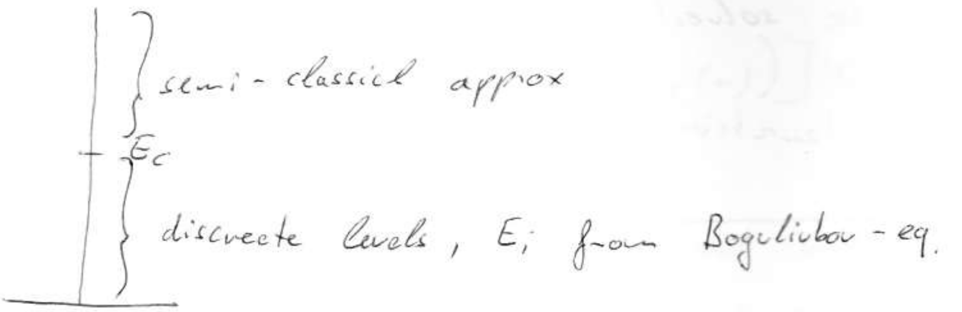
- it is possible that it converges to a non-physical solution.
- only solving a little bit at once
- problematic part: $\sum_i$ in $n_T(r)$

↓

if you cut the sum at the wrong point you may loose some important part of the infinite sum.

→ finite-size correction.

↳ semi-classical approx:



→ add the contribution to the density together
→ this way above E_c stuff isn't lost.

→ $E_c \gg \mu$

→ there are many lvl-s and above E_c the lvl-s are denser,

⇝ the Bose-distribution can populate the lvl-s with a (surprisingly) high probability if the DOS is high there.

Trapped Fermions

$T = 0$, no interaction, HO trap.

$$\left[-\frac{\hbar^2}{2m}\Delta + \frac{1}{2}m\left(\omega_1 x^2 + \omega_2 y^2 + \omega_3 z^2\right)\right]\Psi_{n_1,n_2,n_3}(\underline{r}) = E_{n_1 n_2 n_3}\Psi_{n_1,n_2,n_3}(\underline{r})$$

$$E_{n_1 n_2 n_3} = \hbar\omega_1\left(n_1 + \frac{1}{2}\right) + \hbar\omega_2\left(n_2 + \frac{1}{2}\right) + \hbar\omega_3\left(n_3 + \frac{1}{2}\right)$$

⇝ if there is no degeneracy in the system.

- there are N atoms, ↑↓
- many body grnd. state: (single) Slater-determinant

$$|\Psi\rangle = \Big(\varphi_{101}\,\alpha(s),\ \varphi_{111}\,\beta(s),\ \varphi_{211}\,\alpha,\ \varphi_{211}\,\beta \\ \vdots \\ \Big)$$

$$\rho(\vec{r}) = \langle\Psi|\hat{\rho}(\vec{r})|\Psi\rangle\ ;\ \hat{\rho}(\vec{r}) = \prod_{i=1}^{N}\delta(\vec{r} - \vec{r}_i)$$

$$\Psi(r_1,s_1,r_2,s_2,\dots,r_N,s_N) = \frac{1}{\sqrt{N!}}\sum_{i_1=1}^{N}\dots\sum_{i_N=1}^{N} \varepsilon_{i_1 i_2 \dots i_N}\, \varphi_{i_1}(r_1,s_1)\,\varphi_{i_2}(r_2,s_2)\dots\varphi_{i_N}(r_N,s_N)$$

ordered in a way $\varphi_{111}\ \uparrow$, $\varphi_{111}\ \downarrow$, $\varphi_{211}\ \uparrow$, $\vdots$ — E

⤳ some identities

$$\sum_{i_1=1}^{N}\dots\sum_{i_N=1}^{N} \varepsilon_{i_1\dots i_N}\,\varepsilon_{i_1\dots i_N} = N!$$

$$\sum_{i_2=1}^{N}\dots\sum_{i_N=1}^{N} \varepsilon_{i_1\dots i_N}\,\varepsilon_{j_1 i_2\dots i_N} = \delta_{i_1 j_1}\,(N-1)!$$

⤳ orthogonal basis functions: $\delta_{ij} = \sum_s \int d^3\vec{r}\ \varphi_i^*(\vec{r},s)\,\varphi_j(\vec{r},s)$

$$\langle\Psi|\Psi\rangle = \frac{1}{N!}\sum_{\substack{i_1\\j_1}}\sum_{\substack{i_2\\j_2}}\dots\sum_{\substack{i_N\\j_N}} \varepsilon_{i_1\dots i_N}\,\varepsilon_{j_1\dots j_N}\sum_{s_1}\sum_{s_2}\dots\int d^3\vec{r}_1\dots d^3\vec{r}_N\Big(\varphi_{i_1}(r_1,s_1)\,\varphi_{j_1}(r_1,s_1)\dots\varphi_{i_N}(r_N,s_N)\,\varphi_{j_N}(r_N,s_N)\Big)$$

orthogonality

$$= \frac{1}{N!}\sum_{\substack{i_1\\j_1}}\sum_{\substack{i_2\\j_2}}\dots\sum_{\substack{i_N\\j_N}} \varepsilon_{i_1\dots i_N}\,\varepsilon_{j_1\dots j_N}\,\delta_{i_1 j_1}\,\delta_{i_2 j_2}\dots\delta_{i_N j_N} =$$

$$= \frac{1}{N!}\sum_{i_1}\dots\sum_{i_N}\varepsilon_{i_1\dots i_N}\,\varepsilon_{i_1\dots i_N} = \frac{N!}{N!} = 1$$

• the correct normalization for slaters, if the 1 part wf is orthogonal

$$\langle\Psi|\hat{\rho}(\vec{r},s)|\Psi\rangle = \sum_{s_1}\dots\sum_{s_N}\int d^3\vec{r}_1\dots d^3\vec{r}_N\Big(\Psi^*(r_1,s_1,\dots r_N,s_N)\sum_i\delta(\vec{r}-\vec{r}_i)\,\delta_{ss_i}\cdot\Psi(r_1,s_1\dots r_N,s_N)\Big) =$$

$$= \sum_i\sum_{s_1}\dots\sum_{s_N}\int d^3\vec{r}_1\dots d^3\vec{r}_N\Big(\Psi^*(r_1,s_1\dots \overset{i\text{th}}{r,s}\dots r_N s_N)\,\Psi(r_1,s_1\dots \overset{i\text{th}}{r,s}\dots r_N,s_N)\Big) \overset{(-1)^2}{=}$$

moving $r_i s$ to be the first

$$= N \cdot \sum_{s_2} \dots \sum_{s_N} \int d^3\vec{r}_2 \dots d^3\vec{r}_N \left(\Psi^*(r, s, r_2, s_2 \dots r_N, s_N) \Psi(r, s, r_2, s_2 \dots r_N s_N) \right) =$$

$$= N \cdot \sum_{s_2} \dots \sum_{s_N} \int d^3\vec{r}_2 \dots d^3 r_N \left(\sum_{i_1} \dots \sum_{i_N} \varepsilon_{i_1 \dots i_N} \varphi^*_{i_1}(r, s) \varphi_{i_2}(r_2, s_2) \dots \right) \left(\sum_{j_1} \dots \sum_{j_N} \varepsilon_{j_1 \dots j_N} \varphi_{j_1}(r, s) \varphi_{j_2}(r_2, s_2) \dots \right) \cdot \frac{1}{N!}$$

$$= \frac{1}{(N-1)!} \sum_{\substack{i_1 \\ j_1}} \varphi^*_{i_1}(r, s) \varphi_{j_1}(r, s) \cdot \sum_{\substack{i_2 \dots i_N \\ j_2 \dots j_N}} \varepsilon_{i_1 \dots i_N} \varepsilon_{j_1 \dots j_N} \delta_{i_2 j_2} \dots \delta_{i_N j_N} =$$

$$= \frac{1}{\cancel{(N-1)!}} \sum_{\substack{i_1 \\ j_1}} \varphi^*_{i_1}(r, s) \varphi_{j_1}(r, s) \, \delta_{i_1 j_1} \cancel{(N-1)!} = \sum_i \varphi^*_i(r, s) \varphi_i(r, s)$$

- all 1 part lvl.-s give a contribution to the density with a weight function of uniform 1-s.

$$\rho(r, s) = \sum_i |\varphi_i(r, s)|^2$$

- exact density of the non-interacting system.
- approximate density for large N:
  - ⤳ homogenious system ($V = 0$)
  - ⤳ chemical pot $= \mu$ $n = n(\mu)$

<u>local density approximation:</u>

$$\mu \Leftarrow \mu - V(r)$$

locally changes the chemical potential

$$n(r) = n(\mu - V(r))$$

$\int n(r) \, d^3r = N$ ⤳ fixing the N

$V = \frac{1}{2} m \sum_i \omega_i x_i^2$

- non-int. fermions
- $T = 0$.

- first homogenious problem (periodic boundary)

$-\frac{\hbar^2}{2m} \Delta = H$

$\Psi = e^{i \sum_i k_i x_i}$

$E = \frac{\hbar^2 k^2}{2m} \qquad k^2 = \sum_i k_i^2$

- fill up levels up to μ_F

$$N = 2 \frac{V}{(2\pi)^3} \int d^3k \frac{1}{e^{\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)} + 1} \underset{T=0}{=} 2 \frac{V}{(2\pi)^3} \underbrace{\int_{|k|<k_F} d^3k}_{4\pi \int_0^{k_F} k^2 dk = 4\pi \frac{k_F^3}{3}}$$

$\mu = \frac{\hbar^2 k_F^2}{2m} \rightsquigarrow k_F = \sqrt{\frac{2m\mu}{\hbar^2}}$

$N = \frac{V}{3\pi^2} k_F^3 \qquad / \frac{1}{V}$

$$\boxed{n = \frac{1}{3\pi^2} k_F^3 = \frac{1}{3\pi^2} \frac{(2m\mu)^{3/2}}{\hbar^3}}$$

- now $\mu \to \mu - V(r)$

$$n(r) = \frac{1}{3\pi^2} \left(\frac{2m(\mu - V(r))}{\hbar^2} \right)^{3/2} \cdot \Theta(\mu - V(r))$$

so it does not become imaginary

- fixing μ:

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

this will give μ_{TF}

$$N = \int_{\mu > V(r)} d^3r \, \frac{1}{3\pi^2} \left(\frac{2m\left(\mu - \frac{1}{2}\omega_1 x^2 - \frac{1}{2}\omega_2 y^2 - \frac{1}{2}\omega_3 z^2\right)}{\hbar^2} \right)^{3/2} =$$

new length:

$$a = \sqrt{\frac{2\mu}{m\omega_1^2}} \qquad b = \sqrt{\frac{2\mu}{m\omega_2^2}} \qquad c = \sqrt{\frac{2\mu}{m\omega_3^2}}$$

$$= \int_{\mu > V(r)} d^3r \, \frac{1}{3\pi^2} \left(\frac{2m\mu_{TF}\left(1 - \frac{x^2}{a^2} - \frac{y^2}{b^2} - \frac{z^2}{c^2}\right)}{\hbar^2} \right)^{3/2} =$$

$$x' = \frac{x}{a} \quad dx = a\,dx'$$
$$y' = \frac{y}{b} \quad dy = b\,dy'$$
$$z' = \frac{z}{c} \quad dz = c\,dz'$$

$$= \frac{1}{3\pi^2} \left(\frac{2m\mu_{TF}}{\hbar^2} \right)^{3/2} \left(\frac{2\mu}{m\omega_1^2} \right)^{1/2} \left(\frac{2\mu}{m\omega_2^2} \right)^{1/2} \left(\frac{2\mu}{m\omega_3^2} \right)^{1/2} \cdot$$

$$\cdot \int_{1 > x'^2 + y'^2 + z'^2} dx'dy'dz' \left(1 - x'^2 - y'^2 - z'^2 \right)^{3/2} =$$

integral is rotationally invariant:

$$\underbrace{4\pi \int_0^1 r'^2 dr' \left(1 - r'^2\right)^{3/2}}_{\frac{\pi}{32}}$$

$$= \frac{1}{3} \frac{\mu_{TF}^3}{\underbrace{\hbar^3 \omega_1 \omega_2 \omega_3}_{\hbar^3 \bar{\omega}^3}} = N$$

where $\bar{\omega} = (\omega_1 \omega_2 \omega_3)^{1/3}$

$$\boxed{\mu_{TF} = (3N)^{1/3} \cdot \hbar\bar{\omega}}$$