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SECOND EUROPEAN SUMMER SCHOOL on
MICROSCOPIC QUANTUM MANY-BODY THEORIES
and their APPLICATIONS

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VARIATIONAL MANY-BODY THEORY AND HELIUM PHYSICS
PART IV and V

Arturo POLLS
Universidad de Barcelona
D. Estructura y Cons. de La Mat.
Facultat de Fisica
Barcelona
SPAIN

Fermi-HyperNetted-Chain theory (FHNC)

To treat identical fermions we must use an antisymmetric wave function.

We will start with:

$$\Psi(1,\dots A) = \prod_{i<j} f(r_{ij}) \quad \phi(1,\dots,A)$$

$\phi(1,\dots,A)$ is the function that describes the system in absence of interactions, in our case: a uniform Fermi system and symmetrical (with equal population of the spin-states), $\phi(1,\dots,A)$ is the Slater determinant

$$\phi(1,\dots,A) = \det |\varphi_{\alpha_i}(r_j)|$$

where the w.f. $\varphi_{\alpha_i}(r_i)$ (the subindex refers to the state)

$$\varphi_{\alpha_i}(i) = \eta_{p(\alpha_i)}(i) \frac{1}{\Omega^{1/2}} e^{i\bar{k}_{\alpha_i}\bar{r}_i}$$

are plane waves normalized to volume, and $\eta_p(i)$, $p = 1,\dots,\nu$ are the spin-isospin functions.

For ^3He $s=\frac{1}{2}$, $\nu = 2$ $(2s+1)$ we have two possible spin functions for a single particle state.

For Nuclear Matter, one has to consider also the isospin. Then we have

$s = 1/2$ $t = 1/2 \Rightarrow$ $\begin{matrix} p\uparrow & n\uparrow \\ p\downarrow & n\downarrow \end{matrix}$ in this case $\nu = 4 = (2s+1)(2t+1)$

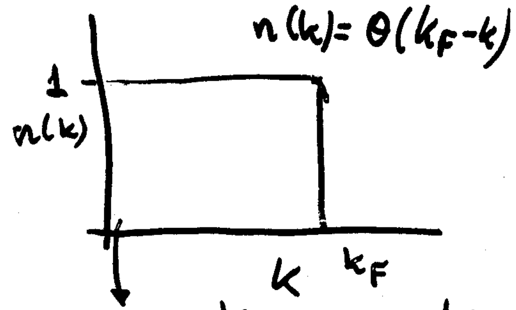
⊛ The plane waves satisfy boundary conditions in a large cube of volume Ω, and $\Omega \to \infty$ in the thermodynamic limit, as well as $A \to \infty$ keeping, $\rho = \frac{A}{\Omega}$ constant.

* The allowed momenta fill the Fermi sphere of radius k_F.

$$A = \nu \cdot \frac{\Omega}{(2\pi)^3} \int d^3k \; n(k)$$

$$\boxed{\sum_k \to \frac{\Omega}{(2\pi)^3} \int d^3k}$$

$$\rho = \frac{\nu \, k_F^3}{6\pi^2}$$



occupation number or momentum distribution.

* The average kinetic energy associated to this w.f.

$$\frac{T}{A} = \frac{\nu \frac{\Omega}{(2\pi)^3} \int_{k<k_F} d^3k \, \frac{\hbar^2 k^2}{2m}}{\nu \frac{\Omega}{(2\pi)^3} \int_{k<k_F} d^3k} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m}$$

$\sim 3\,K$ $\;{}^3He$

~ 20 MeV N.M $\;k_F = 1.36\, fm^{-1}$

* As in the case of bosons, we need the two-body distribution function to calculate the energy!

Let's assume (as it is the case of ^3He) that the interaction depends only on the distance.

we need to calulate the pair distribution function

$$g(r) = \frac{A(A-1)}{\rho^2} \frac{\int dr_3 \ldots dr_A \; \phi^*(1..A)(\Pi f)(\Pi f)\phi}{\int dr_1 \ldots dr_A \; |\Psi(1...A)|^2}$$

where a trace over the spin or the spin-isospin variables is understood.

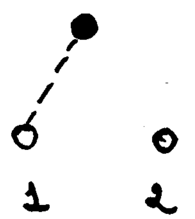
$$\frac{\langle V \rangle}{A} = \frac{1}{2}\rho \int d\bar{r}_{12} \; v(r_{12}) \; g(r_{12})$$

Let's do the same that we did for bosons, and introduce $h = f^2 - 1$, then

$$|\Psi|^2 = \left(1 + \sum' h_{ij} + \sum' h_{ij} h_{kl} + \cdots\right) |\phi|^2$$

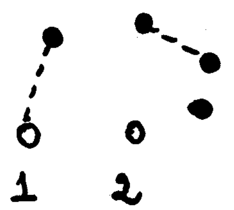
we need to evaluate the square of the Slater determinant. Now, in order to treat the $|\phi|^2$ we will need to introduce new graphical elements!

- In a given term, I can integrate over all internal coordinates that are not touch by a dynamical correlation!



I choose the particle • (could be N-2) and I can integrate over the rest.

How to perform this integration?



Before doing this integration, we will show a pedestrian way to get $g(r)$ for the free Fermi sea.

$$\frac{\langle V\rangle}{N} = \frac{1}{N}\frac{1}{2}\langle\phi|V|\phi\rangle = \frac{1}{2}\frac{1}{N}\sum_{\alpha\beta}\langle \varphi_\alpha(1)\varphi_\beta(2)\,|\,\vartheta(r_{12})\,|\,\varphi_\alpha(1)\varphi_\beta(2)-\varphi_\beta(1)\varphi_\alpha(\ldots$$

$$\varphi_\alpha(1) = \frac{1}{\sqrt{\Omega}}\, e^{i\vec{k}_\alpha\vec{r}_1}\, \underbrace{s_1\, t_1}_{}$$ → spin-isospin functions

$$= \frac{1}{2}\frac{1}{N}\cancel{\frac{\Omega^2}{(2\pi)^6}}\cancel{\frac{1}{\Omega^2}}\int_0^{k_F} d^3k\int_0^{k_F} d^3k'\sum_{s_1 s_2}\sum_{t_1 t_2}\langle e^{-i\bar{k}\bar{r}_1} s_1 t_1\, e^{-i\bar{k}'\bar{r}_2} s_2 t_2\,|\,\vartheta(r)\,|$$

$$e^{i\bar{k}\bar{r}_1} s_1 t_1\, e^{i\bar{k}'\bar{r}_2} s_2 t_2 - e^{i\bar{k}'\bar{r}_1} s_2(1)\, t_2(1)\, e^{i\bar{k}\bar{r}_2} s_1(2)\, t_1(2\ldots$$

$$= \frac{1}{2}\frac{1}{N}\frac{1}{(2\pi)^6}\int_0^{k_F} d^3k\int_0^{k_F} d^3k'\int d^3r_1\int d^3r_2\,\vartheta(r_{12})\Big(\sum_{s_1 s_2}\sum_{t_1 t_2} 1 - \Big(\sum_{s_1 s_2}\delta_{s_1 s_2}\sum_{t_1 t_2}\delta_{t_1 t_2}\Big)\, e^{i(\bar{k}-\bar{k}')(\bar{r}_2-\bar{r}_1)}\Big)$$

$$\sum_{s_1 s_2}\sum_{t_1 t_2} 1 = \mathrm{Tr}(I) = \nu^2$$ Dimension of the spin-isospin space of 2 particles. $\nu = 4$ (Nuclear Matter) $\nu = 2$ ^{3}He, Neutr. matter

$$\sum_{s_1 s_2}\sum_{t_1 t_2}\langle s_1 t_1\, s_2 t_2\,/\,s_2 t_2\, s_1 t_1\rangle = \sum_{s_1 s_2}\sum_{t_1 t_2}\delta_{s_1 s_2}\delta_{t_1 t_2} = \sum_{s_1 s_2} 1 = \nu$$

$$= \mathrm{Tr}(P_\sigma P_\tau) \qquad P_\sigma = \frac{1+\bar{\sigma}_1\bar{\sigma}_2}{2} \qquad P_\tau = \frac{1+\bar{\tau}_1\bar{\tau}_2}{2}$$

Integrate first over k and k'

$$\frac{\langle V\rangle}{N} = \frac{1}{2}\frac{1}{N}\frac{1}{(2\pi)^6}\,\nu^2\int d^3r_1\, d^3r_2\,\vartheta(r_{12})\int_0^{k_F} d^3k\int_0^{k_F} d^3k'\Big(1 - \frac{1}{\nu}\, e^{i\bar{k}(\bar{r}_2-\bar{r}_1)}\, e^{-i\bar{k}'(\bar{r}_2-\bar{r}_1)}\Big)$$

$$\int_0^{k_F} d^3k = \frac{4}{3}\pi k_F^3 = (2\pi)^3\frac{\rho}{\nu}$$

$$\int_0^{k_F} d^3k \; e^{i\bar{k}\bar{r}} \int_0^{k_F} d^3k' \; e^{-i\bar{k}'\bar{r}} = \left[(2\pi)^3 \frac{\rho}{\nu} \, \ell(k_F r) \right]^2$$

$$\Rightarrow \frac{\langle V \rangle}{N} = \frac{1}{2} \frac{1}{N} \frac{1}{\Omega^2} \frac{\Omega^2}{(2\pi)^6} \nu^2 \iint d^3r_1 \, d^3r_2 \; V(r) \int_0^{k_F} d^3k \int_0^{k_F} d^3k' \left(1 - \frac{1}{\nu} e^{i\bar{k}(\bar{r}_2-\bar{r}_1)} e^{i\bar{k}'(\bar{r}_2-\bar{r}_1)}\right)$$

$$= \frac{1}{2} \frac{1}{N} \frac{1}{\cancel{\Omega^2}} \frac{\cancel{\Omega^2}}{\cancel{(2\pi)^6}} \cancel{\nu^2} \left[\cancel{(2\pi)^3} \frac{\rho}{\cancel{\nu}} \right]^2 \iint d^3r_1 \, d^3r_2 \; V(r) \left(1 - \frac{1}{\nu} \ell^2(k_F r)\right)$$

$$= \frac{1}{2} \frac{1}{N} \rho^2 \int d^3r_1 \, d^3r_2 \; V(r) \left(1 - \frac{1}{\nu} \ell^2(k_F r)\right) =$$

$$\bar{r}_2 - \bar{r}_1 = \bar{r}$$

$$= \frac{1}{2} \rho \int d^3r \; V(r) \left(1 - \frac{\ell^2(k_F r)}{\nu}\right)$$

$$\boxed{g(r) = 1 - \frac{\ell^2(k_F r)}{\nu}}$$

PAULI CORRELATIONS!

$\ell(0) = 1$

$g(0) = 1 - \frac{1}{\nu} \Rightarrow$

$\nu = 1 \quad g(0) = 0$

$\nu = 2 \quad g(0) = 1/2$

$\nu = 4 \quad g(0) = 3/4$

$\hookrightarrow$ n° of total states 16, n° of forbidden 4 $\Rightarrow g(0) = \frac{12}{16} = \frac{3}{4}$

$$g(r) = \frac{A(A-1)}{\rho^2} \frac{\int d\Omega_{12} \, \Psi^* \Psi}{\int d\Omega \, \Psi^* \Psi}$$

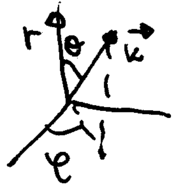
Sequential property: $\rho \int g(r) \, d^3r = A - 1 \Rightarrow$

$$\boxed{\rho \int \left(g(r) - 1\right) d^3r = -1}$$

$$\Rightarrow \int_0^{k_F} d^3k = \frac{4}{3}\pi k_F^3 \; ; \qquad \nu \sum_k 1 = N = \nu \frac{\Omega}{(2\pi)^3}\int d^3k = \nu\frac{\Omega}{(2\pi)^3}\frac{4}{3}\pi k_F^3$$

$$\int_0^{k_F} d^3k \int_0^{k_F} d^3k' = \left(\frac{8\pi^3\rho}{\nu}\right)^2 \qquad \rho = \frac{\nu k_F^3}{6\pi^2} \qquad \boxed{k_F^3 = \frac{6\pi^2\rho}{\nu}}$$

$$\int_{k<k_F} d^3k \; e^{i\bar{k}\bar{r}} = \int dk\, k^2 \int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta)\,\big(\cos kr(\cos\theta) + i\sin kr(\cos\theta)\big)$$



$$\int_{-1}^{1} dx\,(\cos krx + i\sin krx) = \int_{-1}^{1} dx \cos krx$$

$$= \frac{\sin krx}{kr}\Big]_{-1}^{1} = \frac{2\sin kr}{kr}$$

$$\int_{k<k_F} d^3k\; e^{ikr} = 2\pi \int_{k<k_F} dk\, k^2 \,\frac{2\sin kr}{kr} = \frac{4\pi}{r}\int_0^{k_F} dk\; k\sin kr =$$

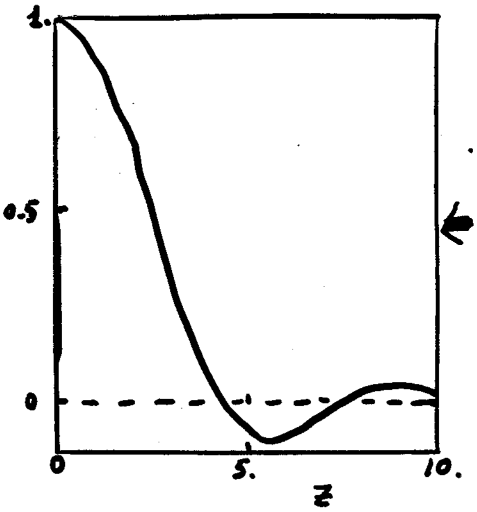
$$= \frac{4\pi}{r}\left[\frac{\sin k_F r}{r^2} - \frac{k_F\cos k_F r}{r}\right]$$

$$\boxed{j_1(k_F r) = \frac{\sin k_F r}{(k_F r)^2} - \frac{\cos k_F r}{k_F r} \qquad \ell(k_F r) = \frac{3\, j_1(k_F r)}{k_F r}} \; !$$

$$= \frac{4\pi k_F^3}{k_F r}\left[\frac{\sin k_F r}{(k_F r)^2} - \frac{\cos k_F r}{k_F r}\right] = 4\pi k_F^3\,\frac{j_1(k_F r)}{k_F r}$$

$$= \frac{6\pi^2\rho}{\nu}\, 4\pi\,\frac{j_1(k_F r)}{k_F r} = (2\pi)^3\frac{\rho}{\nu}\,\frac{3 j_1(k_F r)}{k_F r} = (2\pi)^3\frac{\rho}{\nu}\,\ell(k_F r)$$

$$\boxed{\ell(k_F r) = \frac{\nu}{(2\pi)^3\rho}\int_{k<k_F} d^3k\; e^{i\bar{k}\bar{r}}} \; !$$



$$\ell(z) = \frac{3}{z^3}\left(\sin z - z\cos z\right)$$

$$\downarrow$$

$$g(r) = 1 - \frac{\ell^2(k_F r)}{\nu}$$

Pauli correlations are long range!

Several things to be used:

$$\ell(k_F r) = \frac{\nu}{(2\pi)^3\rho}\int_{k<k_F} d^3k\, e^{i\bar{k}\bar{r}} = \frac{3\, j_1(k_F r)}{k_F r}$$

$$\int d^3r\, \ell(k_F r) = \frac{\nu}{(2\pi)^3\rho}\int d^3r \int_{k<k_F} d^3k\, e^{i\bar{k}\bar{r}} = \frac{\nu}{\rho}\int_{k<k_F} d^3k\, \frac{1}{(2\pi)^3}\int d^3r\, e^{i\bar{k}\bar{r}} = \frac{\nu}{\rho}\int d^3k\, \delta(\bar{k}) = \boxed{\frac{\nu}{\rho}}$$

$$\int d^3r\, \ell^2(k_F r) = \int d^3r\, \frac{\nu}{(2\pi)^3\rho}\,\frac{\nu}{(2\pi)^3\rho}\left[\int_{k<k_F} d^3k\, e^{i\bar{k}\bar{r}}\right]\left[\int_{k'<k_F} d^3k'\, e^{i\bar{k}'\bar{r}}\right]$$

$$= \int d^3k\, d^3k'\, \frac{\nu^2}{\rho^2(2\pi)^3}\,\frac{1}{(2\pi)^3}\int d^3r\, e^{i(\bar{k}+\bar{k}')\bar{r}} = \int d^3k\, d^3k'\, \frac{\nu^2}{\rho^2(2\pi)^3}\,\delta(\bar{k}+\bar{k}')$$

$$= \frac{\nu^2}{\rho^2(2\pi)^3}\int_0^{k_F} d^3k = \boxed{\frac{\nu}{\rho}}$$

$$\rho\int d^3r\, \ell(k_F r)\, e^{i\bar{k}\bar{r}} = \rho\,\frac{\nu}{\rho(2\pi)^3}\int d^3r \int_{k'<k_F} d^3k'\, e^{i\bar{k}'\bar{r}}\, e^{i\bar{k}\bar{r}} =$$

$$= \nu\int_{k'<k_F} d^3k'\, \frac{1}{(2\pi)^3}\int d^3r\, e^{i(\bar{k}+\bar{k}')\bar{r}} = \nu\int_{k'<k_F} d^3k'\, \delta(\bar{k}+\bar{k}') = \boxed{\nu\,\Theta(k_F-k)}$$

$$\rho\int d^3r\, \ell^2(k_F r)\, e^{i\bar{k}\bar{r}} = \boxed{\nu\,\Theta(2k_F-k)\,\left(k^3 - 12\,k\,k_F^2 + 16\,k_F^3\right)/16\,k_F^3}$$

$$\int$$

$$\int d^3y\, \ell(k_F y)\, \ell(k_F |\vec{y}-\vec{z}|) = \int d^3y \frac{\nu}{(2\pi)^3 \rho} \int_{k<k_F} d^3k\, e^{i\vec{k}\vec{y}} \frac{\nu}{(2\pi)^3 \rho} \int_{k'<k_F} d^3k'\, e^{i\vec{k}'(\vec{z}-\vec{y})} =$$

$$= \frac{\nu^2}{\rho^2} \frac{1}{(2\pi)^3} \int d^3k'\, d^3k\, e^{i\vec{k}'\vec{z}} \frac{1}{(2\pi)^3} \int d^3y\, e^{i(\vec{k}-\vec{k}')\vec{y}} =$$

$$= \frac{\nu^2}{\rho^2} \frac{1}{(2\pi)^3} \int_{k'<k_F} d^3k'\, e^{i\vec{k}'\vec{z}} \underbrace{\int_{k<k_F} d^3k\, \delta(\vec{k}-\vec{k}')}_{= 1} = \boxed{\frac{\nu}{\rho}\, \ell(k_F z)}$$

__Structure function:__

$$S(q) = 1 + \rho \int d^3r\, (g(r)-1)\, e^{i\vec{q}\vec{r}} = \frac{1}{A} \langle 0 | \rho_{-\vec{q}}\, \rho_{\vec{q}} | 0 \rangle$$

$$g(r) = 1 - \frac{\ell^2(k_F r)}{\nu}$$

$$S(q) = 1 + \rho \int d^3r \left(\cancel{1} - \frac{\ell^2(k_F r)}{\nu} - \cancel{1}\right) e^{i\vec{q}\vec{r}}$$

$$= \boxed{1 - \theta(2k_F - q)\, \frac{q^3 - 12 q k_F^2 + 16 k_F^3}{16 k_F^3}}$$

__The sequential condition is exactly fulfilled:__

$$\rho \int (g(r)-1)\, d^3r \overset{?}{=} -1 \qquad \Big\{ \quad S(0) = 1 + \rho \int d^3r\, (g(r)-1)$$

$$S(0) = 0$$

$$S(q) = \begin{cases} \frac{3}{4}\frac{q}{k_F} - \frac{1}{2}\left(\frac{1}{2}\frac{q}{k_F}\right)^3 & q < 2k_F \\ 1 & q > 2k_F \end{cases} \Bigg\} \Rightarrow \overline{g(r)}_{r\to\infty} \simeq 1 - \frac{b}{r^4}$$

We need to evaluate $\phi^* \phi$

$$\phi = \begin{vmatrix} e^{i\bar{k}_1\bar{r}_1} S_\uparrow(1) & e^{i\bar{k}_1\bar{r}_2} S_\uparrow(2) & \cdots & e^{i\bar{k}_1\bar{r}_A} S_\uparrow(A) \\ e^{i\bar{k}_1\bar{r}_1} S_\downarrow(1) & e^{i\bar{k}_1\bar{r}_2} S_\downarrow(2) & & \vdots \\ e^{i\bar{k}_2\bar{r}_1} S_\uparrow(1) & e^{i\bar{k}_2\bar{r}_2} S_\uparrow(2) & & \vdots \\ e^{i\bar{k}_2 r_1} S_\downarrow(1) & e^{i\bar{k}_2\bar{r}_2} S_\downarrow(2) & & \vdots \\ \vdots & \vdots & & \end{vmatrix} \frac{1}{\Omega^{A/2}}$$

$$\phi^* = \begin{vmatrix} e^{-i\bar{k}_1\bar{r}_1} S^+_\uparrow(1) & e^{-i\bar{k}_1\bar{r}_1} S^+_\downarrow(1) & e^{-i\bar{k}_2\bar{r}_1} S^+_\uparrow(1) & e^{-i\bar{k}_2\bar{r}_1} S^+_\downarrow(1) \cdots \\ e^{-i\bar{k}_1\bar{r}_2} S^+_\uparrow(2) & e^{-i\bar{k}_1 r_2} S^+_\downarrow(2) & e^{-i\bar{k}_2 r_2} S^+_\uparrow(2) & e^{-i\bar{k}_2\bar{r}_2} S^+_\downarrow(2) \cdots \\ & & & \\ e^{-i\bar{k}_1\bar{r}_A} S^+_\uparrow(A) & e^{-i\bar{k}_1\bar{r}_A} S^+_\downarrow(A) & \cdots & \end{vmatrix} \frac{1}{\Omega^{A/2}}$$

$\phi^*\phi$ is also a determinant!

$$\phi^*\phi = \begin{vmatrix} \sum_k e^{-i\bar{k}\bar{r}_1} e^{i\bar{k}\bar{r}_1} \left(\sum_{p=1}^{\nu} s^+_p(1) s_p(1)\right) & \sum_k e^{-i\bar{k}\bar{r}_1} e^{i\bar{k}\bar{r}_2} \left(\sum_{p=1}^{\nu} S^+_p(1) S_p(2)\right) \cdots \\ \sum_k e^{-i\bar{k}\bar{r}_2} e^{i\bar{k}\bar{r}_2} \left(\sum_{p=1}^{\nu} s^+_p(2) s_p(1)\right) & \sum_k e^{-i\bar{k}\bar{r}_2} e^{i\bar{k}\bar{r}_2} \left(\sum_{p=1}^{\nu} S^+_p(2) S_p(2)\right) \cdots \\ \vdots & \vdots \end{vmatrix} \frac{1}{\Omega}$$

$$\Delta_A(1\ldots A) = \phi^*\phi = \det|\rho(i,j)| \qquad \sum_k \equiv \frac{\Omega}{(2\pi)^3}\int d^3k$$

$$\rho(i,j) = \left(\sum_{p=1}^{\nu} s^+_p(i) s_p(j)\right) \Omega^{-1} \sum_k e^{-i\bar{k}\bar{r}_i} e^{i\bar{k}\bar{r}_j}$$

$$= \left(\sum s^+_p(i) s_p(j)\right) \frac{\rho}{\nu}\, \ell(k_F|\bar{r}_j - \bar{r}_i|) \qquad \ell(k_F r) = \frac{\nu}{(2\pi)^3 \rho}\int_{k<k_F} d^3k\, e^{i}$$

Now we can define sub-determinants involving p-particles:

$$\Delta_p(1 \dots p) = \det |\rho(i,j)|$$

and we have the relation:

$$\int \Delta_{p+1} \, d\bar{x}_{p+1} = (A-p)\, \Delta_p$$

there is a summation over the spin variables of particle p+1

This is the relation that we will use to integrate over all particles that are not affected by any dynamical correlation!

Let's see how the relation works:

⊛ $$\int \Delta_A \, dx_2 \dots dx_A = 1 \cdot 2 \cdots (A-1)\; \Delta(1,1)$$

$$\Delta(1,1) = \rho(1,1) = \rho$$

$$\int \Delta_A \, dx_1 \dots dx_A = (A-1)! \; \frac{A}{\Omega}\, \Omega = A!$$

⊛ $$g_{2F}(r_{12}) = \frac{A(A-1)}{\mathcal{N}\rho^2} \int d\Omega_{12}\, \phi^* \phi = \frac{A(A-1)}{A!\,\rho^2} (A-2)!\; \Delta_2(1,2)$$

$\mathcal{N} = A!$
$$= \frac{1}{\rho^2}\left[\rho(1,1)\,\rho(2,2) - \rho(1,2)\,\rho(2,1)\right] = 1 - \frac{\ell^2(k_F r_{12})}{\nu}$$

$$\rho(1,1) = \rho = \rho(2,2)$$

$$\rho(1,2)\,\rho(2,1) = \underbrace{\left(\sum_p \sum_{p'} s^+_p(1)\, s_p(2)\, s^+_{p'}(2)\, s_{p'}(1)\right)}_{\nu} \frac{\rho^2}{\nu^2}\, \ell^2(k_F r_{12})$$
$$= \frac{\rho^2}{\nu}\, \ell^2(k_F r_{12})$$

I

A crucial property to derive the previous relation:

$$\int \rho(i,j)\,\rho(j,p)\,d^3r_j = \rho(i,p) \quad \Bigg\}\ \text{there is a summation over the spins of particle } j$$

$$\int d^3r_j \sum_{\ell=1}^{\nu} s_\ell^+(i)\, s_\ell(j)\, \frac{\rho}{\nu}\, \ell(k_F(\bar r_i-\bar r_j)) \sum_{\ell'=1}^{\nu} s_{\ell'}^+(j)\, s_{\ell'}(p)\, \frac{\rho}{\nu}\, \ell(k_F|r_j-r_p|)$$

$$= \left(\sum_{\ell=1}^{\nu} s_\ell^+(i)\, s_\ell(p)\right) \frac{\rho^2}{\nu^2}\left(\frac{\nu}{(2\pi)^3\rho}\right)^2 \int d^3r_j \int_{k<k_F} d^3k\, e^{i\bar k(\bar r_i-\bar r_j)} \int_{k'<k_F} d^3k'\, e^{i\bar k'(\bar r_j-\bar r_p)}$$

$$= \left(\sum_{\ell=1}^{\nu} s_\ell^+(i)\, s_\ell(p)\right) \frac{1}{(2\pi)^3} \int d^3k\, d^3k'\, e^{i\bar k\bar r_i}\, e^{-i\bar k' r_p}\, \underbrace{\frac{1}{(2\pi)^3}\int e^{i(\bar k'-\bar k)r_j} d^3r_j}_{\delta(\bar k'-\bar k)}$$

$$= \left(\sum_1 s_\ell^+(i)\, s_\ell(p)\right) \frac{\rho}{\nu}\, \frac{1}{(2\pi)^3}\, \frac{\nu}{\rho} \int_{k<k_F} d^3k\, e^{i\bar k(\bar r_i-\bar r_p)} = \left(\sum_1 s_\ell^+(i)\, s_\ell(p)\right) \frac{\rho}{\nu}\, \ell(k_F(\bar r_i$$

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$g_F(1,2,3)$?

$$g_3^F(1,2,3) = \frac{A(A-1)(A-2)}{\mathcal{N}\rho^3} \int \phi^*\phi\, d\Omega_{123} = \frac{A(A-1)(A-2)}{A!\,\rho^3}(A-3)!\,\Delta_3$$

$$\Delta_3 = \begin{vmatrix} \rho(1,1) & \rho(1,2) & \rho(1,3) \\ \rho(2,1) & \rho(2,2) & \rho(2,3) \\ \rho(3,1) & \rho(3,2) & \rho(3,3) \end{vmatrix} = \big[\rho(1,1)\rho(2,2)\rho(3,3) + \rho(1,2)\rho(2,3)\rho(3,1) + \rho(1,3)\rho(2,1)\rho(3,2) - \rho(1,3)\rho(3,1)\rho(2,2) - \rho(3,2)\rho(2,3)\rho(1,1) - \rho(3,3)\rho(2,1)\rho(1,2)\big]$$

$$= 1 - \frac{1}{\nu}\ell^2(k_F r_{12}) - \frac{1}{\nu}\ell^2(k_F r_{13}) - \frac{1}{\nu}\ell^2(k_F r_{23}) + \frac{2}{\nu^2}\ell(k_F r_{12})\,\ell(k_F r_{13})\,\ell(k_F r_{23})$$

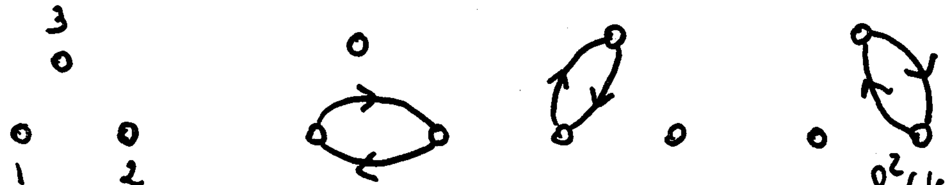
In expanding the determinant, there are loops and products of separate loops of $\left(-\frac{\ell}{\nu}\right)$ functions each loop brings a factor -2ν. The only exception is the two-particle loop, which has a factor $-\nu$.

We represent these functions by means of oriented lines, which will represent $-\frac{\ell}{\nu}$ and indicate the exchange of two particles.

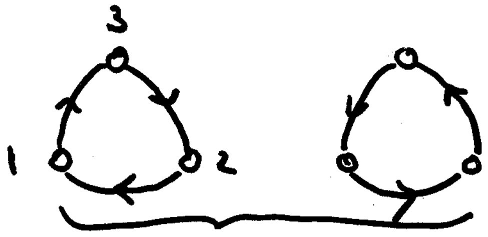
$g_F(r_{12}) =$ 

$1 \qquad - \dfrac{\ell^2(k_F r_{12})}{\nu}$

Each oriented line brings a $-\frac{\ell}{\nu}$. As it is a two particle loop, we have a factor $-\nu$

$g_F(1,2,3) =$ 

$1 \qquad - \dfrac{\ell^2(k_F r_{23})}{\nu}$



$\dfrac{2}{\nu^2}\, \ell(k_F r_{12})\, \ell(k_F r_{13})\, \ell(k_F r_{23})$

Each oriented line brings a $-\frac{\ell}{\nu}$, as it is a loop there is an aditional -2ν. Later we will draw only 1 of those diagrams, and incorporate the factor 2.

(13)

$$g(r_{12}) = \frac{A(A-1)}{\rho^2} \frac{\int \Delta_A F^2 \, d\bar{r}_3 \ldots d\bar{r}_A}{\int \Delta_A F^2 \, d\bar{r}_1 \ldots d\bar{r}_A}$$

include $(A!)^{-1}$ both in the numerat and the denominato So, to normalize ϕ_{FS}

<u>Perform the cluster expansion of F^2</u>

<u>concentrate in the numerator</u>!

We prefere to put in evidence $f^2(r_{12})$!

$$F^2(1\ldots A) = f^2(r_{12}) \left(1 + \sum_{i \neq 1,2} X^{(3)}(12;i) + \sum_{i<j \neq 1,2} X^{(4)}(12;ij) + \ldots\right)$$

$f^2(r_{12}) X^{(p)}$ → correlates particles 1 and 2 with $p-2$ medium particles!

Now, as Δ_A is symmetric under the exchange of coordinates, ⇒ all the terms of $X^{(p)}$ which differ only in the labels of their arguments can be relabelled and summed up! A typical term ⇒

$$\frac{A(A-1)}{\rho^2} \frac{1}{A!} f^2(r_{12}) \int \Delta_A \frac{(A-2)!}{(p-2)!\,(A-p)!} X^{(p)}(12;3\ldots p)\, d\bar{r}_3 \ldots d\bar{r}_A$$

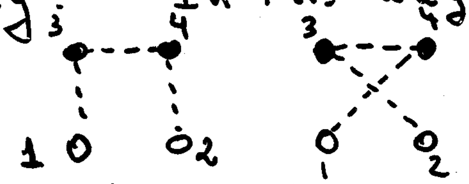
now I <u>can integrate over $(A-p)$ coordinates</u> not affected by $X^{(p)}(12;3\ldots p)$, to get an <u>$(A-p)!\ \Delta_p$</u>,

$\Delta_p = \rho^p \cdot g^F(1\ldots p)$

$$\Rightarrow \frac{\cancel{A!}}{\rho^2 \cancel{A!}} f^2(r_{12}) \cdot \frac{\cancel{(A-p)!}}{(p-2)!\,\cancel{(A-p)!}}\ \rho^p \int d\bar{r}_3 \ldots d\bar{r}_p\ X^{(p)}(12;3\ldots p)\ g^F(1,\ldots p)$$

$$\text{Numerator} = f^2(r_{12})\, g^F(r_{12}) + f^2(r_{12}) \sum_{p=3} \frac{\rho^{p-2}}{(p-2)!} \int d\bar{r}_3 \dots d\bar{r}_p \; X^{(p)}(12;3\dots p)\, g^F(1,\dots,p)$$

Warning! In this way, we are considering



which give the same value and after we divide by 2 ⇒ Take all correlations and draw all diagrams ⇒ The symmetry factors come automatically.

The other strategy: (Similar to what we did in bosons) ⇒ Multiply by $(p-2)!$ draw only

and worry about the symmetry factors of each diagram!

Actually this is the way used later on!

Diagrammatical rules:

We have two types of points:

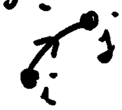
* external points: open circles ○
* internal points: solid circles ●

two types of lines:

* dynamical correlations: dashed lines f^2-1

A dashed line connecting two points i and j gives a factor $h(r_{ij}) = f^2(r_{ij}) - 1$

ii) Statistical correlation lines:

oriented solid line 

The oriented solid line connecting two points i and j gives a factor $-\frac{\ell(k_F r_{ij})}{\nu}$

Rules:

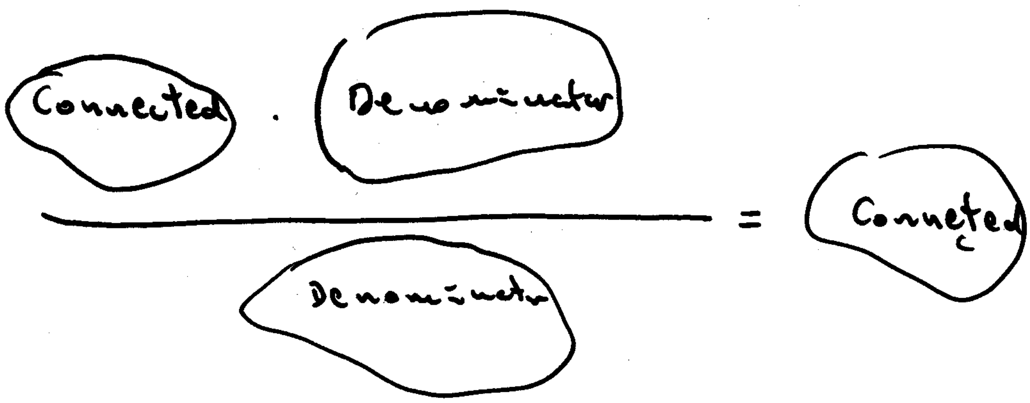
* Every internal point is extremity of at least one dynamical line. Solid points (internal) imply an integration over the corresponding coordinates times a factor ρ.

* The exchange lines form closed loops and different loops do not have common points.
  (As a consequence of the expansion of the determinant)

  Each line brings a factor: $-\frac{\ell(k_F r)}{\nu}$

  Each closed loop brings a factor: -2ν
  except the two particle loop: $-\nu$

The expansion is linked! All the disconnected diagrams cancel exactly with the denominator.



We can add an additional rule:

- ⊛ Each internal point, besides being the extremity of at least one dynamical line, should be connected to the external points by at least one path of correlation (dynamical and statistical) lines.

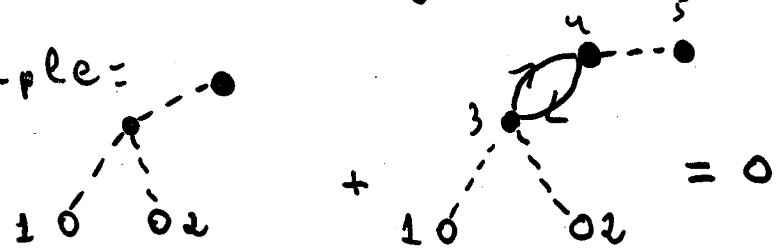
- ⊛ As $f^2(r_{12})$ will be added later, ~~no~~ there are no dynamical lines connecting the external points.

The expansion is IRREDUCIBLE

(Fantoni and Rosati, Nuovo Cimento A20 (1974) 179)

The reducible diagrams cancel in the numerator!

Example:

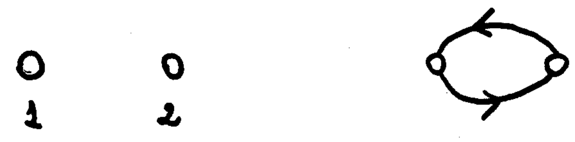


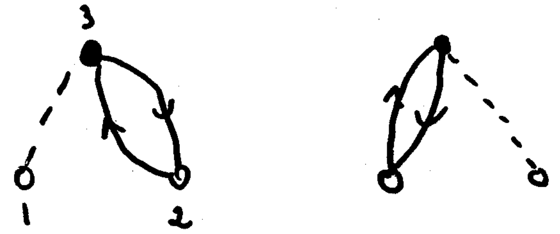
Which can be extended to any articulation point affected ~~by~~ only by dynamical correlations.

$$\rho \int dr_3\, h(r_{13})\, h(23) \cdot \rho \int d^3r\, h(r) \quad +$$

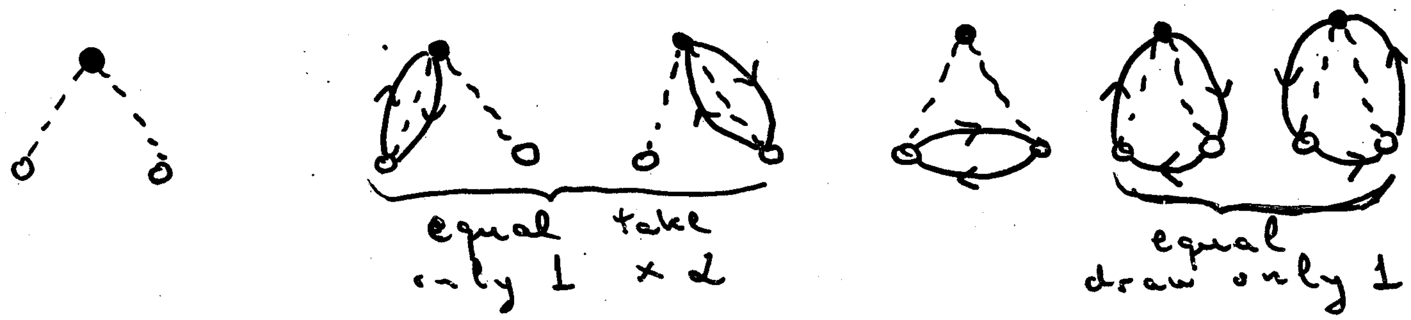
$$+ \ \rho \int dr_3\, h(r_{13})\, h(r_{23}) \underbrace{\left[\rho \int d^3r \left(-\frac{\ell^2(k_F r)}{\nu}\right)\right]}_{-1} \rho \int d^3r\, h(r) = 0$$

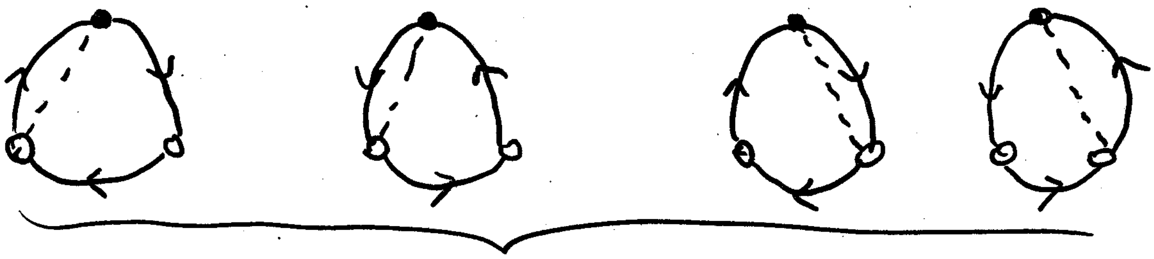
Besides the Bose type diagrams there are new ones containing exchanges!





are equal
later I will take only 1
times a factor 2.





all equal.

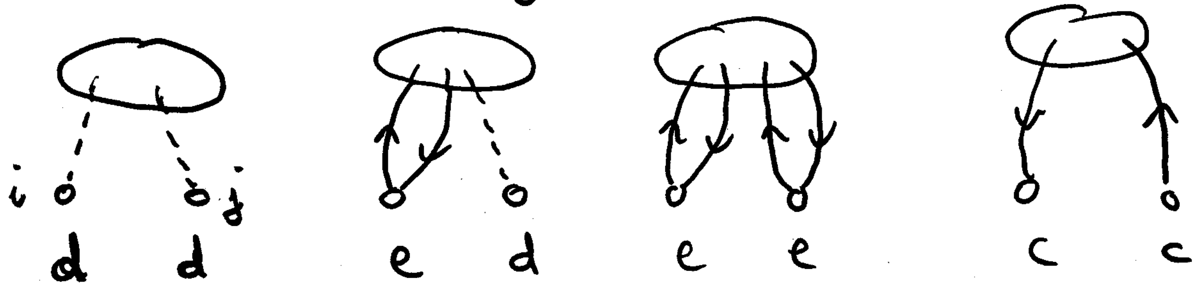
Hypernetted-chain equations:

We need again the concepts of:

i-j subdiagram
i-j composite subdiagram

i-j subdiagram < nodal / non-nodal

Any i-j subdiagram $\Gamma(i,j)$ may be classified by looking at the type of correlation lines affecting the points i and j.



The blob stands for any irreducible diagram having the proper external lines.

$\Gamma_{dd}(i,j)$ (dd ≡ dynamical, dynamical) Both points i and j are not affected by statistical lines.

$\Gamma_{de}(i,j)$ (de ≡ dynamical-exchange)
Point "i" is not affected by statistical lines, whilst point "j" is a common extremity of two statistical lines, superimposed or not with dynamical lines.

$\Gamma_{ee}(i,j)$ (ee ≡ exchange, exchange)
Both points i and j are extremities of two statistical lines. (superimposed or not with dynamical lines)

$\Gamma_{cc}(i,j)$ (cc ≡ cyclic, cyclic)
Both points i and j are extremities of one statistical line. (

Starting from some given subdiagrams one can construct more involved subdiagrams by connecting them (<u>convolution product</u>) or by superposition (<u>algebraic product</u>). Of course, the diagrammatic rules must be satisfied!

* Now we can define $N_{mn}(r_{12})$ the sum of all the 1-2 nodal subdiagrams of the type specified by the subscripts mn. Moreover, $X_{mn}(r_{12})$ represents the sum of all non-nodal 1-2 subdiagrams of the type mn.

* These $N_{mn}(r_{12})$ functions may be constructed by means of chain connection of the various $X_{mn}(r)$. The diagrammatic rules allow only for those connections:

X_{dd} with X_{dd}, X_{ee} or X_{de}
X_{de} with X_{dd} or X_{de}
X_{ee} with X_{dd} or X_{de}
X_{cc} with X_{cc} or $-\frac{1}{2}\ell$.

<u>Remember</u>! Chain connection:

$$(a(r_{ij}) \mid b(r_{jk})) = \rho \int d\bar{r}_j \; a(r_{ij})\, b(r_{jk})$$

Chain connections between two N_{mn} functions are not allowed! would produce many times the same diagram!

However, it is clear that connecting N_{dd} and X_{dd} reproduces part of N_{dd}!

<u>Remember for Bosons:</u> $(X_{dd} \mid N_{dd}) = N_{dd} - (X_{dd} \mid X_{dd})$

$$\Rightarrow \quad N_{dd} = (X_{dd} \mid N_{dd} + X_{dd})$$

<u>Now we can try for Fermions:</u>

$$N_{dd}(r_{12}) = (X_{dd}(r_{13}) + X_{de}(r_{13}) \mid N_{dd}(r_{32}) + X_{dd}(r_{32})) + $$
$$+ (X_{dd}(r_{13}) \mid N_{ed}(r_{32}) + X_{ed}(r_{32}))$$

$$N_{de}(r_{12}) = (X_{dd}(r_{13}) + X_{de}(r_{13}) \mid N_{de}(r_{32}) + X_{de}(r_{32}))$$
$$+ (X_{dd}(r_{13}) \mid N_{ee}(r_{32}) + X_{ee}(r_{32}))$$

$$N_{ee}(r_{12}) = (X_{ed}(r_{13}) \mid N_{ee}(r_{32}) + X_{ee}(r_{32}))$$
$$+ (X_{ed}(r_{13}) + X_{ee}(r_{13}) \mid N_{de}(r_{32}) + X_{de}(r_{32}))$$

For N_{cc}, the situation is more delicate!

N_{cc} correspond to all nodal diagrams constructed with X_{cc} and $-\ell/\nu$

* In those chains, the factor $-\ell/\nu$ can appear without having superimposed any dynamical correlation!

* The value of the chain does not change if the order of the components of the chain is changed! ⇒ Therefore we can put all the factors $-\frac{1}{\nu}\ell(k_F r)$ together

* Now we can use the relation:

$$\left(-\frac{1}{\nu}\ell(k_F r_{im}) \,\middle|\, -\frac{1}{\nu}\ell(k_F r_{mj})\right) = \frac{1}{\nu}\ell(k_F r_{ij})$$

Therefore we can collapse all factors $-\frac{1}{\nu}\ell$ (without having superimposed dynamical correlations) in only one or none! ⇒ This is compatible with:

$$\left(X_{cc}(r_{13}) \,\middle|\, N_{cc}(r_{32})\right) = N_{cc}(r_{12}) - \left(X_{cc}(r_{13}) \,\middle|\, X_{cc}(r_{32})\right) - \\ - \left(X_{cc}(r_{13}) \,\middle|\, -\frac{1}{\nu}\ell(k_F r_{32})\right)$$

⊛ Notice that X_{cc} do not contain $-\frac{1}{\nu}\ell$

$$N_{cc}(r_{32}) = \left(X_{cc}(r_{13}) \,\middle|\, N_{cc}(r_{32}) + X_{cc}(r_{32}) - \frac{1}{\nu}\ell(k_F r_{32})\right)$$

$$X_{cc}(r) = \underbrace{f^2(r)\, e^{N_{dd}(r) + E_{dd}(r)}}_{F(r)} \left\{N_{cc}(r) + E_{cc}(r) - \frac{1}{\nu}\ell(k_F r)\right\}$$

$$+ \frac{1}{\nu}\ell(k_F r) - N_{cc}(r)$$

↓

we substract $-\frac{1}{\nu}\ell(k_F r)$, that was introduced in $F(r)$ $\left(-\frac{1}{\nu}\ell(k_F r)\right)$.

Finally, $\boxed{F(r) = f^2(r)\, e^{N_{dd}(r) + \mathcal{E}_{dd}(r)}}$ (22)

$$X_{dd}(r) = F(r) - N_{dd}(r) - 1$$

$$X_{de}(r) = F(r)\left\{N_{de}(r) + \mathcal{E}_{de}(r)\right\} - N_{de}(r)$$

$$X_{ee}(r) = F(r)\Big\{N_{ee}(r) + \mathcal{E}_{ee}(r) + \left[N_{de}(r) + \mathcal{E}_{de}(r)\right]^2 - \nu\left[N_{cc}(r) + \mathcal{E}_{cc}(r)\right]^2 + 2\,\ell(k_F r)\left[N_{cc}(r) + \mathcal{E}_{cc}(r)\right] - \frac{1}{\nu}\ell^2(k_F r)\Big\} - N_{ee}(r)$$

$$X_{cc}(r) = F(r)\left\{N_{cc}(r) + \mathcal{E}_{cc}(r) - \frac{1}{\nu}\ell(k_F r)\right\} + \frac{1}{\nu}\ell(k_F r) - N_{cc}(r)$$

$\mathcal{E}_{mn}(r)$ indicates the contribution of all elementary sub-diagrams of the type mn

$$N_{dd}(r_{12}) = \left(X_{dd}(r_{13}) + X_{de}(r_{13}) \mid N_{dd}(r_{32}) + X_{dd}(r_{32})\right) + \left(X_{dd}(r_{13}) \mid N_{ed}(r_{32}) + X_{ed}(r_{32})\right)$$

$$N_{de}(r_{12}) = \left(X_{dd}(r_{13}) + X_{de}(r_{13}) \mid N_{de}(r_{32}) + X_{de}(r_{32})\right) + \left(X_{dd}(r_{13}) \mid N_{ee}(r_{32}) + X_{ee}(r_{32})\right)$$

$$N_{ee}(r_{12}) = \left(X_{ed}(r_{13}) \mid N_{ee}(r_{32}) + X_{ee}(r_{32})\right) + \left(X_{ed}(r_{13}) + X_{ee}(r_{13}) \mid N_{de}(r_{32}) + X_{de}(r_{32})\right)$$

$$N_{cc}(r_{12}) = \left(X_{cc}(r_{13}) \mid N_{cc}(r_{32}) + X_{cc}(r_{32}) - \frac{1}{\nu}\ell(k_F r_{32})\right)$$

System of coupled non-linear integral equations

$$X_{cc}(r) = f^2(r)\, e^{N_{dd} + E_{dd}} \left\{ N_{cc} + E_{cc} - \frac{\ell}{\nu} \right\} + \frac{\ell}{\nu} - N_{cc}$$

Let's take $E_{dd} = 0$, $E_{cc} = 0$

$$\simeq (h+1)(1 + N_{dd} + \dots) \left\{ N_{cc} - \frac{\ell}{\nu} \right\} + \frac{\ell}{\nu} - N_{cc}$$

$\Rightarrow$ The simplest diagram:

$h\left(-\frac{\ell}{\nu}\right)$

$$N_{cc}(r_{12}) = \left(X_{cc}(r_{13}) \,\middle|\, N_{cc}(r_{32}) + X_{cc}(r_{32}) - \frac{1}{\nu}\,\ell(k_F r_{32}) \right)$$

$\tilde{X}_{cc}$ $\tilde{X}_{cc}$

$\tilde{X}_{cc}$ $\widetilde{-\frac{\ell}{\nu}}$

<u>The next</u>:

$X_{cc} \Rightarrow$

$h\left(-\frac{1}{\nu}\ell\right)$

$h\left(N_{dd}\left(-\frac{1}{\nu}\ell\right)\right)$

$h \cdot N_{cc}$

The radial distribution function is given by:

$$g(r) = f^2(r)\, e^{N_{dd}(r) + \mathcal{E}_{dd}(r)} \Big\{ 1 - \frac{1}{\nu}\, \ell^2(k_F r) + N_{ee}(r) + E_{ee}(r)$$

$$+ \left[N_{de}(r) + E_{de}(r)\right]^2 + 2\left[N_{de}(r) + \mathcal{E}_{de}(r)\right]$$

$$- \nu\left[N_{cc}(r) + E_{cc}(r)\right]^2 + 2\,\ell(k_F r)\left[N_{cc}(r) + E_{cc}(r)\right]\Big\}$$

which has the correct factors given by the diagrammatic rules.

For Bosons, $g(r) = f^2(r)\, e^{N(r) + \mathcal{E}(r)} \Rightarrow g(r) = 1 + X(r) + N(r)$

non-nodal: $X(r) = f^2(r)\, e^{N(r) + \mathcal{E}(r)} - 1 - N(r)$

For Fermions:

$$\boxed{g(r) = 1 + X_{dd}(r) + N_{dd}(r) + X_{ee}(r) + N_{ee}(r) + 2\,X_{de}(r) + 2\,N_{de}}$$

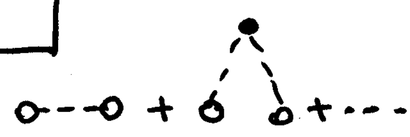
introducing $L(r) = \ell(k_F r) - \nu\left[N_{cc}(r) + \mathcal{E}_{cc}(r)\right]$

$$\boxed{g(r) = f^2 e^{N_{dd} + \mathcal{E}_{dd}} \left\{ -\frac{1}{\nu} L^2(r) + N_{ee}(r) + E_{ee}(r) + \left[1 + N_{de}(r) + E_{de}(r)\right]^2 \right\}}$$

and the static structure function: $S(k) = 1 + \widetilde{g - 1}$

$$\boxed{\begin{aligned} S(k) &= 1 + \widetilde{X_{dd} + N_{dd} + X_{ee} + N_{ee} + 2X_{de} + 2N_{de}} \\ &= \frac{1 + \tilde{X}_{ee}}{\left[1 - \tilde{X}_{de}\right]^2 - \left[1 + \tilde{X}_{ee}\right]\tilde{X}_{dd}} \end{aligned}}$$

Also used: $\Gamma_{dd} = X_{dd} + N_{dd}$

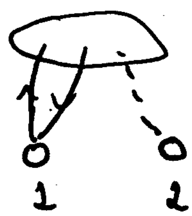


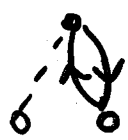
Some factors:

$2\ \ell\ N_{cc} \Rightarrow$  $\Rightarrow -2\nu \left(-\frac{\ell}{\nu}\right) N_{cc}$

$-\nu\ N_{cc}^2 \Rightarrow$  $-2\nu\ \frac{1}{2}\ N_{cc}^2$

$\frac{1}{2} \downarrow$ symmetry factor

$2\ N_{de} \Rightarrow$  $+$ 

$\Rightarrow$  $+$  $+$  $+$  $+ \cdots$

$\left(N_{de}(r) + \mathcal{E}_{de}\right)^2 \Rightarrow$  $+$  $+$  $+ \cdots$

The calculation of the kinetic energy is more complicated than in the bosonic case.

$$\frac{\langle T\rangle}{N} = -\frac{\hbar^2}{2m}\,\frac{1}{N}\,\frac{1}{\mathcal{N}^{-1}}\sum_{i=1}^{N}\int \phi^* F\,\nabla_i^2\,F\phi \; d\bar{x}_1\ldots d\bar{x}_A$$

$$F = \prod_{i<j} f(r_{ij})$$

integration over positions and summation over spin

* there are several ways to apply ∇_i^2.

Using the Jackson-Feenberg identity as we did for bosons:

$$\left.\frac{\langle T\rangle}{N}\right|_{JF} = -\frac{\hbar^2}{2m}\,\frac{1}{N}\,\frac{1}{\mathcal{N}^{-1}}\sum_{i=1}^{A}\int d\Omega \Big[\overset{①}{\phi^* F^2\nabla_i^2\phi} - \overset{②}{\tfrac{1}{4}F^2\nabla_i^2(\phi^*\phi)} +$$

$$+\overset{③}{\tfrac{1}{2}\phi^*\left\{F\nabla_i^2 F - (\vec{\nabla}_i F)^2\right\}\phi}\Big]$$

now $$F\nabla_i^2 F - (\vec{\nabla}_i F)^2 = \sum_{\substack{j=1\\ \neq i}}^{A}\left[\frac{\nabla_i^2 f(r_{ij})}{f(r_{ij})} - \left(\frac{\vec{\nabla}_i f(r_{ij})}{f(r_{ij})}\right)^2\right]F^2$$ as for Bosons!

$$\left.\frac{\langle T\rangle}{N}\right|_{JF} = \underset{①}{\overset{\frac{3}{5}\frac{\hbar^2 k_F^2}{2m}}{\uparrow}}{T_F} \quad \underbrace{-\frac{\hbar^2}{4m}\rho\int d^3r\, g(r)\left(\nabla^2 \ln f(r)\right)}_{③}$$

ϕ was an eigenstate of T (kinetic energy operator)

$$\underbrace{-\frac{\hbar^2}{2m}\,\frac{1}{\mathcal{N}^{-1}}\int d\bar{x}_1\ldots d\bar{x}_A\; F^2\left(-\frac{1}{4}\nabla_1^2|\phi|^2\right)}_{②}$$

$$t_2^s + t_3^s$$

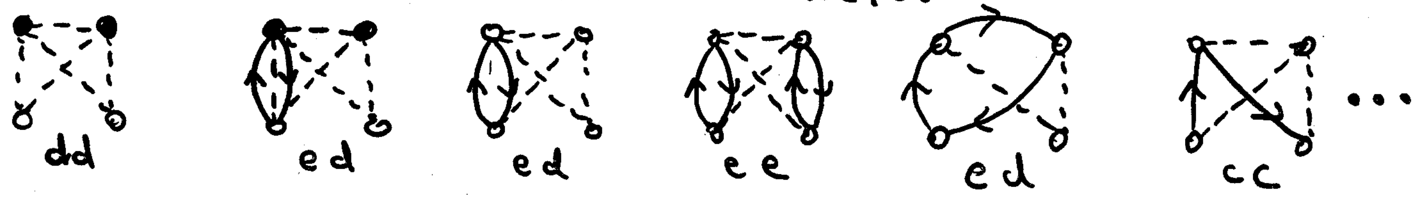
two-body term $\quad$ three-body term (small)

Fantoni & Rosati Phys. Lett. B84 (1979) 2[illegible]

$$t_2^s = -\frac{\hbar^2}{8m}\rho\int d^3r\, f^2 e^{N_{dd}+E_{dd}}\left[\frac{1}{\nu}\nabla^2\ell^2(k_F r) - 2N_{cc}(r)\,\nabla^2\ell(k_F r)\right]$$

Due to the exchange there are many more elementary diagrams : $\mathcal{E}_{dd}$, $\mathcal{E}_{ee}$, $\mathcal{E}_{de}$, $\mathcal{E}_{cc}$

In the bosonic case we had 1 elementary diagram with 4 points:  now we have many more.

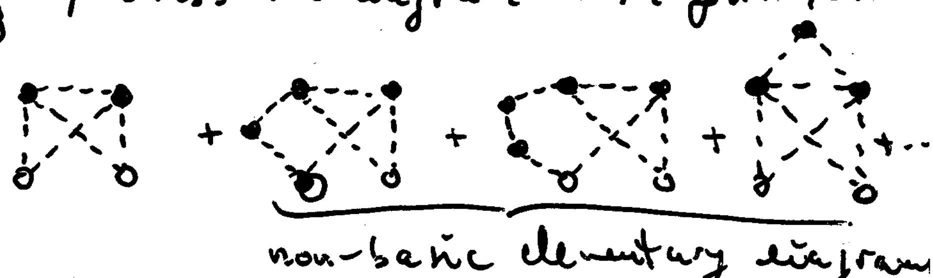


and there are several thousand with 5 points.

Can we still make an expansion in the order of the elementary diagrams?

In the Bosonic case:

1) $E(r) = 0$
2) Solve HNC equations
3) Select a set of basic diagrams (no "ij" subdiagram different than $h(r)$)
   For instance  , dress the diagram with $g(r)-1 = \Gamma$ as above $\Rightarrow$



4) Go to step 2 , and iterate until convergence

With  we get HNC/4

Fermi Cancellations

Independently if $f(r)$ is short-range or long-range there are cancellations among diagrams with a given number of "h" factors and exchange correlations, involving elementary diagrams and different number of particles.

$D_1(r)$ $D_2(r)$ $D_3(r)$ elementary.

$$D_1(r) = -\frac{1}{\nu}\,\ell^2(k_F r)\,h(r)$$

$$D_2(r) = \frac{2\rho}{\nu^2}\,\ell(k_F r)\int d r_3\; h(r_3)\,\ell(k_F r_3)\,\ell(k_F|r - r_3|)$$

$$D_3(r) = -\frac{2\rho}{\nu^3}\int d^3 r_3 \int d^3 r_4\; h(|\bar r_3 - \bar r_4|)\,\ell(k_F r_3)\,\ell(k_F r_4)\,\ell(k_F|\bar r_3 - \bar r|)\,\ell(k_F|\bar r_4 - \bar r|)$$

Their contribution to $S(0)$ involves an integration!

$$\int d^3 r\, D_1(r) = \int d^3 r\, D_3(r) = -\frac{1}{2}\int D_2(r)\, d^3 r.$$

Therefore the sum of the three diagrams at $k=0$ is zero! $\Rightarrow$ We should include those diagrams at the same time! The cancellations involve diagrams with different number of points but the same number of dynamic correlations. (Dressing the dynamic correlations with exchange lines!)

* FHNC/0 will violate the sum-rule $S(0)=0$
* This cancellation happens only at $k=0$? or there are strong cancellations between the diagrams and therefore would question the expansion in terms of elementary diagrams!

$$\left.\begin{array}{l} D_2(k) \\ D_3(k) \end{array}\right\} = 0 \quad k \geq 2k_F$$

$D_1(k)$ may have arbitrary high Fourier component

→ The cancellation concerns mainly low k.

* Short-range correlations in r-space ⇒ high-k components should be more important ⇒ we still have a good estimate of the energy with FHNC/n. Probably problems with the long-range behaviour.

<u>There is one scheme</u> (Krostcheck & Ristig) <u>which takes the Fermi cancellation into account:</u>

One defines a $L_{ee}(r_{ij})$ an insertion function

$$L_{ee}(r_{ij}) = \rho^{-1}\delta(r_{ij}) + X_{ee}(r_{ij})$$
$$= \tilde{S}_F(r_{ij}) + [\Delta X_{ee}(r_{ij})]^{(1)} + \dots + [\Delta X_{ee}(r_{ij})]^{(n)}$$

↓ There is not integral equation for these terms.

X_{ee} at the end should be the sum of all non nodal diagrams of type X_{ee}, properly decomposed

$$\tilde{S}_F(r_{ij}) = \frac{1}{\rho}\,\delta(r_{ij}) - \frac{\ell^2(k_F r)}{\nu}$$

Inserting process!

Also I have:

$\Gamma_{dd}(r)$ sum of all dd diagrams not including exchanges at the reference points.

$E_{dd}(r)$ elementary.

$X_{de}(r)$ all non nodal 1-2 diagrams properly grouped to consider cancellations

$$\tilde{N}_{dd}(k) = \tilde{X}_{dd}\left[\frac{1}{(1-\tilde{X}_{de})^2 - \tilde{X}_{dd}\tilde{L}_{ee}} - 1\right]$$

$$S(k) = \tilde{L}_{ee}\,\frac{[1+\tilde{\Gamma}_{dd}\tilde{L}_{ee}]}{(1-\tilde{X}_{de})^2}$$

At any order:

$\tilde{L}_{ee}(k) = S_F(k) + O(k^2)$ $\quad k\to 0^+$

$[\Delta X_{ee}(k)]^{(n)} \sim k^2$ $\quad k\to 0^+$

$\tilde{X}_{de}(k) = O(k)$ $\quad k\to 0^+$

$E_{dd}(k)$ is bounded $\quad k\to 0^+$

$\Rightarrow S(0^+)=0$ holds order by order in the number of dressed dashed lines!
True also for a S.R.C. (Short Range Correl

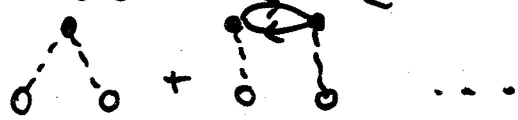
$$\left.\begin{aligned}\tilde{L}_{ee} &= S_F(k)\\ \tilde{X}_{de} &= 0\\ \tilde{E}_{dd} &= 0\end{aligned}\right\} \quad \text{FHNC//0}$$

$$\tilde{N}_{dd}(k) = \tilde{X}_{dd}\left[\frac{1}{(1-X_{de})^2 - \tilde{X}_{dd}\tilde{L}_{ee}} - 1\right] \underset{\text{FHNC//0}}{\Rightarrow} \tilde{X}_{dd}\left[\frac{1}{1-\tilde{X}_{dd}\tilde{L}_{ee}} - 1\right]$$

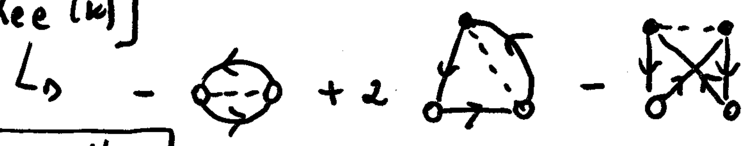
$$S(k) = \tilde{L}_{ee}\,\frac{[1+\tilde{\Gamma}_{dd}\tilde{L}_{ee}]}{(1-\tilde{X}_{de})^2} \underset{\text{FHNC//0}}{=} \tilde{L}_{ee}\,(1+\tilde{\Gamma}_{dd}\tilde{L}_{ee})$$

$$\tilde{N}_{dd} = \tilde{X}_{dd}\,[\cancel{1} + \tilde{X}_{dd}\tilde{L}_{ee} + \cdots - \cancel{1}] = \tilde{X}_{dd}\,\tilde{L}_{ee}\,\tilde{X}_{dd}$$

$\tilde{X}_{dd} =$  $\qquad \tilde{L}_{ee} = 1 +$ 

$\tilde{X}_{dd}\,\tilde{L}_{ee}\,\tilde{X}_{dd} \Rightarrow$ 

$$\tilde{L}_{ee}(k) = S_F(k) + [\Delta X_{ee}(k)]^{(1)}$$

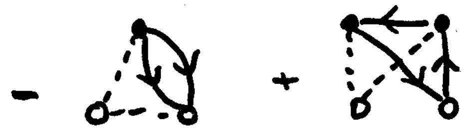


$X_{de}(k) = 0$

$E_{dd}(k) = 0$

$\boxed{\text{FHNC//1}}$

$$L_{ee}(k) = S_F(k) + [\Delta X_{ee}(k)]^{(1)} + [\Delta X_{ee}(k)]^{2}$$

$X_{de}(k) = [\Delta X_{de}(k)]^{(2)} \longrightarrow$ 

$\boxed{\text{FHNC//2}}$

* This scheme is useful to study $S(k)$ $k \to 0$, also for the optimization (this week).

However, the $g(r)$ obtained from $S(k)$ by F.T. does not factorize $f^2(r)$! at a given FHNC//n

$\Rightarrow$ problem when calculating in "r" with a short range repulsion.

$\Rightarrow$ The 1 and h factors to build f^2 in all the diagrams are distributed in different orders of approximation!

* In the Fantoni & Rosati scheme we have f^2 explicitly. Pays more attention to the short-range behaviour ! $S(k)$ $k \to 0$ is not guarantee !

Applications

^3He $\rho_{sat} = 0.277\ \sigma^{-3}$ $e_{exp} = -2.47\ K$

$$\Psi(r_1 \dots r_A) = \prod_{i<j} f(r_{ij})\ \phi_{FS}$$

Notice that the nodal structure of Ψ and ϕ_{FS} is the same!

* $f(r_{ij})$ is taken to be the optimal Jastrow of the underlying mass-three Boson system $f(r) \underset{r\to\infty}{=} 1 - \beta/r^2$. During this week you will see how to optimize $f(r)$ for Fermions

* The interaction is the HFDHE2, Aziz potential.

FHNC RESULTS Elementary diagrams in the interpolating appr

Jastrow $\boxed{K}$	$\langle T \rangle$	$\langle V \rangle$	$\langle E \rangle$
0.237	10.58	-12.12	-1.54
0.277	13.25	-14.55	-1.31
0.301	14.93	-15.92	-0.99

Too low saturation density and not enough binding.

Situation improves with triplet correlations, back-flow correlations, spin-correlations, propagator corrections. It will be explained during this week.

* Recent DMC calculations reproduce the EOS up to the solidification density.

– Remember the talk of Dalfovo about the susceptibility

Nuclear Matter (non-relativistic treatment!)

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

$$\frac{\hbar^2}{2m} \simeq 20 \text{ MeV-fm}^2$$

* The interaction v_{ij} is not completly known. The knowledge of V_{ijk} is worse

* Important to have good and precise Many-body calculations to constraint the interactions!

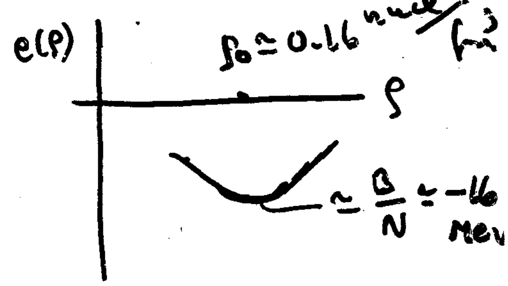
* Realistic potentials have an operatorial structure
  $\Rightarrow$ The correlation should also have operatorial structure.

* S. Fantoni will present an overview of the present situation.

  * There are calulations with FHNC both for finite nuclei and nuclear matter!

$$v_{ij} = \sum_{\ell}\sum_{i<j=1}^{N} v_\ell(r_{ij})\,\hat{O}^\ell(i,j)$$

$$\hat{O}^\ell(i,j) = 1,\ \bar\sigma_i\cdot\bar\sigma_j,\ \bar t_i\cdot\bar t_j,\ (\bar\sigma_i\cdot\bar\sigma_j)(t_i\cdot t_j),$$
$$S(ij),\ S(ij)\,t_i\cdot t_j,\ \bar L\cdot\bar S,\ \bar L\cdot\bar S\ \bar t_i\cdot\bar t_j,$$
$$L^2,\ L^2(\bar t_i\cdot\bar t_j),\ (\bar L\cdot\bar S)^2,\ (\bar L\cdot\bar S)^2(t_i\cdot t_j),$$
$$L^2(\bar\sigma_i\cdot\bar\sigma_j),\ L^2(\bar\sigma_i\cdot\bar\sigma_j)(\bar t_i\cdot\bar t_j)$$



$\boxed{\text{Jastrow is clearly not enough!}}$

Dynamic structure function

$$\boxed{S(q,\omega) = \frac{1}{N} \sum_{\{n\}} |\langle n | \rho^{+}_{q} | 0 \rangle|^2 \, \delta(E_n - E_0 - \omega)}$$

$$\rho^{+}_{q} = \sum_i e^{i\bar{q}\bar{r}_i} \qquad \hat{\rho}_{\bar{q}} = \sum_{ij} \langle i | e^{i\bar{q}\bar{r}} | j \rangle \, c^{+}_{i} c_j$$

$$\langle \vec{r} | j \rangle = \frac{1}{\sqrt{\Omega}} e^{i\bar{k}_j\bar{r}} \quad , \quad \frac{1}{(2\pi)^{3/2}} e^{i\bar{k}_j\bar{r}}$$

Finite volume — Continuum

$$\langle i | e^{i\bar{q}\bar{r}} | j \rangle = \frac{1}{(2\pi)^3} \int d^3r \; e^{-i(\bar{k}_i - \bar{q} - \bar{k}_j)\vec{r}} = \delta(\bar{k}_i - \bar{q} - \bar{k}_j)$$

I can only excite ph states

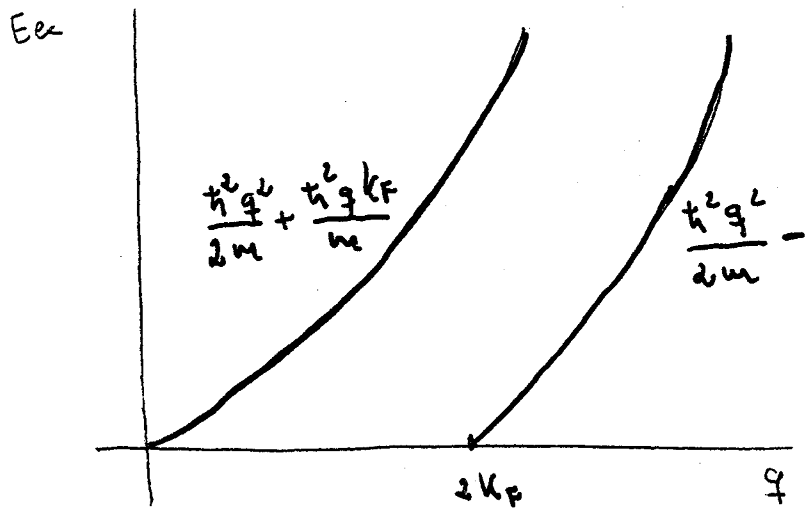
$\hat{\rho}_{\bar{q}} = \sum_{ij} \delta(\bar{k}_i - \bar{q} - \bar{k}_j) \, c^{+}_{i} c_j$. Solo puedo excitar ph estados, is limited to those states therefore the summation over $\{n\}$, is limited to those states! por lo tanto la suma sobre $\{n\}$, se limita a estos estados!

For the Free Fermi Sea!

$$\boxed{S(q,E) = \frac{\nu}{(2\pi)^3 \rho} \int d^3k \; \Theta(k_F - k) \, \Theta(|\bar{k}+\bar{q}| - k_F) \, \delta\left(E - \frac{\hbar^2(\bar{k}+\bar{q})^2}{2m} + \frac{\hbar^2 k^2}{2m}\right)}$$

Energy excitation — Particle-hole band

Energía de excitación : Banda Partícula-agujero



$$0 \leq E \leq \frac{\hbar^2 q^2}{2m} + \frac{\hbar^2 q k_F}{m} \qquad q < 2k_F$$

$$-\frac{\hbar^2 q k_F}{m} + \frac{\hbar^2 q^2}{2m} \leq E \leq \frac{\hbar^2 q^2}{2m} + \frac{\hbar^2 q k_F}{m} \qquad q > 2k_F$$

is superfluous

Para $q > 2k_F$, $\Theta(|\bar{k}+\bar{q}| - k_F)$ es superflua y

$$S(q,E) = \frac{\nu}{(2\pi)^3 \rho} \int d^3k \; \Theta(k_F - k) \; \delta\left(E - \frac{\hbar^2(\bar{k}+\bar{q})^2}{2m} + \frac{\hbar^2 k^2}{2m}\right)$$

$$= \frac{\nu}{(2\pi)^2 \rho} \int_0^{k_F} dk\, k^2 \int_{-1}^{1} dx \; \frac{m}{\hbar^2 k q} \; \delta\left(\frac{Em}{\hbar^2 kq} - \frac{q}{2k} - x\right)$$

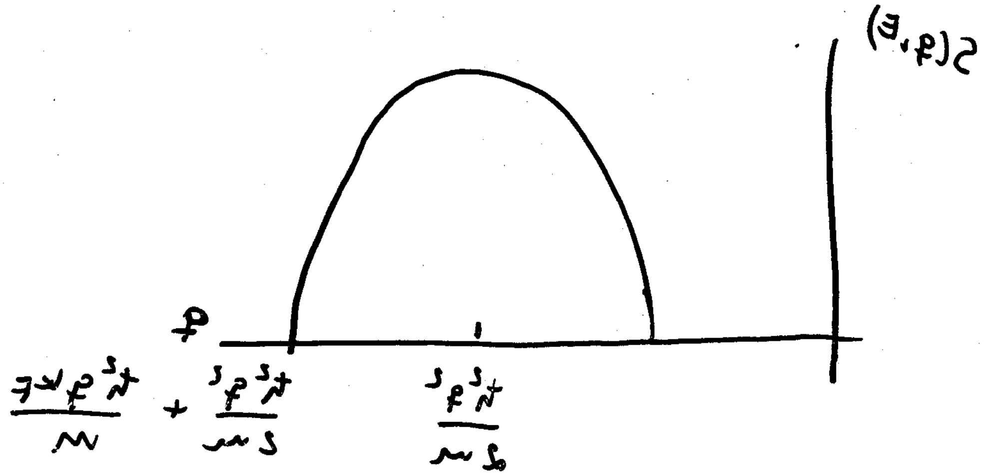
$$\delta(f(x)) = \sum_i \frac{\delta(x - x_i)}{\left(\frac{df}{dx}\right)_{x=x_i}}$$

$$\delta\left(E - \frac{\hbar^2(\bar{k}+\bar{q})^2}{2m} + \frac{\hbar^2 k^2}{2m}\right) =$$

$$= \delta\left(E - \frac{\hbar^2 q^2}{2m} - \frac{\hbar^2 kq}{m} x\right) = \frac{m}{\hbar^2 kq}\, \delta\left(\frac{Em}{\hbar^2 kq} - \frac{q}{2k} - x\right)$$

$$S(q,E) = \frac{V}{4\pi^2\rho}\,\frac{m}{\hbar^2}\,\frac{1}{2q}\left[k_F^2 - \frac{q^2}{4}\left(\frac{2mE}{\hbar^2 q^2} - 1\right)^2\right]$$

$q > 2k_F$



Notice :

$$S(q,E) = \frac{V}{4\pi^2\rho}\,\frac{m}{\hbar^2 q}\int_{|y|} k\, n(k)\, dk$$

$$|y| = \frac{mE}{\hbar^2 q} - \frac{q}{2}$$

One can define Compton profile, which depends only on y, y-scaling!

$$J(q,y) = \frac{\hbar^2 q}{m}\, S(q,\omega)$$

Para un "q" dado, $k < k_F$ y la pregunta es para que valores de E, se cumplirá $-1 \leq x \leq 1$? Para estos valores tendré contribución.

$$-1 \leq \frac{Em}{\hbar^2 kq} - \frac{q}{2k} \leq 1$$

$$-1 + \frac{q}{2k} \leq \frac{Em}{\hbar^2 kq} \leq 1 + \frac{q}{2k} \Rightarrow -\frac{\hbar^2 kq}{m} + \frac{\hbar^2 q^2}{2m} \leq E \leq \frac{\hbar^2 kq}{m} + \frac{\hbar^2 q^2}{2m}$$

ahora bien $k < k_F$, por lo tanto para cada $q > 2k_F$, podemos decir que:

$$\boxed{\frac{\hbar^2 q^2}{2m} - \frac{\hbar^2 q}{m} k_F \leq E \leq \frac{\hbar^2 q^2}{2m} + \frac{\hbar^2 q}{m} k_F}$$

For each q and E, even if E fulfill the previous condition,
Para cada q, E, aunque E cumpla la condición anterior,
the integral over k has a lower limit of integration.
la integral sobre k viene limitada inferiormente!

$$S(q,E) = \frac{\nu}{(2\pi)^2 \rho} \int_0^{k_F} dk\, k^2 \int_{-1}^{1} dx \frac{m}{\hbar^2 kq} \delta\left(\frac{Em}{\hbar^2 kq} - \frac{q}{2k} - x\right)$$

$$|x| < 1 \Rightarrow \left|\frac{Em}{\hbar^2 kq} - \frac{q}{2k}\right| < 1 \Rightarrow \left|\frac{1}{k}\left(\frac{Em}{\hbar^2 q} - \frac{q}{2}\right)\right| < 1$$

$$\Rightarrow k > \left|\frac{Em}{\hbar^2 q} - \frac{q}{2}\right|$$

$$S(q,E) = \frac{\nu}{(2\pi)^2 \rho} \int_{\frac{q}{2}\left|\frac{E}{\frac{\hbar^2 q^2}{2m}} - 1\right|}^{k_F} dk\, \cancel{k^2} \frac{m}{\hbar^2 \cancel{k} q} = \frac{\nu}{(2\pi)^2 \rho} \frac{m}{\hbar^2} \frac{1}{2q} k^2 \Bigg|_{\frac{q}{2}\left[\frac{E}{\frac{\hbar^2 q^2}{2m}} - 1\right]}^{k_F}$$

Reglas de Suma: Para $q > 2k_F$. m_0 y m_1

Recordemos su valor

$$m_0(q) = S(q) \quad , \text{ En nuestro caso } q > 2k_F \Rightarrow \underline{\underline{S(q) = 1}}$$

$$m_1(q) = \frac{\hbar^2 q^2}{2m}$$

$$m_0(q) = \int_0^\infty S(q,E)\, dE \qquad m_1(q) = \int_0^\infty S(q,E)\, E\, dE$$

$$\int S(q,E)\, dE = \int dE \, \frac{\nu}{(2\pi)^3 \rho} \int d^3k \; \Theta(k_F - k) \; \delta\left(E - \frac{\hbar^2(\bar{k}+\bar{q})^2}{2m} + \frac{\hbar^2 k^2}{2m}\right)$$

I perform first the integral over E,

$$\int dE \; \delta\left(E - \frac{\hbar^2(\bar{k}+\bar{q})^2}{2m} + \frac{\hbar^2 k^2}{2m}\right) = 1 \quad \Rightarrow$$

$$\int S(q,E)\, dE = \frac{\nu}{(2\pi)^3 \rho} \int d^3k \; \Theta(k_F - k) = 1$$

O.K. porque $S(q,E) = 1$ $\quad q > 2k_F$ en el Mar de Fermi libre.

* Haciendo la integral explícitamente se obtiene lo mismo

$$m_1(q) = \int E\, S(q,E)\, dE = \int dE\; E\; \frac{\nu}{(2\pi)^3 \rho} \int d^3k\; \theta(k_F - k)$$

$$\cdot\, \delta\left(E - \frac{\hbar^2 (\bar{k}+\bar{q})^2}{2m} + \frac{\hbar^2 k^2}{2m}\right).$$

$$\int dE\; E\; \delta\left(E - \frac{\hbar^2 (\bar{k}+\bar{q})^2}{2m} + \frac{\hbar^2 k^2}{2m}\right) = \frac{\hbar^2 (\bar{k}+\bar{q})^2}{2m} - \frac{\hbar^2 k^2}{2m}$$

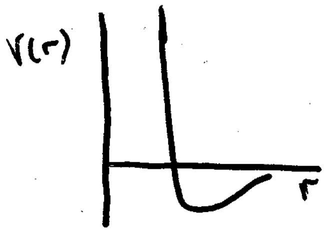
$$= \frac{\hbar^2\, \bar{k}\cdot\bar{q}}{m} + \frac{\hbar^2 q^2}{2m}$$

$$m_1(q) = \frac{\nu}{(2\pi)^3 \rho} \int d^3k\; \theta(k_F - k) \left(\underset{\downarrow\, 0}{\frac{\hbar^2\, \bar{k}\cdot\bar{q}}{m}} + \frac{\hbar^2 q^2}{2m} \right)$$

$$= \frac{\hbar^2 q^2}{2m} \underbrace{\frac{\nu}{(2\pi)^3 \rho} \int d^3k\; \theta(k_F - k)}_{= 1} = \frac{\hbar^2 q^2}{2m}$$

SUMMARY

* We have learned how to calculate the ground-state energy and the low excitation energies of strongly correlated systems.



⊛ Strong short-range repulsion weak long-range attraction.

⊗ Difficult to perform perturbative theory.

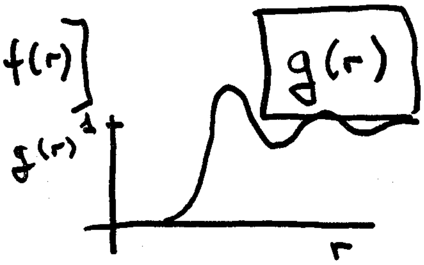
* VARIATIONAL METHOD

$$\Psi_0^T = \Pi f(r_{ij})$$
$$\Psi_0^T = \Pi f(r_{ij}) \; \phi_{FS}(1 \dots A)$$

$$\frac{1}{N} \frac{\langle \Psi_0 | H | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = E_0^V > E_0$$

* For Bose systems

$$\frac{E}{N} = \frac{1}{2} \rho \int d^3r \; g(r) \left[V(r) - \frac{\hbar^2}{2m} \Delta \ln f(r) \right]$$

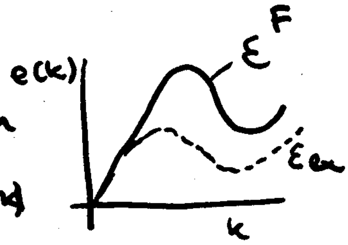


$$\frac{\delta}{\delta f} \left(\frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right)$$ Optimal condition

* Good long range behavior of $g(r) \Leftrightarrow$ Right $\underset{k \to 0}{S(k)} \propto k$

* Good low-energy spectrum

$$\Psi_k = \rho_k \Psi_0 \qquad \rho_k = \sum_j e^{i k r_j} \qquad \varepsilon^F(k) = \frac{\hbar^2 k^2}{2m S(k)}$$



* First extension: IMPURITY Problem
  - Chemical potential
  - Spectrum < variational / Perturbation theory with correlated basis

* Fermions:
  - FHNC equations
  - Optimization
  - Spectrum