Correlated Basis Function theory of the fermion hard-sphere fluid

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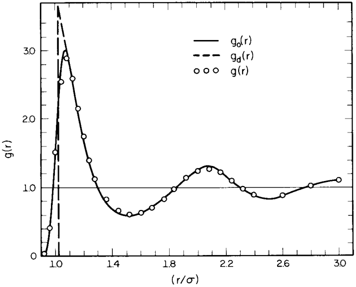
Outline

- ⋆ Why hard spheres ?
- ⋆ The hard core problem
- ⋆ Perturbative expansion at low density
- ⋆ Correlated Basis Function (CBF) theory
- ⋆ Diagrammatic cluster expansion
- ⋆ The Hyper-Netted-Chain approximation for the radial distribution function of a classical liquid
- ⋆ Extension to the case of quantum fluids: Bose statistics

Why hard spheres?

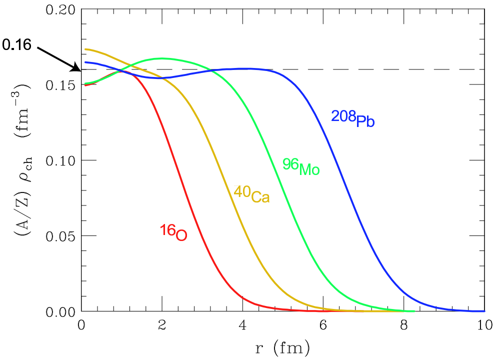
- ⋆ The presence of a strong repulsive core is a prominent feature of the pair potentials describing the dynamics of a variety of systems, ranging from classical and quantum liquids to nuclear matter
- ⋆ Compare the distribution functions corresponding to Lennard-Jones and hard core potentials

$$v_{\rm LJ}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{12} \right]$$

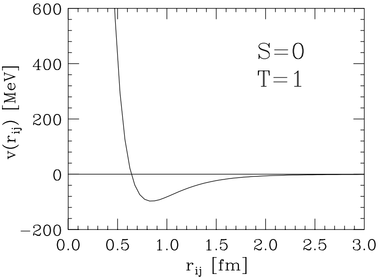


Why hard spheres? (continued)

⋆ The nucleon-nucleon interaction is known to be strongly repulsive at short distances, as clearly shown by the saturation of the measured charge-density distributions



★ Radial dependence of the nucleon-nucleon potential in the $S = 0$, $T = 1$ and $\ell = 0$ channel



★ A system of pointlike fermions at uniform density ρ, interacting through the potential

$$v(r) = \begin{cases} \infty & r < a \\ 0 & r > a \end{cases}$$

is a very useful model for investigating concepts and approximations employed to study the properties of nuclear matter

Taming the hard core

- Problem: "standard" perturbation theory in the Fermi gas basis cannot be used
- The matrix elements of the hard-core potential

$$\langle \mathbf{p}' | v | \mathbf{p} \rangle \ ,$$

where the states $|\mathbf{p}\rangle$ and $|\mathbf{p}'\rangle$ describe non interacting particle pairs carrying relative momenta $\mathbf{p}$ and $\mathbf{p}'$, respectively, are divergent.

- The perturbative series can be rearranged replacing v with the T-matrix, describing scattering between free particles

$$\langle \mathbf{p}' | T | \mathbf{p} \rangle = \langle \mathbf{p}' | v | \mathbf{p} \rangle + \sum_{\mathbf{p}''} \langle \mathbf{p}' | v | \mathbf{p}'' \rangle \frac{m}{\mathbf{p}^2 - \mathbf{p}''^2} \langle \mathbf{p}'' | T | \mathbf{p} \rangle \ ,$$

where m is the particle mass.

- T is well behaved, and in a dilute system can be treated in perturbation theory.

Results of perturbation theory

- Including the first four terms of the low-density expansion, the energy per particle can be written in the form

$$\frac{E}{N} = \frac{k_F^2}{2m}\left[\frac{3}{5} + \frac{2}{\pi}x + \frac{12}{35\pi^2}(11 - 2\ln 2)x^2 + 0.78x^3\right]$$

with $x = k_F a$ and $k_F = (6\pi^2\rho/\nu)^{1/3}$, ν being the degeneracy of the system ($\nu = 2,\ 4$ for pure neutron matter and symmetric nuclear matter, respectively)

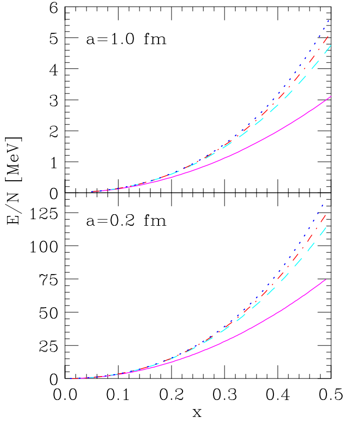
- The *estimated* error is

$$\Delta = \frac{k_F^2}{2m}\frac{x^4}{1-x}$$

- Note: denoting by r_0 the unit radius, defined through $4\pi\rho r_0^3/3 = 1$ we find

$$\frac{r_0}{a} = \frac{1}{x}\left(\frac{18\pi}{4\nu}\right)^{1/3} \approx \frac{1}{x}(1.5 \div 1.9)$$

Convergence of the low-density expansion



- ⋆ How do we extend the description to the high-density region, relevant for many astrophysical applications?

Correlated Basis Function (CBF) theory

- ⋆ A complete set of *correlated* states are obtained from the Fermi gas states through the transformation

$$|n\rangle = F\,|n_{FG}\rangle = \prod_{j>i} f(r_{ij})\,|n_{FG}\rangle$$

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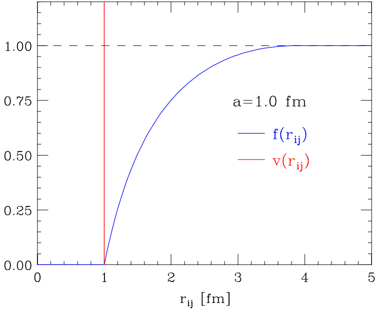
▷ The shape of $f(r_{ij})$ reflects the behavior of the potential.



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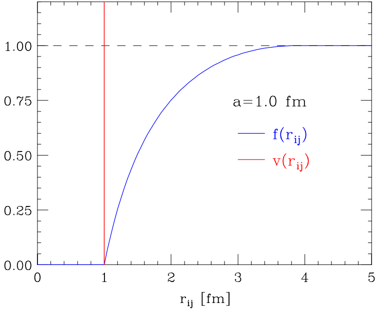


★ Problem: compute

$$\frac{\langle 0_{FG}|F^\dagger \left(\sum_{i=1}^{N} -\frac{\nabla^2}{2m}\right) F|0_{FG}\rangle}{\langle 0_{FG}|F^\dagger F|0_{FG}\rangle}$$

Statistical mechanics of classical liquids

⋆ Canonical Ensamble : fixed particle number (N), volume (V) and temperature (T)

- Equilibrium probability density $(R \equiv \{\mathbf{r}_1, \ldots, \mathbf{r}_N\},\ P \equiv \{\mathbf{p}_1, \ldots, \mathbf{p}_N\})$:

$$n_0(R,P) = \frac{1}{N!} \frac{e^{-\beta H_N(R,P)}}{Q_N(V,T)} \ ,$$

where $\beta = 1/T$, H_N is the hamiltonian

$$H_N(R,P) = T_N(P) + V_N(R) = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{j>i=1}^{N} v(r_{ij}) \ ,$$

with $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, and Q_N is the canonical partition function

$$Q_N(V,T) = \frac{1}{N!} \int \frac{dP}{(2\pi)^{3N}} \, dR \, e^{-\beta H_N(R,P)} = \frac{\Lambda^{-3N}}{N!} Z_N(V,T)$$

$$\Lambda = \left(\frac{2\pi\beta}{m} \right)^{1/2} \ , \quad Z_N(V,T) = \int dR \, e^{-\beta V_N(R)}$$

⋆ Link between statistical mechanics and thermodinamycs:

▷ At equilibrium the free energy F

$$F = E - TS = -\frac{1}{\beta} \ln Q_N(V,T) \ ,$$

where E and S denote energy and entropy, respectively, is minimum.

$$P = -\left(\frac{\partial F}{\partial V}\right)_T \quad , \quad S = -\left(\frac{\partial F}{\partial T}\right)_V \quad , \quad E = -\left(\frac{\partial (F/T)}{\partial (1/T)}\right)_V$$

⋆ n-particle density:

$$\begin{aligned}\rho_N^{(n)}(\mathbf{r}_1,\ldots,\mathbf{r}_n) &= \frac{1}{(N-n)!}\frac{1}{Q_N(V,T)}\int\frac{dP}{(2\pi)^{3N}}\int d^3r_{n+1}\ldots d^3r_N\, \mathrm{e}^{-\beta H_N} \\ &= \frac{N!}{(N-n)!}\frac{1}{Z_N(V,T)}\int d^3r_{n+1}\ldots d^3r_N\, \mathrm{e}^{-\beta V_N}\end{aligned}$$

Distribution functions

- Normalization of the n-particle density

$$\int d^3r_1 \ldots d^3r_n \, \rho_N^{(n)}(\mathbf{r}_1, \ldots, \mathbf{r}_n) = \frac{N!}{(N-n)!}$$

- Homogeneous system

$$\rho_N^{(1)}(\mathbf{r}_1) = \frac{N}{V} = \rho$$

- Ideal gas: $V_N(R) = 0, \; Z_N(V,T) = V^N$

$$\rho_N^{(n)}(\mathbf{r}_1, \ldots, \mathbf{r}_n) = \rho^n \frac{N!}{N^n (N-n)!} = \rho^n \left[1 + O\left(\frac{n}{N} \right) \right]$$

$$\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \rho^2 \left(1 - \frac{1}{N} \right)$$

- Definition of distribution functions

$$g_N^{(n)}(\mathbf{r}_1,\ldots,\mathbf{r}_n) = \frac{1}{\rho^n}\rho_N^{(n)}(\mathbf{r}_1,\ldots,\mathbf{r}_n)$$

Note: interaction effects factor out.

- $g_N^{(n)}$ describes deviations from independent (random) motion
- $n = 2$

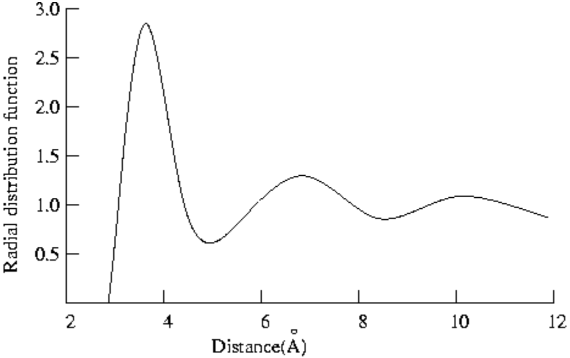
$$g_N^{(2)} = g(r_{12}) \quad , \quad \lim_{r_{12}\to\infty} g(r_{12}) = \left(1 - \frac{1}{N}\right)$$

- $g(r_{12})$ determines the interaction energy

$$E = E_{\rm kin} + E_{\rm int} \quad , \quad E_{\rm int} = \frac{1}{2}\int d^3r_{12}\ v(r_{12})g(r_{12})$$

- Warning : the simple structure of the above equation is deceiving, as the integration over the coordinates of $(N-2)$-particles is hidden in the definition of the two-particle distribution function.
- Problem : how do we compute $g(r_{12})$?

Typical behavior of the radial distribution function



⋆ $g(r)$ of liquid Argon at temperature 100 K and density 1.396 g/cm^3, obtained from a molecular dynamics simulation

Enter the diagrammatic expansion

- Starting point

$$e^{-\beta \sum_{j>i=1}^{N} v(r_{ij})} = \Pi_{j>i=1}^{N} e^{-\beta v(r_{ij})} = \Pi_{j>i=1}^{N} f^2(r_{ij}) = \Pi_{j>i=1}^{N} \left[1 + h(r_{ij})\right]$$

- $v(r_{ij})$ short ranged $\Rightarrow \lim_{r\to\infty} f^2(r) = 1 \Rightarrow \lim_{r\to\infty} h(r) = 0$
- Two-particle density

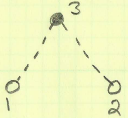
$$\rho_N^{(2)}(r_{12}) = N(N-1)\, \frac{\int d^3r_3 \ldots d^3r_N\, \Pi_{j>i=1}^{N}[1 + h(r_{ij})]}{\int d^3r_1 \ldots d^3r_N\, \Pi_{j>i=1}^{N}[1 + h(r_{ij})]} =$$

- Expand numerator and denominator in "powers" of the short-ranged function $h(r)$, the volume integral of which is small

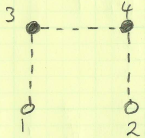
$$\Pi_{j>i=1}^{N}[1+h(r_{ij})] = f^2(r_{12}) \left[1 + \sum_{(ij)\neq(12)} h(r_{ij}) + \sum_{(ij),(kl)\neq(12)} h(r_{ij})\, h(r_{kl}) + \ldots \right]$$

* Associate diagrams to the terms resulting from the expansion of numerator and denominator

$$\int d^3r_3 \, h(r_{13}) \, h(r_{32}) =$$

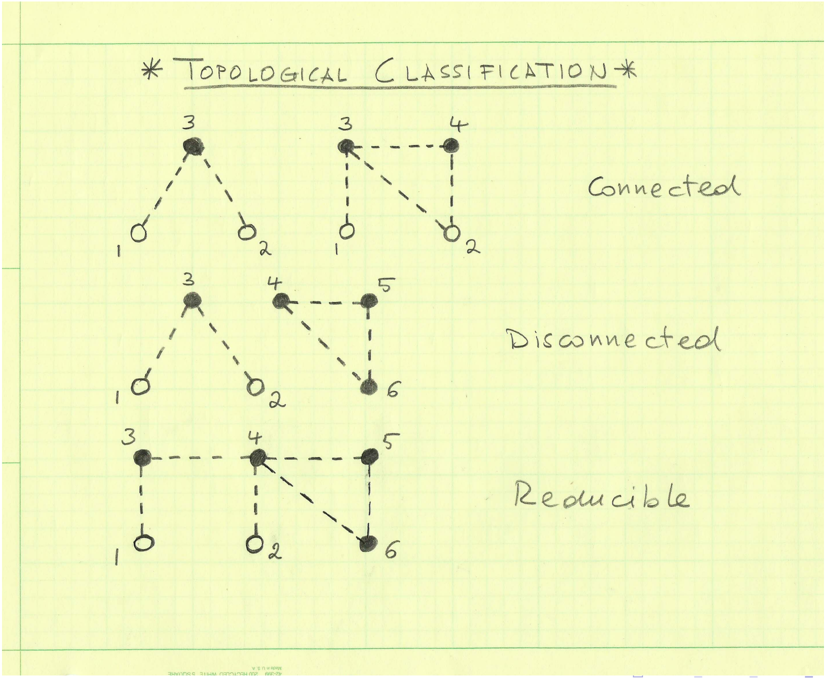


$$\int d^3r_3 \, d^3r_4 \, h(r_{13}) \, h(r_{34}) \, h(r_{42}) =$$



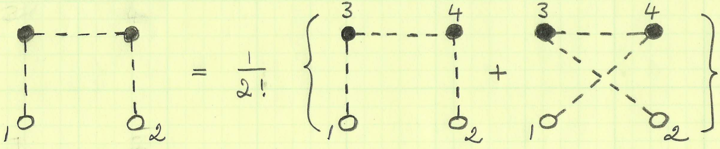
- ○ <u>External point</u> : represents particles 1 or 2
- ● <u>Internal point</u> : represents any of particles 3, ... , N, the coordinates of which are integrated over.

i ○- - - - - -● j <u>Correlation line</u> : represents a factor $h(r_{ij})$, where the indices i and j may label either internal or external points.


* TOPOLOGICAL CLASSIFICATION *
Connected
Disconnected
Reducible

* From labelled to unlabelled diagrams

The black dots correspond to dummy integration variables. Hence, labelling is irrelevant and can be omitted



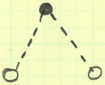
$\Gamma = \frac{1}{2!}$ { Sum of all topologically distinct diagrams obtained assigning labels 3 & 4 to the internal points. }

* Diagrammatic expansion of the pair distribution function $g(r_{12})$.

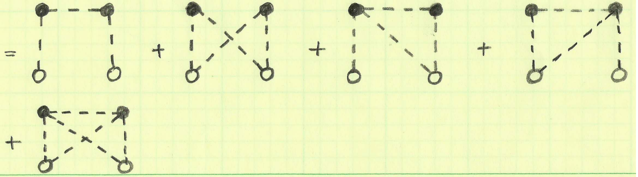
$$g(r_{12}) = f^2(r_{12}) \left[1 + \sum_{n=1}^{\infty} \rho^n g_n(r_{12}) \right]$$

* The sum includes the contributions of all connected and irreducible diagrams

$g_1(r_{12}) =$

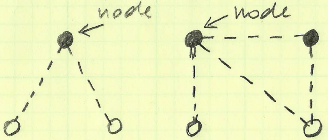


$g_2(r_{12}) =$

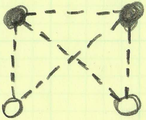


Further classification

* Nodal (or series) diagrams: all paths connecting the external points 1 & 2 go through (at least) one of the internal points (nodes)



* Elementary (or bridge) diagrams: there are several independent paths (with no internal points in common) connecting the external points



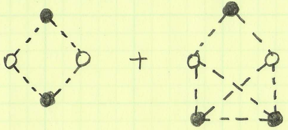
$$g(r_{12}) = e^{-\beta v(r_{12})} \, e^{[N(r_{12}) + E(r_{12})]}$$

$$= e^{-\beta v(r_{12})} \left\{ 1 + [N(r_{12}) + E(r_{12})] + \frac{1}{2}[N(r_{12}) + E(r_{12})]^2 + \cdots \right\}$$

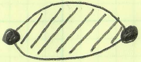
$$= e^{-\beta v(r_{12})} [1 + N(r_{12}) + E(r_{12})] + X(r_{12})$$

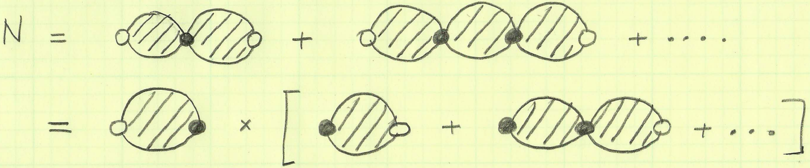
* <u>Composite</u> (or parallel) diagrams

$$X = e^{-\beta v(r_{12})} \left\{ \quad + \quad + \cdots \right\}$$



Define

 sum of all <u>non-nodal</u> diagrams



<u>Hypernetted Chain</u> (HNC) approximation: neglect elementary diagrams (may be reasonable at "not too high" density

$$N(r_{12}) = \rho \int dr_3^3 \, X(r_{13}) \left[X(r_{32}) + N(r_{32}) \right]$$

HNC integral equation for $g(r)$

- Neglecting elementary diagrams

$$g(r_{12}) = \mathrm{e}^{-\beta v(r_{ij})}\ \mathrm{e}^{N(r_{ij})}$$

$$X(r_{12}) = \mathrm{e}^{-\beta v(r_{12})}\mathrm{e}^{N(r_{12})} - N(r_{12}) - 1 = g(r_{12}) - 1 - N(r_{12})$$

$$\mathrm{e}^{\beta v(r_{12})} g(r_{12}) = \mathrm{e}^{N(r_{12})} \Rightarrow N(r_{12}) = \beta v(r_{12}) + \ln g(r_{12})$$

$$X(r_{12}) = g(r_{12}) - 1 - \beta v(r_{12}) - \ln g(r_{12})$$

- The integral equation of the previous slide becomes

$$\beta v(r_{12}) + \ln g(r_{12}) = \rho \int d^3 r_3 [g(r_{13}) - 1 - \beta v(r_{13}) - \ln g(r_{13})][g(r_{32}) - 1]$$

Distribution function of the bosonic hard sphere liquid

- Replace the phase-space distribution with $|\Psi(R)|^2$

$$g(r_{12}) = \frac{N(N-1)}{\rho^2} \frac{\int d^3 r_{n+1} \ldots d^3 r_N \, |\Psi_0(R)|^2}{\int dR \, |\Psi_0(R)|^2}$$

- Ground state wave function

$$\Psi_0(R) = \Pi_{j>i=1}^{N} f^2(r_{ij})$$

- Same diagrammatic expansion as in the case of classical liquids: replace $\exp[-\beta v(r_{ij})] \to f^2(r_{ij})$

$$X(r_{12}) = f^2(r_{12}) e^{N(r_{12})} - N(r_{12}) - 1$$

$$N(r_{12}) = \rho \int d^3 r_3 X(r_{13}) [N(r_{32}) + X(r_{32})]$$

$$g(r_{12}) = N(r_{12}) + X(r_{12}) + 1$$

- For any given $f(r)$, $g(r)$ can be obtained iteratively

(1) Compute the first approximation to $X(r)$, setting $N(r) = 0$

$$X^{(0)}(r) = f^2(r)$$

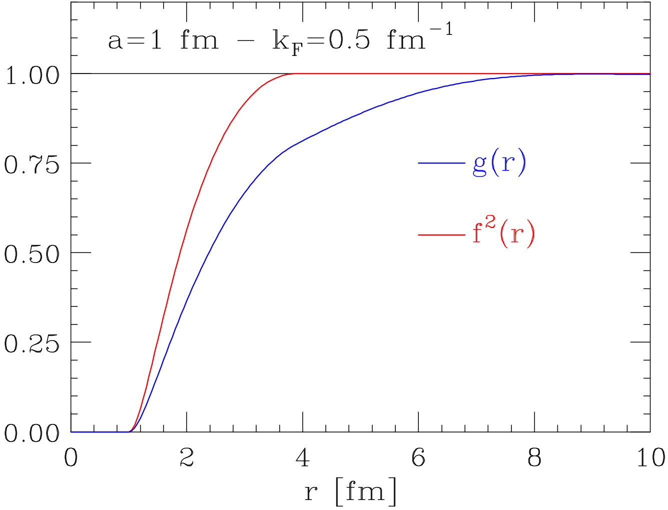
(2) solve the integral equation for $N(r)$ numerically, either through matrix inversion in coordinate space or in Fourier space, using

$$N^{(0)}(k) = \frac{\rho X^{(0)}(k)}{1 - \rho X^{(0)}(k)}$$

(3) Compute

$$X^{(1)}(r) = f^2(r) \exp[N^{(0)}(r)] - N^{(0)} - 1$$

(4) Go back to step (3) and continue till convergence is reached


a=1 fm – k_F=0.5 fm^-1
1.00
0.75
0.50
0.25
0.00
0
2
4
6
8
10
r [fm]
g(r)
f^2(r)

Enter Fermi statistics

- Ground state wave function of the Fermion hard sphere liquid

$$\Psi_0(R) = \Pi_{j>i=1}^{N} f^2(r_{ij})\ \Phi_0(1,\ldots,N)$$

- Φ_0 is the ground state wave-function of the Fermi gas at density ρ

$$\Phi_0(1,\ldots,0) = \frac{1}{\sqrt{N!}}\det[\phi_i(x_i)]\ ,$$

$$\phi_i(x_i) = \frac{1}{\sqrt{V}}\ e^{i\mathbf{k}_i\cdot\mathbf{r}_i}\ \eta_i \quad , \quad |\mathbf{k}_i| < k_F = \left(\frac{6\pi^2\rho}{\nu}\right)^{1/3}$$

- Antisymmetrization of the ground state wave function leads to significant changes in the diagrammatic cluster expansion of the distribution function

Ditribution function of the free Fermi gas

- Consider (dx_i denotes $\mathbf{r}_i$ integration and sum over discrete degrees of freedom)

$$g_{FG}(r_{12}) == \frac{N(N-1)}{\rho^2} \frac{\int dx_3 \ldots dx_N |\Phi_0(x_1, \ldots, x_N)|^2}{\int dx_1 \ldots dx_N |\Phi_0(x_1, \ldots, x_N)|^2}$$

- Exploiting the properties of determinants the above equation can be rewritten (recall: $|\mathbf{k}_i|$, $|\mathbf{k}_j| < k_F$)

$$g_{FG}(r_{12}) = \sum_{i,j} \phi_i(\mathbf{r}_1)\phi_j(\mathbf{r}_2)[\phi_i(\mathbf{r}_1)\phi_j(\mathbf{r}_2) - \phi_j(\mathbf{r}_1)\phi_i(\mathbf{r}_2)]$$

$$= \frac{\nu^2}{(2\pi)^6} \left[\left(\frac{4\pi k_F^3}{3} \right)^2 - \frac{1}{\nu} \left| \int_{|\mathbf{k}|<k_F} d^3k \, e^{i\mathbf{k}\cdot\mathbf{r}_{12}} \right|^2 \right] = \rho^2 \left[1 - \frac{1}{\nu} \ell^2(k_F r_{12}) \right]$$

$$\ell(x) = \frac{3}{x^3} [\sin x - x \cos x]$$

$g_{FG}(r)$ in symmetric nuclear matter at equilibrium density