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

(3 - 14 September 2001)

MICROSCOPIC DESCRIPTION OF QUANTUM LIQUIDS
PART 1 & II

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"Microscopic description of quantum liquids"

Quantum liquids → Good lab. for Many-body theori

- * They exist
- * The interaction is simple.
- * All kinds of statistics: boson, fermion and mix.
- * A lot of experimental information well stablishe

  e.o.s , chemical potentials, Transport propertie superfluidity, etc...
- * A lot of experimental activity:
  - * polarized ^{3}He, polarized mixtures
  - * Inelastic scattering of neutrons by ^{4}He, ^{3}He and mixtures. at very high momentum.
  - * Inhomogeneous systems: Surface properties, density profile, surface tension, films, slabs, surface impurities ... clusters.

References

* "Microscopic Quantum Many-Body Theories and their Applications".
Lecture Notes in Physics Vol. 510
Springer 1998

* J.W. Clark, "Variational theory of Nuclear Matter"
Progress in Particle and Nuclear Physics, Vol. 2, (1979)
(Pergamon)

* E. Feenberg, "Theory of Quantum Liquids"
(Springer, New York, 1969).

* "The Many-Body Problem: Jastrow Correlations Versus Brueckner Theory", Lectures Notes in Physics,
(Vol. 138) Springer 1981.

*

Helium (1868)

After the hydrogen (75%) is the most abundant element in the universe with a ≃ 25%. However not so much in the earth.

* Two isotops

^{4}He (99'99986 %) 2p 2n $2e^-$ boson
^{3}He (0,00014 %) 2p 1n $2e^-$ fermion

* Difficult to get ^{3}He. As a subproduct in nuclear reactions.

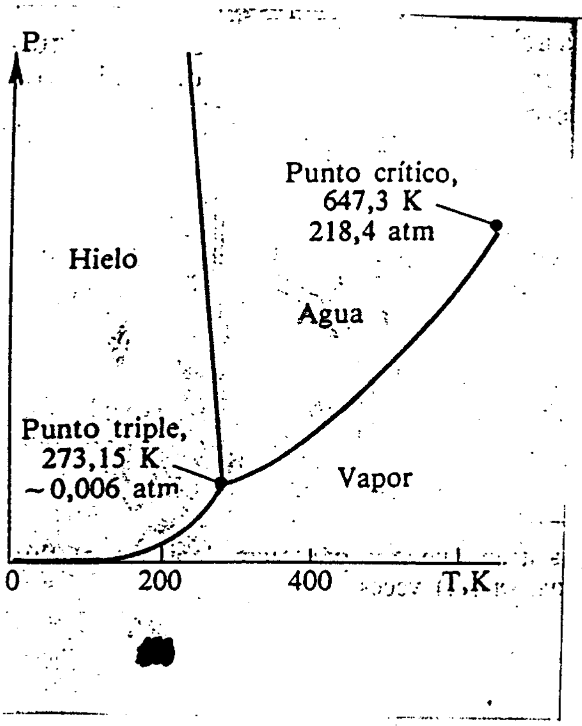
* It is the lighter of the noble gases.

  * It has a couple of electrons in a 1s orbital in a spin singlet state!

  * The first excited state is ≃ 20 eV
  * The first ionization energy is ≃ 24.56 eV

He atoms do not form stable diatomic molecules!

* I can forget the internal structure and consider them as particles which interaction shows a strong repulsion at short distances and a weak attraction.



At a given T,
if $P > P_{sat} \Rightarrow$ liquid
$P < P_{sat} \Rightarrow$ gas

$P = P_{sat}$ coexistence liquid-vapor

- $T > T_c$ no liquid even under high compression
- Triple point, coexistence of three phases
- Usually at low T and P there is the solid phase.
- Cooling a substance reduces the average kinetic energy of its atoms; if the temperature is made low enough ⇒ they lose their mobility and are confined to a fixed positions: becomes solid

^{4}He Phase diagram

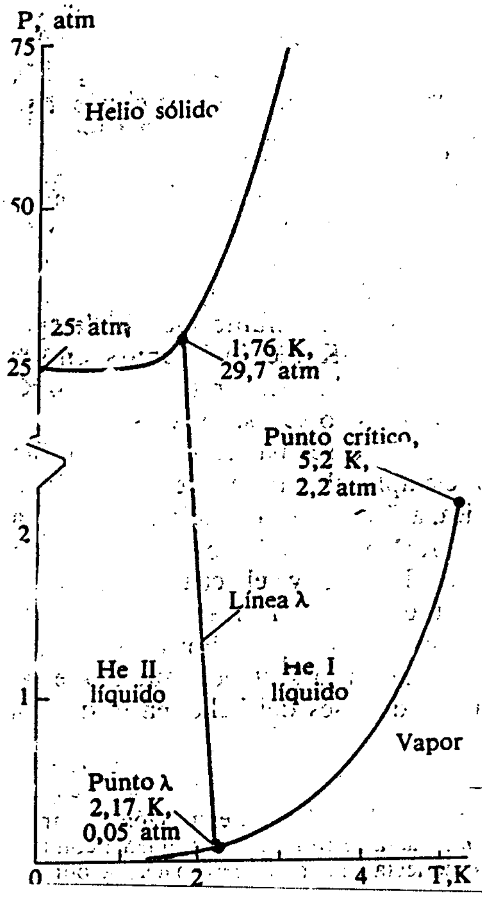


FIG. 5.2. *Diagrama de estado del helio (a lo largo del eje y, para evidenciar el diagrama, la escala en la parte superior del dibujo ha sido reducida).*

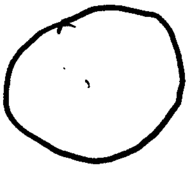
Remains liquid down to T=

Zero point motion !

$\Updownarrow$

Uncertainty Principle

$\rho_0 = 0.0218 \ \frac{\text{Atoms}}{Å^3} \Rightarrow \frac{\Omega}{N_4} = 45'9 \ Å^3$



$\Rightarrow \quad \frac{4}{3}\pi R^3 = V_a$

$R \propto V_a^{1/3} = 2.22 \ Å$

$E_0 \sim \frac{\hbar^2}{2m} \frac{1}{V_a^{2/3}}$

* ^{4}He liquified 1908 Onnes *NP (1913)

solidified 1926 Keesom

superfluidity 1928
1932 keesom
(heat capacity)

1938 Kapitza *NP (1978)

- Two-fluid model :
- Landau Theory $(\overset{41-}{1947})$ *NP (1962)
- Feynman Theory :(1954-56) *NP (1965)

T=0 properties

^4He

$\boxed{e_0 = -7.17 \text{ K}}$

$\rho_0 = 0.365\ \sigma^{-3} = 0.0218$ Atoms/Å^3

$\frac{\hbar^2}{2m_4} = 6.02$ K· Å^2

$\langle U \rangle \simeq -21$ K $\langle T \rangle \simeq 14$ K

big cancellation

$V_s = 238$ m/seg

$\frac{\Omega}{N_4} = 45.9$ Å^3

$V_A = \frac{4}{3}\pi R^3 = 9.20$ Å^3

$R \simeq 1'3$ Å

$P_s = 25$ atm

$\frac{V_A}{V} = 0'2$

$\rho_c =$

$T_c = 5.2$ K

$P_c = 2.26$ Atm

$T_B = 4.215$ K

^3He

$\boxed{e_0 = -2.47 \text{ K}}$

$\rho_0 = 0.277\ \sigma^{-3} = 0.0164$ Atoms/Å^3

$\frac{\hbar^2}{2m_3} = 8.03$ K· Å^2

$\langle U \rangle \simeq -15$ K $\langle K \rangle \simeq 12$ K

$V_s = 182.90$ m/seg.

$P_s = 34$ atm

$\frac{\Omega}{N_3} = 60.9$ Å^3

$\boxed{\frac{V_A}{V} = 0'15}$

$K_F = 0.78$ Å^{-1} $\rightarrow \langle E_F \rangle = \frac{3}{5}\frac{k_F^2}{2m} \simeq 3$ K

$\rho_c =$

$T_c = 3.32$ K

$P_c = 1.15$ atm

$T_B = 3.191$ K

1 ^3He impurity in ^4He

???

$\boxed{\mu_0 = -2.78 \text{ K}}$

$m_I^* = 2.3$ $\boxed{2.2\, m_I}$

$$e_{L.F} = \frac{\hbar^2 q^2}{2m_I^*}$$

$$e_{M.F} = \frac{\hbar^2 q^2}{2m_I^*}\frac{1}{1+\chi q^2}$$

$\alpha = 0.284$

Nuclear Matter

$e \simeq -16$ MeV

$\rho_0 = 0'17$ N/fm^3

$\frac{1}{\rho_0} = 5'88$ fm^3

$V_N \underset{r \simeq 0'4}{\simeq} 0'268$ fm^3

$\frac{V_N}{V} \simeq 0'05$

* Microscopic description means to solve the Schrödinger equation for a Hamiltonian defined in terms of the masses and the interaction between the atoms.

$$\boxed{H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j}^{A} V(r_{ij})} \qquad \boxed{T = 0\ ^\circ K}$$

$$\left.\begin{array}{l} A \to \infty \\ \Omega \to \infty \end{array}\right\} \quad \rho = \frac{A}{\Omega} = cte$$

$\boxed{\text{Homogeneous system}}$

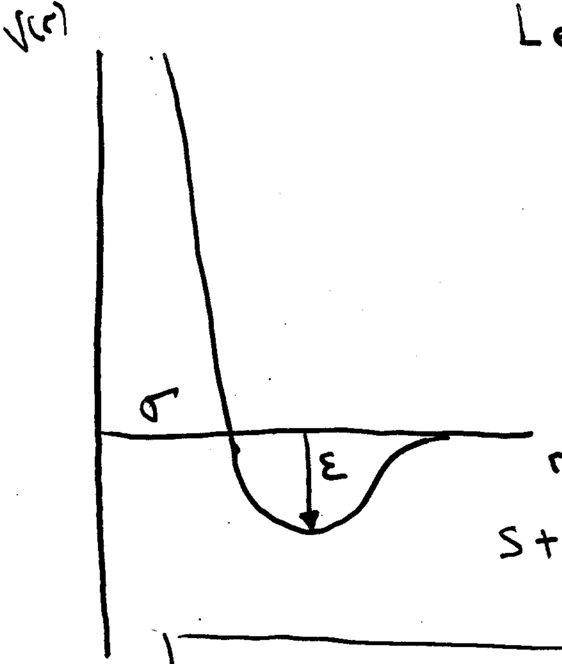
Statistics !

Symmetric ^4He Bosons

Antisymmetric ^3He Fermions!

Same interaction : $\left\{\begin{array}{l} ^4He - ^4He \\ ^3He - ^3He \\ ^4He - ^3He \end{array}\right.$

The interaction :



Lennard-Jones:

$$V(r) = 4\,\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

$$\varepsilon = 10.22\ K$$

$$\sigma = 2.556\ \mathring{A}$$

Strong repulsion ⇒ SRC
Short Range Correlations

$$\boxed{1\,eV \simeq 11000\ K}$$

Aziz potential

* The ionization potential $\simeq 2.45$ e.V
the first excitation energy $\simeq 20$ e.V

⇒ The constituents are the atoms !
which can be considered as hard-spheres with 2.6 Å of diameter

POTENCIAL DE AZIZ (J. Chem Phys 70 (1979) 4330)

$$V(r) = \varepsilon \left\{ A \, e^{-\alpha \, r/r_m} - \left[C_6 \left[\frac{r_m}{r}\right]^6 + C_8 \left[\frac{r_m}{r}\right]^8 + C_{10} \left[\frac{r_m}{r}\right]^{10} \right] F(r) \right\}$$

$$F(r) = \begin{cases} \exp\left[-\left(\frac{D\, r_m}{r} - 1\right)^2\right] & \frac{r}{r_m} \leq D \\ 1 & \frac{r}{r_m} > D \end{cases}$$

$A = 0.5448504 \cdot 10^6$

$\alpha = 13.353384$

$D = 1.241314$

$r_m = 2.9673$ Å

$\varepsilon = 10.8$

$C_6 = 1.37032412$

$C_8 = 0.4253785$

$C_{10} = 0.178100$

VARIATIONAL PRINCIPLE

$$\boxed{\frac{1}{N}\;\frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} = E^v \geqslant E_0}$$

$$\Psi_T(\bar{r}_1,\ldots,\bar{r}_A) = \underset{\substack{\downarrow \\ \text{correlation} \\ \text{operator}}}{F(\bar{r}_1,\ldots,\bar{r}_A)}\;\underset{\substack{\downarrow \\ \text{zero order} \\ \text{description}}}{\phi(\bar{r}_1,\ldots,\bar{r}_A)}$$

F incorporates the correlations produced by the interactions between the particles.

ϕ describes the system without interaction

$= 1$ for bosons

$=$ free Fermi sea for fermions

$$F = \prod_{i<j} f(r_{ij}) \prod_{i<j<k} f(\bar{r}_i,\bar{r}_j,\bar{r}_k) \ldots$$

a good starting point is

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

$$\boxed{\text{How to calculate } \frac{1}{N}\frac{\langle \Psi_0 | V | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \; ?}$$

$$V = \sum_{i<j}^{N} V(r_{ij})$$

$$\frac{\langle \Psi_0 | V | \Psi_0 \rangle}{N} = \frac{1}{N} \frac{\langle \Psi_0 | \sum V(r_{ij}) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} =$$

* all pairs of particles give the same contribution!

$$= \frac{N(N-1)}{2} \frac{1}{N} \frac{\langle \Psi_0 | V(r_{12}) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} =$$

$$= \frac{N(N-1)}{2} \frac{1}{N} \int d\bar{r}_1 \, d\bar{r}_2 \; V(r_{12}) \; \frac{\int d\Omega_{12} \; \Psi^* \Psi}{\int d\Omega \; \Psi^* \Psi}$$

$$= \frac{1}{N} \frac{1}{2} \rho^2 \int d\bar{r}_1 \, d\bar{r}_2 \; V(r_{12}) \; \frac{N(N-1)}{\rho^2} \frac{\int d\Omega_{12} \; \Psi^* \Psi}{\int d\Omega \; \Psi^* \Psi}$$

$$= \frac{1}{N} \frac{1}{2} \rho^2 \, \Omega \int d^3 r \; V(r) \cdot g(r) = \frac{1}{2} \rho \int d^3 r \; V(r) g(r)$$

$$\boxed{g(r) = \frac{N(N-1)}{\rho^2} \frac{\int |\Psi|^2 \, d\bar{r}_3 \ldots d\bar{r}_A}{\int |\Psi|^2 \, d\bar{r}_1 \ldots d\bar{r}_A}}$$

Sequential condition

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

Remember!

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

$$\rho \int d^3r \, g(r) = \rho \, \frac{A(A-1)}{\rho^2} \int d^3r \, \frac{\int d\Omega_{12} \, \Psi^* \Psi}{\int d\Omega \, \Psi^* \Psi}$$

$$= \rho \, \frac{A(A-1)}{\rho^2} \cdot \underbrace{\frac{1}{\Omega} \int d^3r_1}_{\substack{\equiv \\ 1}} \cdot \int d^3r_2 \, \frac{\int d\Omega_{12} \, \Psi^* \Psi}{\int d\Omega \, \Psi^* \Psi}$$

$$= \rho \, \frac{A(A-1)}{\rho^2} \, \frac{1}{\Omega} \, \underbrace{\int d^3r_1 \int d^3r_2 \, \frac{\int d\Omega_{12} \, \Psi^* \Psi}{\int d\Omega \, \Psi^* \Psi}}_{\substack{\equiv \\ 1}}$$

$$= \rho \, \frac{A(A-1)}{\rho^2} \, \frac{1}{\Omega} = A - 1$$

$$\rho \int d^3r \, g(r) = A - 1 \Rightarrow \boxed{\rho \int d^3r \, [g(r) - 1] = -1}$$

normalized such that if I put a particle at the origin and I integrate $g(r) * \rho$ I get the rest of the particles.

$$\Rightarrow \frac{\langle V \rangle}{N} = \frac{1}{2} \rho \int d^3r \, V(r) \, g(r)$$

KINETIC ENERGY. (several ways to apply the laplacians)!

$$\langle T \rangle_{JF} = -\frac{\hbar^2}{2m} \frac{\langle \Psi | \sum_i \nabla_i^2 | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

$$\int \Psi^* \nabla_1^2 \Psi \, d\Omega \equiv \frac{1}{4} \int \left[\Psi^* (\bar{\nabla}_1^2 \Psi) + (\bar{\nabla}_1^2 \Psi^*) \Psi - 2 (\bar{\nabla}_1 \Psi^*)(\bar{\nabla}_1 \Psi) \right].$$

Ψ real.

$$\equiv \frac{1}{2} \int \left[(\nabla_1^2 \Psi) \Psi - (\bar{\nabla}_1 \Psi)(\bar{\nabla}_1 \Psi) \right] d\Omega$$

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

$$F(\nabla_1^2 F) - (\nabla_1 F)^2 \quad ?$$

$$\vec{\nabla}_1 F = \sum_{i=2}^{N} \frac{\vec{\nabla}_1 f(r_{1i})}{f(r_{1i})} F$$

three body terms.

$$\vec{\nabla}_1^2 F = \sum_{i=2}^{N} \frac{(\vec{\nabla}_1^2 f_{1i}) f_{1i} - (\bar{\nabla}_1 f_{1i})^2}{f_{1i}^2} + \left(\sum_{i=2}^{A} \frac{\bar{\nabla}_1 f_{1i}}{f_{1i}} \right) \left(\sum_{i=2}^{A} \frac{\bar{\nabla}_1 f_{1i}}{f_{1i}} \right) F$$

cancelled by $-(\nabla_1 \Psi)(\nabla_1 \Psi)$

all particles give the same contribution!

$$\frac{1}{N} \langle T \rangle_{JF} = -\frac{\hbar^2}{2mN} \frac{1}{\langle \Psi | \Psi \rangle} \frac{1}{2} \overset{\downarrow}{N} \int d\Omega \, F^2 \sum_{i=2}^{N} \frac{(\nabla_1^2 f_{1i}) f_{1i} - (}{f_{1i}^2}$$

$$= -\frac{\hbar^2}{2mN} \frac{1}{\langle \Psi | \Psi \rangle} \frac{1}{2} N(N-1) \int d\Omega F^2 \frac{(\nabla_1^2 f_{12}) f_{12} - (\nabla_1 f_{12})^2}{f_{12}^2}$$

$$\frac{(\nabla_1^2 f_{12}) f_{12} - (\nabla_1 f_{12})^2}{f_{12}^2} = \frac{2f'}{rf} + \frac{f''}{f} - \frac{f'^2}{f^2} = \Delta_{\bar{r}_{12}} \ln f(r_{12})$$

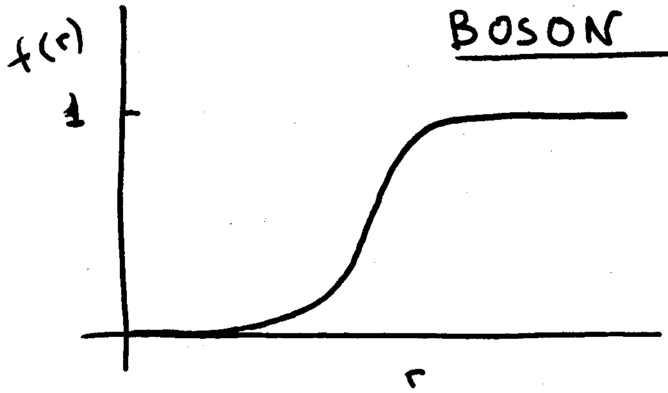
$$\frac{1}{N} \langle T \rangle_{JF} = -\frac{1}{N} \frac{\hbar^2}{2m} \frac{1}{2} N(N-1) \int dr_1 dr_2 \, \Delta \ln f(r_{12}) \cdot \frac{\int d\Omega_{12} F^2}{\int d\Omega F^2}$$

$$= \frac{1}{2} \rho \frac{\hbar^2}{2m} \int d\bar{r} \; g(r_{12}) \left(-\Delta \ln f(r_{12}) \right)$$

for $f(r) = e^{-\frac{1}{2}\left(\frac{b\sigma}{r}\right)^5} \Rightarrow \Delta_r \ln f(r) = -\left(\frac{b\sigma}{r}\right)^5 \frac{1}{r^2} 10$

* I need the two-body distribution function to calulate $\langle T \rangle$. T is a one body operator but due to the correlations I need the two-body distribution function in the case that the correlation operator is the product of two-body correlation functions.

BOSON SYSTEM



$$f(r) \doteq 0 \quad r \to 0$$

$$f(r) \to 1 \quad r \to \infty$$

With only 2-body correlations:

$$\frac{1}{N} \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{1}{2} \rho \int d^3 r \, g(r) \left[V(r) - \frac{\hbar^2}{2 m_4} \Delta \ln f \right]$$

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

* Calculated performing cluster expansio summed up by means of integr equations: HNC, FHNC,

Two alternatives:

⊛ Trial f(r).

for ^4He and ^3He

$$f(r) = e^{-\left[\frac{b\sigma}{r}\right]^5 \frac{1}{2}}$$

⊛ Optimal f(r) → Right long range behavior!

$$\frac{\delta}{\delta f} \left(\frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right) = 0$$

- Three body correlations
- HNC

VMC Variational Monte Carlo

- DMC Diffusion Monte Carlo

The ground state wave function of a many-body boson system has two important features:

i) It has no nodes ⇒ Can be chosen real and positive

ii) It is non degenarate

$$\Psi_0(\bar{r}_1,\dots,\bar{r}_N) = \exp\left[\frac{1}{2}\chi(\bar{r}_1,\bar{r}_2,\dots,\bar{r}_N)\right]$$

and suppose that χ may be complex

$$\chi(\bar{r}_1,\bar{r}_2,\dots\bar{r}_N) = \chi_R(\bar{r}_1,\bar{r}_2,\dots,\bar{r}_N) + i\,\chi_I(\bar{r}_1,\bar{r}_2,\dots,\bar{r}_N)$$

χ_R and χ_I are real and symmetric.

* This wave function is general enough.

$$\Psi_0^*\,\Psi_0 = e^{\frac{1}{2}[\chi_R - i\chi_I]}\;e^{1/2[\chi_R+i\chi_I]} = e^{\chi_R}$$

Depends only on χ_R.

* Potential energy:

$$\frac{\langle\Psi_0|\sum_i V(r_{ij})|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} = \frac{\int d\bar{r}_1\dots d\bar{r}_N\; e^{\chi_R}\sum_{i<j} V(r_{ij})}{\int d\bar{r}_1\dots d\bar{r}_N\; e^{\chi_R}}$$

Depends only on χ_R

* Kinetic energy:

$$\frac{\langle\Psi_0|-\frac{\hbar^2}{2m}\sum_i\nabla_i^2|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} = -\frac{\hbar^2}{8m}\sum_{i=1}^{N}\frac{\int dr_1\dots dr_N\left[\Psi^*\nabla_i^2\Psi + \Psi\nabla_i^2\Psi^* - 2(\vec{\nabla}_i\Psi^*)(\vec{\nabla}_i\right.}{\langle\Psi|\Psi\rangle}$$

$$= \frac{\int d\bar{r}_1\dots d\bar{r}_N\; e^{\chi_R}\left[-\frac{\hbar^2}{8m}\sum_{i=1}^{N}(\nabla_i^2\chi_R) + \frac{\hbar^2}{8m}\sum_{i=1}^{N}(\vec{\nabla}_i\chi_I)^2\right]}{\int d\bar{r}_1\dots d\bar{r}_N\; e^{\chi_R}}$$

The kinetic energy has two pieces, only the second term depends on χ_I and is <u>positive</u>

Therefore the energy is minimized (Variational Principle) by setting $\chi_I = 0$.

Ψ_0 is non-degenerate : is a consequence of the fact that there are <u>no</u> nodes. If there were another eigenstate with energy E_0, then it can be taken orthogonal to Ψ_0.

This new state should have a node (in order to be orthogonal to Ψ_0) $\Rightarrow$ $\chi_I \neq 0$.

However his energy can be lowered by setting $\chi_I =$

$\Rightarrow$ then we violate the assumption that E_0 is the lowest energy.

The exact form of the wave function:

The function $\chi = \chi_R$ can be decomposed into n-body functions u_n $\quad 1 \leq n \leq N$

$$\chi(\bar{r}_1 .. \bar{r}_N) = \sum_{n=1}^{N} \sum_{(i_1..i_n)} u_n(\bar{r}_{i_1} \ldots \bar{r}_{i_n})$$

summation over all distinct choices of the $\underline{n}$ coordinates from the N coordinates.

$$\Psi_0(\bar{r}_1 .. \bar{r}_N) = \exp\left[\sum_{i<j} u_2(r_{ij}) + \sum_{i<j<k} u_3(\bar{r}_i, \bar{r}_j, \bar{r}_k) + \ldots\right]$$

Known as Feenberg wave function

an equivalent form is:

$$\Psi_0(\bar r_1 \dots \bar r_N) = \prod_{n=2}^{N} \prod_{i_1<i_2<\dots<i_n} f_n(\bar r_{i_1} \dots \bar r_{i_n})$$

$$= \prod_{i<j} f_2(r_{ij}) \prod_{i<j<k} f_3(\bar r_i, \bar r_j, \bar r_k) \dots$$

$$\Psi_0(r_1 \dots r_N) = \prod_{i<j} f_2(r_{ij}) \quad \text{(Jastrow wave function)}$$

may be viewed as a first step in a systematic approach to the exact ground-state wave function.

Requirements: Ψ_0 real, positive, no nodes
translationally invariant
u_n uniquely defined

implications: u_n should be:

⊛ real * symmetric under interchange of the particle coordinates

⊛ invariant under translation of the center of mass

$$\bar R = \frac{1}{n} \sum_{i=1}^{n} r_i$$

⊛ invariant under rigid rotation around the center of mass $\bar R$

⊛ invariant under simultaneous inversion of all coordinates

$$r_i \rightarrow -r_i$$

⊛ "<u>cluster property</u>" u_n vanishes whenever any one of the coordinate differences becomes arbitrarily large ⇒ <u>it makes the function</u> (the decomposition) <u>unique</u>!

It excludes the possibility of symmetrized u_p type terms in u_n, with $n > p$.

Example: $u_3(\bar{r}_1, \bar{r}_2, \bar{r}_3)$ may not contain a term of the form $\vartheta(r_1, r_2) + \vartheta(r_2, r_3) + \vartheta(r_3, r_1)$ this term belongs to u_2.

Cluster property in terms of $F(1 \dots N)$:

If any subset, say $i_1 \dots i_p$, of the particles is removed far from the rest, $i_{p+1} \dots i_N$, then F decomposes into a product of two factors:

$$F(1 \dots A) = F_p(i_1 \dots i_p) \quad F_{A-p}(i_{p+1} \dots i_N)$$

Therefore: the correlation operators F_n, $1 < n \leq A$ may be determined by dispersing $A-n$ particles separately to infinity and invoking the cluster property.

* In particular the cluster property requires that

$$f_2(r) \xrightarrow[r \to \infty]{} 1$$

Finally: Notice that all those properties apply also to the case that we are working with an approximate w.f.

$$\Psi_0(r_1 \dots r_N) = e^{\sum_{i<j} u_2(r_{ij})} \equiv \prod_{i<j} f^{(2)}(r_{ij})$$

How to calculate E^V? "only two-body correlations"

For a boson system:

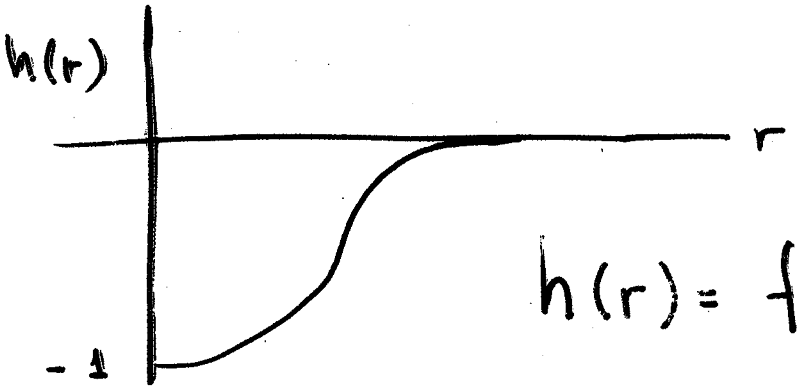
$$\frac{E}{N} = \frac{1}{2} \rho \int d^3r \, g(r) \left[V(r) - \frac{\hbar^2}{2m_4} \Delta \ln f \right]$$

$g(r)$ is the two-body distribution function

$$\boxed{g(r) = \frac{A(A-1)}{\rho^2} \frac{\int |\Psi|^2 \, d\bar{r}_3 \dots d\bar{r}_A}{\int |\Psi|^2 \, d\bar{r}_1 \dots d\bar{r}_A}}$$

If we know $g(r)$ it is easy to calculate E/N!

How to calculate $g(r)$?



$$h(r) = f^2(r) - 1$$

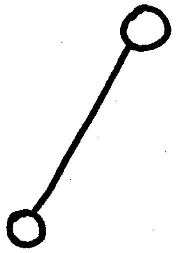
$$g(r) = \frac{A(A-1)}{\rho^2} \quad \frac{\int d\Omega_{12}\,(1+h_{12}+h_{13}+\ldots+h_{12}h_{13}+\ldots}{\int d\Omega \;\ldots\ldots}$$

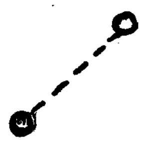
- Tremendous problem, but we observe many simplifications:

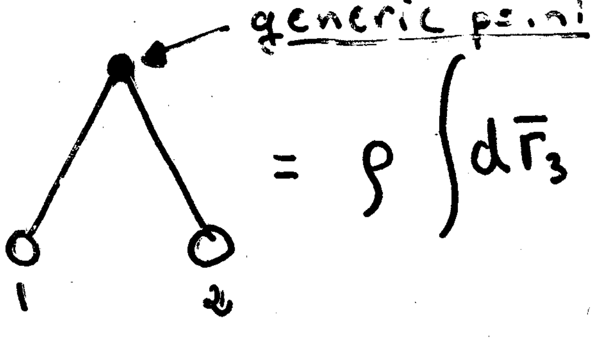
  a) Many integrals give the same result.

  b) There are big cancelations.

- It is useful a diagrammatic notation!

$h \equiv$


later on we will use the notation:




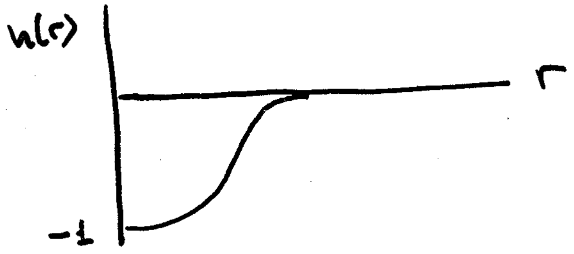
$$= \rho \int d\bar{r}_3 \; h(r_{13})\, h(r_{23})$$

To classify integrals ≡ To classify diagrams.

$$g(r) = \frac{\rho^{-2}\, N(N-1)\ \Omega^{-N} \int d\,\Omega_{12}\ (1 + h_{12} + \dots + h_{12} h_{13} + \dots}{\Omega^{-N} \int d\,\Omega\ (1 + h_{12} + \dots + h_{12}\, h_{13} + \dots)}$$

g(r) becomes a quotient of two integrals of infinite series.

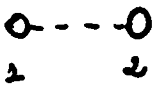
$$h = f^2 - 1$$



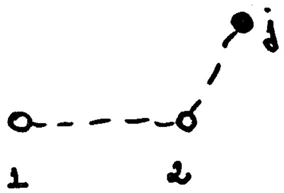
Numerator : Do not integrate over 1 and 2.

a)


1 coordinates which are not integration variables $(\bar{r}_1, \bar{r}_2)$ appear as open circles.

b)


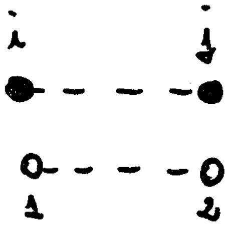
h_{12} correlation factors h_{ij} joining particles i and j appear as dashed lines

c)


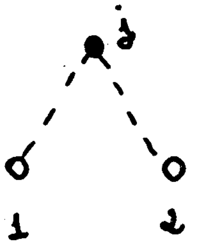
$$h_{12} \frac{N-2}{\Omega} \int d^3r \; h(r)$$

coordinates which are integration variables appear as solid dots. later will bring a density factor.

* unlinked

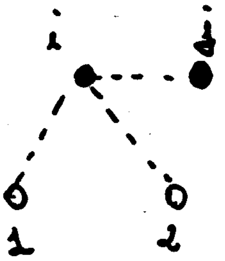
d)


$$h_{12} \frac{(N-2)(N-3)}{2\,\Omega} \int d^3r \; h(r)$$

e)


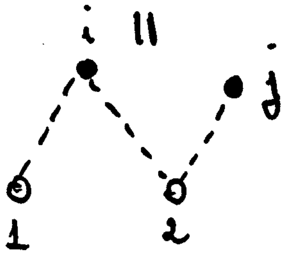
$$\frac{N-2}{\Omega} \int d^3 r_j \; h(r_{1j}) \; h(r_{2j})$$

* reducible or factorable

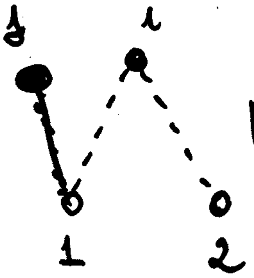
f)


$$\frac{N-2}{\Omega} \int d^3r_i \; h(r_{1i})\, h(r_{2i}) \cdot \frac{N-3}{\Omega} \int d^3r \; h(r)$$

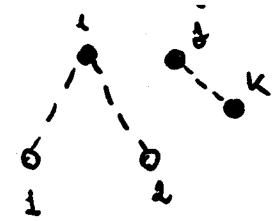
*"i" is an articulation point

g)


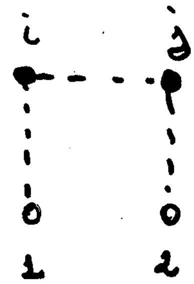
=



h)

i) 

$$\frac{(N-2)}{\Omega}\int d^3r_i\, h(r_{1i})\, h(r_{2i}) \cdot \frac{(N-3)(N-4)}{2\,\Omega}\int d^3r\, h(r)$$

e) 

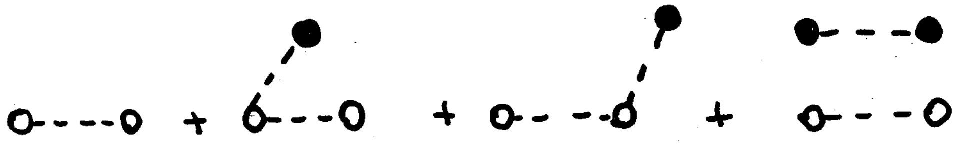
$$\frac{(N-2)\,(N-3)}{\Omega^2}\int d^3r_i\; d^3r_j\;\; h(1i)\; h(ij)\; h(j2)$$

Denominator:

a) 1

b)  $\frac{N(N-1)}{2\,\Omega}\int h(r)\, d^3r$

All unlinked and reducible diggrams of the numerator cancel the denominator to order $1/N$

 $=$

$$= h_{12}\left[1 + 2\,\frac{N-2}{\Omega}\int d^3r\, h(r) + \frac{(N-2)(N-3)}{2\,\Omega}\int d^3r\, h(r)\right] =$$

$$= h_{12}\left[1 + \frac{N(N-1)}{2\,\Omega}\int d^3r\, h(r) - \frac{1}{\Omega}\int d^3r\, h(r)\right]$$

The factor in square brackets is equal to the denominator up to 1 correlation line, except

* To classify diagrams <=> to classify integrals

* **LINKED**: One can not separate the pencil from the paper to draw them

$$\left[1 + \frac{N(N-1)}{2\Omega}\int d^3r\, h(r) + \frac{1}{\Omega}\int d^3r\, h(r) + \right]$$

* **UNLINKED**: consist of two or more completely separate pieces.

$$= \frac{N-2}{\Omega}\int d^3r_i\, h(r_{1i})\, h(r_{2i})\,Ⓐ \left[1 + 3\,\frac{N-3}{\Omega}\int d^3r\, h(r) + \frac{(N-3)(N-4)}{2\Omega}\int h(r)\, d^3r\right]$$

Reducible called factorable because it factors into two independent contributions though it is linked. (Translational invariance)

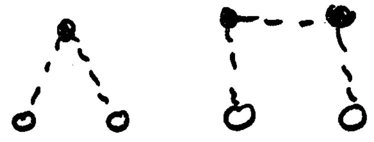
LINKED

Ⓐ is called articulation point: [illegible] diagram can [illegible] into two pieces without disrupting any correlation lines or disconnecting the external points.

$$= \frac{N-2}{\Omega}\int d^3r_i\, [illegible] \left[1 + \frac{N(N-1)}{2\Omega}\int d^3r\, h(r) - \frac{1}{\Omega}\int h(r)\, d^3r\right]$$

Irreducible

Nodal :



Composite :

Elementary:

simple

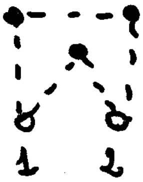
Nodal point: a point through which all paths from ① to ② must pass.

i-j sub-diagram : is a part of a diagram joined to the rest only at points "i" and "j".

1-2 sub-diagram

1-2 sub-diagram

i-j composite subdiagram : consist of two or more i-j subdiagrams. Simple



← Composite 1-2 diagram, A composite diagram factors into their constituent i-j subdiagrams.

i-j nodal diagram: if there is at least one nodal point.

Simple diagram ⟨ Nodal

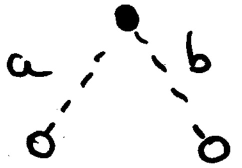
non-nodal ≡ Elementary.

Non-nodal, non-composite

Building diagrams:

Nodal diagrams ⇒ convolution product.

$$(a(r_{1i})\,|\,b(r_{i2})) = \rho \int dr_i \; a(r_{1i})\, b(r_{i2})$$

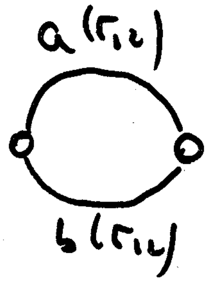


in the thermodynamic limit

a black point ⇒ density factor

Product ⇒ Composite diagrams

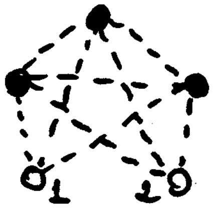
$$a(r_{12})\; b(r_{12}) \Rightarrow$$

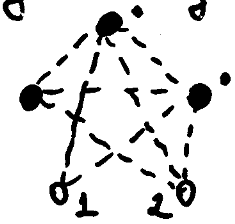


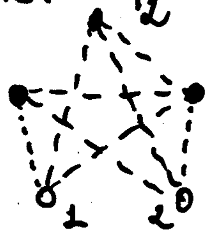
Elementary diagrams

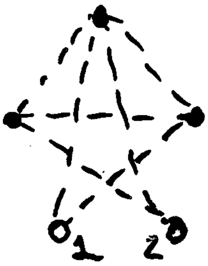
only 1 with 4 points

symmetry factor 1/2









5 elementary diagrams with 5 points

s=6 , 2 1 1 1

THEOREM: We need to consider only the irreducible diagrams of the numerator.

[illegible] diagrams?

for bosons: HNC VAN LEEUWEN, GROENEVELD, DE BOER (1959)

for fermions: FHNC $\begin{cases}\text{Krotscheck - Ristig (1974-75)} \\ \text{Fantoni - Rosati (197~~5~~7)}\end{cases}$

for mixtures: HNC/FHNC A.F & A.P. (1981)

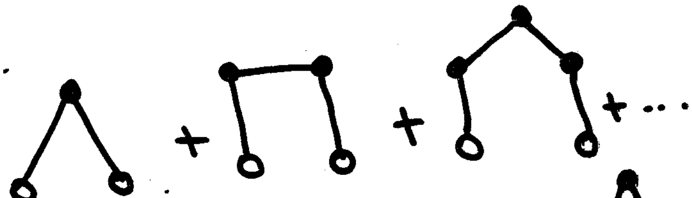
(X(r)) later notation

α(r) The sum of all non-nodal diagrams

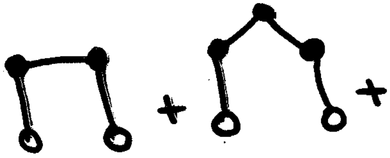
N(r) " " " " nodal diagrams

$$(\alpha(r)\,|\,N(r)) = N(r) - (\alpha(r)\,|\,\alpha(r))$$

; N(r) =



(h | N(r)) =



= N(r) −

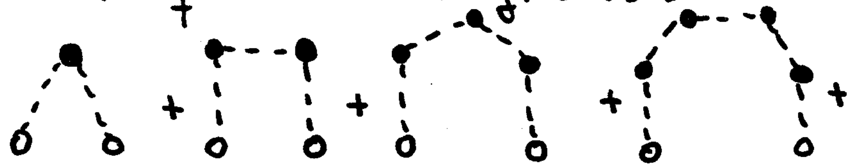
= N(r) − (h|h)

$$\alpha(r) = f(r)\, \underbrace{e^{N(r)+E(r)}}_{1 + N(r) + \frac{1}{2!}N^2(r) + \ldots} - 1$$

Diagrammatic contents of the iterative process

1º) iteration : $X = h = f^2 - 1 =$ 

Construction of nodal diagrams:

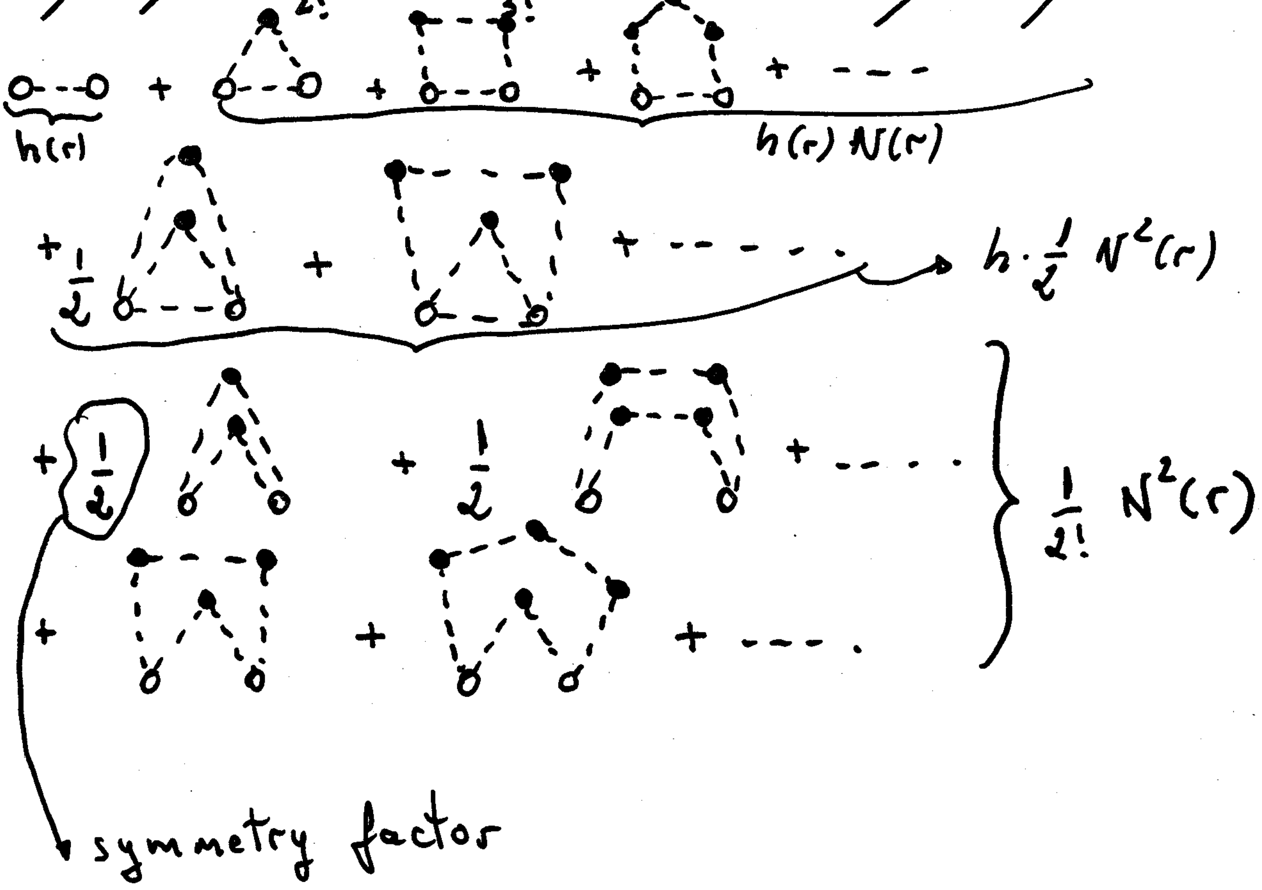
$N(r_{12}) =$  $= \frac{\tilde{h}^2}{1-\tilde{h}}$

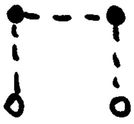
2º) iteration : $X(r) = f^2(r)\, e^{N(r)} - N(r) - 1 =$

$$= \big(h(r)+1\big)\left(1 + N(r) + \frac{1}{2!}N^2(r) + \frac{1}{3!}N^3(r) + \dots\right) - N(r) - 1$$

$$= h(r) + h(r)N(r) + h(r)\frac{1}{2!}N^2(r) + h(r)\frac{1}{3!}N^3(r) + \dots$$

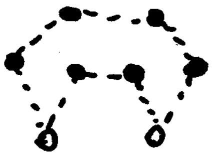
$$+\cancel{1} + \cancel{N(r)} + \frac{1}{2!}N^2(r) + \frac{1}{3!}N^3(r) + \dots \quad -\cancel{N(r)} - \cancel{1} =$$



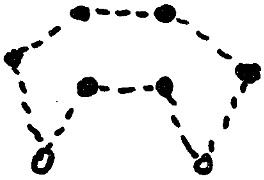
$N^2(r) = \Big($  $+$  $+$  $+$  $+ \cdots \Big)^2$

$= \Big($  $+$  $+ \ldots +$

$+2$  $+2$  $+2$  $+ \ldots$

$+2$  $+ \cdots \Big)$

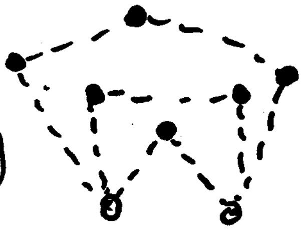
$\frac{1}{2} N^2(r) = \frac{1}{2}$  $+ \frac{1}{2}$  $+ \cdots$

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

symmetry factor

$\frac{1}{3!} N^3(r) = \frac{1}{3!}$  $+ \ldots$ symmetry factor $\frac{1}{6}$

$+ \frac{1}{3!} \cdot 3$  $+ \frac{1}{3!}\ 3$  $+ \cdots$

$+ \frac{1}{3!}\ 6$  $+ \cdots$ symmetry factor $\frac{1}{2}$

symmetry factor 1

ITERATIVE SCHEME

$f^2(r)$

$X(r)$ ~~Composite~~ Non-nod
$N(r)$ Nodals
$\mathcal{E}(r)$ Elementary

$h = f^2(r) - 1$

$$\begin{tikzcd}
\tilde{h}(k) = \widetilde{f^2(r)-1} \arrow[r, "\tilde{X}=\tilde{h}"] & \tilde{N}(k) = \dfrac{\tilde{X}^2(k)}{1-\tilde{X}(k)} \arrow[r, "F.T."] & N(r) \arrow[d] \\
 & \tilde{X}(k) \arrow[u] & X(r) = f^2 e^N - N - \cdots \arrow[l, "F.T."']
\end{tikzcd}$$

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

$$S(k) = 1 + \rho \int e^{i\bar{k}\bar{r}} \left(g(r) - 1\right) d^3r$$

$$= 1 + \tilde{X}(k) + \tilde{N}(k)$$

$$\tilde{N} = \frac{\tilde{X}^2}{1-\tilde{X}} \Rightarrow S(k) = \frac{1}{1-\tilde{X}} \rightarrow \tilde{X} = \frac{S-1}{S}$$

$$\Rightarrow \tilde{N} = \frac{(S-1)^2}{S}$$

$$\boxed{\tilde{X} = \frac{S(k)-1}{S(k)} \quad ; \quad \tilde{N} = \frac{\left(S(k)-1\right)^2}{S(k)}}$$

$\downarrow$

valid with and without elementary diagrams

RESULTS FOR ^4He

$$f(r) = e^{-\frac{1}{2}\left(\frac{b\sigma}{r}\right)^5}$$

$b = 1.17$

$\langle T \rangle \simeq 14\,K$, $\langle V \rangle \simeq 20\,K$

$\rho = 0.365\,\sigma^{-3}$

HNC/S	(MC)	HNC/ST	(MC)
-5.71	(-5.73)	-6.54	(-6.53)

Equilibrium density and binding energy:

	$\rho\,(\sigma^{-3})$	E/N (K)
HNC/0	0.291	-5.12
HNC/S	0.330	-5.82
HNC(ST)	0.364	-6.55
MC (J+T)	0.360	-6.53
* GFMC	0.365	-6.85
Exp	0.365	-7.17

For global analysis.

$$e(\rho) = e_0 + b\left(\frac{\rho-\rho_0}{\rho_0}\right)^2 + c\left(\frac{\rho-\rho_0}{\rho_0}\right)^3$$

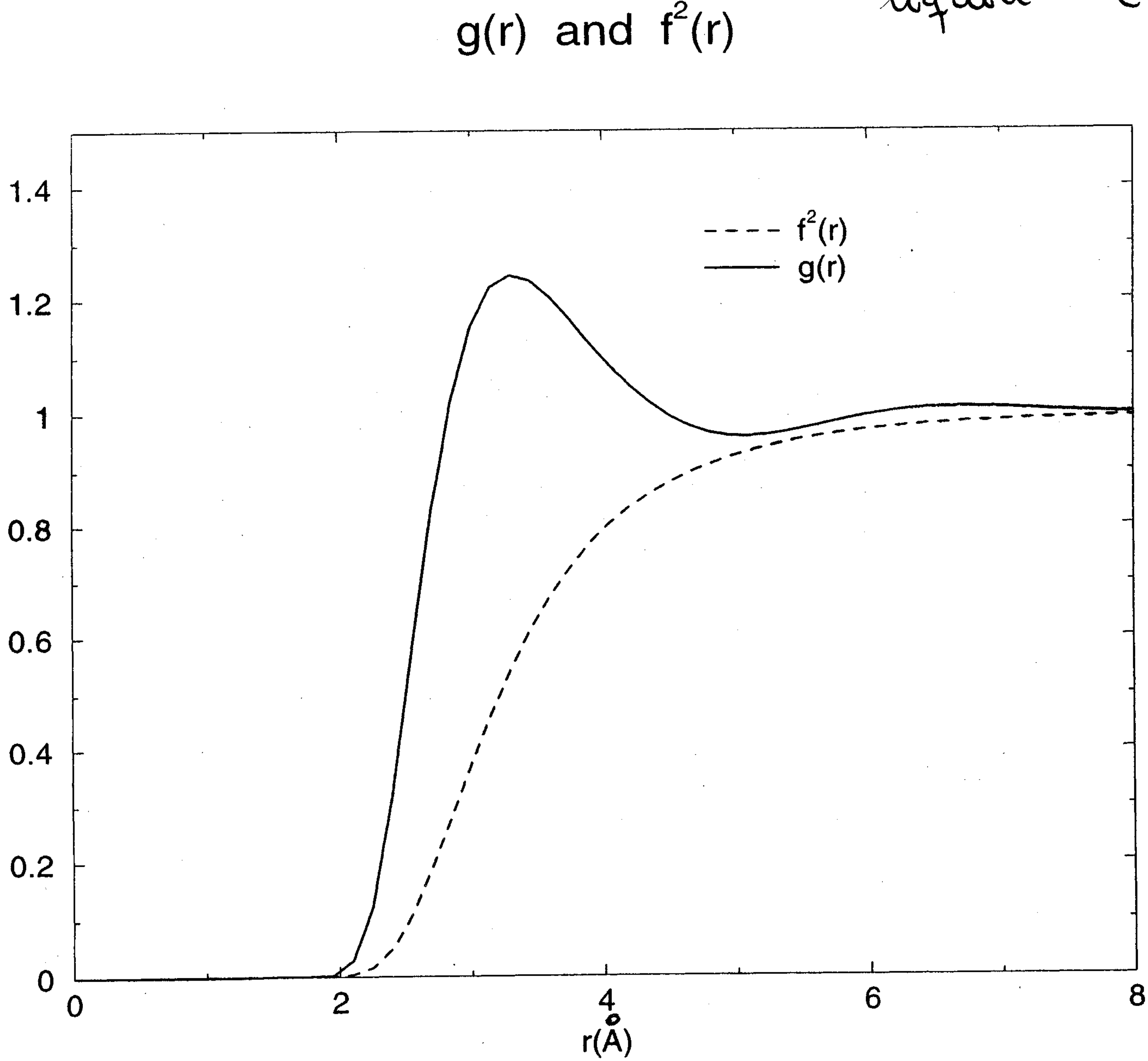
	e_0	ρ_0	b	c
Exp:	-7.17	0.3648	13.65	7.67
LJ HNC/S :	-5.824	0.3304	10.690	1.976
LJ HNC/ST:	-6.547	0.3644	15.529	22.048
Aziz. GFMC:	-7.11	0.360	10.08 ± 3.2	12.59 ± 8.5
Aziz. UFP :	-6.898	0.3624	12.72	12.16

$$P = -\left(\frac{\partial E}{\partial \Omega}\right)_N = \rho^2 \frac{de(\rho)}{d\rho} \quad ; \quad \mu = \left(\frac{\partial E}{\partial N}\right) = e(\rho) + \frac{P(\rho)}{\rho}$$

$$k_T = -\frac{1}{\Omega}\left(\frac{\partial \Omega}{\partial P}\right) \Rightarrow \frac{1}{\rho}\left(\frac{\partial \rho}{\partial P}\right) \Rightarrow k_T^{-1} = \Omega \frac{\partial^2 E}{\partial \Omega^2}$$

$$k_T^{-1} = 2\rho^2 \frac{\partial e(\rho)}{\partial \rho} + \rho^3 \frac{\partial^2 e(\rho)}{\partial \rho^2}$$

$c^2(\rho) = \frac{1}{\rho m k_T} \Rightarrow$ Aziz & Pathria
Phys. Rev. A7 (1973) 809



liquid ^4He

$$f(r) = e^{-\left[\frac{b\sigma}{r}\right]^5 \frac{1}{2}} \quad b = 1.17$$

$$g(r) = f^2 e^{N(r)}$$

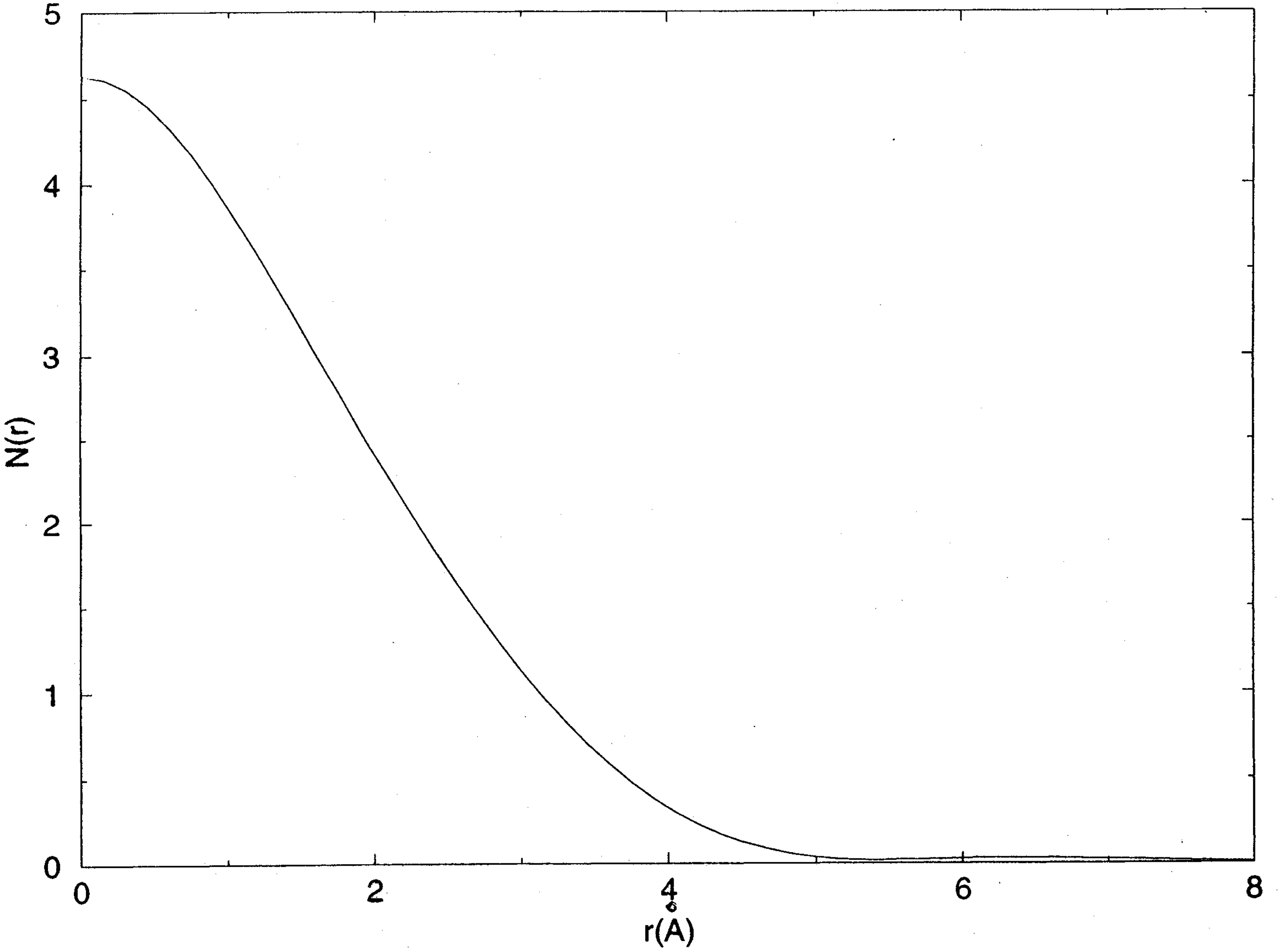
$$\rho = \rho_0 = 0.02186 \ \frac{\text{Atom}}{\mathring{A}^3}$$

HNC/0 Nodals liquid ^4He

$\rho = \rho_0 = 0.02186$ Atom/$\mathring{A}^3$

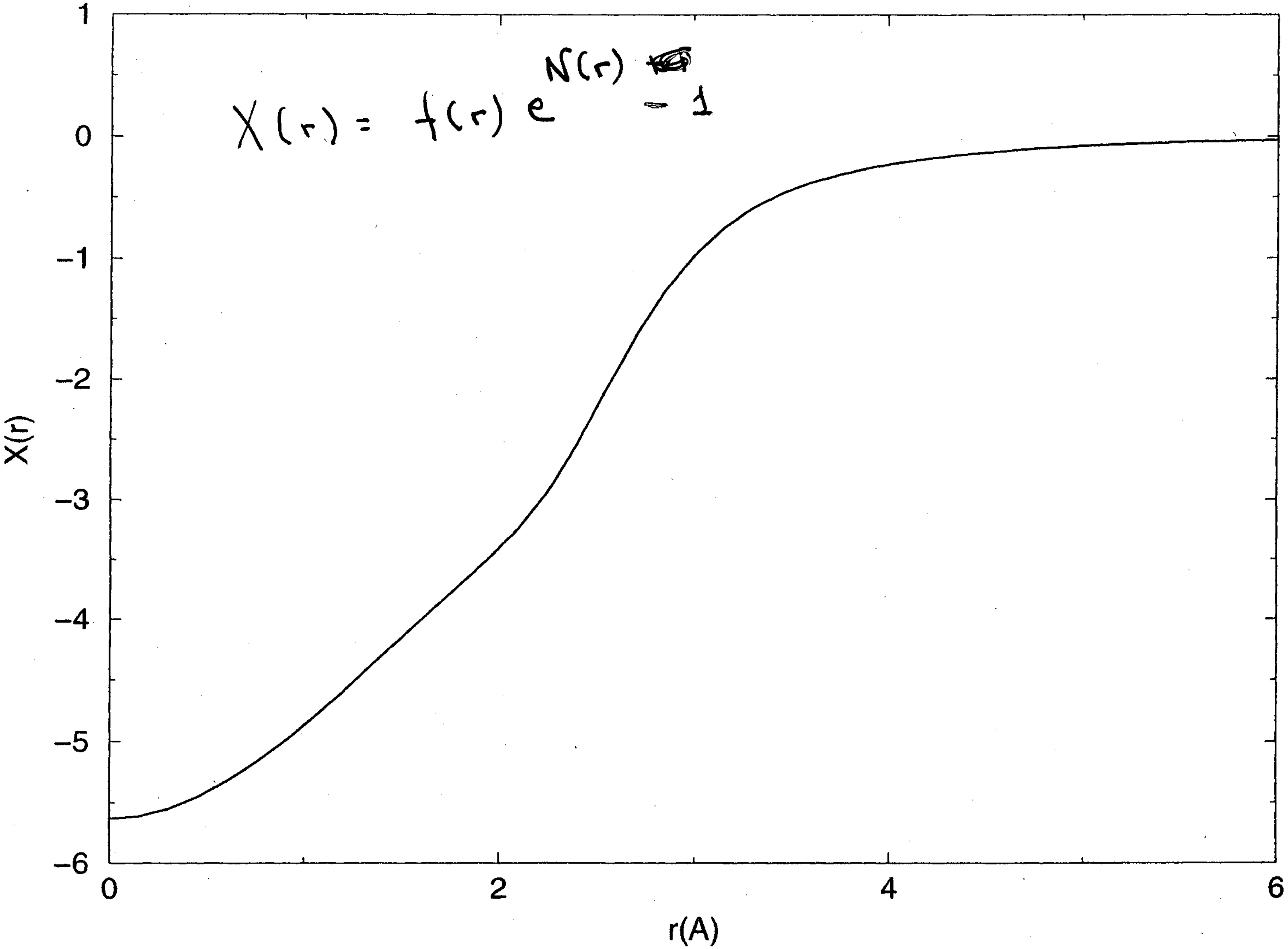
$f(r) = e^{-\left[\frac{b\sigma}{r}\right]^{5}\frac{1}{2}}$

$b = 1.17$



Composite liquid ⁴He

HNC/0

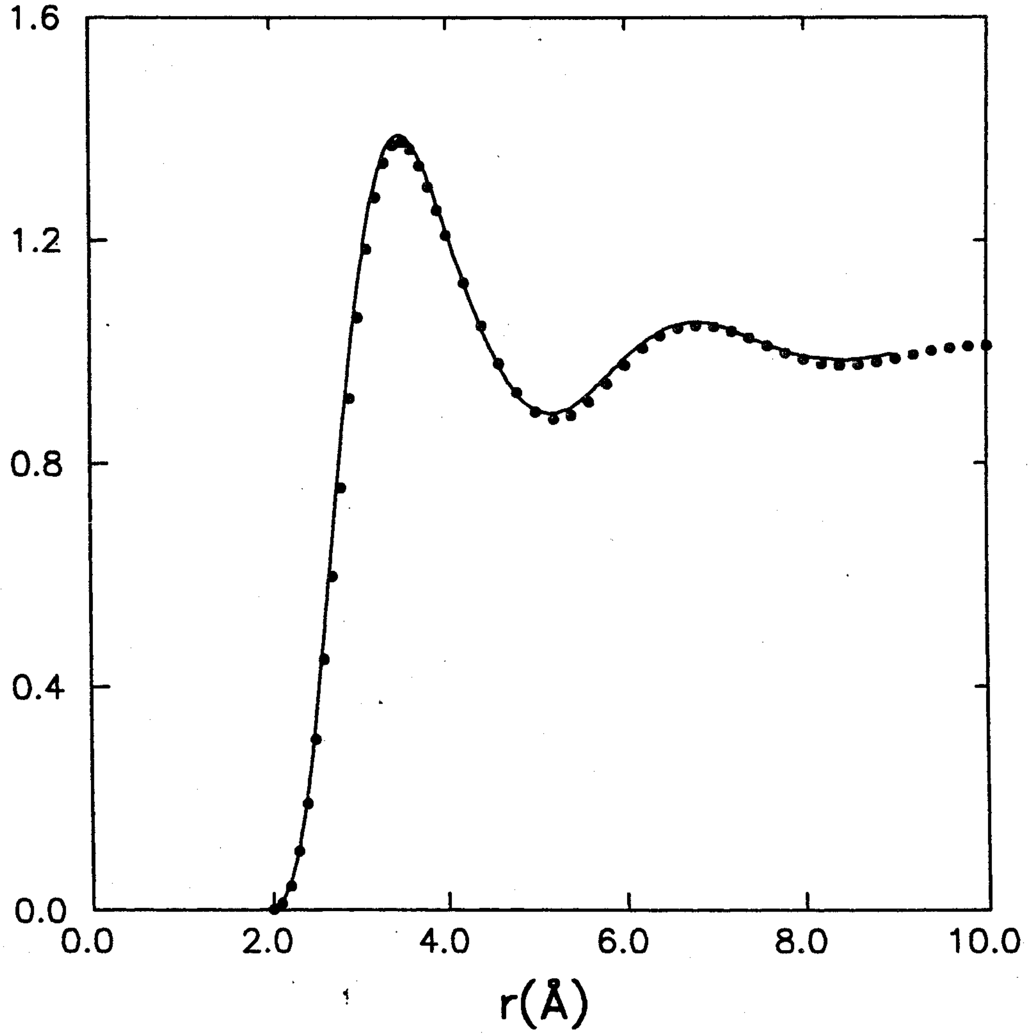


$X(r) = f(r)\, e^{N(r)} - 1$

$g(r)$, $\rho_0 = 0.365\,\sigma^{-3}$, GFMC ———

Exp. ● ● ●

$$g(r) = \frac{A(A-1)}{\rho^2} \frac{\int d\Omega_{12}\, \Psi^*(\bar{r}_1,\ldots,\bar{r}_A)\, \Psi(\bar{r}_1,\ldots,\bar{r}_A)}{\int d\Omega\, \Psi^*(\bar{r}_1,\ldots\bar{r}_A)\, \Psi(\bar{r}_1,\ldots,\bar{r}_A)}$$



J. Boronat , K. Casulleras
PRB 49 (1994) 8920

HFD-B(HE) (Aziz II) DMC ^{4}He

	3d	2d	1d
ρ_0	0.02186 $Å^{-3}$	0.04347 $Å^{-2}$	0.062 $Å^{-1}$
e_0 (K)	-7.27 (-7.17) exp	-0.89	-0.0036
$\langle T \rangle$ (K)	14.32	4.00	0.2706
$\langle V \rangle$ (K)	-21.59	-4.89	-0.2742
c m/s	238.3	92'8	8.0
n_0	0.084	0.23	/

3d : J. Boronat & J. Casulleras PRB 49 (1994) 8920

2d : S. Giorgini, J. Boronat, J. Casulleras PRB 54 (1996) 669

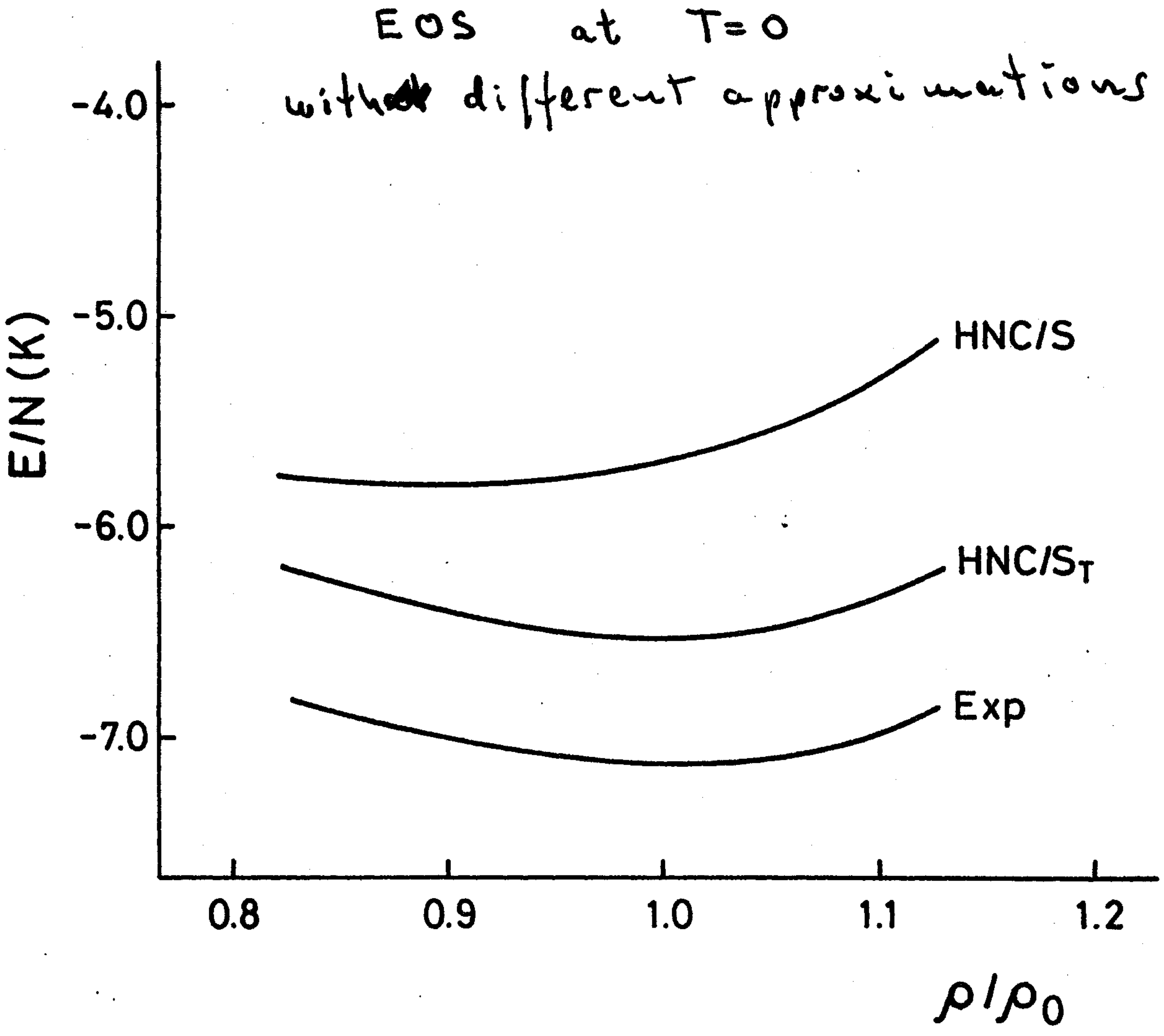
1d : Preprint, – C. Gordillo, J. Boronat, J. Casulleras
– Krotscheck & Miller (CBF optimal

* Reasonable agreement between all methods when :

CBF : Optimal correlations : 2body + 3body elementary diagrams

Shadow + VMC : The trial w.f. properly chose

* Pressure and chemical potential are more delicate quantities



EOS at T=0
with different approximations

What to do with the elementary diagrams?

$$g(r) = 1 + X(r) + N(r)$$

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

$$N(r_{12}) = \rho \int dr_3\; X(r_{23}) \left(X(r_{13}) + N(r_{13}) \right)$$

Ⓐ HNC/0 $\qquad \mathcal{E}(r) = 0$

Ⓑ PY assumes a full cancellation between elementary and composite!

$$e^{N+\mathcal{E}} \underset{PY}{\simeq} 1 + N + \underbrace{\frac{1}{2} N^2 + \dots + \mathcal{E} + \mathcal{E}^2 + \dots}_{\overset{\shortparallel}{0}}$$

$$e^{N+\mathcal{E}} \simeq 1 + N \Rightarrow \mathcal{E}_{PY} = \ln(1+N) - N(r)$$

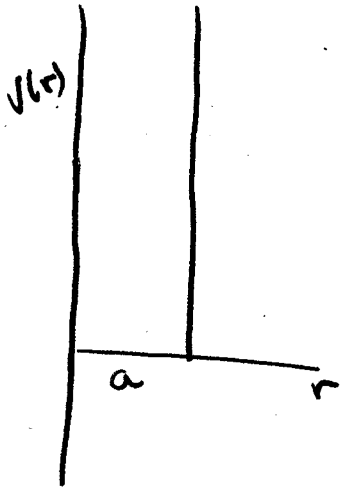
Percus-Yevick:

$$g_{PY}(r) = 1 + X_{PY}(r) + N_{PY}(r)$$

$$X_{PY}(r) = f^2(r) \left(1 + N_{PY}(r)\right) - 1 - N_{PY}(r)$$

$$N_{PY}(r) = \rho \int dr_3\; X_{PY}(r_{23}) \left(X_{PY}(r_{13}) + N_{PY}(r_{13}) \right)$$

Correlation function



$$f(r) = 0 \qquad r<a$$

$$f(r) = 1 \qquad r>d$$

$$f(r) = \frac{d}{r} \; \frac{\sin(k(r-a))}{\sin(k(d-a))}$$

the healing condition

$$f_J'(r=d) = 0 \Rightarrow \cot(k(d-a)) = \frac{1}{kd}$$

d is a variational parameter.

$$\boxed{\text{Bose hard-spheres}}$$

The relevant parameter is $x = \rho a^3$

$$\frac{E}{\Omega} = \frac{2\pi\rho^2 a \hbar^2}{m} \left[1 + \frac{128}{15} \left(\frac{\rho a^3}{\pi} \right)^{1/2} + 8\left(\frac{4}{3}\pi - \sqrt{3} \right)(\rho a^3) \ln(\rho a^3) + O(\rho a^3) \right]$$

Up to this order, we do not see the details of the potential, we are sensitive only to the scattering length!

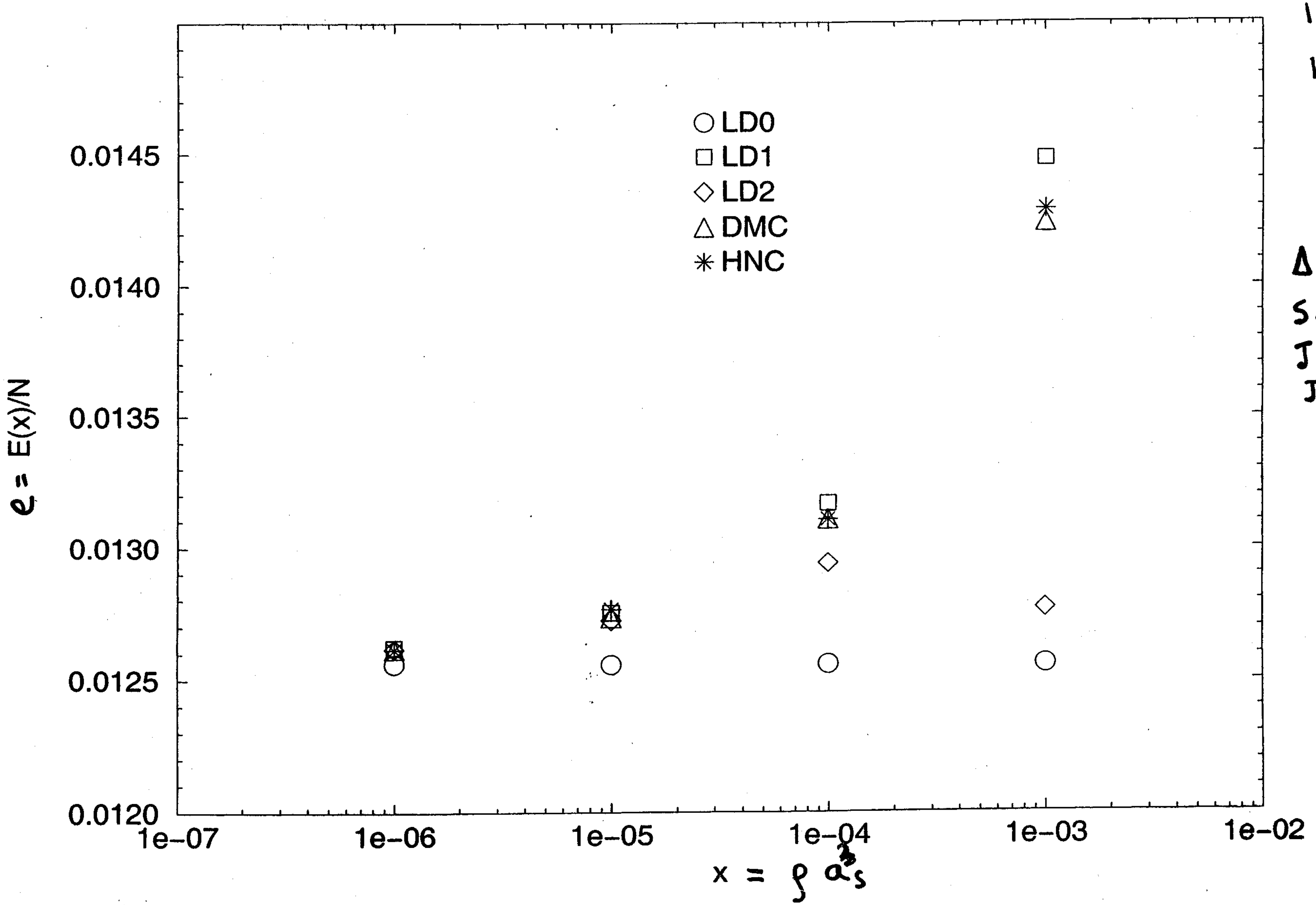
$$e = \frac{\frac{E}{\Omega}\frac{\Omega}{N}}{\frac{\hbar^2}{2ma^2}} = 4\pi\rho a^3 \left[1 + \ldots \right.$$

$$\boxed{e = \frac{\bar{e}}{\frac{\hbar^2}{2ma_s^2}}}$$

Remember: $LD0 = 4\pi\rho a_s^3$

HS gas Bose gas

The energies have been multiplied by 10^3 at $x=1.e\text{-}6$
10^2 at $x=1.e\text{-}5$
10 at $x=1.e\text{-}4$



△ DMC,
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Optimal equation

$$\Psi = \prod_{i<j} f^{(2)}(r_{ij})$$

Starting from the Jackson-Feenberg

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

we have

$$\left.\begin{array}{l} E = E(f,g) \\ g = g(f) \end{array}\right\}$$

one possible way is to eliminate "g" from $E = E(f,g$

then we get $E = \bar{E}(f)$, and then we ~~have~~ make variations of "f" to get:

$$\frac{\delta \bar{E}[f]}{\delta f} = 0$$ optimal correlation function!

However, it is easier to express "f" in terms of "g" and make the variations respect to "g".

I will work in HNC/0, elementary diagram

$E(r) \equiv 0$

$$g(r) = 1 + X(r) + N(r) \longrightarrow S(k) = 1 + \widetilde{g-1}$$

$$\tilde{N} = \frac{\tilde{X}^2}{1-\tilde{X}}$$

$$\boxed{\tilde{h}(k) = \rho \int d^3r \; e^{i\bar{k}\bar{r}} \, h(r) \quad \text{harbitrary function}}$$

$$\tilde{S} = \frac{1}{1-\tilde{X}} \quad ; \quad \tilde{N} = \frac{(S-1)^2}{S} \quad ; \quad \tilde{X} = \frac{S-1}{S}$$

in HNC/0, $g(r) = f^2(r)\, e^{N(r)}$

$$\Rightarrow \ln\left(\frac{g(r)}{f^2(r)}\right) = N(r) = \frac{1}{(2\pi)^3\rho}\int d^3k\, \frac{(S-1)^2}{S}\, e^{i\bar{k}\bar{r}}$$

therefore I can express $\ln f(r)$ in terms of $S(k)$ and g.

$$\ln f(r) = \frac{1}{2}\left\{\ln g(r) - \frac{1}{(2\pi)^3\rho}\int \frac{(S-1)^2}{S}\, e^{i\bar{k}\bar{r}}\, d^3k\right\}$$

and therefore

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

$$= \frac{\rho}{2}\int d^3r\, g(r)\, V(r) + \frac{\rho}{2}\int d^3r\, g(r)\, \frac{\hbar^2}{4m}\int \frac{(S-1)^2}{S}\, \Delta_{\bar{r}}\, e^{i\bar{k}\bar{r}}$$

$$d^3k\, \frac{1}{(2\pi)^3\rho} - \frac{\rho}{2}\frac{\hbar^2}{4m}\int d^3r\, g(r)\, \Delta \ln g(r)$$

applying $\Delta_{\bar{r}}$ to $e^{i\bar{k}\bar{r}}$ and performing first the integration over "r",

$$\frac{E}{N} = \frac{\rho}{2}\int d^3r\, g(r)\, V(r) - \frac{\hbar^2}{8m}\frac{1}{(2\pi)^3\rho}\int d^3k\, k^2\, \frac{(S-1)^2}{S}\, \underbrace{\rho\int d^3r\, e^{i\bar{k}\bar{r}}\, g(}_{\overbrace{g(r)-1} = S-1}$$

$$-\frac{\rho}{2}\frac{\hbar^2}{4m}\int d^3r\, g(r)\, \nabla^2 \ln g(r)$$

$$\boxed{\frac{E}{N} = \frac{\rho}{2}\int g(r)\, V(r)\, d^3r - \frac{\hbar^2}{8m}\frac{1}{(2\pi)^3\rho}\int d^3k\, k^2\, \frac{(S-1)^3}{S} - \frac{\rho}{2}\frac{\hbar^2}{4m}\int d^3r\, g(r)\cdot \nabla^2 \ln g(r}$$

it is convenient to intraduce $G^2 = g$,

$$-\frac{\hbar^2}{4m}\frac{\rho}{2}\int d^3r\, g(r)\,\nabla^2 \ln g(r) = \frac{\hbar^2}{4m}\frac{\rho}{2}\int d^3r\,(\vec{\nabla} G^2)\,(\vec{\nabla} \ln G^2)$$

$$= \frac{\hbar^2}{\cancel{4}m}\frac{\rho}{2}\int d^3r\,\cancel{2}\,(\vec{\nabla} G)\,\cancel{G}\,\cancel{2}\,\frac{(\vec{\nabla} G)}{\cancel{G}} = \frac{\hbar^2\rho}{2m}\int d^3r\,(\vec{\nabla} G)^2$$

variations of S respect to G ?

$S = 1+\rho\int d^3r\,[g(r)-1]\,e^{i\bar{k}\bar{r}}$ $\qquad g(r) = G^2(r)$

$$\delta S = 1+\rho\int d^3r\,[(G+\delta G)^2-1]\,e^{i\bar{k}\bar{r}} - 1-\rho\int d^3r\,[G^2(r)-1]\,e^{i\bar{k}\bar{r}}$$

$$= 2\rho\int d^3r\; G\,\delta G\, e^{i\bar{k}\bar{r}} = 2\,\widetilde{G\,\delta G}$$

$$\frac{\delta}{\delta G}\left(\frac{E}{N}\right) = \frac{\delta}{\delta G}\left[\frac{\rho}{2}\int G^2(r)\,V(r)\,d^3r - \frac{\hbar^2}{8m}\frac{1}{(2\pi)^3\rho}\int d^3k\,k^2\,\frac{(S-1)^3}{S} + \right.$$

$$\left. + \frac{\hbar^2}{2m}\,\rho\int d^3r\,(\vec{\nabla} G)^2\right]$$

a) $$\frac{\delta}{\delta G}\left[\frac{\rho}{2}\int G^2(r)\,V(r)\,d^3r\right] = \frac{\rho}{2}\int 2\,G(r)\,V(r)\,\delta G(r)\,d^3r$$

b) $$\frac{\delta}{\delta G}\left[\frac{\hbar^2}{2m}\,\rho\int d^3r\,(\vec{\nabla} G)^2\right] = \frac{\hbar^2}{2m}\,\rho\int d^3r\,(\vec{\nabla}(G+\delta G))^2 -$$

$$- \frac{\hbar^2}{2m}\,\rho\int d^3r\,(\vec{\nabla} G)^2 = \cancel{\frac{\hbar^2}{2m}\,\rho\int d^3r\,(\vec{\nabla} G)^2} + \frac{\hbar^2}{2m}\,2\rho\int d^3r\,\vec{\nabla} G\,\vec{\nabla}$$

$$+ \ldots - \cancel{\frac{\hbar^2}{2m}\,\rho\int d^3r\,(\vec{\nabla} G)^2} = -\frac{\hbar^2}{2m}\,2\rho\int d^3r\,(\nabla^2 G)\,\delta$$

c) $$\frac{\delta}{\delta G}\left[-\frac{\hbar^2}{8m}\frac{1}{(2\pi)^3\rho}\int d^3k\; k^2\;\frac{(S-1)^3}{S}\right] =$$

$$= -\frac{\hbar^2}{8m}\frac{1}{(2\pi)^3\rho}\int d^3k\; k^2\;\frac{\delta}{\delta S}\left(\frac{(S-1)^3}{S}\right)\frac{\delta S}{\delta G} =$$

$$= -\frac{\hbar^2}{8m}\frac{1}{(2\pi)^3\rho}\int d^3k\; k^2\left(\frac{S-1}{S}\right)^2(2S+1)\;2\;\widetilde{G\delta G}$$

now we use : $\rho\int d^3r\, f(r)\, g(r) = \frac{1}{(2\pi)^3\rho}\int \tilde{f}(k)\,\tilde{g}(k)\, d^3k$

to write the last expression in coordinate space, and we define what is called "induced interaction"

$$\tilde{W}_0 = -\frac{1}{2}\underset{\displaystyle\downarrow\ \frac{\hbar^2k^2}{2m}}{t(k)}\left(2\,S(k)+1\right)\left(1-\frac{1}{S(k)}\right)^2$$

$$\frac{1}{(2\pi)^3\rho}\int d^3k\left(-\frac{\hbar^2k^2}{4m}(2\,S(k)+1)\left(1-\frac{1}{S(k)}\right)^2\right)\widetilde{G\delta G} =$$

$$= \rho\int d^3r\; W_0(r)\; G\,\delta G$$

finally:

$$\boxed{\begin{array}{c}\frac{\delta}{\delta G}\left(\frac{E}{N}\right) \Longleftrightarrow\quad -\frac{\hbar^2}{m}\nabla^2G(r) + \left[V(r)+W_0(r)\right]G(r) = 0 \\[2ex] G = g^{1/2}(r) \qquad \tilde{W}_0(k) = -\frac{\hbar^2k^2}{4m}(2S+1)\left(1-\frac{1}{S(k)}\right)^2\end{array}}$$

An equivalent way to express the optimization condition, useful to study the momentum-space structure of the different functions is given by:

$$\frac{\delta E}{\delta S} = 0 \implies S(k) = \frac{1}{\sqrt{1 + \frac{2}{t(k)} \tilde{V}_{ph}(k)}}$$

$$t(k) = \frac{\hbar^2 k^2}{2m}$$

$$V_{ph}(k) = g(r)\, v(r) + \frac{\hbar^2}{m} \left| \vec{\nabla} \sqrt{g(r)} \right|^2 + \left[g(r) - 1 \right] w_I(r)$$

$V_{ph}(r)$ is a so called particle-hole effective interaction.

In order to have an acceptable solution one requires $\tilde{V}_{ph}(k) > 0$, in particular $\tilde{V}_{ph}(0^+) > 0$

$$\left.\begin{cases} \underset{k\to 0}{\varepsilon(k)} = \dfrac{t(k)}{S(k)} \sim \dfrac{\hbar k}{m} \sqrt{m \tilde{V}_{ph}(0^+} \\[2ex] \varepsilon(k) = \hbar c k \qquad k \to 0^+ \end{cases}\right\} \Rightarrow \tilde{V}_{ph}(0^+) = mc$$

Long-range behaviour

General sum-rule arguments show that:

$$\lim_{k\to 0} S(k) = \frac{\hbar k}{2mc}$$ linear in k

c velocity of sound

which reflects the long-wavelength density fluctuation

* This fact implies a long-range behaviour of $g(r)$ and also of $f(r)$. Actually a short-range $f(r)$, i.e. $e^{-1/2\left(\frac{b}{r}\right)^5}$ produces a finite value of $\lim_{k\to 0} S(k)$.

* Two behaviours that are of interest to us are:

$$\tilde{f}(k) \xrightarrow[k\to 0]{} ak \quad \text{and} \quad \tilde{f}(k) \xrightarrow[k\to 0]{} \frac{b}{k}$$

how they behave in $\underset{r\to\infty}{r}$?

Remember:

$$\tilde{f}(k) = \rho \int_0^\infty f(r) \frac{\sin kr}{kr} 4\pi r^2 dr \quad ; \quad f(r) = \frac{1}{(2\pi)^3 \rho} \int_0^\infty \tilde{f}(k) \frac{\sin kr}{kr} 4\pi k^2 dk$$

$$\int_0^\infty F(k)\,\sin kr\,dk = \frac{F(0)}{r} - \frac{F''(0)}{r^3} + \frac{F^{IV}(0)}{r^5} \dots$$

when $F(k)$ and its derivatives are well behaved!

* $\tilde{f}(k) \xrightarrow[k\to 0]{} ak$ what happens in r?

$$\frac{1}{(2\pi)^3\rho}\int_0^\infty (ak+..)\,\frac{\sin kr}{kr}\,4\pi k^2 dk = \frac{4\pi}{(2\pi)^3\rho}\,\frac{1}{r}\int_0^\infty (ak^2+--)\,\sin kr\,dk =$$

$$= \frac{4\pi}{(2\pi)^3\rho}\,\frac{1}{r}\left[\frac{0}{r} - \frac{2a}{r^3} + --\right] \simeq -\frac{a}{\pi^2\rho}\,\frac{1}{r^4}$$

$$\boxed{\begin{array}{lll} \tilde{f}(k) \xrightarrow[k\to 0]{} ak & \Rightarrow & f(r) \xrightarrow[r\to\infty]{} -\dfrac{a}{\pi^2\rho}\,\dfrac{1}{r^4} \\[2ex] \tilde{f}(k) \xrightarrow[k\to 0]{} \dfrac{b}{k} & \Rightarrow & f(r) \to \dfrac{b}{2\pi^2\rho}\,\dfrac{1}{r^2} \end{array}}$$

* $$\boxed{\boxed{S(k) \underset{k\to 0}{\sim} \frac{\hbar k}{2mc} \quad \Rightarrow \quad g(r) \underset{r\to\infty}{=} 1 - \frac{\hbar}{2\pi^2\rho Mc}\,\frac{1}{r^4}}}$$

$$g(r) = 1 + \underbrace{\frac{1}{(2\pi)^3\rho}\int_0^\infty (S(k)-1)\,\frac{\sin kr}{kr}\,4\pi k^2 dk}$$

$$\frac{1}{(2\pi)^3\rho}\,4\pi\,\frac{1}{r}\int_0^\infty (S(k)-1)\,k\,\underline{\sin kr}\;dk$$

$F(0)=0 \qquad F''(0) = \dfrac{\hbar}{Mc}$

$$= \frac{1}{(2\pi)^3\rho}\,4\pi\,\frac{1}{r}\int_0^\infty \frac{\hbar k^2}{2Mc} - k \dots\dots =$$

$$= -\frac{\hbar}{2\pi^2\rho Mc}\,\frac{1}{r^4} + \dots$$

What about X and N?

$$S(k) = 1 + \tilde{X} + \tilde{N}$$

$$\tilde{X} = 1 - \frac{1}{S} \quad \Rightarrow \quad \lim_{k\to 0} \tilde{X} = 1 - \frac{2mc}{\hbar}\frac{1}{k}$$

$$\tilde{N} = \frac{\tilde{X}^2}{1-\tilde{X}} \quad \Rightarrow \quad \lim_{k\to 0} \tilde{N} \Rightarrow -2 + \frac{2mc}{\hbar}\frac{1}{k} + \frac{\hbar}{2mc} k$$

Check!

$$S(k) = 1 + \underbrace{1 - \frac{2mc}{\hbar}\frac{1}{k}}_{\tilde{X}} \underbrace{-2 + \frac{2mc}{\hbar}\frac{1}{k} + \frac{\hbar}{2mc} k}_{\tilde{N}} \simeq \frac{\hbar}{2mc} k$$

$$\boxed{\underset{r\to\infty}{N(r)} \to \frac{mc}{\hbar \pi^2 \rho}\frac{1}{r^2}}$$

And $\underset{r\to\infty}{f(r)} \sim 1 - \frac{mc}{2\pi^2 \hbar \rho}\frac{1}{r^2} + \cdots$

reproduces the correct linear behaviour of $\underset{k\to 0}{S(k)}$.

$$f(r) - 1 \underset{r\to\infty}{\simeq} -\frac{mc}{2\pi^2\hbar\rho}\frac{1}{r^2} \qquad (f^2-1) \underset{r\to\infty}{\simeq} -\frac{mc}{\pi^2\hbar\rho}\frac{1}{r^2}$$

$$\widetilde{(f^2-1)} \simeq -\frac{2mc}{\hbar}\frac{1}{k}$$

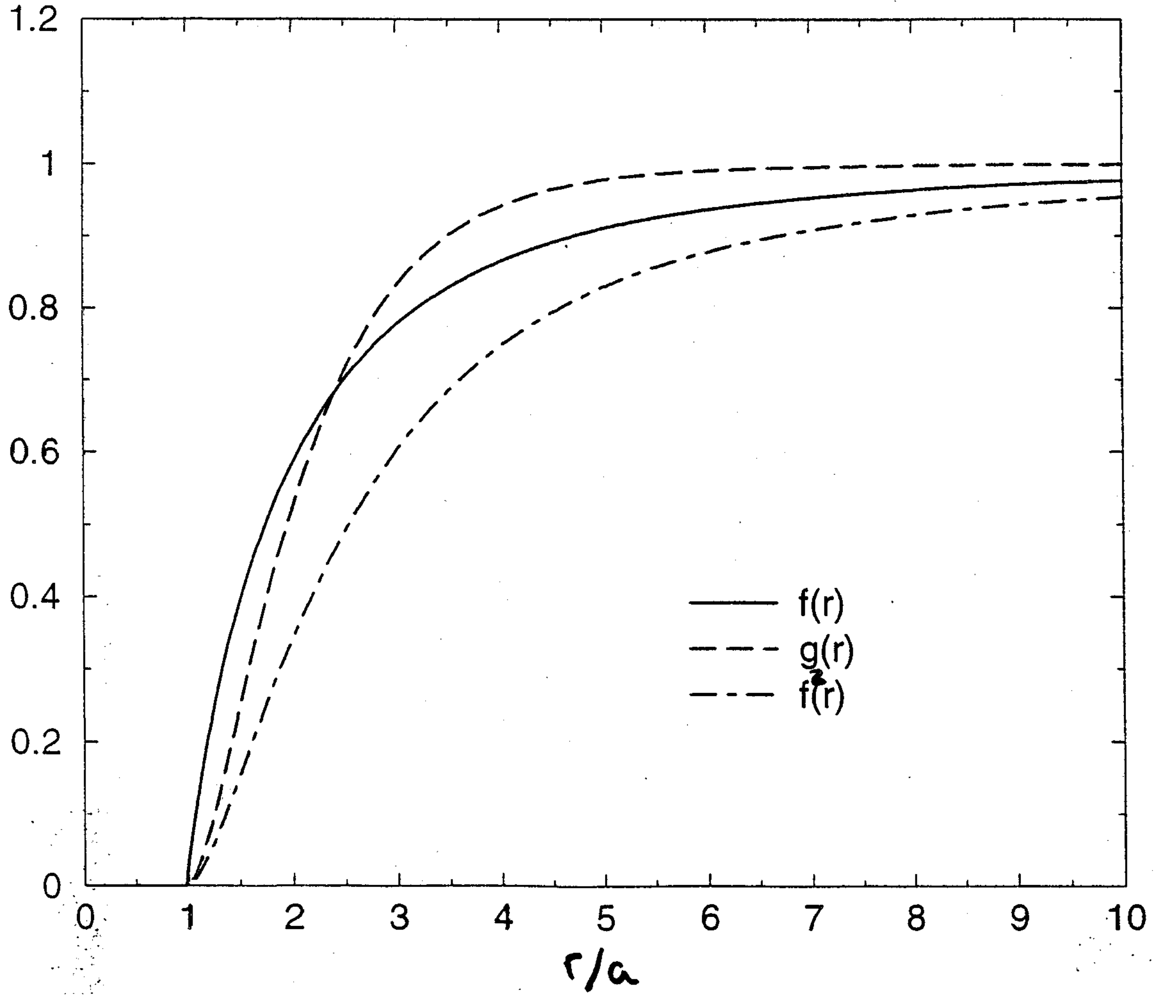
$$\tilde{N}(k) = \frac{\tilde{X}^2}{1-\tilde{X}} \Rightarrow \underset{k\to 0}{\tilde{N}(k)} \simeq \frac{\frac{4m^2c^2}{\hbar^2}\frac{1}{k^2}}{\frac{2mc}{\hbar}\frac{1}{k}} \simeq \frac{2mc}{\hbar}\frac{1}{k}$$

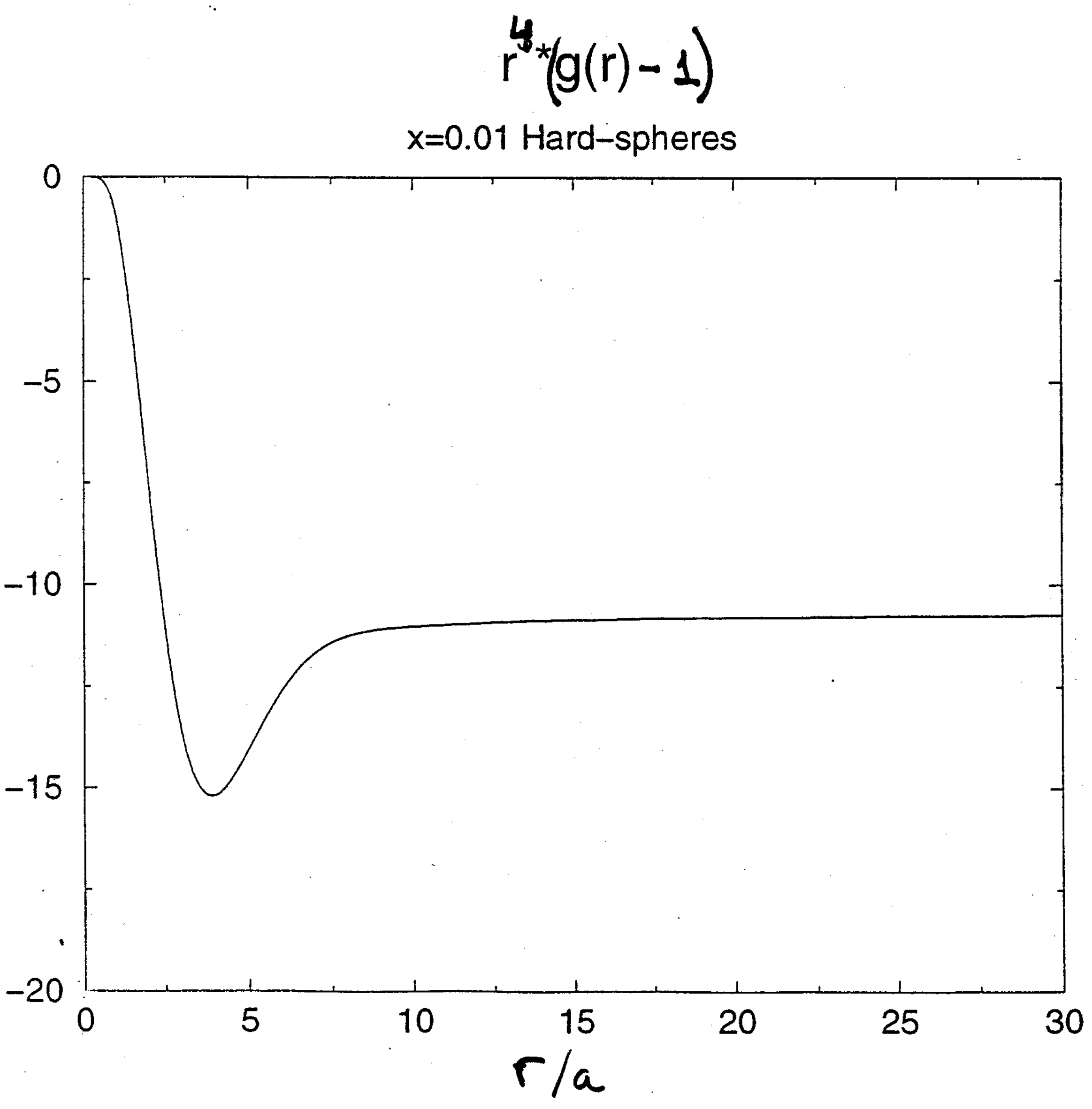
$$X = f^2 e^{N+\mathcal{E}} - N - 1 = (h^2+1)(1+N+\mathcal{E}+\cdots) - N - 1$$

$$\tilde{h}^2 \underset{k\to 0}{=} -\frac{2mc}{\hbar}\frac{1}{k} \qquad = h^2 + h^2 N + \cdots = h^2(1+N+\cdots) + \cdots$$

Hard-spheres   Optimal correlation

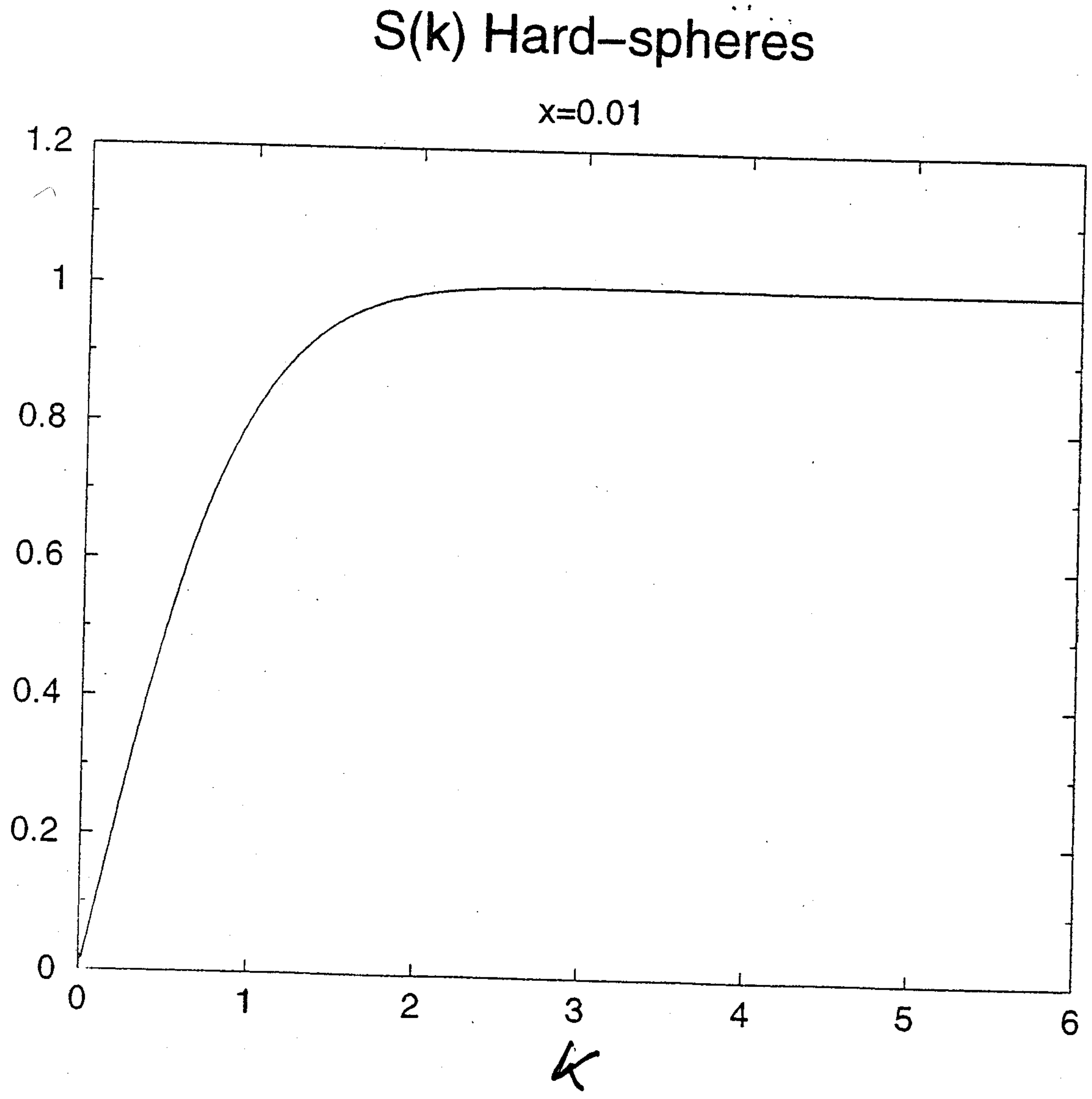
$\boxed{x = 0.01}$




r^4*(g(r)-1)
x=0.01 Hard-spheres
0
-5
-10
-15
-20
0
5
10
15
20
25
30
r/a

Structure function

Linear behaviour $k \to 0$



Doing the variations respect to $\ln f(r)$!

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

$$\frac{\delta}{\delta(\ln f(r))}\left(\frac{E}{A}\right) = 0$$

we have two terms:

$$\frac{\delta}{\delta(\ln f(r))}\left(\frac{E}{A}\right) = \frac{1}{2}\rho\int d^3r \overset{\text{Ⓐ}}{\left(\frac{\delta}{\delta(\ln f(r))}[g(r)]\right)}\left[V(r) - \frac{\hbar^2}{2m}\nabla^2 \ln f(r)\right]$$

$$+ \frac{\rho}{2}\int d^3r\, g(r)\, \overset{\text{Ⓑ}}{\frac{\delta}{\delta(\ln f(r))}\left[V(r) - \frac{\hbar^2}{2m}\nabla^2 \ln f(r)\right]}$$

Ⓑ $\frac{\rho}{2}\int d^3r\, g(r)\,\frac{\delta}{\delta(\ln f(r))}\left[V(r) - \frac{\hbar^2}{2m}\nabla^2 \ln f(r)\right] =$

$$= -\frac{\rho}{2}\frac{\hbar^2}{2m}\int d^3r\, g(r)\,\frac{\delta}{\delta(\ln f(r))}\left(\nabla^2 \ln f(r)\right) =$$

$$= -\frac{\rho}{2}\frac{\hbar^2}{2m}\int d^3r\,\left(\nabla^2 g(r)\right)\,\delta(\ln f(r))$$

$$\int d^3r\, g(r)\,\nabla^2\left[\ln f(r) + \delta \ln f(r)\right] - \int d^3r\, g(r)\,\nabla^2 \ln f(r) =$$

$$= \int d^3r\, g(r)\,\nabla^2 \delta \ln f(r) = \int d^3r\,\left(\nabla^2 g(r)\right)\,\delta(\ln f(r))$$

Ⓐ $\frac{\delta g}{\delta \ln f}\,\delta(\ln f) = \frac{\delta g}{\delta f}\,\frac{\delta f}{\delta \ln f}\,\delta \ln f = \frac{\delta g}{\delta f}\, f\,\delta(\ln f)$

Assuming HNC/0 $\quad g(r) = f^2 e^{N(r)}$

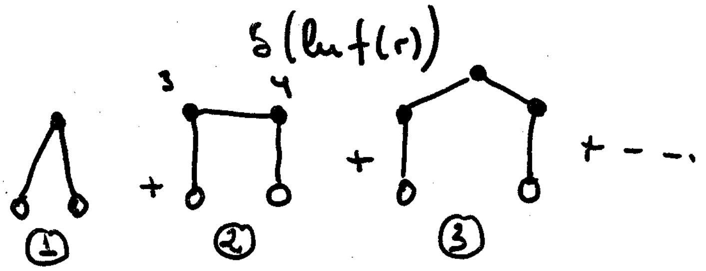
$$\frac{\delta g}{\delta f} = 2 f e^{N} + f^2\,\frac{\delta\left(e^{N(f^2)}\right)}{\delta f}$$

$$\frac{\delta(e^{N(f^2)})}{\delta f} = \frac{\delta(e^{N(f^2)})}{\delta f^2}\frac{\delta f^2}{\delta f} = 2f\ e^{N(f^2)}\ \frac{\delta N(f^2)}{\delta f^2}$$

introducing the notation: $\vartheta_{JF}(r) = V(r) - \frac{\hbar^2}{2m}\nabla^2 \ln f(r)$

$$\frac{\rho}{2}\int d^3r\ \frac{\delta g(r)}{\delta(\ln f(r))}\ \vartheta_{JF}(r)\overset{\delta(\ln f(r))}{\downarrow} = \frac{\rho}{2}2\int d^3r\ f^2\ e^N\ \vartheta_{JF}\ \delta(\ln f(r))$$

$$+\frac{\rho}{2}2\int d^3r_{12}\ \vartheta_{JF}(r_{12})\ f^2(r_{12})\ e^{N(f^2(r'_{ij}))}\ \frac{\delta N(f^2(r'_{ij}))}{\delta f^2}\ f^2(r'_{ij}$$

N =  + - - -

$$② = \rho^2\int(f^2(r_{13})-1)\ (f^2(r_{34})-1)(f^2(r_{42})-1)d\bar{r}_3\,d\bar{r}_4 = h(r_{12})$$

now I must perform the variation in all sides!

i.e. $f^2(r_{34}) \Rightarrow \rho^2\int(f^2(r_{13})-1)\ (f^2(r_{42})-1)\,d\bar{r}_3\,d\bar{r}_4$

Therefore, we should derive respect all internal sides, besides we have the term $f^2\vartheta_{JF}$ in the side (12) ⇒ Then, we let for the end the integral over the side where we perform the variation ⇒ This is equivalent to calculate all the diagrams where $f^2\,\vartheta_{JF}(r)$ appears in all the possible positions.

$$\boxed{\frac{\rho}{2}\int d^3r\ \frac{\delta g(r)}{\delta(\ln f(r))}\ \vartheta_{JF}(r)\ \delta(\ln f(r)) = \rho\int d^3r\ g(r)\left[\vartheta_{JF}(r) + N'(r)\right]\delta\ln f(r)}$$

$N'(r)$ are the nodal diagrams with the term $\boxed{V_{JF}(r)\, f^2(r)}$ in ~~its in~~ one of its internal sides!

$$\frac{\delta}{\delta(\ln f(r))}\left(\frac{E}{A}\right) = \rho\int d^3r\left(-\frac{\hbar^2}{4m}\nabla^2 g(r) + g'(r)\right)\delta \ln f(r)$$

$g'(r)$ is the distribution function in which $\vartheta_{JF}(r)\, f^2$ appears in the side ~~12~~ and in all the internal ones, but only once.

$$\boxed{\begin{array}{l}\dfrac{\delta}{\delta(\ln f(r))}\left(\dfrac{E}{A}\right) = 0 \quad \Rightarrow \\[2ex] g'(r) - \dfrac{\hbar^2}{4m}\nabla^2 g(r) = 0 \iff \tilde g'(k) + \dfrac{\hbar^2}{4m} k^2 (S(k)-1) = 0\end{array}}$$

$$\Downarrow$$

$$\langle\Psi|\rho_{\vec k}\,\rho_{-\vec k}\,(H-E)|\Psi\rangle = 0$$

$$\rho_{\vec k} = \sum_j e^{i\vec k \vec r_j}$$

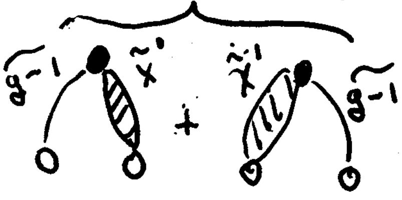
How to calculate g' ?

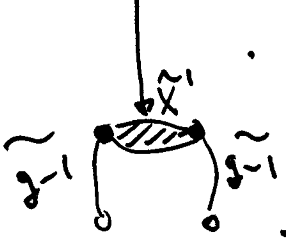
$g'(r)$ is the sum of all diagrams in which $V_{JF}(r)\, f^2(r)$ appears only once in all possible positions

$g'(r) = X' + N'$ Sum of non-nodal and nodal diagrams

$$\tilde N' = \tilde X'\,(\widetilde{g-1})\,2 + \tilde X'\,(\widetilde{g-1})^2 = \tilde X'\left[2(S-1) + (S-1)^2\right]$$

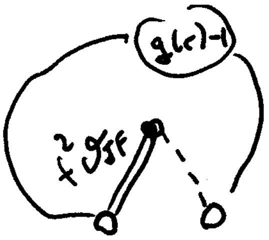
$$= \tilde X'\left[S^2 - 1\right]$$





$$g'(r) = X'(r) + N'(r)$$

$$\tilde{N}'(k) = \tilde{X}'(k)\ \left[S^2(k)-1\right]$$



besides : $X'(r) = \vartheta_{JF}(r)\ g(r) + N'(r)\ \left(g(r)-1\right)$

therefore : $g'(r) = \vartheta_{JF}(r) g(r) + N'(r)\ \left(g(r)-1\right) + N'(r)$

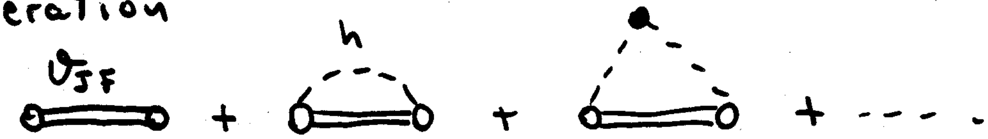
$$= \left(\vartheta_{JF} + N'\right) g(r)$$

iterative scheme: $g(r),\ S(k) \longrightarrow g',\ X',\ N'$

$$\begin{tikzcd}
\text{1st. iteration:} \arrow[d] & & \\
X' = \vartheta_{JF}\ g \arrow[d, "\text{F.T.}"] & & \\
\tilde{X}' \arrow[r] & \tilde{N}' = \tilde{X}'\left[S^2-1\right] \arrow[r, "\text{F.T.}"] & N'(r) \arrow[d] \\
& \tilde{X}' \arrow[u] & X'(r) = \vartheta_{JF}(r)\, g(r) + N'(r)\, (g(r)-1) \arrow[l, "\text{F.T}"']
\end{tikzcd}$$

1st. iteration

$X' =$



$$= \vartheta_{JF} \cdot g$$

Optimal condition for $\Psi = \prod f(r_{ij})$

- The change in energy is small.
- Right asymptotic behavior!

$$\begin{cases} S(k) \underset{k\to 0}{\sim} \dfrac{\hbar k}{2mc} \\[2ex] g(r) \underset{r\to\infty}{=} 1 - \dfrac{\hbar}{2\pi^2 \rho m c}\dfrac{1}{r^4} \end{cases}$$

$$\boxed{\begin{aligned} &-\frac{\hbar^2}{m}\nabla^2\sqrt{g(r)} + \left[\vartheta(r) + W_0(r)\right]\sqrt{g(r)} = 0 \\ &\qquad \tilde{W}_0(k) = -\frac{\hbar^2 k^2}{4m}\left(2S(k)+1\right)\left(1 - \frac{1}{S(k)}\right)^2 \end{aligned}}$$

$$\boxed{\begin{aligned} &S(k) = \frac{1}{\sqrt{1 + \frac{2}{t(k)}\tilde{V}_{ph}(k)}} \qquad t(k) = \frac{\hbar^2 k^2}{2m} \\ &V_{ph}(r) = g(r)\,\vartheta(r) + \frac{\hbar^2}{m}\left|\vec{\nabla}\sqrt{g(r)}\right|^2 + \left[g(r) - 1\right] w_I(r) \end{aligned}}$$

$$g'(r) - \frac{\hbar^2}{4m}\nabla^2 g(r) = 0 \iff \tilde{g}'(k) + \frac{\hbar^2}{4m}k^2\left(S(k) - 1\right) = 0$$

$$\Updownarrow$$

$g'(r)$ distribution function in which $\vartheta_{JF}(r)\, f^2(r)$ appears only once in each diagram in the internal positions.

$$\langle \Psi | \rho_{\bar{k}}\, \rho_{-\bar{k}}\, (H - E) | \Psi \rangle = 0$$

$$\rho_{\bar{k}} = \sum_j e^{i \bar{k} \bar{r}_j}$$

"Feynman Phonon"

$$|\Psi_{\vec k}\rangle = \rho_F(\vec k)\,|\Psi_0\rangle \qquad \rho_F = \sum_{i=1}^{A} e^{i\bar k\bar r_i}$$

Eigenstate of momentum $\vec k$

$$\rho_F^+(\vec k)\,\rho_F(\vec k) = \sum_i e^{-i\bar k\bar r_i}\sum_j e^{i\bar k\bar r_j} = A + \sum_{i\neq j} e^{i\vec k(\bar r_j-\bar r_i)}$$

Normalization:

$$\frac{\langle\Psi_{\vec k}|\Psi_{\vec k}\rangle}{\langle\Psi_0|\Psi_0\rangle} = \frac{\langle\Psi_0|\rho_k^+\,\rho_k|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} = \frac{\langle\Psi_0|A+\sum_{i\neq j} e^{i\bar k(r_j-r_i)}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} =$$

$$= A + A(A-1)\,\frac{\langle\Psi_0|e^{i\bar k(\bar r_2-\bar r_1)}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} =$$

$$= A + \rho^2\int d\bar r_1\,d\bar r_2\; e^{i\bar k\bar r_{12}}\;\frac{A(A-1)}{\rho^2}\;\frac{\int d\Omega_{12}\,|\Psi_0|^2}{\langle\Psi_0|\Psi_0\rangle}$$

$$= A + A\rho\int d\bar r_{12}\; e^{i\bar k\bar r_{12}}\; g(r) = A\,S(k)$$

Excitation energy:

$$e(k) = \frac{\langle\Psi_{\bar k}|H-E_0|\Psi_{\bar k}\rangle}{\langle\Psi_{\bar k}|\Psi_{\bar k}\rangle} = \frac{\langle\Psi_0|\rho_{\bar k}^+\,\{H-E_0\}\,\rho_{\bar k}|\Psi_0\rangle}{\langle\Psi_0|\rho_{\bar k}^+\,\rho_{\bar k}|\Psi_0\rangle} =$$

$$= \underset{\substack{\| \\ 0}}{\frac{\langle\Psi_0|\rho_{\bar k}^+\,\rho_{\bar k}\,\{H-E_0\}|\Psi_0\rangle}{\langle\Psi_0|\rho_k^+\,\rho_k|\Psi_0\rangle}} + \frac{\langle\Psi_0|\rho_{\bar k}^+\,[H-E_0,\rho_{\bar k}]|\Psi_0\rangle}{\langle\Psi_0|\rho_k^+\,\rho_k|\Psi_0\rangle}$$

if $|\Psi_0\rangle$ is the ground state

$[E_0, \rho_q] = 0$; $\left[\sum U(r_{ij}),\ \rho_q\right] = 0$

↳ If the interaction is momentum independent !

$$\frac{\langle \Psi_0 | \rho_k^+ [H - E_0, \rho_k]\, | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \frac{\langle \Psi_0 | \rho_k^+ \left[-\frac{\hbar^2}{2m} \sum_i \nabla_i^2, \rho_k\right] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

$$\left[-\frac{\hbar^2}{2m} \sum_i \nabla_i^2, \rho_{\bar{q}}\right] = -\frac{\hbar^2}{2m} \sum_i \left[\nabla_i^2, \rho_{\bar{q}}\right]$$

$$\Psi_0 \rho_k^+ [\bar{\nabla}_i^2, \rho_k] \Psi_0 \Rightarrow \Psi_0 \rho_k^+ (\nabla_i^2 \rho_k) \Psi_0 + \Psi_0 \cancel{\rho_k^+ \nabla} \rho_k (\nabla_i^2 \Psi_0)$$
$$- \cancel{\Psi_0 \rho_k^+ \rho_k (\nabla_i^2 \Psi_0)} + \Psi_0 \rho_k^+\, 2 (\bar{\nabla}_i \rho_k)(\bar{\nabla}_i \Psi_0)$$

but $\boxed{\int g\, f(\vec{\nabla} g) = -\frac{1}{2} \int g (\vec{\nabla} f) g \qquad \text{"}g\text{" real}}$

$$= \Psi_0 \rho_{\bar{k}}^+ (\nabla_i^2 \rho_{\bar{k}}) \Psi_0 - \frac{1}{2}\, 2\, \Psi_0\, \vec{\nabla}_i (\rho_k^+ \bar{\nabla}_i \rho_k) \Psi_0$$

$$= \cancel{\Psi_0 \rho_k^+ (\bar{\nabla}_i^2 \rho_{\bar{k}})} \Psi_0 - \Psi_0 (\vec{\nabla}_i \rho_{\bar{k}}^+)(\vec{\nabla}_i \rho_{\bar{k}}) \Psi_0 - \cancel{\Psi_0 \rho_k^+ (\bar{\nabla}_i^2 \rho_k)} \Psi_0$$

$$e(k) = -\frac{\hbar^2}{2m} \sum_{i=1}^{A} - \frac{\langle \Psi_0 | (\vec{\nabla}_i \rho_{\cancel{q}k}^+)(\vec{\nabla}_i \rho_k) \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \left(\frac{\langle \Psi_k | \Psi_k}{\langle \Psi_0 | \Psi_0 \rangle} \right)^{-1}$$

$$= \frac{\hbar^2}{2m} k^2 \sum_{i=1}^{A} \left(\frac{\langle \Psi_k | \Psi_k \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \right)^{-1} = \frac{\hbar^2}{2m} k^2\, A\, \frac{1}{A\, S(\cancel{q}k)}$$

$$= \frac{\hbar^2}{2m} \frac{k^2}{S(k)}$$

$$e_F(k) = \frac{\hbar^2}{2m} \sum_{i=1}^{A} \frac{\langle \Psi_0 | \left(\vec{\nabla}_i \rho_F^+(k)\right) \left(\vec{\nabla}_i \rho_F(k)\right) | \Psi_0 \rangle}{\langle \Psi_0 | \rho_F^+(k)\, \rho_F(k) | \Psi_0 \rangle} = \frac{\hbar^2 k^2}{2m\, S(k)}$$

behaviour at low k !

$$\lim_{k \to 0} S(k) = \frac{\hbar k}{2 m v_s}$$ v_s sound velocity!

$$\boxed{\underset{k\to 0}{e_F(k)} = \hbar\, k\, v_s}$$

linear in k

typical phonon spectrum.

good description up to $\underline{k \simeq 0.6\ \text{Å}^{-1}}$

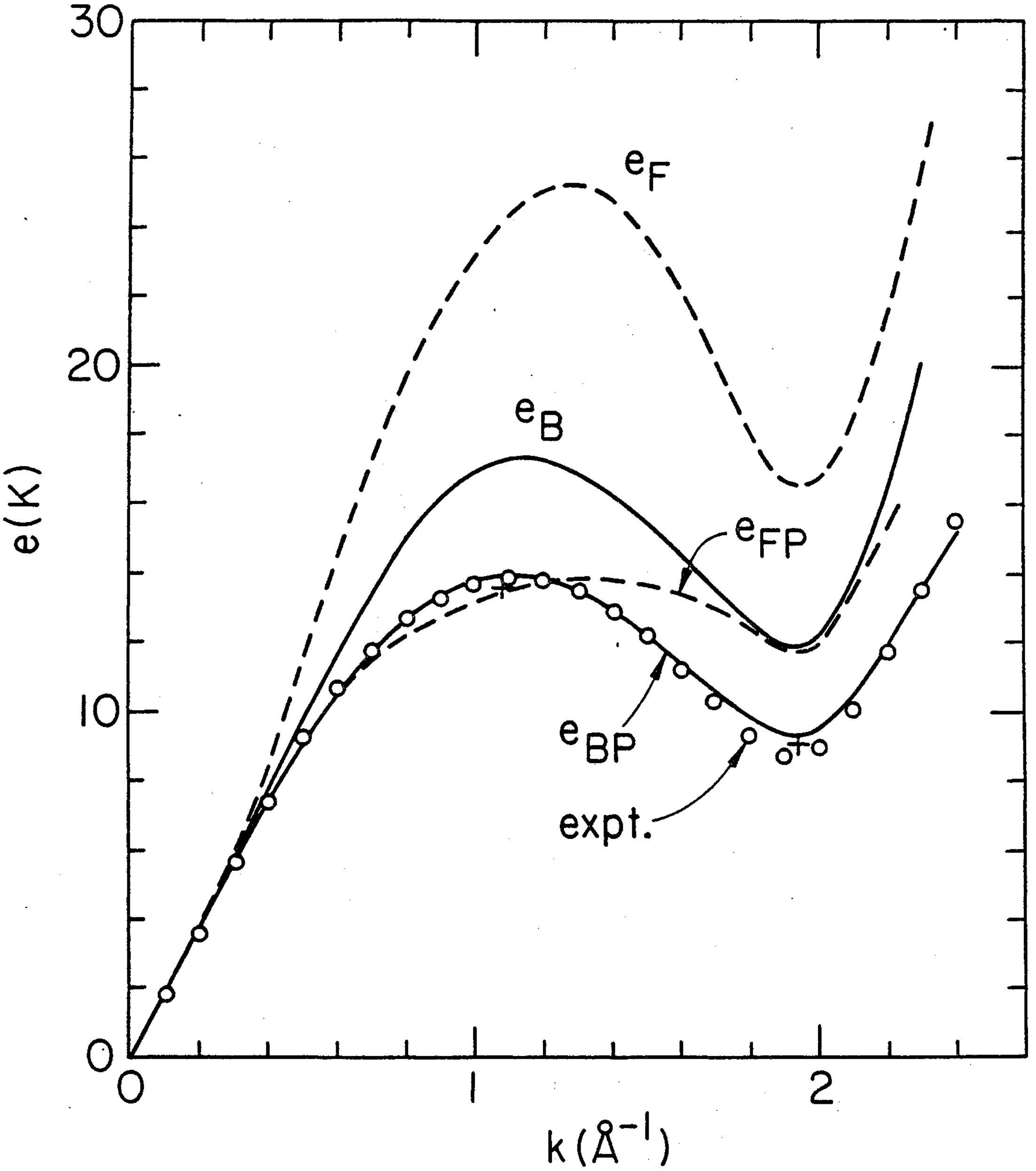
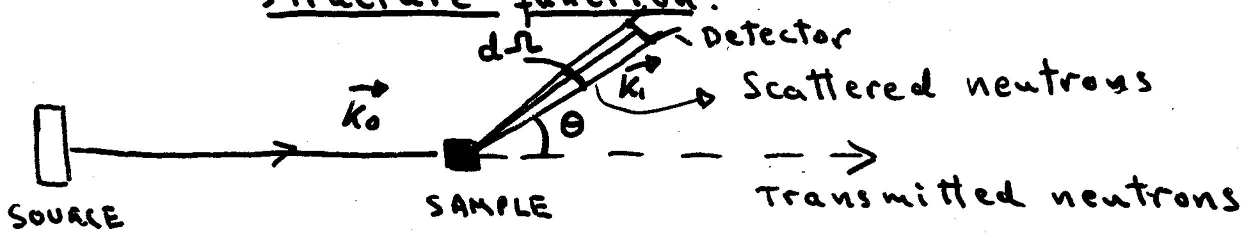


Fig. 18

Relation between the cross section and the dynamic structure function.



$$\frac{d^2\sigma}{dE\,d\Omega} = \frac{k_1}{k_0}\, b^2\left[\frac{1}{N}\sum_n \left|\langle n|\sum_j e^{-i(\bar{k}_1-\bar{k}_0)\vec{r}_j}|0\rangle\right|^2 \delta(E-(E_n-E_0))\right]$$

* The nuclear interaction is very short range in front of the wave length of the incident beam

(25 meV → 1.8 Å or 600 meV → 0.4 Å)

Kinetic energy incident neutrons

↓

Only s-scattering is possible → Use of Fermi pseudo pot.

$$V(r) = \frac{2\pi\hbar^2}{m}\, b \sum_{j=1}^{N} \delta(\bar{r}-\bar{r}_j)$$

↓

Use of the Golden Rule (i.e. first order perturbation theory)

to calculate the cross section.

$$\frac{d^2\sigma}{dE\,d\Omega} = \frac{k_1}{k_0}\, b^2\, S(q,E)$$

$$\begin{cases} \vec{q} = \vec{k}_1 - \vec{k}_0 & \text{momentum transfer} \\ E = \dfrac{\hbar^2 k_0^2}{2m} - \dfrac{\hbar^2 k_1^2}{2m} & \text{energy trans.} \end{cases}$$

$$S(q,E) = \frac{1}{N}\sum_n{}' \left|\langle n|\hat{\rho}_{\bar{q}}|0\rangle\right|^2 \delta(E-(E_n-E_0))$$

$$\hat{\rho}_{\bar{q}} = \sum_{i} e^{i\bar{q}\bar{r}_i}$$ fluctuation density operat

Dynamic Structure function:

$$S(q,E) = \frac{1}{A} \sum_n |\langle n | \rho_{\bar q} | 0 \rangle|^2 \, \delta(E - (E_n - E_0))$$

Sum-rules:

$$\left.\begin{aligned} \int_0^\infty S(q,E)\, dE &= S(q) \\ \int_0^\infty S(q,E)\, E\, dE &= \frac{\hbar^2 q^2}{2m} \end{aligned}\right\}$$ They help in understanding S(q,E).

$S(q,\omega)$ in a one phonon approach!

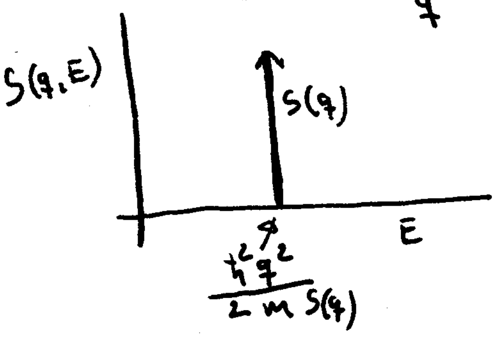
$$|n\rangle = |\Psi_{\bar k}\rangle = \frac{\rho_{\bar k} |\Psi_0\rangle}{(\langle \Psi_0 | \rho_k^+ \rho_k | \Psi_0 \rangle)^{1/2}} = \frac{\rho_{\bar k} |\Psi_0\rangle}{A^{1/2} S(q)^{1/2}}$$

$$\langle \Psi_{\bar k} | \rho_{\bar q} | 0 \rangle = \delta_{\bar k \bar q} \frac{A\, S(q)}{A^{1/2} S(q)^{1/2}} = \delta_{\bar k \bar q} (A\, S(q))^{1/2}$$

$$S(q,E) = \frac{1}{A} \sum_{\bar k}{}' |\langle \bar k | \rho_{\bar q} | 0 \rangle|^2 \, \delta(E - (E_{\bar k} - E_0))$$

$$= \frac{1}{A} \sum_{\bar k}{}' \delta_{\bar k \bar q} \frac{1}{A S(k)} A^2 S^2(k) \, \delta\left(E - \frac{\hbar^2 \bar k^2}{2m S(k)}\right)$$

$$= S(q) \, \delta\left(E - \frac{\hbar^2 q^2}{2m S(q)}\right)$$



Detail of the sum-rules !

$$S(q,E) = \frac{1}{N} \sum_n |\langle n| \rho_{\bar{q}} |0\rangle|^2 \, \delta(E-(E_n-E_0))$$

$$\int \overset{\underline{m_0}}{S(q,E)} \, dE = \frac{1}{N} \int dE \sum_n |\langle n| \rho_{\bar{q}} |0\rangle|^2 \, \delta(E-(E_n-E_0))$$

$$= \frac{1}{N} \sum_n |\langle n| \rho_{\bar{q}} |0\rangle|^2 = \frac{1}{N} \sum_n \langle 0| \rho_q^+ |n\rangle \langle n| \rho_q |0\rangle =$$

$$= \frac{1}{N} \langle 0| \rho_q^+ \rho_q |0\rangle = S(q)$$

$$\underline{m_1}$$

$$m_1 = \int S(q,E)\, E \, dE = \frac{1}{N} \int dE \; E \sum_n |\langle n| \rho_{\bar{q}} |0\rangle|^2 \, \delta(E-(E_n-E_0))$$

$$= \frac{1}{N} \sum_n (E_n-E_0) \langle 0| \rho_q^+ |n\rangle \langle n| \rho_q |0\rangle =$$

$$= \frac{1}{N} \sum_n \langle 0| \rho_q^+ |n\rangle \langle n| H \rho_q - \rho_q H |0\rangle =$$

$$= \frac{1}{N} \sum_n \langle 0| \rho_q^+ |n\rangle \langle n| [H, \rho_{\bar{q}}] |0\rangle =$$

$$= \frac{1}{2} \frac{1}{N}$$ [redacted] $$\langle 0| [\rho_{\bar{q}}^+, [H, \rho_{\bar{q}}]] |0\rangle$$

Let's calculate the commutator !

Only kinetic energy contributions !

$$\frac{1}{2}\left[A, [T, B]\right] F \qquad\qquad T = \sum_{i=1}^{N} -\frac{\hbar^2}{2m} \nabla_i^2$$

$F =$ is a generic correlation operator

$$A = \sum_i f(r_i) \quad ; \quad B = \sum_i g(r_i)$$

$$\frac{1}{2}\left[A, [T, B]\right] F = \frac{1}{2}\left(-\frac{\hbar^2}{2m}\right) \sum_{i=1}^{N} \left[A, [\bar{\nabla}_i^2, B]\right] F =$$

$$= -\frac{\hbar^2}{4m} \sum_i \left[A, \nabla_i^2 B - B \nabla_i^2\right] F = -\frac{\hbar^2}{4m} \sum_i \left\{ A \nabla_i^2 B - A B \nabla_i^2 - \nabla_i^2 B A + B \nabla_i^2 A \right\} F$$

$$= -\frac{\hbar^2}{4m} \sum_i \Big\{ A (\nabla_i^2 B) F + 2 A (\bar{\nabla}_i B)(\bar{\nabla}_i F) + A B (\nabla_i^2 F)$$

$$- A B (\nabla_i^2 F) - (\nabla_i^2 B) A F - B (\nabla_i^2 A) F - B A (\nabla_i^2 F)$$

$$- 2 (\bar{\nabla}_i B)(\bar{\nabla}_i A) F - 2 B (\vec{\nabla}_i A)(\vec{\nabla}_i F) - 2 (\bar{\nabla}_i B) A (\bar{\nabla}_i F)$$

$$+ B (\nabla_i^2 A) F + 2 B (\bar{\nabla}_i A)(\bar{\nabla}_i F) + B A (\nabla_i^2 F) \Big\}$$

$$= -\frac{\hbar^2}{4m} \sum_i -2 (\bar{\nabla}_i B)(\bar{\nabla}_i A) F$$

$$\frac{1}{2}\left[A, [T, B]\right] F = \frac{\hbar^2}{2m} \sum_i (\bar{\nabla}_i B)(\bar{\nabla}_i A) F$$

taking: $A = \rho_q^{+} = \sum_j e^{-i\bar{q}\bar{r}_j}$ $\qquad \vec{\nabla}_i \rho_q^{+} = -i\bar{q}\, e^{-i\bar{q}\bar{r}_i}$

$\rho_q = \sum_k e^{i\bar{q}\bar{r}_k}$ $\qquad \vec{\nabla}_i \rho_q = i\vec{q}\, e^{i\bar{q}\bar{r}_i}$

$$m_1 = \frac{1}{2} \langle 0 | \left[\rho_q^{+}, [H, \rho_q]\right] | 0 \rangle =$$

$$= \frac{\hbar^2}{2m} \sum_i \frac{\langle 0 | (i\vec{q})(-i\vec{q})\, e^{i\bar{q}\bar{r}_i}\, e^{-i\bar{q}\bar{r}_i} | 0 \rangle}{\langle 0 | 0 \rangle}$$

$$= \frac{1}{\;} N \frac{\hbar^2 q^2}{\;} = \frac{\hbar^2 q^2}{2m} \quad !$$

Sum-rules ?

$$S^{1ph}(q,\omega) = S(q)\ \delta\left(E - \frac{\hbar^2 q^2}{2m\,S(q)}\right)$$

$$\int_0^\infty S(q,E)\,dE = S(q) \quad \text{ok!}$$

$$\int_0^\infty S(q,E)\,E\,dE = S(q)\ \frac{\hbar^2 q^2}{2m\,\cancel{S(q)}} = \frac{\hbar^2 q^2}{2m} \quad \text{ok!}$$

In general, if the sum rule is exhausted by <u>one</u> energy then:

$$S(q,E) = Z_q\,\delta(E - E_q)$$

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

$$m_1 = \int_0^\infty S(q,E)\,E\,dE = \frac{q^2}{2m} = Z_q\,E_q$$

$$E_q = \frac{m_1}{m_0} = \frac{\frac{q^2}{2m}}{S(q)} = \frac{q^2}{2m\,S(q)}$$