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

(3 - 14 September 2001)

MICROSCOPIC CALCULATION OF THE EXCITATION SPECTRUM OF A ^{3}He IMPURITY IN LIQUID ^{4}He
PART III

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"MICROSCOPIC CALCULATION OF THE EXCITATION SPECTRUM OF A ^3He IMPURITY IN LIQUID ^4He"

- The impurity problem (^3He-impurity in liquid ^4He) is crucial to understand ^3He - ^4He mixtures.
- ^4He (boson) and ^3He (fermion) remain liquids at $T=0$.
- They mix forming a quantum liquid where coexist both types of statistics $\Rightarrow$ very interesting excitation spectrum!
- The maximum solubility of ^3He in ^4He is $X^m \simeq 6'6\%$ at zero pressure. As the concentrations are small $\Rightarrow$ Interesting to study the limit of zero concentration!

STATIC PROPERTIES: Chemical potential, Structure function, excess volume

EXCITATION SPECTRUM: Effective mass

"Late developments in the microscopic study of Helium liquids"

One ^3He impurity in liquid ^4He at $T=0$ is used as a prototype system to report on the late developments of several microscopic many-body theories:

* **CBFT** (Correlated Basis function Theory)
  "^3He impurity excitation spectrum in liquid ^4He"
  A. Fabrocini & A. Polls ; Phys. Rev. B58 (1998) 5209

* Equations of motion of time dependent correlation
  "Single-particle and Fermi-liquid properties of ^3He-^4He mixtures: A microscopic analysis", E. Krotscheck et al; Phys. Rev. B58 (1998) 1228?

* Shadow Wave Functions & Variational Monte Carl
  "Variational calculation of excited state properties of a ^3He impurity in superfluid ^4He"
  D. E. Galli, G. L. Masserini, L. Reatto; Phys. Rev. B (1999)

* DMC (Diffusion Monte Carlo)
  "Quantum Monte Carlo study of static properties of one ^3He atom in superfluid ^4He"
  J. Boronat, J. Casulleras, Phys. Rev. B 59 (1999) 8844

IMPURITY

Hamiltonian:

$$H(N+1) = H_4(N) + H_I(N+1) =$$

$$= -\frac{\hbar^2}{2m_4}\sum_i \nabla_i^2 + \sum_{i<j}^{N} v(r_{ij}) - \frac{\hbar^2}{2m_I}\nabla_I^2 + \sum_{j=1}^{N} v(r_{Ij})$$

Wave function: Ground-state

$$\Psi(\bar{r}_1 \dots \bar{r}_N, \bar{r}_I) = F_J \; F_T$$

$$F_J = \prod_{i<j}^{N} e^{-u_{ij}/2} \prod_{i=1}^{N} e^{-u_{iI}/2}$$

$$F_T = \prod_{i<j<k}^{N} e^{-q_{ijk}/2} \prod_{i<j}^{N} e^{-q_{ijI}/2}$$

$$q_{ijk} = \sum_{cyc} \xi(r_{ij})\,\xi(r_{ik})\;\hat{r}_{ij}\,\hat{r}_{ik}$$

We want to calculate : μ_I

$$\mu_I(\rho) = \frac{\langle \Psi(N+1) | H(N+1) | \Psi(N+1) \rangle}{\langle \Psi(N+1) | \Psi(N+1) \rangle} - \frac{\langle \Psi(N) | H(N) | \Psi(N) \rangle}{\langle \Psi(N) | \Psi(N) \rangle}$$

- Both quantities of order N
- μ_I is of order 1. Big cancellations!

$$\mu_I^{exp}(\rho_0) = -2.785 \text{ K}$$

$$E^V(A+1) = E_4^V(A) + \mu_I^V$$

$E_4^V(A)$ (term of order A). Energy of the medium.
Will be cancelled.

μ_I^V : (order of unity). Chemical potential of the impurity

Using Jackson-Feenberg identity for T:

$$\frac{E_4^V}{A} = \frac{\rho}{2}\int d\bar{r}_{12}\, g_{2,12}\left(v_{12} + \frac{\hbar^2}{4m_4}\nabla^2 u_{12}\right) +$$

$$+ \frac{\hbar^2}{16 m_4}\rho^2 \int d\bar{r}_{12}\, d\bar{r}_{13}\, g_{3,123}\, \nabla_1^2 q_{123} \equiv v(\rho) + t^{(2)}(\rho) + t^{(3)}(\rho)$$

$$\underline{\mu_I^V(\rho) = e_i(\rho) + e_r(\rho)}$$

$$e_r(\rho) = \frac{\rho^2}{2}\int d\bar{r}_{12}\, g^r_{2,12}\left(v_{12} + \frac{\hbar^2}{4m_4}\nabla^2 u_{12}\right) + \frac{\hbar^2}{16 m_4}\rho^3 \int d\bar{r}_{12}\, d\bar{r}_{13}\, g^r_{3,123}\, \nabla_1^2 q_{123}$$

$$e_i(\rho) = \rho \int d\bar{r}_{I1}\, g_{2,I1}\left(v_{I1} + \frac{\hbar^2}{4\mu_2}\nabla^2 u_{I1}\right) + \frac{\hbar^2}{8\mu_3}\rho^2 \int d\bar{r}_{I1}\, d\bar{r}_{I2}\, g_{3,I12}\, \nabla_I^2 q_{I12}$$

$$\frac{1}{\mu_2} = \frac{1}{2}\left(\frac{1}{m_4} + \frac{1}{m_I}\right) \qquad \frac{1}{\mu_3} = \frac{1}{2}\left(\frac{2}{m_4} + \frac{1}{m_I}\right)$$

$\boxed{\text{A.C.A.}}$

$$h = f^2 - 1$$

$$\rho \int d^3r\, h(r_{1j})\, h(r_{2j})$$

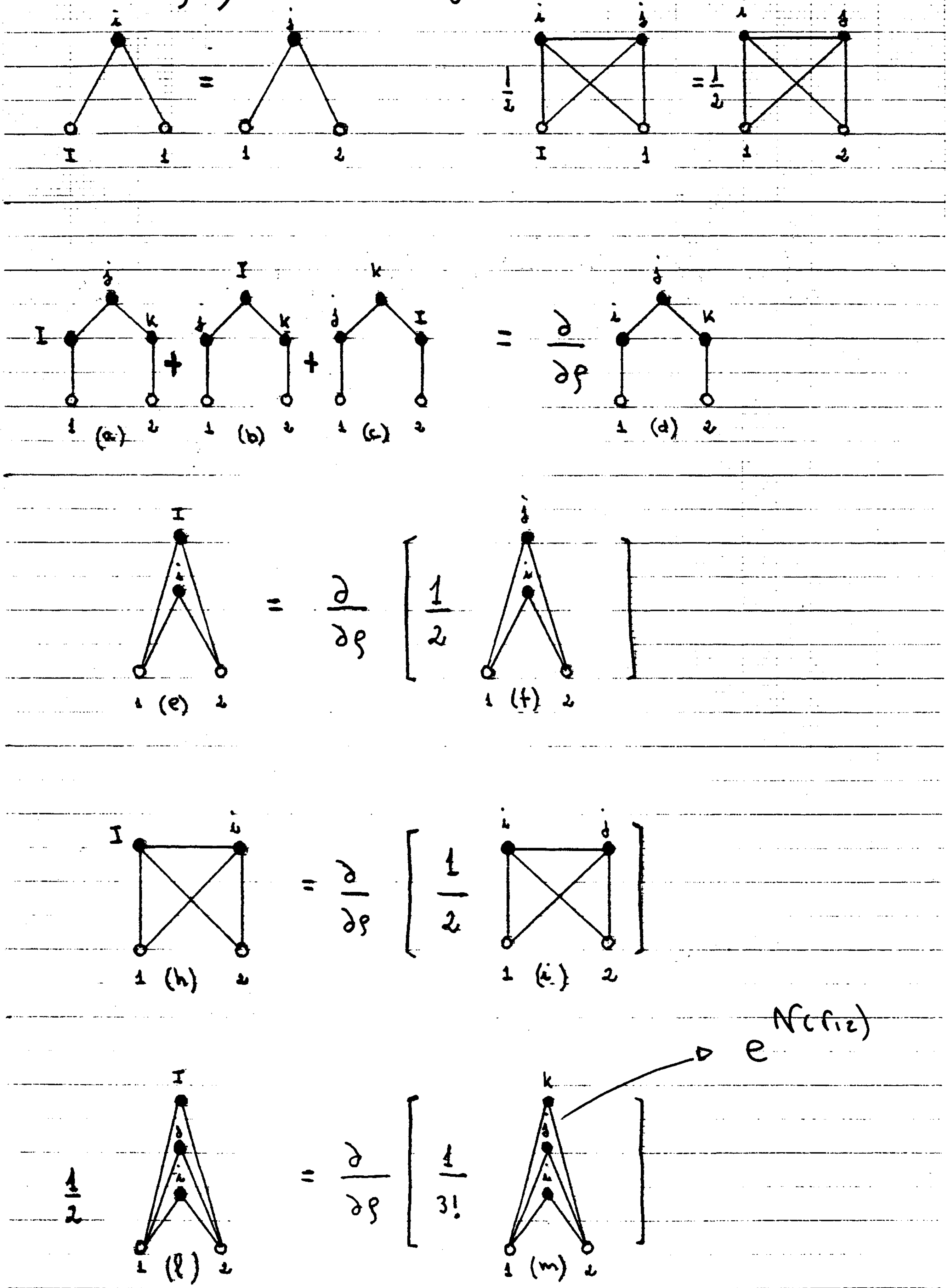


Fig. 1.

DISTRIBUTION FUNCTIONS:

$$g^{(4)}_{n,12\ldots n} + \frac{1}{\Omega}\, g^{r}_{n,12\ldots n} = \frac{A(A-1)\ldots(A-n+1)}{\rho^{n}} \; \frac{\int d\Omega_{12\ldots n}\, |\Psi(A+1)|^2}{\int d\Omega\, |\Psi(A+1)|^2}$$

$$g_{n,I12\ldots n-1} = \frac{\Omega\, A(A-1)\ldots(A-n+2)}{\rho^{n-1}} \; \frac{\int d\Omega_{I12\ldots n-1}\, |\Psi(A+1)|^2}{\int d\Omega\, |\Psi(A+1)|^2}$$

$$g^{r}_{n,12\ldots n} = \left.\frac{\partial}{\partial \rho_I}\, g_{n,12\ldots n}\right)_{\rho_I = 0}$$

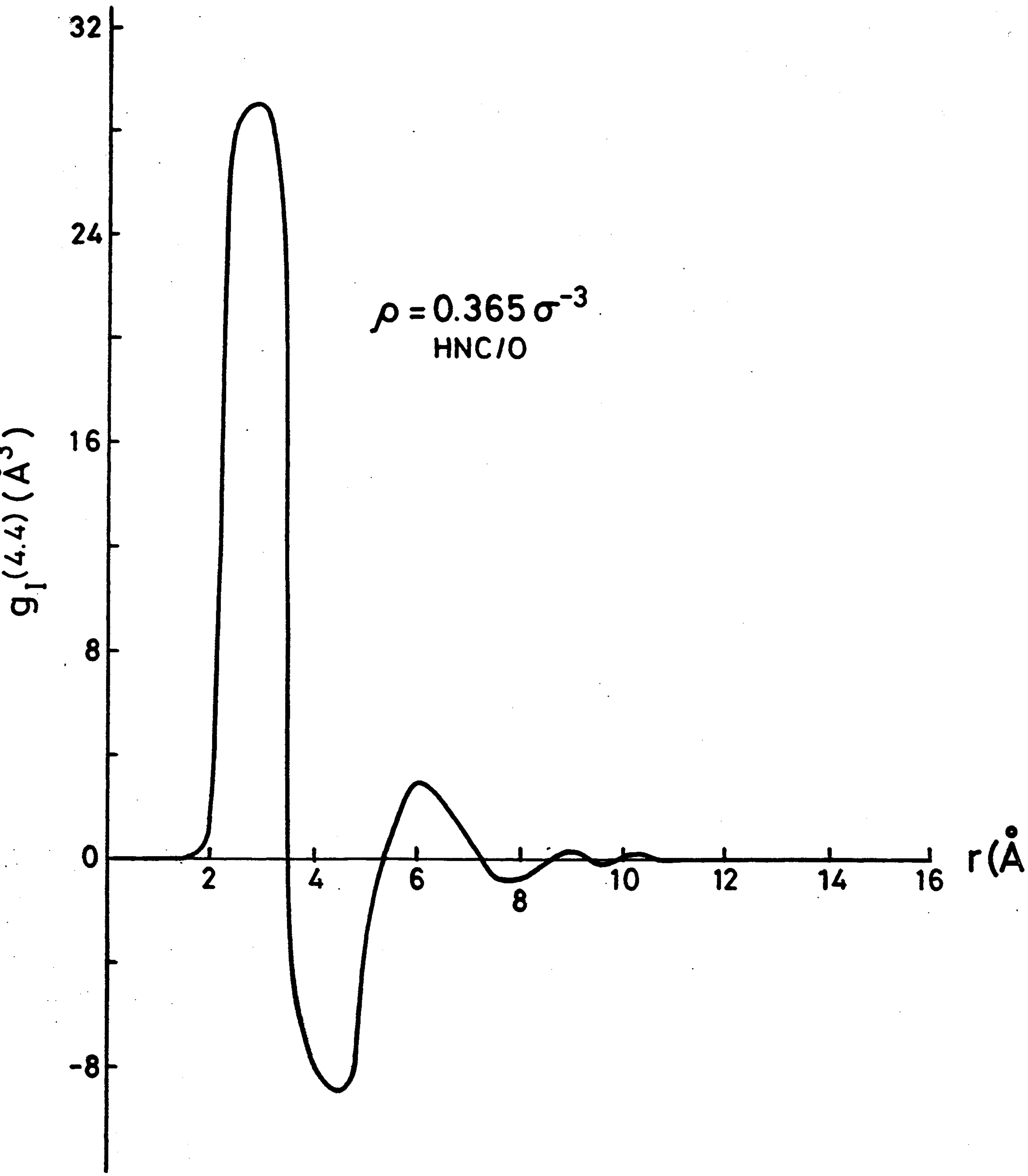
$$g_{2,I1} = \frac{A\cdot}{\rho\,\frac{1}{\Omega}} \; \frac{\int d\Omega_{I1}\, |\Psi(A+1)|^2}{\int d\Omega\, |\Psi(A+1)|^2}$$

AVERAGE CORRELATION APPROXIMATION

As $V_{44} \equiv V_{43}$ $\Rightarrow$ good approximation $\Rightarrow$ $u_{ij} \equiv u_{iI}$, $q_{ijk} \equiv q_{Ijk}$

$$g_{n,I23\ldots n-1}(\rho) = g^{4}_{n,12\ldots n}(\rho)$$

$$g^{r}_{\ldots 12\ldots n}(\rho) = \frac{\partial g^{(4)}_{n,12\ldots n}(\rho)}{\partial \rho}$$



⑦

$$\boxed{e_I(\rho) = 2e(\rho) + \left(\frac{m_4}{m_I} - 1\right) t^{(2)}(\rho) + \frac{m_4}{m_I} t^{(3)}(\rho)}$$

to get $e_r(\rho)$:

$$\frac{P(\rho)}{\rho} = e(\rho) - t^{(3)}(\rho) + \frac{\rho^2}{2} \int d^3r \, \frac{\partial g_2^{(4)}(\rho, r)}{\partial \rho} \left(v(r) + \frac{\hbar^2}{4m} \nabla^2 u_{12} \right) +$$

$$+ \frac{\hbar^2}{16m} \rho^3 \int d^3r_{12} \, d^3r_{13} \, \frac{\partial g_3^{(4)}(\rho, r_{12}, r_{13})}{\partial \rho} \nabla_1^2 q_{123}$$

$$\Rightarrow \boxed{e_r(\rho) = \frac{P(\rho)}{\rho} - e(\rho) + t^{(3)}(\rho)}$$

$$\mu_I(\rho) = e_r(\rho) + e_I(\rho) = \mu_4(\rho) + \left(\frac{m_4}{m_I} - 1\right) t(\rho)$$

$$t(\rho) = t^{(2)}(\rho) + t^{(3)}(\rho)$$

$$\mu_4(\rho) = e(\rho) + \frac{P(\rho)}{\rho}.$$

Baym's formula!

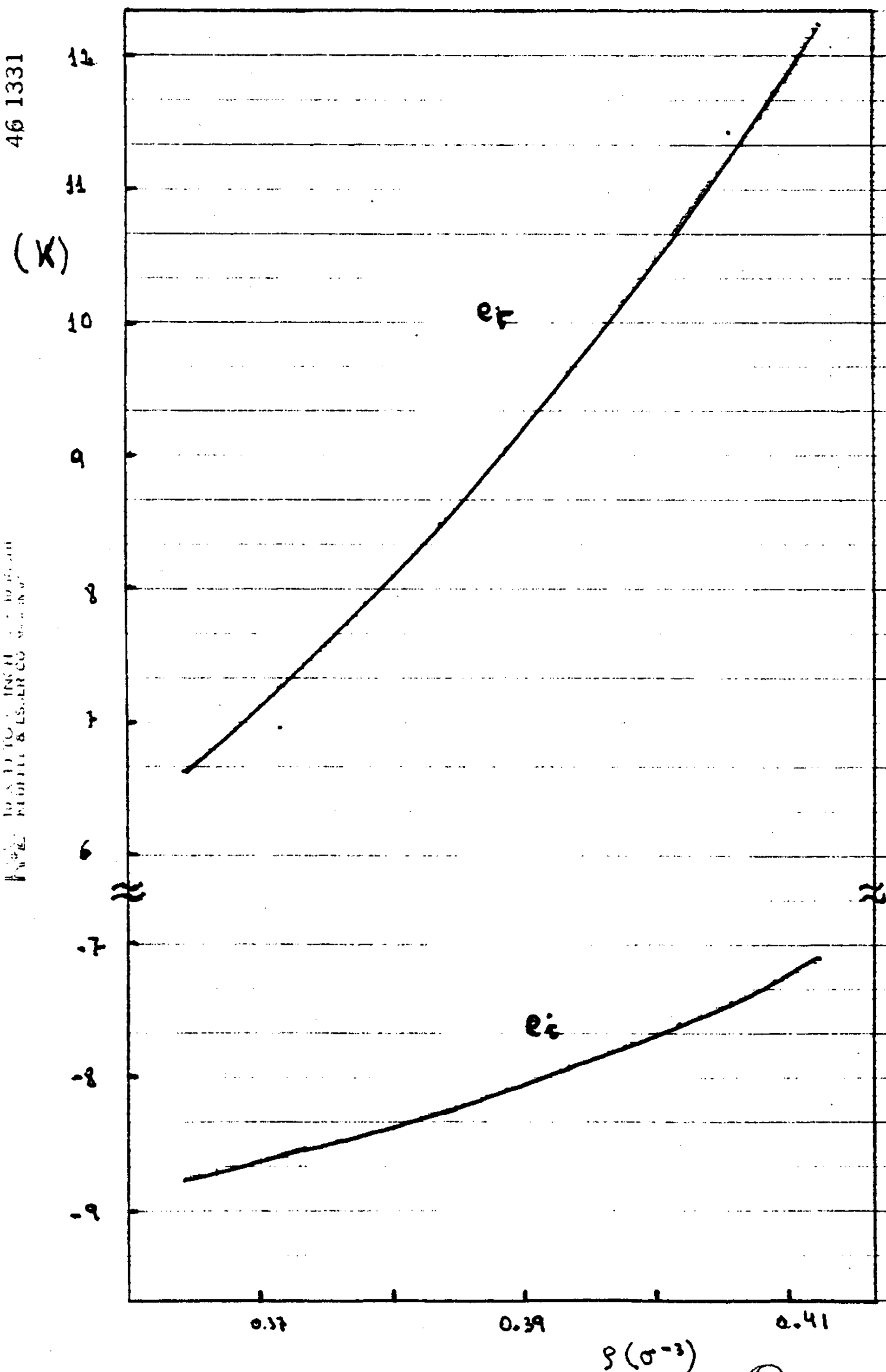
<u>Baym results</u>.

$t(\rho) = 14.16$ McMillan. (Montecarlo calculation) L.J.
twobody correlation

With $t\_(\rho) \Rightarrow \boxed{\mu_I = -[illegible]}$
[illegible] with three-body correlations L.J, $\boxed{t(\rho) = 13.52 \Rightarrow u_I \simeq [illegible]}$

Renormalization and interaction pieces of μ_I.

Calculated in HNC/ST. Lennard-Jones.



P=0	ρ	e_r	e_i
HNC/S	0.330	5.82	-7.69
HNC/ST	0.364	6.63	-8.76

A. C. A. Average Correlation Approximation.

$$\mu_I^{ACA}(\rho) = \frac{m_4}{m_I}\, e(\rho) + \left(1 - \frac{m_4}{m_I}\right) V(\rho) + \frac{P(\rho)}{\rho}$$

valid for n-body correlations.

Equivalent to Baym's phormula:

$$H(N+1) = H_4(N+1) + \underbrace{H(N+1) - H_4(N+1)}_{\left(\frac{m_4}{m_I} - 1\right) \frac{\nabla_I^2}{2m_4}}$$

$$\mu_I = \frac{\langle \Psi(N+1) | H(N+1) | \Psi(N+1) \rangle}{\langle \Psi(N+1) | \Psi(N+1) \rangle} - \frac{\langle \Psi(N) | H(N) | \Psi(N) \rangle}{\langle \Psi(N) | \Psi(N) \rangle} =$$

$$= \mu_4 + t_4(\rho) \left(\frac{m_4}{m_I} - 1\right)$$

$$\boxed{\mu_I^{ACA} = \underbrace{e(\rho) + \frac{P(\rho)}{\rho}}_{\mu_4(\rho)} + t_4(\rho) \left(\frac{m_4}{m_I} - 1\right)}$$

Taking DMC values, (J. Boronat & J. Casulleras PRB 59 (1999) 8844)

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

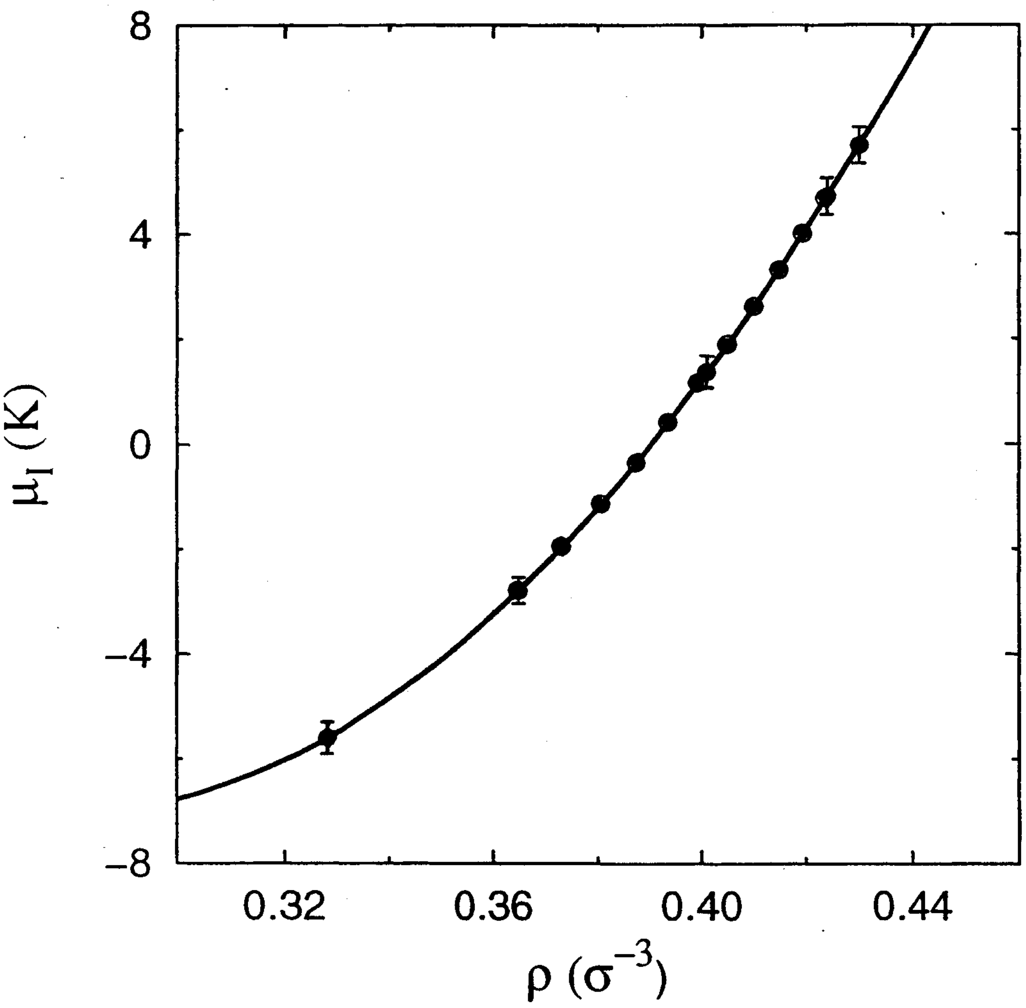
P (atm)	μ_4 (K)	μ_I^{ACA} (K)	$t_4(\rho)$ (K)
0	-7.27	-2.58	14.32
		↓	
		-2.79	

-2.79 { DMC value allowing different correlation

$$\boxed{\text{Remember! } \mu_I^{exp} = -2.785\ K}$$

FIG. 5. Chemical potential of the ^{3}He impurity as a function of the density (full circles). The solid line is a polynomial fit to the DMC results. The open circles are experimental data from Ref. 1.

J. Boronat & J. Casulleras
PRB 59 (1999) 8844



● Experimental results

DMC results

The ^3He impurity as a probe in liquid ^4He

$$\left.\begin{aligned}\frac{\langle\Psi(N+1)\,|\,H(N+1)\,|\,\Psi(N+1)\rangle}{\langle\Psi(N+1)\,|\,\Psi(N+1)\rangle} &= E(N+1)\\ \frac{\langle\Psi(N)\,|\,H(N)\,|\,\Psi(N)\rangle}{\langle\Psi(N)\,|\,\Psi(N)\rangle} &= E(N)\end{aligned}\right\}\quad \mu_I(\rho) = E(N+1) - E(N)$$

in general μ_I is not an upperbound, but if $E(N)$ is the exact energy of the ground-state then $\mu_I(\rho)$ is an upper-bound.

<u>In A.C.A.</u>

$$\mu_I^{A.C.A}(\rho) = \mu_4^{exp}(\rho) + \left(\frac{m_4}{m_I} - 1\right) t_4^{exp}(\rho)$$

$$\mu_I^{A.C.A}(\rho) > \mu_I^{exp}(\rho) \Rightarrow \mu_I^{A.C.A} - \mu_I^{exp} \geq 0$$

$$\boxed{t_4^{exp}(\rho) \geq \left(\frac{m_4}{m_I} - 1\right)^{-1} \left(\mu_I^{exp}(\rho) - \mu_4^{exp}(\rho)\right)}$$

LOWER-BOUND

$$\boxed{\langle V\rangle_{exp} \leq e_{exp} - \langle t\rangle_{LB}} \qquad \frac{m_4}{m_3} = 1.3273$$

Upper-bound

At saturation density: $\rho = 0.3648\,\sigma^{-3}$

$$\mu_4^{exp}(\rho) = e_4^{exp} = -7.17\ K \qquad \mu_I^{exp} = -2.785$$

$$t_4^{LB}(\rho_0) = 13.4\ K$$

$$V^{UB}(\rho_0) = -20.6\ K$$

One ^4He atom in liquid ^3He.

* No mixture.

$\cancel{e_4} = -7.17K$

$\mu_3^{exp} = -2.47$ K

$\mu_4^{exp} \approx -6.6$ K

Lahuerte
J. Low temp. Phys.
12 (1973) 127

1) $\mu_4(\rho) = \mu_3(\rho) + \left(\frac{m_3}{m_4} - 1\right) t(\rho)$

$$\simeq -2.47 - \underbrace{0.24648}_{1/4} \cdot \underset{UFP}{11.85} = -5.39 \text{ K}$$

2) as $m_I > m$ I get an upperbound

$$t_3(\rho) \leq \left|\frac{m_3}{m_4} - 1\right|^{-1} \left(\mu_3^{exp} - \mu_4^{exp}\right) \simeq 16.7[illegible]$$

$t^{UC}(\rho^{ex.}) \simeq 16.78$

$V^{LB}(\rho) \simeq -19.26$

→ The quality of the wave function is worse.

⇒ T_F is a lower bound

$\rho_0 = 0.[illegible]47\ \sigma^{-3}$

$\Rightarrow \langle V \rangle^{U.C} \simeq -[illegible]7K$

$\langle T_F \rangle = 3$ K

$\Big\}$ not useful

Excitation spectrum of one ^{3}He impurity and the effective mass.

Variational approach

$$\Psi_v(\vec{k}) = \rho_I(\vec{k})\, \Psi_0(A+1)$$

$$\boxed{\rho_I(\vec{k}) = e^{i\vec{k}\vec{r}_I}}$$

$$E_k = \frac{\langle \Psi_v(\vec{k}) \,|\, H(A+1) \,|\, \Psi_v(\vec{k}) \rangle}{\langle \Psi_v(\vec{k}) \,|\, \Psi_v(\vec{k}) \rangle} =$$

$$= \frac{\langle \Psi_0(A+1) \,|\, \rho_I^+ \rho_I \, H(A+1) \,|\, \Psi_0(A+1) \rangle}{\langle \Psi_0(A+1) \,|\, \Psi_0(A+1) \rangle} +$$

$$\frac{\langle \Psi_0(A+1) \,|\, \rho_I^+ \,[H, \rho_I]\, |\, \Psi_0(A+1) \rangle}{\langle \Psi_0(A+1) \,|\, \Psi_0(A+1) \rangle} =$$

$$= E_0(A+1) + \frac{\hbar^2 k^2}{2 m_I}$$

$$\boxed{\frac{m_I^*}{m_I} = 1 \quad \text{k-independent}}$$

$$\boxed{\frac{m_I}{m_I^*} = \frac{m_I}{\hbar^2} \frac{1}{k} \frac{\partial e(k)}{\partial (k)}}$$

LP: $\frac{\hbar^2 k^2}{2 m_I^*}$ $\qquad$ MLP: $\frac{\hbar^2 k^2}{2 m_I^*} \frac{1}{1 + b k^2}$

$\downarrow$

At $k=0$, Krotscheck et al. PRL 80 (1998) 4709 $\Rightarrow$ $m_I^* \simeq 2.18\, m$

Adding back-flow correlations

$$\Psi_v(\vec{k}) = \rho_I(\vec{k})\; F_B\; \Psi_0(A+1)$$

$$F_B(\vec{k}, A+1) = \prod_{i=1} \exp\left\{ i\,\vec{k}\,(\bar{r}_i - \bar{r}_I)\,\eta(r_{Ii}) \right\}$$

$$\eta(r) = A_0 \exp\left\{ -\left[\frac{(r-r_0)}{w_0} \right]^2 \right\}$$

A_0 variational paremeter, $r_0 = 0.8\,\sigma$, $w_0 = 0.44\,\sigma$

$$E_v(\vec{k}) = \frac{\langle \Psi_0(A+1) \,|\, F_B^+ \rho_I^+ \rho_I F_B\; H(A+1) \,|\, \Psi_0(A+1) \rangle}{\langle \Psi_0(A+1) \,|\, \Psi_0(A+1) \rangle} + $$

$$+ \frac{\langle \Psi_0 \,|\, F_B^+ \rho_I^+ \left[H, \rho_I F_B \right] \,|\, \Psi_0 \rangle}{\langle \Psi_0 \,|\, \Psi_0 \rangle}$$

$$\boxed{E_v(\vec{k}) = E_0(A+1) + \frac{\hbar^2 k^2}{2 m_I} \left[1 + e_2 + \frac{m_I}{\mu_2} e_m + e_3 \right]}$$

$$e_2 = \rho \int d r_{I1}\; g^{(2)}_{I1} \left(2\,\eta_{I1} + \frac{2}{3}\, r_{I1}\, \eta'_{I1} \right)$$

$$e_m = \rho \int d r_{I1}\; g^{(2)}_{I1} \left(\eta^2_{I1} + \frac{1}{3} \left[r^2_{I1} (\eta'_{I1})^2 + 2\, \eta_{I1}\, r_{I1}\, \eta'_{I1} \right] \right)$$

$$e_3 = \rho^2 \int d r_{I1}\, d r_{I2}\; g^{(3)}_{I12} \left\{ \eta_{I1}\, \eta_{I2} + \frac{1}{3} \left[r_{I1}\, \eta'_{I1}\, \eta'_{I2}\, r_{I2} \right.\right.$$

$$\left.\left. (\hat{r}_{I1}\, \hat{r}_{IK})^2 + 2\, \eta_{I1}\, \eta'_{I2}\, r_{I2} \right] \right\}$$

$\mu_2 = \dfrac{m_I\, m_4}{m_I + m_4}$ reduced mass

$$\frac{m_I^*}{m_I} = \frac{1}{1 + e_2 + \left(\frac{m_I}{\mu}\right) e_m + e_3}$$

At $\rho_0 = 0.02185\ \mathring{A}^{-3} = 0.365\ \sigma^{-3}$

Lennard-Jones

$\frac{m_I^*}{m_I}$	J	J+T
CA	1.45	1.44
KSA	1.46	1.44
HNC/S	1.48	1.46

Back-flow correlations are not enough !

- The spectrum is parabolic ⇒

  The effective mass is k-independent

- Back-flow correlations do not bring any correction to the binding energy of the impurity

PERTURBATION THEORY

$$\rho_I(K) = e^{i\bar{k}\bar{r}_I}$$
$$\rho(q) = \sum_{i=1}^{A} e^{i\bar{q}\bar{r}_i}$$

Basis: $|\bar{k}\rangle = \rho_I(\bar{k})\,|0\rangle$

$$|\bar{k}-\bar{q}\,;\bar{q}\rangle = \rho_I(\bar{k}-\bar{q})\,\rho(\bar{q})\,|0\rangle$$

$$|\bar{k}-\bar{q}_1-\bar{q}_2\,;\bar{q}_1,\bar{q}_2\rangle = \rho_I(\bar{k}-\bar{q}_1-\bar{q}_2)\,\rho(\bar{q}_1)\,\rho(\bar{q}_2)\,|0\rangle$$

* Hope: low order will be enough!

NON ORTHOGONAL. $\boxed{\text{CBF}}$

Correlated Basis Function

HAMILTONIAN:

Unperturbed: $$H_{0,ij} = \delta_{ij}\,\frac{\langle\Psi_i|H|\Psi_i\rangle}{\langle\Psi_i|\Psi_i\rangle} = \delta_{ij}\,E_i^v$$

Interaction: $$H_{I,ij} = (1-\delta_{ij})\,\frac{\langle\Psi_i|H-E_K|\Psi_j\rangle}{(\langle\Psi_i|\Psi_i\rangle\langle\Psi_j|\Psi_j\rangle)^{1/2}}$$

$$= (1-\delta_{ij})\,(H_{ij} - E_K N_{ij})$$

where $E_K = E_0 + \varepsilon_K$ is the eigenvalue of H for the eingenstate $|\Psi(\vec{k})\rangle$

BRILLOUIN - WIGNER series:

$$\Delta E_K = \sum_{j\neq k}\frac{(H_{kj}-E_K N_{kj})(H_{jk}-E_K N_{jk})}{E_K - E_j^v} +$$

$$+\sum_{\substack{j,i\neq k\\ i\neq j}}\frac{(H_{kj}-E_K N_{kj})(H_{ji}-E_K N_{ji})(H_{ik}-E_K N_{ik})}{(E_K-E_j^v)(E_K-E_i^v)} + \dots$$

ORTHOGONALIZATION $\qquad$ 1 phonon space.

$$|\bar{k}\rangle = \rho_I(k)\,|0\rangle$$

$$|\bar{k}-\bar{q},\bar{q}\rangle = \frac{1}{A^{1/2}\,S(q)^{1/2}}\left\{|k-q;q) - |\bar{k}\rangle\langle\bar{k}|\bar{k}-\bar{q},\bar{q})\right\}$$

$$|\bar{k}-\bar{q};\bar{q}) = \rho_I(\bar{k}-\bar{q})\,\rho(\bar{q})\,|0\rangle$$

Overlaps

$$\langle\bar{k}|\bar{k}\rangle = 1 \qquad \langle\bar{k}|\bar{k}-\bar{q},\bar{q}\rangle = 0$$

$$\langle\bar{k}-\bar{q};\bar{q}|\bar{k}-\bar{q};\bar{q}\rangle = 1$$

Hamiltonian

$$\langle\bar{k}|H(A+1)|\bar{k}\rangle = E(A+1) + \frac{\hbar^2k^2}{2m_I}$$

$$\langle\bar{k}-\bar{q};\bar{q}|H(A+1)|\bar{k}-\bar{q};\bar{q}\rangle = E(A+1) + \frac{\hbar^2q^2}{2mS(q)} + \frac{\hbar^2(\bar{k}-\bar{q})^2}{2m_I}$$

$$\langle\bar{k}|H(A+1)|\bar{k}-\bar{q};\bar{q}\rangle = -\frac{\hbar^2}{2m_I}\,\bar{k}\cdot\bar{q}\;\frac{S_I(q)}{A^{1/2}\,S(q)^{1/2}}$$

$$\frac{\langle\Psi(A+1)|\rho^*(q)\,\rho(q)|\Psi(A+1)\rangle}{\langle\Psi(A+1)|\Psi(A+1)\rangle} = \frac{\langle\Psi(A+1)|A+\sum_{i\neq j}e^{i\bar{q}(\bar{r}_i-\bar{r}_j)}|\Psi(A+1)\rangle}{\langle\Psi(A+1)|\Psi(A+1)\rangle}$$

$$= A + A(A-1)\frac{\langle\Psi(A+1)|e^{i\bar{q}(\bar{r}_2-\bar{r}_1)}|\Psi(A+1)\rangle}{\langle\Psi(A+1)|\Psi(A+1)\rangle} =$$

$$= A + \rho^2\int d\bar{r}_1\,d\bar{r}_2\;e^{i\bar{q}(\bar{r}_1-\bar{r}_2)}\;\frac{A(A-1)}{\rho^2}\;\frac{\int d\Omega_{12}\,\Psi^*(A+1)\,\Psi(A+1)}{\int d\Omega\,\Psi^*\,\Psi}$$

$$= A\cdot S(q) + O(1)$$

$$\langle \bar{k} | \bar{k}-\bar{q}, \bar{q}) = \langle 0 | \rho^{I}_{-\bar{k}} \; \rho^{I}_{\bar{k}-\bar{q}} \; \rho_{\bar{q}} | 0 \rangle =$$

$$= \frac{\langle \Psi(A+1) | \cancel{e^{-i\bar{k}\bar{r}_I}} \; \cancel{e^{i\bar{k}\bar{r}_I}} \; e^{-i\bar{q}\bar{r}_I} \sum_{i=1}^{A} e^{i\bar{q}\bar{r}_i} | \Psi(A+1) \rangle}{\langle \Psi(A+1) | \Psi(A+1) \rangle} =$$

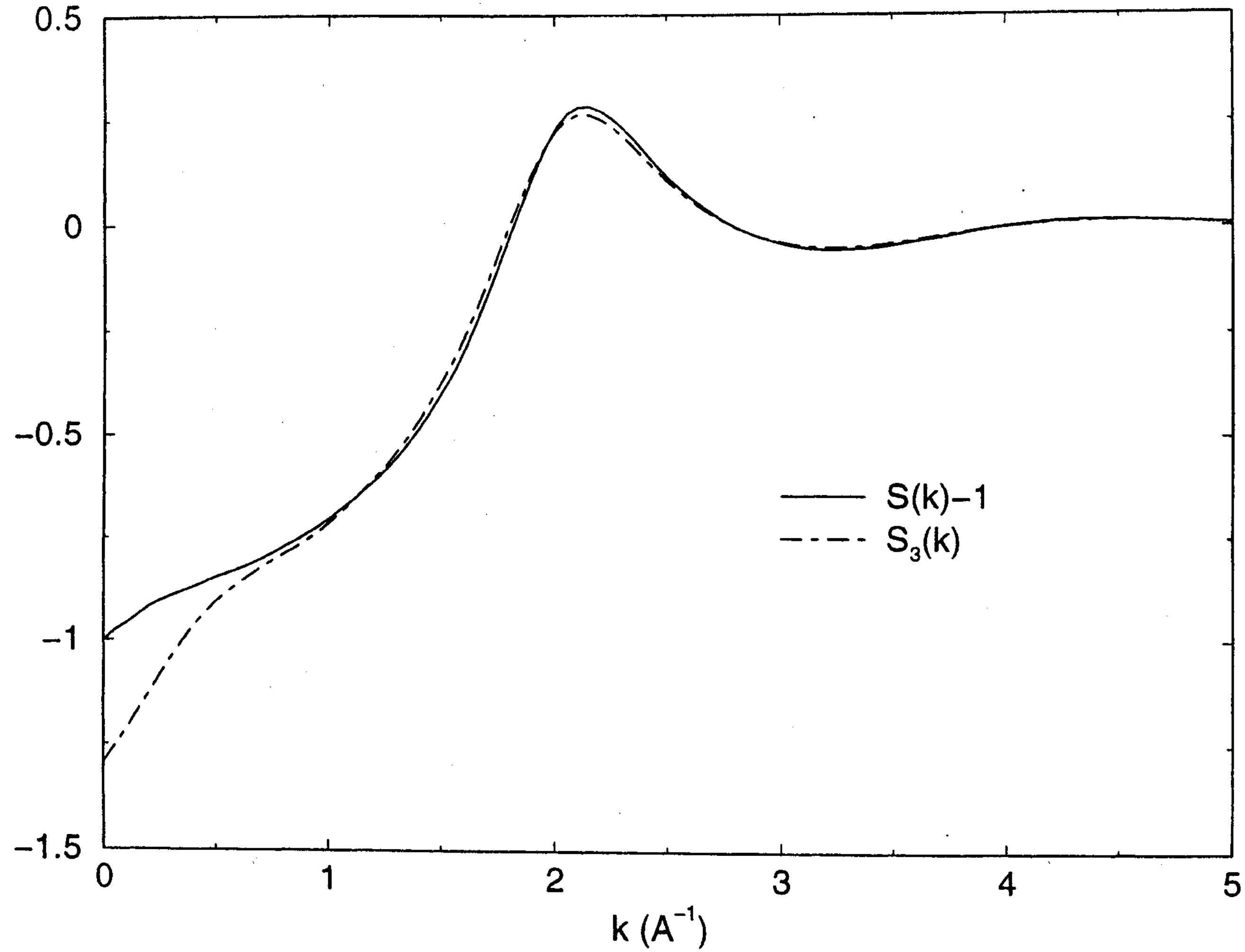
$$= A \; \frac{\langle \Psi(A+1) | e^{i\bar{q}(\bar{r}_1 - \bar{r}_I)} | \Psi(A+1) \rangle}{\langle \Psi(A+1) | \Psi(A+1) \rangle}$$

$$= \frac{\rho}{\Omega} \int d\bar{r}_1 \, d\bar{r}_I \; e^{i\bar{q}(\bar{r}_1 - \bar{r}_I)} \; \frac{A \cdot \Omega}{\rho} \; \frac{\int d\Omega_{1I} \; \Psi^{*}(A+1) \Psi(A+1)}{\int d\Omega \; \Psi(A+1) \Psi(A+1)}$$

$$= \rho \int d\bar{r}_{1I} \; e^{i\bar{q}\bar{r}_{1I}} \; g(\bar{r}_{1I}) = S_I(q)$$

$$\boxed{\langle \bar{k} | \bar{k}-\bar{q}, \bar{q}) = S_I(q)}$$

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



$$S^{(4,4)}(k) = 1 + \rho \int d\bar{r}\, e^{i\bar{k}\bar{r}} (g(r) - 1)$$

$$S^{(I,4)}(k) = \rho \int d\bar{r}\, e^{i\bar{k}\bar{r}} (g^{(I,4)}(r) - 1)$$

$$S^{(I,4)}(0^+) = -(1+\alpha)$$

$$\alpha = \frac{\vartheta}{\vartheta_4} \quad \text{molar volumes}$$

$$= 0.284$$

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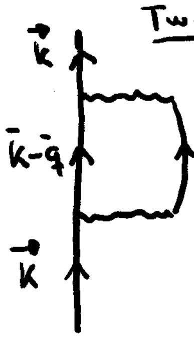
$\boxed{\text{OIP}}$



Two types of diagrams!

$$E(k) = E_0(A+1) + e_0(k) + \Delta e(k)$$

$$e_0(k) = \frac{\hbar^2 k^2}{2m_I}$$

$$\Delta e(k) = \Delta e_{OIP} + \Delta e_{TIP} + \Delta e_{ROP}$$

$$\Delta e_{OIP}(k) = \sum_{\vec{q}} \frac{\left| \langle \vec{k} \,|\, H(A+1) - E(k) \,|\, \vec{k}-\vec{q}, \vec{q} \rangle \right|^2}{\cancel{E_0} + e_0(k) + \Delta_{OIP}(k) - \cancel{E_0} - e_0(|\vec{k}-\vec{q}|) - \omega_F(\ldots}$$

$$= \frac{\Omega}{(2\pi)^3} \int d^3q \; \frac{S_I^2(q)}{A \cdot S(q)} \; \frac{\left(-\frac{\hbar^2}{2m_I}\right)^2 \left(\vec{k}\cdot\vec{q}\right)^2}{\Delta e_{OIP}(k) + \frac{\hbar^2 k^2}{2m_I} - \frac{\hbar^2(\vec{k}-\vec{q})^2}{2m_I} - \frac{\hbar^2 q^2}{2m\,S(q)}}$$

$$\langle \vec{k} \,|H(A+1) - E(k)\,|\, \vec{k}-\vec{q}; \vec{q} \rangle = -\frac{\hbar^2}{2m_I} \, \vec{k}\,\vec{q} \; \frac{S_I(q)}{A^{1/2} S(q)^{1/2}}$$

* We use Brillouin-Wigner $\Rightarrow$ Self-consistent solution in $\Delta e_{OIP}(k)$ at each k.

If we work in one phonon space $\Rightarrow$

* For Δe_{OIP} we need only $S_I(q)$ and $S(q)$!

The m^* at $k=0$ is even simpler:

$$\boxed{\frac{m^*}{m_I} \simeq 1.8}$$

$$\frac{m^*}{m_I} = \frac{1}{1 - \frac{1}{4\pi^2\rho}\,\frac{\hbar^2}{2m_I}\,\frac{2}{3}\int_0^\infty dq \; \frac{q^2 S_I(q)^2}{\frac{S(q)\,\hbar^2}{2m_I} + \frac{\hbar^2}{2m_I}}}$$

The other diagrams are more complicated and require three-body structure functions !

Two common approximations:

* Convolution approx: (CA)

* Kirkwood superposition approx: (KSA)

$$S^{(3)}(\bar{q}_1, \bar{q}_2, \bar{q}_3) = \frac{1}{N_4} \frac{\langle \Psi_0 | \rho_4^+(\bar{q}_1)\, \rho_4^+(\bar{q}_2)\, \rho_4(\bar{q}_3) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

with $\bar{q}_3 = \bar{q}_1 + \bar{q}_2$

$$S^{(3)}_{CA}(\bar{q}_1, \bar{q}_2, \bar{q}_3) = S(q_1)\, S(q_2)\, S(q_3)$$

factorizes in momentum space

SA factorizes in r-space

$$g^{(3)}_{KSA}(\bar{r}_1, \bar{r}_2, \bar{r}_3) = g^{(2)}(r_{12})\, g^{(2)}(r_{13})\, g^{(2)}(r_{23})$$

* Sensitivity of the calculation to the approximation used for $S^{(3)}$!

* The two phonon states $|\bar{k}-\bar{q}_1-\bar{q}_2 ; \bar{q}_1 \bar{q}_2\rangle$ have been orthogonalized to: $|\bar{k}\rangle$

$|\bar{k}-\bar{q}_1-\bar{q}_2 ; \bar{q}_1+\bar{q}_2\rangle$

$|\bar{k}-\bar{q}_1, \bar{q}_1\rangle$

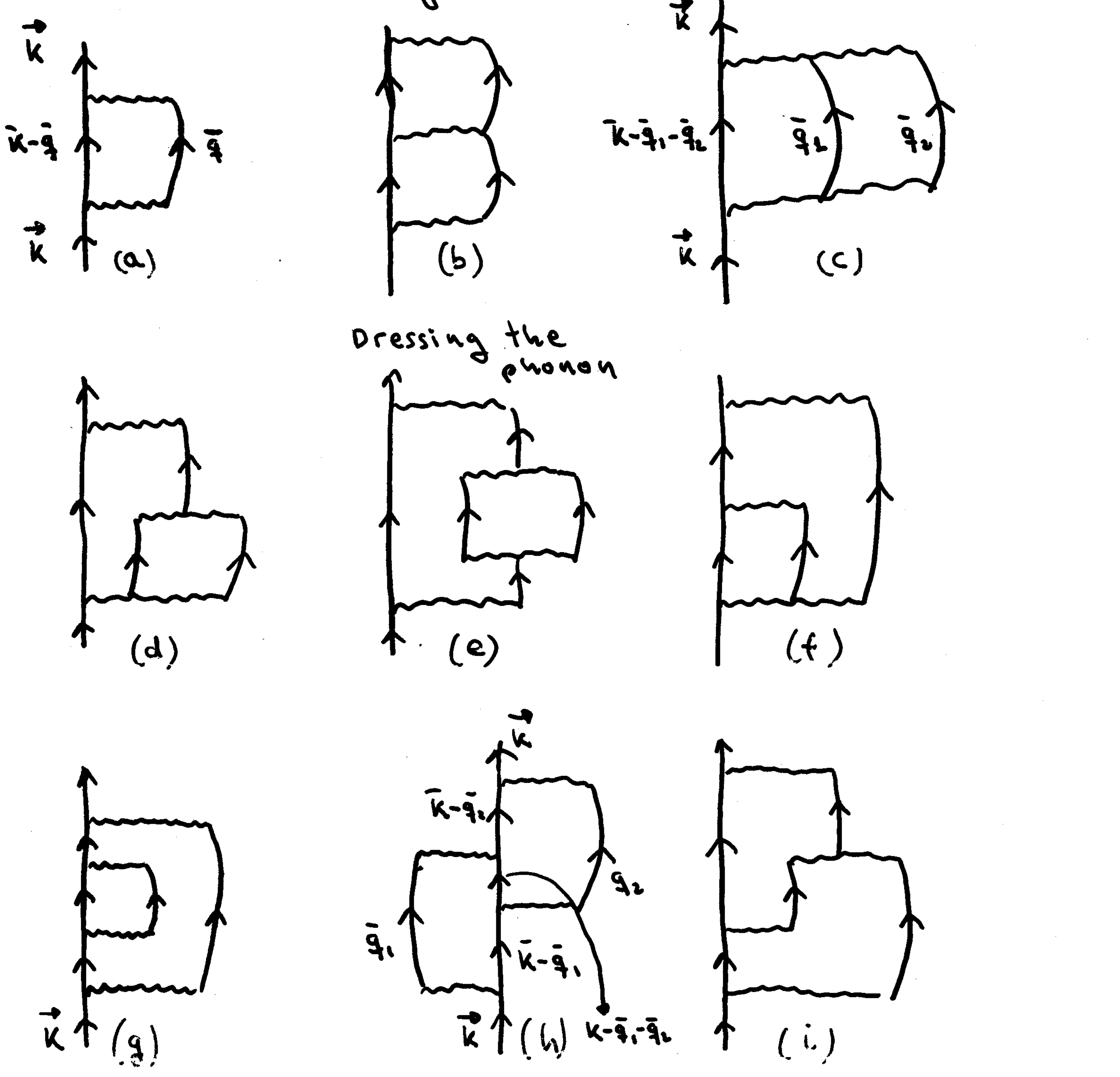
$|\bar{k}-\bar{q}_2, \bar{q}_2\rangle$

All OIP (one independent phonon) and

TIP (two independent phonons)!

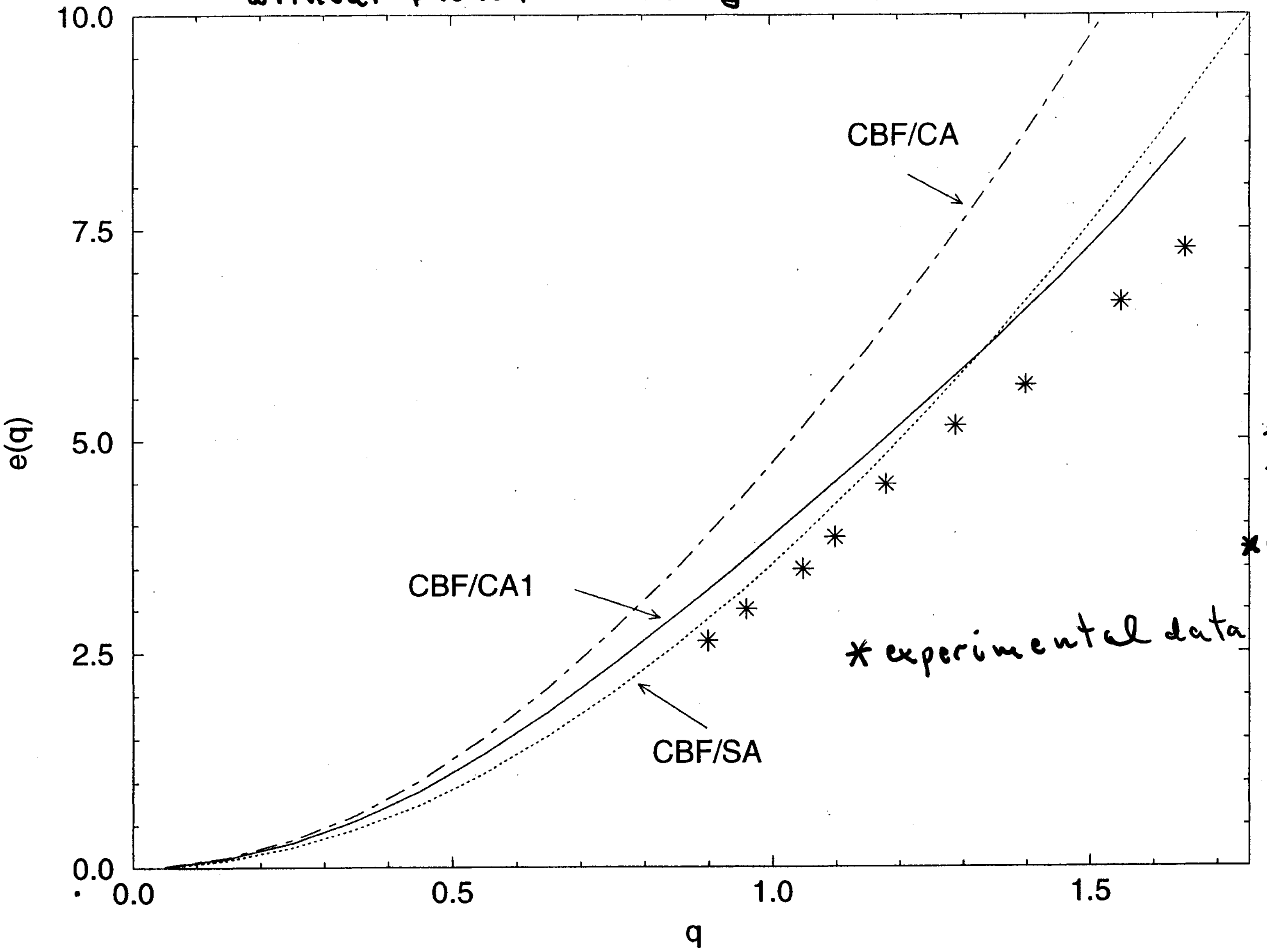
We have two levels of diagrams:

- perturbative diagrams
- HNC diagrams to calculate the matrix elemen



^{3}He single particle energies, in CA, KSA, CA1 without phonon rescattering.

CA1 is obtained in CA but using the experimental ^{4}He spectrum. Diagram (e) is not included!



$m_I^*(CA) = 1.6\, m_3$

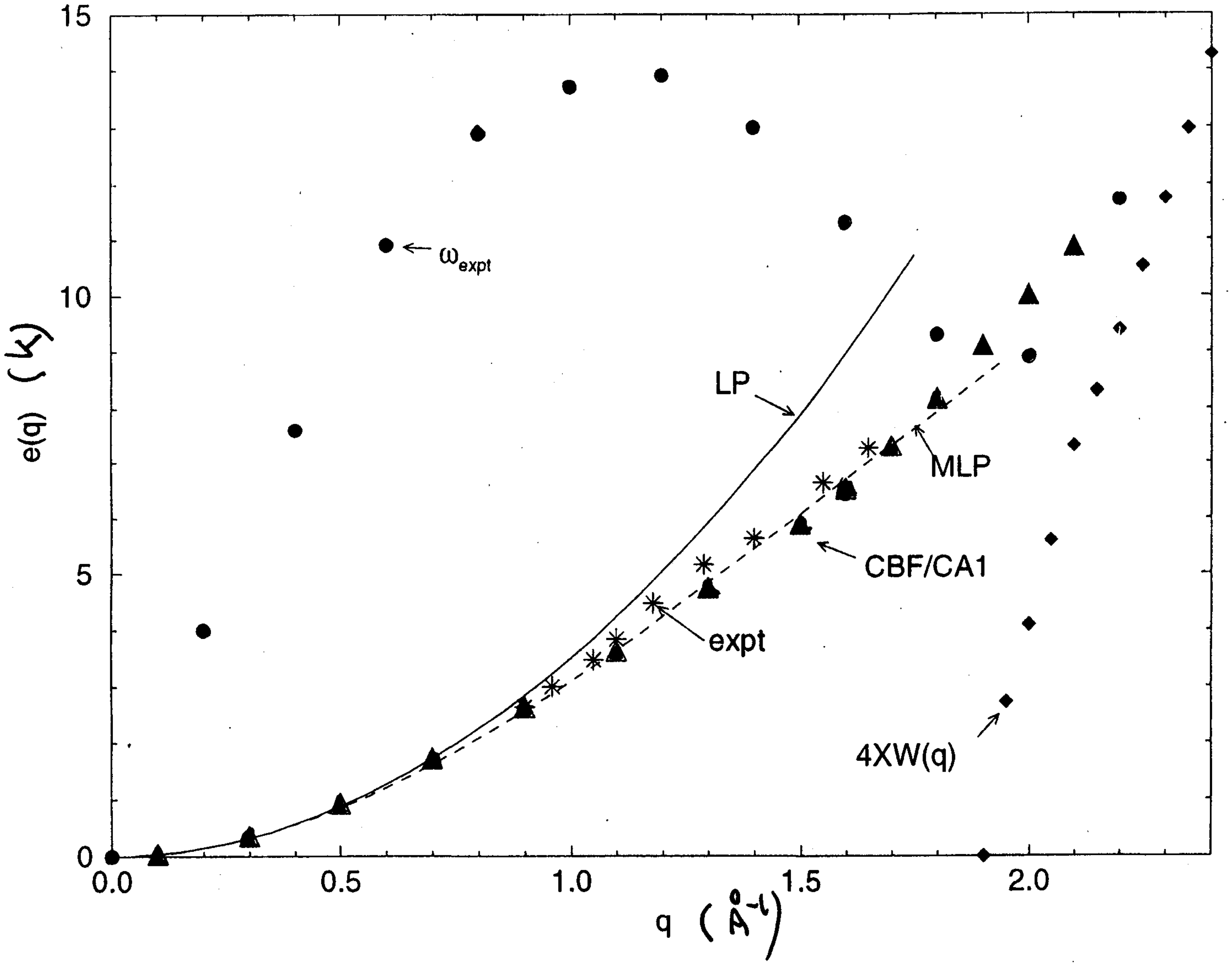
$m_I^*(KSA) = 2.1\, m_3$

ROP not included

* KSA is closer to expt. at large q

* CA1 and KSA are closer at large q => good description of the roton in ^{4}He

* The blue dots are the ^{4}He excitation spectrum



When the energy denominator is zero the self-energy becomes complex.

The impurity quasi-particle can decay into ^{4}He phonon-roton while making a transition into a low-energy impurity mode $\Rightarrow$ The quasiparticle acquires a finite lifetime.

The imaginary part : $W(q) = \mathrm{Im} \sum(q, e(q))$

The OIP contribution:

$$W_{OIP}(q) = \pi \sum_{q_1}' \left| \langle \bar{q} \,|\, H - E_0 - e(q) \,|\, \bar{q} - \bar{q}_1 ; \bar{q}_1 \rangle \right|^2 \delta\left(e(q) - e_0(|\bar{q} - \bar{q}_1|) - W(q_1) \right)$$

where we have used the MLP impurity spectrum and the experimental ^{4}He $W(q)$.

The experimental results compatible with neutron scattering measurements at low q are parametrized by:

$$e_{MLP}(q) = \frac{\hbar^2 q^2}{2m_3^*} \frac{1}{1+\gamma q^2}$$

$$\boxed{m^* \sim 2'2\, m_3 \qquad \gamma \sim 0.13\ \mathring{A}^2}$$

$$e_{LP}(q) = \frac{\hbar^2 q^2}{2m_3^*}$$

one can also parametrize

$$e(q) = \frac{\hbar^2 q^2}{2m_3^*(q)}$$

$$\frac{1}{m_3^*(q)} = \frac{1}{\hbar^2 q} \frac{\partial}{\partial q}\left(e(q)\right)$$

In this way $m_3^*(0) = m_3^*$

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

	$m_3^*(0)$
OIP	$1.8\ m_3$
+ TIP	$2.1\ m_3$
+ ROP	$2.2\ m_3$

and $\boxed{m_3^*(q = 1'7\ \mathring{A}^{-1}) = 3.2\ m_3}$

other results.

$m_3^*(0)$	$\rho = 0.365\ \sigma^{-3}$
$2'2$	(a)
$2'09$	(b)
$2'18$	(c)

(a) DMC Boronat et al PRB 59 (1999) 8844

(b) Krotscheck et al PRB 58 (1998) 12282

(c) Extracted from specific heat measurements. R. Simons. E. Krotscheck et al PRL 80 (1998) 4709

$$\boxed{\gamma(CBF) \simeq 0.19\ \mathring{A}^2}$$

B. Fak et al. PRB41 (1990) [illegible] Low "q" J Low Temp. Phys. 93 (1993) 57

Neutron scattering

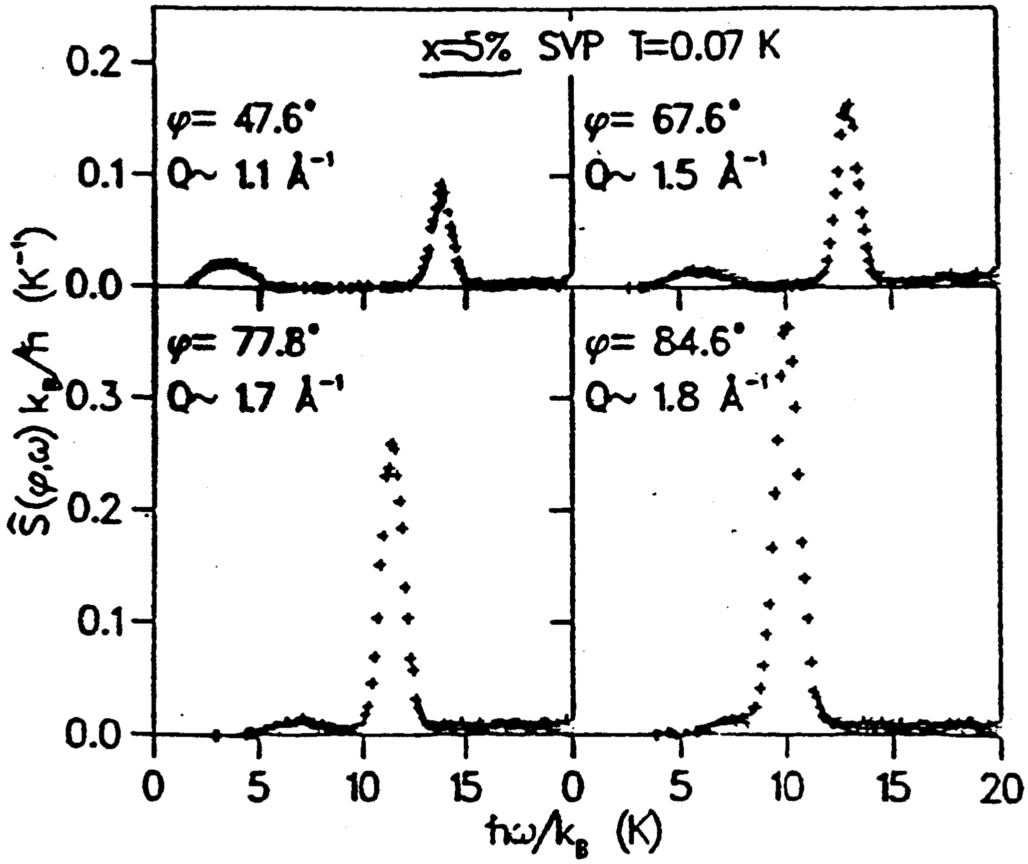
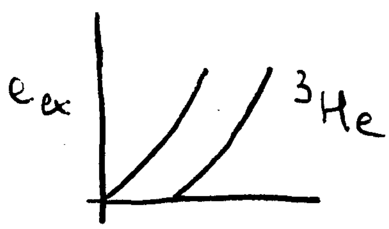
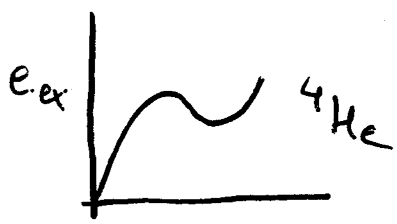


FIG. 2. Neutron-scattering function $\hat{S}(\phi,\omega)$ for selected angles. With increasing wave vector the low-energy particle-hole peak becomes weaker as it approaches the large phonon-roton peak.

$x = 5\%$ $k_F \simeq 0.3\ \mathrm{\AA}^{-1}$

$q > 2k_F$





The ph-peak defines the m^*.

The ph-peak is well fitted with a Lindhard function with $e(k) = \frac{\hbar^2 q^2}{2m_3^*}\frac{1}{1+\gamma q^2}$ and a quenching factor ~ 0.37.

$m_3^* \simeq 2.3\, m_I$

$\gamma \simeq 0.13$

They take $S^{(3,4)}(q,\omega) = 0$??