Static and Dynamic Many-Body Correlations

Overview and Prospects

E. Krotscheck

Institute for Theoretical Physics
Johannes Kepler University, A-4040 Linz, Austria

July 18, 2006

Outline

1. Ground state theory: (Fermi) HNC summations and optimization
   - View from the top: Parquet diagrams
   - View from above the top: The strength of correlated wave functions
2. Fermions – another problem
   - Fermions in the parquet language
   - ^{3}He-^{4}He-mixtures: Where parquet tells us something
3. Boson Dynamics
   - Equations of motion and dynamic response
   - Sum rules and limits

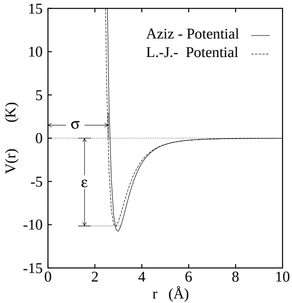
Wave functions, diagrams, and optimization

Where most many-body talk starts...

Postulate a microscopic, strongly interacting Hamiltonian

Calculate macroscopic properties from no other information.

$$H = -\sum \frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} V(i,j)$$



1. Structure
2. Energetics
3. Excitations
4. (Thermo)dynamics
5. Surface properties
6. Name it we have it. . .

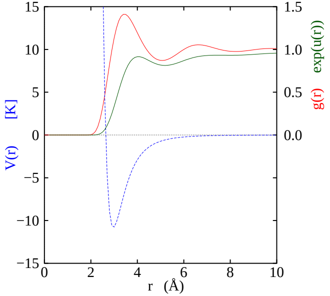
Why it became necessary: Neutron stars didn't let us fit any data.

Correlated wave functions

What looked like a “simple quick and dirty” method (Jastrow):

$$\Psi(1,\ldots,N) = \exp\frac{1}{2}\left[\sum_i u_1(\mathbf{r}_i) + \sum_{i<j} u_2(\mathbf{r}_i,\mathbf{r}_j)\right]\Phi_0(1,\ldots,N)$$
$$\equiv F(1,\ldots,N)\Phi_0(1,\ldots,N)$$

$\Phi_0(1,\ldots,N)$ “Model wave function”



- An intuitive way to include core exclusion;
- Diagram summation methods from classical statistics (HNC, PY, BGY);
- Optimization $\delta E/\delta u_n = 0$ makes correlations unique.
- HNC is the only diagram classification that is in all orders compatible with optimization;

Two-body Euler equations: $\delta E / \delta u_2 = 0$

Summarizing its two faces

- "RPA" version (Campbell, Feenberg 1969)

$$S(q) = \left[1 + 4m\tilde{V}_{p-h}(q)/\hbar^2 q^2\right]^{-1/2}$$

Two-body Euler equations: $\delta E / \delta u_2 = 0$

Summarizing its two faces

- "RPA" version (Campbell, Feenberg 1969)

$$S(q) = \left[1 + 4m\tilde{V}_{p-h}(q)/\hbar^2 q^2\right]^{-1/2}$$

- "Bethe-Goldstone" version (Lantto, Siemens 1977)

$$\frac{\hbar^2}{m}\nabla^2\sqrt{g(r)} = [v(r) + w(r)]\sqrt{g(r)}$$

Two-body Euler equations: $\delta E / \delta u_2 = 0$

Summarizing its two faces

- "RPA" version (Campbell, Feenberg 1969)

$$S(q) = \left[1 + 4m\tilde{V}_{p-h}(q)/\hbar^2 q^2\right]^{-1/2}$$

- "Bethe-Goldstone" version (Lantto, Siemens 1977)

$$\frac{\hbar^2}{m}\nabla^2\sqrt{g(r)} = \left[v(r) + w(r)\right]\sqrt{g(r)}$$

- "particle–hole interaction"

$$\begin{aligned} V_{p-h}(r) &\equiv g(r)v(r) + \frac{\hbar^2}{m}\left|\nabla\sqrt{g(r)}\right|^2 \\ &+ w(r)\left[g(r) - 1\right] \end{aligned}$$

Two-body Euler equations: $\delta E / \delta u_2 = 0$

Summarizing its two faces

- “RPA” version (Campbell, Feenberg 1969)

$$S(q) = \left[1 + 4m\tilde{V}_{p-h}(q)/\hbar^2 q^2\right]^{-1/2}$$

- “Bethe-Goldstone” version (Lantto, Siemens 1977)

$$\frac{\hbar^2}{m}\nabla^2\sqrt{g(r)} = [v(r) + w(r)]\sqrt{g(r)}$$

- “particle–hole interaction”

$$\begin{aligned} V_{p-h}(r) &\equiv g(r)v(r) + \frac{\hbar^2}{m}\left|\nabla\sqrt{g(r)}\right|^2 \\ &+ w(r)\left[g(r) - 1\right] \end{aligned}$$

- “induced interaction” $\tilde{w}(k)$.

“...it appears that the optimized Jastrow function is capable of summing all rings and ladders, and partially all other diagrams, to infinite order.”

H.-K. Sim, C.-W. Woo and J. R. Buchler, Phys Rev. A2, 2024 (1970).

Two-body Euler equations: $\delta E/\delta u_2 = 0$

The power of unconstrained optimization

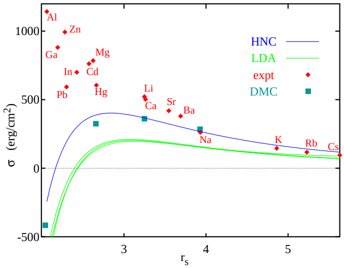
- All reference to a “Jastrow” wave function has disappeared. Easier and much faster than optimizing parameters;
- Generalization to simple non-uniform (plane surface or spherical) geometry is easy and efficient;
- Restriction to $u_2(|\mathbf{r}_i - \mathbf{r}_j|)$ unnecessary and not helpful;
- Generalizible of FHNC-EL to non-uniform Fermi systems

Two-body Euler equations: $\delta E / \delta u_2 = 0$

The power of unconstrained optimization

- All reference to a “Jastrow” wave function has disappeared. Easier and much faster than optimizing parameters;
- Generalization to simple non-uniform (plane surface or spherical) geometry is easy and efficient;
- Restriction to $u_2(|\mathbf{r}_i - \mathbf{r}_j|)$ unnecessary and not helpful;
- Generalizible of FHNC-EL to non-uniform Fermi systems

- Excellent agreement of FHNC-EL for metallic surface energies with GFMC;
- Physically intuitive explanation for why LDA fails;
- About an order of magnitude better than LDA for closed shell atoms.



View from the top: parquet diagrams

A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rep. **86**, 55 (1982)

In terms of Feynman diagrams

- Sum all ladder diagrams with a local, particle-particle reducible interaction $V_{p-p}(k)$;

View from the top: parquet diagrams

A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rep. **86**, 55 (1982)

In terms of Feynman diagrams

- Sum all ladder diagrams with a local, particle-particle reducible interaction $V_{p-p}(k)$;
- Define a "particle-hole irreducible interaction" $V_{p-h}(k, \omega)$;

View from the top: parquet diagrams
A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rep. **86**, 55 (1982)

In terms of Feynman diagrams

- Sum all ladder diagrams with a local, particle-particle reducible interaction $V_{p-p}(k)$;
- Define a "particle-hole irreducible interaction" $V_{p-h}(k,\omega)$;
- *Localize* $V_{p-h}(k,\omega) \approx V_{p-h}(k,\bar{\omega}(k)) \equiv V_{p-h}(k)$ such that energy dependent and energy independent interactions give the same contribution to $S(k)$;

View from the top: parquet diagrams

A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rep. **86**, 55 (1982)

In terms of Feynman diagrams

- Sum all ladder diagrams with a local, particle-particle reducible interaction $V_{p-p}(k)$;
- Define a "particle-hole irreducible interaction" $V_{p-h}(k,\omega)$;
- *Localize* $V_{p-h}(k,\omega) \approx V_{p-h}(k,\bar{\omega}(k)) \equiv V_{p-h}(k)$ such that energy dependent and energy independent interactions give the same contribution to $S(k)$;
- Sum all ring diagrams with this local particle-hole irreducible interaction;

View from the top: parquet diagrams

A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rep. **86**, 55 (1982)

In terms of Feynman diagrams

- Sum all ladder diagrams with a local, particle-particle reducible interaction $V_{p-p}(k)$;
- Define a "particle-hole irreducible interaction" $V_{p-h}(k,\omega)$;
- *Localize* $V_{p-h}(k,\omega) \approx V_{p-h}(k,\bar{\omega}(k)) \equiv V_{p-h}(k)$ such that energy dependent and energy independent interactions give the same contribution to $S(k)$;
- Sum all ring diagrams with this local particle-hole irreducible interaction;
- Define "particle-particle irreducible interaction" $V_{p-p}(k,\omega)$;

View from the top: parquet diagrams

A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rep. **86**, 55 (1982)

In terms of Feynman diagrams

- Sum all ladder diagrams with a local, particle-particle reducible interaction $V_{p-p}(k)$;
- Define a "particle-hole irreducible interaction" $V_{p-h}(k,\omega)$;
- *Localize* $V_{p-h}(k,\omega) \approx V_{p-h}(k,\bar{\omega}(k)) \equiv V_{p-h}(k)$ such that energy dependent and energy independent interactions give the same contribution to $S(k)$;
- Sum all ring diagrams with this local particle-hole irreducible interaction;
- Define "particle-particle irreducible interaction" $V_{p-p}(k,\omega)$;
- *Localize* $V_{p-p}(k,\omega) \approx V_{p-p}(k,\bar{\omega}(k)) \equiv V_{p-p}(k)$ such that energy dependent and energy independent interactions give the same contribution to $S(k)$;

View from the top: parquet diagrams

A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rep. **86**, 55 (1982)

In terms of Feynman diagrams

- Sum all ladder diagrams with a local, particle-particle reducible interaction $V_{p-p}(k)$;
- Define a "particle-hole irreducible interaction" $V_{p-h}(k,\omega)$;
- *Localize* $V_{p-h}(k,\omega) \approx V_{p-h}(k,\bar{\omega}(k)) \equiv V_{p-h}(k)$ such that energy dependent and energy independent interactions give the same contribution to $S(k)$;
- Sum all ring diagrams with this local particle-hole irreducible interaction;
- Define "particle-particle irreducible interaction" $V_{p-p}(k,\omega)$;
- *Localize* $V_{p-p}(k,\omega) \approx V_{p-p}(k,\bar{\omega}(k)) \equiv V_{p-p}(k)$ such that energy dependent and energy independent interactions give the same contribution to $S(k)$;
- Iterate;

View from the top: parquet diagrams

A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rep. **86**, 55 (1982)

In terms of Feynman diagrams

- Sum all ladder diagrams with a local, particle-particle reducible interaction $V_{p-p}(k)$;
- Define a "particle-hole irreducible interaction" $V_{p-h}(k,\omega)$;
- *Localize* $V_{p-h}(k,\omega) \approx V_{p-h}(k,\bar{\omega}(k)) \equiv V_{p-h}(k)$ such that energy dependent and energy independent interactions give the same contribution to $S(k)$;
- Sum all ring diagrams with this local particle-hole irreducible interaction;
- Define "particle-particle irreducible interaction" $V_{p-p}(k,\omega)$;
- *Localize* $V_{p-p}(k,\omega) \approx V_{p-p}(k,\bar{\omega}(k)) \equiv V_{p-p}(k)$ such that energy dependent and energy independent interactions give the same contribution to $S(k)$;
- Iterate;
- Calculate energy by coupling constant integration.

View from the top: parquet diagrams
A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rep. **86**, 55 (1982)

In terms of Feynman diagrams

- Sum all ladder diagrams with a local, particle-particle reducible interaction $V_{p-p}(k)$;
- Define a "particle-hole irreducible interaction" $V_{p-h}(k,\omega)$;
- *Localize* $V_{p-h}(k,\omega) \approx V_{p-h}(k,\bar{\omega}(k)) \equiv V_{p-h}(k)$ such that energy dependent and energy independent interactions give the same contribution to $S(k)$;
- Sum all ring diagrams with this local particle-hole irreducible interaction;
- Define "particle-particle irreducible interaction" $V_{p-p}(k,\omega)$;
- *Localize* $V_{p-p}(k,\omega) \approx V_{p-p}(k,\bar{\omega}(k)) \equiv V_{p-p}(k)$ such that energy dependent and energy independent interactions give the same contribution to $S(k)$;
- Iterate;
- Calculate energy by coupling constant integration.

Re-derive HNC-EL !

Variational wave function:

$$\Psi(1\ldots N) = \exp\frac{1}{2}\left[\sum_i u_1(\mathbf{r}_i) + \sum_{i<j} u_2(\mathbf{r}_i,\mathbf{r}_j) + \sum_{i<j<k} u_3(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k)\right]$$

Optimization $\delta E/\delta u_3(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k) = 0$ (Campbell PLA **44**, 471 (1973)) clearly lowers energy.

$$\frac{E_3}{N} = -\frac{1}{3!}\int \frac{d^3k d^3p d^3q}{(2\pi)^6\rho^2}\delta(\mathbf{p}+\mathbf{k}+\mathbf{q})\frac{|V_3(\mathbf{p},\mathbf{k},\mathbf{q})|^2}{\varepsilon(k)+\varepsilon(p)+\varepsilon(q)}\,,$$

$V_3(\mathbf{p},\mathbf{k},\mathbf{q})$: effective 3-body vertex

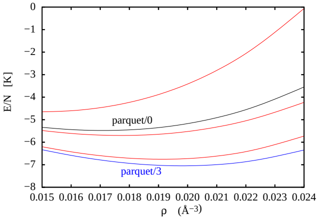
$\varepsilon(k) = \hbar^2 k^2/2mS(k) \equiv t(k)/S(k)$ "Feynman spectrum."

$\Rightarrow$ Energy correction in quantitative agreement with MC !

Triplet parquet
Another view from “above” the top

Perturbation Theory	HNC/EL
$-\frac{5}{16}\int\frac{d^3k}{(2\pi)^3\rho}\frac{\tilde V^4(k)}{t^3(k)}$	$-\frac{5}{16}\int\frac{d^3k}{(2\pi)^3\rho}\frac{\tilde V^4(k)}{t^3(k)}$
$-\frac{1}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t^2(k)t(p)}$	$-\frac{1}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t^2(k)t(p)}$
$-\frac{1}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t^2(k)(t(k)+t(p)+t(\lvert\mathbf{p}+\mathbf{k}\rvert))}$	$-\frac{1}{8}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t^2(k)t(p)}$
$-\frac{1}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t(k)t(p)(t(k)+t(p)+t(\lvert\mathbf{p}+\mathbf{k}\rvert))}$	$-\frac{3}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t(k)t(p)t(\lvert\mathbf{p}+\mathbf{k}\rvert)}$
$-\frac{1}{2}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t(k)t(p)(t(k)+t(p)+t(\lvert\mathbf{p}+\mathbf{k}\rvert))}$	– – –
$-\frac{1}{16}\int\frac{d^3kd^3pd^3q}{(2\pi)^9\rho^3}\frac{\tilde V(k)\tilde V(p)\tilde V(q)}{t(k)t(p)t(q)}$	$-\frac{1}{16}\int\frac{d^3kd^3pd^3q}{(2\pi)^9\rho^3}\frac{\tilde V(k)\tilde V(p)\tilde V(q)}{t(k)t(p)t(q)}$
$-\frac{1}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V^2(p)}{t^2(k)(t(k)+t(p)+t(\lvert\mathbf{p}+\mathbf{k}\rvert))}$	– – –
$-\frac{1}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V^2(p)}{t(k)t(p)(t(k)+t(p)+t(\lvert\mathbf{p}+\mathbf{k}\rvert))}$	– – –
$\frac{1}{8}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V^2(p)}{t^2(k)t(p)}$	– – –

- Many diagrams of random size and sign, large cancellations (Jackson, Lande, Guintnk, Smith, PRB **31**, 403 (1985);

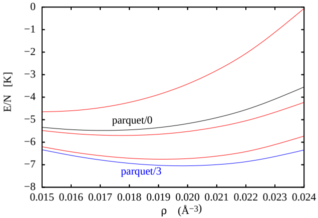


Triplet parquet

Another view from “above” the top

Perturbation Theory	HNC/EL	
$-\frac{5}{16}\int \frac{d^3k}{(2\pi)^3\rho}\frac{\tilde{V}^4(k)}{t^3(k)}$	$-\frac{5}{16}\int \frac{d^3k}{(2\pi)^3\rho}\frac{\tilde{V}^4(k)}{t^3(k)}$	
$-\frac{1}{4}\int \frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde{V}^2(k)\tilde{V}(p)\tilde{V}(\|\mathbf{p}+\mathbf{k}\|)}{t^2(k)t(p)}$	$-\frac{1}{4}\int \frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde{V}^2(k)\tilde{V}(p)\tilde{V}(\|\mathbf{p}+\mathbf{k}\|)}{t^2(k)t(p)}$	
$-\frac{1}{4}\int \frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde{V}^2(k)\tilde{V}(p)\tilde{V}(\|\mathbf{p}+\mathbf{k}\|)}{t^2(k)(t(k)+t(p)+t(\|\mathbf{p}+\mathbf{k}\|))}$	$-\frac{1}{8}\int \frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde{V}^2(k)\tilde{V}(p)\tilde{V}(\|\mathbf{p}+\mathbf{k}\|)}{t^2(k)t(p)}$	
$-\frac{1}{4}\int \frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde{V}^2(k)\tilde{V}(p)\tilde{V}(\|\mathbf{p}+\mathbf{k}\|)}{t(k)t(p)(t(k)+t(p)+t(\|\mathbf{p}+\mathbf{k}\|))}$	$-\frac{3}{4}\int \frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde{V}^2(k)\tilde{V}(p)\tilde{V}(\|\mathbf{p}+\mathbf{k}\|)}{t(k)t(p)t(\|\mathbf{p}+\mathbf{k}\|)}$	
$-\frac{1}{2}\int \frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde{V}^2(k)\tilde{V}(p)\tilde{V}(\|\mathbf{p}+\mathbf{k}\|)}{t(k)t(p)(t(k)+t(p)+t(\|\mathbf{p}+\mathbf{k}\|))}$	– – –	
$-\frac{1}{16}\int \frac{d^3kd^3pd^3q}{(2\pi)^9\rho^3}\frac{\tilde{V}(k)\tilde{V}(p)\tilde{V}(q)}{t(k)t(p)t(q)}$	$-\frac{1}{16}\int \frac{d^3kd^3pd^3q}{(2\pi)^9\rho^3}\frac{\tilde{V}(k)\tilde{V}(p)\tilde{V}(q)}{t(k)t(p)t(q)}$	
$-\frac{1}{4}\int \frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde{V}^2(k)\tilde{V}^2(p)}{t^2(k)(t(k)+t(p)+t(\|\mathbf{p}+\mathbf{k}\|))}$	– – –	
$-\frac{1}{4}\int \frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde{V}^2(k)\tilde{V}^2(p)}{t(k)t(p)(t(k)+t(p)+t(\|\mathbf{p}+\mathbf{k}\|))}$	– – –	
$\frac{1}{8}\int \frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde{V}^2(k)\tilde{V}^2(p)}{t^2(k)t(p)}$	– – –	

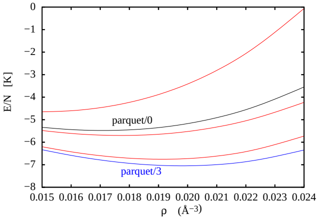
- Many diagrams of random size and sign, large cancellations (Jackson, Lande, Guintnk, Smith, PRB **31**, 403 (1985);



- Some are “natural” terms (e.g. self-energy insertions), some totally irreducible

Perturbation Theory	HNC/EL	
$-\frac{5}{16}\int\frac{d^3k}{(2\pi)^3\rho}\frac{\tilde V^4(k)}{t^3(k)}$	$-\frac{5}{16}\int\frac{d^3k}{(2\pi)^3\rho}\frac{\tilde V^4(k)}{t^3(k)}$	
$-\frac{1}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t^2(k)t(p)}$	$-\frac{1}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t^2(k)t(p)}$	
$-\frac{1}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t^2(k)(t(k)+t(p)+t(\lvert\mathbf{p}+\mathbf{k}\rvert))}$	$-\frac{1}{8}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t^2(k)t(p)}$	
$-\frac{1}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t(k)t(p)(t(k)+t(p)+t(\lvert\mathbf{p}+\mathbf{k}\rvert))}$	$-\frac{3}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t(k)t(p)t(\lvert\mathbf{p}+\mathbf{k}\rvert)}$	
$-\frac{1}{2}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V(p)\tilde V(\lvert\mathbf{p}+\mathbf{k}\rvert)}{t(k)t(p)(t(k)+t(p)+t(\lvert\mathbf{p}+\mathbf{k}\rvert))}$	– – –	
$-\frac{1}{16}\int\frac{d^3kd^3pd^3q}{(2\pi)^9\rho^3}\frac{\tilde V(k)\tilde V(p)\tilde V(q)}{t(k)t(p)t(q)}$	$-\frac{1}{16}\int\frac{d^3kd^3pd^3q}{(2\pi)^9\rho^3}\frac{\tilde V(k)\tilde V(p)\tilde V(q)}{t(k)t(p)t(q)}$	
$-\frac{1}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V^2(p)}{t^2(k)(t(k)+t(p)+t(\lvert\mathbf{p}+\mathbf{k}\rvert))}$	– – –	
$-\frac{1}{4}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V^2(p)}{t(k)t(p)(t(k)+t(p)+t(\lvert\mathbf{p}+\mathbf{k}\rvert))}$	– – –	
$\frac{1}{8}\int\frac{d^3kd^3p}{(2\pi)^6\rho^2}\frac{\tilde V^2(k)\tilde V^2(p)}{t^2(k)t(p)}$	– – –	

- Many diagrams of random size and sign, large cancellations (Jackson, Lande, Guintnk, Smith, PRB **31**, 403 (1985);



- Some are "natural" terms (e.g. self-energy insertions), some totally irreducible
- Combined result identical to variational.

- Fermion-HNC and EL a lot messier

- Fermion-HNC and EL a lot messier
- Rings: FHNC-EL sums ring diagrams in a collective approximation:

$$\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1-\tilde{V}_{p-h}(q,\omega)\chi_0(q,\omega)} \approx \frac{\chi_0^{(coll)}(q,\omega)}{1-\tilde{V}_{p-h}(q,\omega)\chi_0^{(coll)}(q,\omega)}$$

where the pole strength $\hbar\omega_q^{(3)}$ in

$$\chi_0^{(coll)}(q,\omega) = \frac{2t(q)}{(\hbar\omega+i\eta)^2-(\hbar\omega(q))^2}; \qquad \hbar\omega(q) \equiv \frac{t(q)}{S_F(q)} = \frac{\hbar^2q^2}{2mS_F(q)}$$

is chosen such that such that

$$-\Im m \int_{-\infty}^{\infty} \frac{d(\hbar\omega)}{2\pi}\,\chi_0^{(coll)}(q,\omega) = S_F(q), \quad -\Im m \int_{-\infty}^{\infty} \frac{d(\hbar\omega)}{2\pi}\,\hbar\omega\,\chi_0^{(coll)}(q,\omega) = t(q$$

- Ladder diagrams – “parallel connections”
  Not investigated.

- Ladder diagrams – “parallel connections”
  Not investigated.
- Self-energy insertions – “cyclic chain diagrams”:
  A static approximation to “at least” G0W
  . . . as we will see.

Why deal with ^{3}He-^{4}He mixtures ?

Why deal with ^{3}He-^{4}He mixtures ?

- Bose component very well understood
- Low fermion density $\Rightarrow$ Theory should be easy
- Good experiments

Why deal with ^{3}He-^{4}He mixtures ?

- Bose component very well understood
- Low fermion density $\Rightarrow$ Theory should be easy
- Good experiments

Wave function for a mixture

$$\Psi_0(\{\mathbf{r}_i^{(\alpha)}\}) = e^{\frac{1}{2}U(\{\mathbf{r}_i^{(\alpha)}\})}\Phi_0(\{\mathbf{r}_i^{(3)}\})$$

$$U(\{\mathbf{r}_i^{(\alpha)}\}) = \frac{1}{2!}\sum_{\alpha\beta}\sum_{i,j}^{N_\alpha,N_\beta}{}' u^{(\alpha\beta)}(\mathbf{r}_i,\mathbf{r}_j) + \frac{1}{3!}\sum_{\alpha\beta\gamma}\sum_{i,j,k}^{N_\alpha,N_\beta,N_\gamma}{}' u^{(\alpha\beta\gamma)}(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k)\,.$$

Why deal with ^{3}He-^{4}He mixtures ?

- Bose component very well understood
- Low fermion density $\Rightarrow$ Theory should be easy
- Good experiments

Wave function for a mixture

$$\begin{aligned}\Psi_0(\{\mathbf{r}_i^{(\alpha)}\}) &= e^{\frac{1}{2}U(\{\mathbf{r}_i^{(\alpha)}\})}\Phi_0(\{\mathbf{r}_i^{(3)}\})\\ U(\{\mathbf{r}_i^{(\alpha)}\}) &= \frac{1}{2!}\sum_{\alpha\beta}\sum_{i,j}^{N_\alpha,N_\beta}{}' u^{(\alpha\beta)}(\mathbf{r}_i,\mathbf{r}_j) + \frac{1}{3!}\sum_{\alpha\beta\gamma}\sum_{i,j,k}^{N_\alpha,N_\beta,N_\gamma}{}' u^{(\alpha\beta\gamma)}(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k)\,.\end{aligned}$$

- Energetics of the mixture extremely well reproduced by theory (E. K. and M. Saarela, Phys. Rep. **232**, 1 (1993).)

- Define a “correlated particle-hole state”

$$\Psi_{p-h}(\{\mathbf{r}_i^{(\alpha)}\}) = e^{\frac{1}{2}U(\{\mathbf{r}_i^{(\alpha)}\})}\Phi_{p-h}(\{\mathbf{r}_i^{(3)}\})\,;$$

$\Phi_{p-h}(\{\mathbf{r}_i^{(3)}\})$ is a particle-hole excited state model wave function

- Define a CBF single particle spectrum

$$\frac{\left\langle\Psi_{p-h}\middle| H \middle|\Psi_{p-h}\right\rangle}{\left\langle\Psi_{p-h}\,\middle|\,\Psi_{p-h}\right\rangle} \equiv \varepsilon^{(3)}(p) - \varepsilon^{(3)}(h)\,;$$

- Obtain the effective mass from this spectrum.

- Define a "correlated particle-hole state"

$$\Psi_{p-h}(\{\mathbf{r}_i^{(\alpha)}\}) = e^{\frac{1}{2}U(\{\mathbf{r}_i^{(\alpha)}\})}\Phi_{p-h}(\{\mathbf{r}_i^{(3)}\})\,;$$

  $\Phi_{p-h}(\{\mathbf{r}_i^{(3)}\})$ is a particle-hole excited state model wave function

- Define a CBF single particle spectrum

$$\frac{\left\langle \Psi_{p-h}\middle| H \middle|\Psi_{p-h}\right\rangle}{\left\langle \Psi_{p-h} \,\middle|\, \Psi_{p-h}\right\rangle} \equiv \varepsilon^{(3)}(p) - \varepsilon^{(3)}(h)\,;$$

- Obtain the effective mass from this spectrum.

Why naïve ?

Effective mass of ^{3}He-^{4}He mixtures

The naïve method:

- Define a "correlated particle-hole state"

$$\Psi_{p-h}(\{\mathbf{r}_i^{(\alpha)}\}) = e^{\frac{1}{2}U(\{\mathbf{r}_i^{(\alpha)}\})}\Phi_{p-h}(\{\mathbf{r}_i^{(3)}\})\,;$$

  $\Phi_{p-h}(\{\mathbf{r}_i^{(3)}\})$ is a particle-hole excited state model wave function

- Define a CBF single particle spectrum

$$\frac{\left\langle\Psi_{p-h}\middle| H \middle|\Psi_{p-h}\right\rangle}{\left\langle\Psi_{p-h} \mid \Psi_{p-h}\right\rangle} \equiv \varepsilon^{(3)}(p) - \varepsilon^{(3)}(h)\,;$$

- Obtain the effective mass from this spectrum.

Why naïve ?

- Misses hydrodynamic backflow. Fix this "by hand" for the time being by giving the ^{3}He particles a "hydrodynamic effective mass" m^*_{3H}.
- Fermionic effect is "Hartree-Fock like":

$$\varepsilon^{(3)}(k) = U_0 + \frac{\hbar^2 k^2}{2m^*_{3H}} - \frac{\rho^{(3)}}{2}\int d^3r\, W_{\rm eff}(r)\, j_0(r\,k)\,\ell(r\,k_F)$$

The conventional approach

G0W-approximation for a "self-energy" $\Sigma(q,\omega)$:

$$\Sigma(k,\omega) = i\int \frac{d^3k d(\hbar\omega')}{(2\pi)^4\rho^{(3)}} G^{(0)}(|\mathbf{k}-\mathbf{q}|,\omega-\omega')\,\tilde{V}_{eff}(k,\omega')$$

Free Green's function:

$$\begin{aligned} G^{(0)}(q,\omega) &= \frac{n_{\mathbf{q},\sigma}}{\hbar\omega - t^{(3)}(q) - i\eta} + \frac{1-n_{\mathbf{q},\sigma}}{\hbar\omega - t^{(3)}(q) + i\eta} \\ &\equiv G_H^{(0)}(q,\omega) + G_F^{(0)}(q,\omega)\,, \\ G_F^{(0)}(k,\omega) &= \frac{n_{\mathbf{q},\sigma}}{\hbar\omega - t^{(3)}(q) - i\eta} - \frac{n_{\mathbf{q},\sigma}}{\hbar\omega - t^{(3)}(q) + i\eta} \end{aligned}$$

- $\Rightarrow$ "Hydrodynamic part" $G_H^{(0)}(q,\omega)$ survives ar zero ^{3}He concentration;

The conventional approach

G0W-approximation for a “self-energy” $\Sigma(q,\omega)$:

$$\Sigma(k,\omega) = i\int \frac{d^3k d(\hbar\omega')}{(2\pi)^4 \rho^{(3)}} G^{(0)}(|\mathbf{k}-\mathbf{q}|,\omega-\omega')\,\tilde{V}_{eff}(k,\omega')$$

Free Green’s function:

$$\begin{aligned} G^{(0)}(q,\omega) &= \frac{n_{\mathbf{q},\sigma}}{\hbar\omega - t^{(3)}(q) - i\eta} + \frac{1-n_{\mathbf{q},\sigma}}{\hbar\omega - t^{(3)}(q) + i\eta} \\ &\equiv G_H^{(0)}(q,\omega) + G_F^{(0)}(q,\omega)\,, \\ G_F^{(0)}(k,\omega) &= \frac{n_{\mathbf{q},\sigma}}{\hbar\omega - t^{(3)}(q) - i\eta} - \frac{n_{\mathbf{q},\sigma}}{\hbar\omega - t^{(3)}(q) + i\eta} \end{aligned}$$

- $\Rightarrow$ “Hydrodynamic part” $G_H^{(0)}(q,\omega)$ survives ar zero ^{3}He concentration;
- $\Rightarrow$ Treat “hydrodynamic” self-energy by equations of motion method.

Effective interaction in the two-impurity limit:

Energy dependent "effective interaction":

$$\tilde{V}_{eff}(q,\omega) = \tilde{V}^{(33)}_{p-h}(q) + \tilde{V}^{(34)}_{p-h}(q)\,\chi^{(44)}(q,\omega)\,\tilde{V}^{(34)}_{p-h}(q)$$

$$\chi_0^{(\alpha\beta)}(q,\omega) = \frac{2\,t^{(\alpha)}(q)\delta_{\alpha\beta}}{(\hbar\omega)^2 - (\varepsilon^{(\alpha)}(q))^2}$$

Parquet-prescription to "localize" $\tilde{V}_{eff}(q,\omega)$

1. Construct RPA static structure function

$$\begin{aligned} S^{(33)}_{RPA}(q) &= -\int \frac{d(\hbar\omega)}{2\pi} \Im m \left[\chi_0^{(33)}(q,\omega) + \chi_0^{(33)}(q,\omega)\tilde{V}_{eff}(q,\omega)\chi_0^{(33)}(q,\omega)\right] \\ &= 1 - \frac{1}{t^{(3)}(q)}\left[\tilde{V}^{(33)}_{p-h}(q) - 2\,\frac{\left[V^{(33)}_{p-h}(q)\right]^2 S^{(44)}(q)}{\left(t^{(3)}(q) + \varepsilon^{(4)}(q)\right)^2}\right], \end{aligned}$$

2. Construct *ladder approximation* for the same quantity in terms of a different and yet unspecified local effective interaction, say $\tilde{V}_L(q)$

$$
\begin{aligned}
S^{(33)}_{ladder}(q) &= \int \frac{d(\hbar\omega)}{2\pi} \,\Im m \left[\chi_0^{(33)}(q,\omega) + \chi_0^{(33)}(q,\omega)\, \tilde{V}_L(q)\chi_0^{(33)}(q,\omega)\right] \\
&= 1 - \frac{1}{t^{(3)}(q)}\, \tilde{V}_L(q)\,.
\end{aligned}
$$

3. Define the average frequency $\bar{\omega}(q)$ such that these two forms of the static structure function are *identical* for

$$
\tilde{V}_L(q) = \tilde{V}_{eff}(q,\bar{\omega})\,.
$$

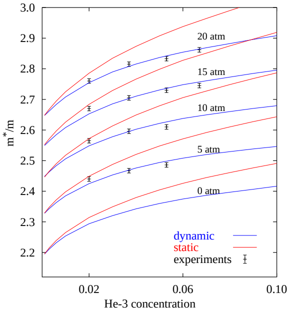
$$
(\hbar\bar{\omega})^2(q) = -\frac{\varepsilon^{(4)}(q)\,(t^{(3)})^2(q)}{\varepsilon^{(4)}(q) + 2t^{(3)}(q)}\,.
$$

4. Insert this $\hbar\bar{\omega}(q)$ into the energy-dependent effective interaction. Obtain

$$
\tilde{W}_{eff}(q) = \tilde{V}_{eff}(q,\bar{\omega}) = \tilde{V}_L(q)\,.
$$

5. The “Fock term” if (F)HNC is a “single pole approximation” to G0W.

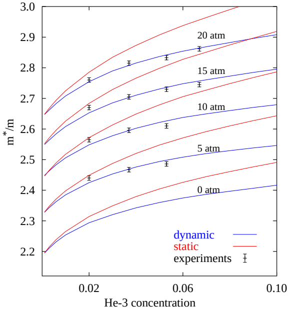
How important is all of this ?



- Zero concentration limit from independent calculation

Experiments: S. Yorozu, H. Fukuyama, and H. Ishimoto, Phys. Rev. B **48**, 9660 (1993)
Theory: E. K., J. Paaso, M. Saarela, K. Schörkhuber, and R. Zillich: Phys. Rev. B **B 58**, 12282 (1998).

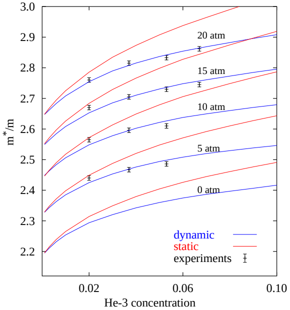
How important is all of this ?



- Zero concentration limit from independent calculation
- “static” or “FHNC” over-estimates Fermi-Liquid effect

Experiments: S. Yorozu, H. Fukuyama, and H. Ishimoto, Phys. Rev. B **48**, 9660 (1993)
Theory: E. K., J. Paaso, M. Saarela, K. Schörkhuber, and R. Zillich: Phys. Rev. B **B 58**, 12282 (1998).

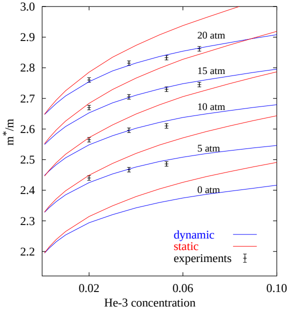
How important is all of this ?



- Zero concentration limit from independent calculation
- “static” or “FHNC” over-estimates Fermi-Liquid effect
- “dynamic” theory in quantitative agreement with experiments

Experiments: S. Yorozu, H. Fukuyama, and H. Ishimoto, Phys. Rev. B **48**, 9660 (1993)
Theory: E. K., J. Paaso, M. Saarela, K. Schörkhuber, and R. Zillich: Phys. Rev. B **B 58**, 12282 (1998).

How important is all of this ?



- Zero concentration limit from independent calculation
- “static” or “FHNC” over-estimates Fermi-Liquid effect
- “dynamic” theory in quantitative agreement with experiments
- Parquet ideas are not completely useless after all :)

Experiments: S. Yorozu, H. Fukuyama, and H. Ishimoto, Phys. Rev. B **48**, 9660 (1993)
Theory: E. K., J. Paaso, M. Saarela, K. Schörkhuber, and R. Zillich: Phys. Rev. B **B 58**, 12282 (1998).

Wave function for excited states:

$$|\Psi(t)\rangle = e^{-iE_0 t/\hbar} \frac{F e^{\frac{1}{2}\delta U} |\Psi_0\rangle}{\langle \Psi_0 | e^{\frac{1}{2}\delta U^\dagger} F^\dagger F e^{\frac{1}{2}\delta U} |\Psi_0\rangle]^{1/2}} ,$$

$|\Psi_0\rangle$: model ground state, $\delta U(t)$: excitation operator

Bosons:

$$\delta U(t) = \sum_{\mathbf{q}} \delta u^{(1)}_{\mathbf{q}}(t) \hat{\rho}_{\mathbf{q}} + \sum_{\mathbf{q},\mathbf{q}'} \delta u^{(2)}_{\mathbf{q},\mathbf{q}'}(t) \hat{\rho}_{\mathbf{q}} \hat{\rho}_{\mathbf{q}'} + \ldots$$

Fermions:

$$\delta U(t) = \sum_{\mathbf{p},\mathbf{h}} \delta u^{(1)}_{\mathbf{p},\mathbf{h}}(t) a^\dagger_{\mathbf{p}} a_{\mathbf{h}} + \sum_{\mathbf{p},\mathbf{h},\mathbf{p}',\mathbf{h}'} \delta u^{(2)}_{\mathbf{p},\mathbf{h},\mathbf{p}',\mathbf{h}'}(t) a^\dagger_{\mathbf{p}} a^\dagger_{\mathbf{p}'} a_{\mathbf{h}} a_{\mathbf{h}'}$$

Action principle:

$$\delta \mathcal{S} = \delta \int_{t_1}^{t_2} dt \left\langle \Psi(t) \middle| H + U_{ext}(t) - i\hbar \frac{\partial}{\partial t} \middle| \Psi(t) \right\rangle = 0.$$

Linear response:

- Linearization:

$$|\Psi(t)\rangle = \delta\,|\Psi(t)\rangle + |\Psi_0\rangle$$

- Induced fluctuations:

$$\delta_1\rho(\mathbf{r};t) \sim \left\langle \Psi_0 \mid \hat{\rho}(\mathbf{r}) \mid \delta\Psi(t) \right\rangle + c.c.$$
$$\delta_1\mathbf{j}(\mathbf{r};t) \sim \left\langle \Psi_0 \mid \hat{\mathbf{j}}(\mathbf{r}) \mid \delta\Psi(t) \right\rangle + c.c.$$

- Dynamic response function:

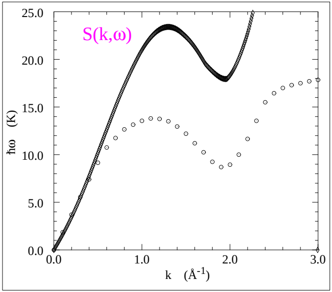
$$\delta\rho(\mathbf{r},\omega) = \int d^3r' \chi(\mathbf{r},\mathbf{r}';\omega) U_{ext}(\mathbf{r}',\omega)$$

- Dynamic structure function:

$$S(\mathbf{r},\mathbf{r}';\omega) = -\frac{1}{\pi}\Im m\,\chi(\mathbf{r},\mathbf{r}';\omega)$$

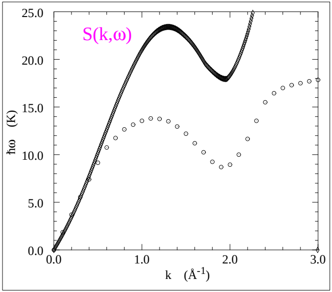
Rationalization of Pair Fluctuations

- "Feynman approximation" $\delta u^{(2)}(\mathbf{q}, \mathbf{q}') = 0$ off by a factor of two;



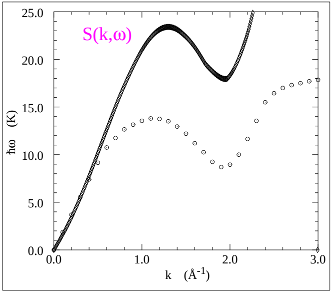
Rationalization of Pair Fluctuations

- "Feynman approximation" $\delta u^{(2)}(\mathbf{q}, \mathbf{q}') = 0$ off by a factor of two;
- One-body fluctuations are insufficient to understand the excitations in ^{4}He;



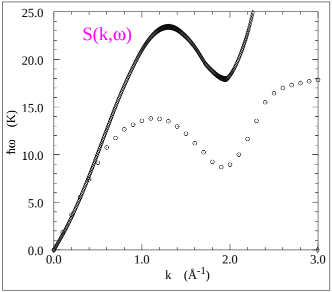
Rationalization of Pair Fluctuations

- "Feynman approximation" $\delta u^{(2)}(\mathbf{q}, \mathbf{q}') = 0$ off by a factor of two;
- One-body fluctuations are insufficient to understand the excitations in ^{4}He;
- Pair fluctuations should become important if the wavelength of excitations is comparable to inter-particle distance.



Rationalization of Pair Fluctuations

- "Feynman approximation" $\delta u^{(2)}(\mathbf{q}, \mathbf{q}') = 0$ off by a factor of two;
- One-body fluctuations are insufficient to understand the excitations in ^{4}He;
- Pair fluctuations should become important if the wavelength of excitations is comparable to inter-particle distance.
- A similar effect is to be expected in ^{3}He.



Include “pair” excitations

- Build a basis of 1 and 2 phonon states (“Correlated Basis Functions”):, let $\delta H = H - E_0$

$$\chi^{CBF}(\mathbf{q},\omega) = \left[G^{CBF}(\mathbf{q},\omega) + G^{*CBF}(\mathbf{q},-\omega)\right]$$

Include “pair” excitations

- Build a basis of 1 and 2 phonon states (“Correlated Basis Functions”):, let $\delta H = H - E_0$

$$\chi^{CBF}(\mathbf{q},\omega) = \left[G^{CBF}(\mathbf{q},\omega) + G^{*CBF}(\mathbf{q},-\omega)\right]$$

- Phonon propagator

$$G^{CBF}(\mathbf{q},\omega) = S(q)\left[\hbar\omega - \varepsilon(q) + i\eta + \Sigma(\mathbf{q},\omega)\right]^{-1}$$

Include "pair" excitations

- Build a basis of 1 and 2 phonon states ("Correlated Basis Functions"):, let $\delta H = H - E_0$

$$\chi^{CBF}(\mathbf{q},\omega) = \left[G^{CBF}(\mathbf{q},\omega) + G^{*CBF}(\mathbf{q},-\omega)\right]$$

- Phonon propagator

$$G^{CBF}(\mathbf{q},\omega) = S(q)\left[\hbar\omega - \varepsilon(q) + i\eta + \Sigma(\mathbf{q},\omega)\right]^{-1}$$

- Self-energy ("renormalized" and "unrenormalized")

$$\Sigma(\mathbf{q},\omega) = \frac{\Sigma_u(\mathbf{q},\omega)}{1-\Sigma_u(\mathbf{q},\omega)/\varepsilon(q)}$$

$$\Sigma_u(\mathbf{q},\omega) = -\frac{1}{2}\sum_{\mathbf{q}_1..\mathbf{q}_4}\langle\mathbf{q}|\,F^\dagger\delta HF\,|\mathbf{q}_1,\mathbf{q}_2\rangle \times$$

$$\times\left[\langle\mathbf{q}_1,\mathbf{q}_2|\,F^\dagger(\delta H-\hbar\omega)F\,|\mathbf{q}_3,\mathbf{q}_4\rangle\right]^{-1}\langle\mathbf{q}_3,\mathbf{q}_4|\,F^\dagger\delta HF\,|\mathbf{q}\rangle$$

Just keep diagonal term:

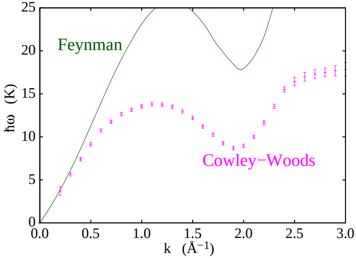
$$\langle \mathbf{q}_1, \mathbf{q}_2 | F^\dagger (\delta H - \hbar\omega) F | \mathbf{q}_3, \mathbf{q}_4 \rangle \approx S(q_1) S(q_2) \left[\varepsilon(q_1) + \varepsilon(q_2) - \hbar\omega \right] \delta_{\mathbf{q}_1,\mathbf{q}_3} \delta_{\mathbf{q}_2,\mathbf{q}_4}$$

Then

$$\Sigma_u(\mathbf{q}, \omega) = -\frac{1}{2} \sum_{\mathbf{q}_1 \mathbf{q}_2} \frac{\left| \langle \mathbf{q} | F^\dagger \delta H F | \mathbf{q}_1, \mathbf{q}_2 \rangle \right|^2}{\varepsilon(q_1) + \varepsilon(q_2) - \hbar\omega}$$

RPA: $\delta u_{2..}(\mathbf{q}_i, \mathbf{q}_j, \ldots; t) = 0$

- Correct long wavelength limit;



Just keep diagonal term:

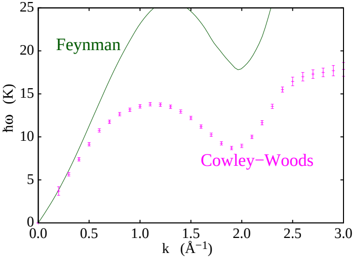
$$\langle \mathbf{q}_1, \mathbf{q}_2 | F^\dagger (\delta H - \hbar\omega) F | \mathbf{q}_3, \mathbf{q}_4 \rangle \approx S(q_1) S(q_2) \left[\varepsilon(q_1) + \varepsilon(q_2) - \hbar\omega \right] \delta_{\mathbf{q}_1,\mathbf{q}_3} \delta_{\mathbf{q}_2,\mathbf{q}_4}$$

Then

$$\Sigma_u(\mathbf{q}, \omega) = -\frac{1}{2} \sum_{\mathbf{q}_1 \mathbf{q}_2} \frac{\left| \langle \mathbf{q} | F^\dagger \delta H F | \mathbf{q}_1, \mathbf{q}_2 \rangle \right|^2}{\varepsilon(q_1) + \varepsilon(q_2) - \hbar\omega}$$

RPA: $\delta u_{2..}(\mathbf{q}_i, \mathbf{q}_j, \ldots; t) = 0$

- Correct long wavelength limit;
- No multi-phonon processes;



Just keep diagonal term:

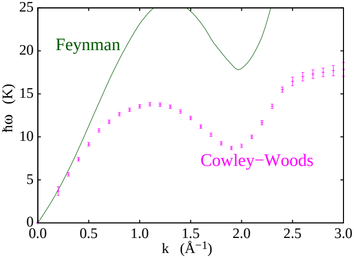
$$\langle \mathbf{q}_1, \mathbf{q}_2 | F^\dagger (\delta H - \hbar\omega) F | \mathbf{q}_3, \mathbf{q}_4 \rangle \approx S(q_1)S(q_2)\left[\varepsilon(q_1) + \varepsilon(q_2) - \hbar\omega\right] \delta_{\mathbf{q}_1,\mathbf{q}_3}\delta_{\mathbf{q}_2,\mathbf{q}_4}$$

Then

$$\Sigma_u(\mathbf{q},\omega) = -\frac{1}{2}\sum_{\mathbf{q}_1\mathbf{q}_2} \frac{\left|\langle \mathbf{q} | F^\dagger \delta H F | \mathbf{q}_1, \mathbf{q}_2 \rangle\right|^2}{\varepsilon(q_1) + \varepsilon(q_2) - \hbar\omega}$$

RPA: $\delta u_{2..}(\mathbf{q}_i, \mathbf{q}_j, \dots; t) = 0$

- Correct long wavelength limit;
- No multi-phonon processes;
- Infinite lifetime.



Just keep diagonal term:

$$\langle \mathbf{q}_1, \mathbf{q}_2 | F^\dagger (\delta H - \hbar\omega) F | \mathbf{q}_3, \mathbf{q}_4 \rangle \approx S(q_1) S(q_2) \left[\varepsilon(q_1) + \varepsilon(q_2) - \hbar\omega\right] \delta_{\mathbf{q}_1, \mathbf{q}_3} \delta_{\mathbf{q}_2, \mathbf{q}_4}$$

Then

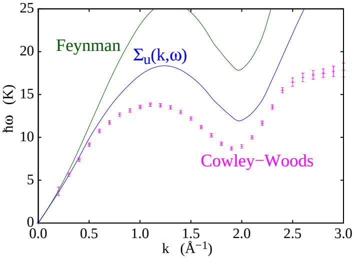
$$\Sigma_u(\mathbf{q}, \omega) = -\frac{1}{2} \sum_{\mathbf{q}_1 \mathbf{q}_2} \frac{\left| \langle \mathbf{q} | F^\dagger \delta H F | \mathbf{q}_1, \mathbf{q}_2 \rangle \right|^2}{\varepsilon(q_1) + \varepsilon(q_2) - \hbar\omega}$$

RPA: $\delta u_{2..}(\mathbf{q}_i, \mathbf{q}_j, \ldots; t) = 0$

- Correct long wavelength limit;
- No multi-phonon processes;
- Infinite lifetime.

Beyond RPA: $\delta u_2(\mathbf{q}_i, \mathbf{q}_j; t) \neq 0$:

- Includes "Phonon-splitting";



Just keep diagonal term:

$$\langle \mathbf{q}_1, \mathbf{q}_2 | F^\dagger (\delta H - \hbar\omega) F | \mathbf{q}_3, \mathbf{q}_4 \rangle \approx S(q_1) S(q_2) \left[\varepsilon(q_1) + \varepsilon(q_2) - \hbar\omega \right] \delta_{\mathbf{q}_1,\mathbf{q}_3} \delta_{\mathbf{q}_2,\mathbf{q}_4}$$

Then

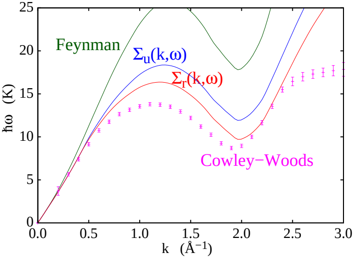
$$\Sigma_u(\mathbf{q},\omega) = -\frac{1}{2} \sum_{\mathbf{q}_1 \mathbf{q}_2} \frac{\left| \langle \mathbf{q} | F^\dagger \delta H F | \mathbf{q}_1, \mathbf{q}_2 \rangle \right|^2}{\varepsilon(q_1) + \varepsilon(q_2) - \hbar\omega}$$

RPA: $\delta u_{2..}(\mathbf{q}_i, \mathbf{q}_j, \ldots; t) = 0$

- Correct long wavelength limit;
- No multi-phonon processes;
- Infinite lifetime.

Beyond RPA: $\delta u_2(\mathbf{q}_i, \mathbf{q}_j; t) \neq 0$:

- Includes "Phonon-splitting";
- "renormalized" BW-CBF gets roton below 10K.



Large momentum limits

Because people ask for it...

The easy ones: m_0 and m_1 sum rules are satisfied *independently of the choice of the self-energy* (H. W. Jackson, PRA **9**, 964 (1974).

$$
\begin{aligned}
m_0(q) &= -\Im m \int_{-\infty}^{\infty} \frac{d(\hbar\omega)}{2\pi} \chi^{(CBF)}(q,\omega) \\
&= -\Im m \int_{-\infty}^{\infty} \frac{d(\hbar\omega)}{2\pi} \chi^{(RPA)}(q,\omega) = S(q) \\
m_1(q) &= -\Im m \int_{-\infty}^{\infty} \frac{d(\hbar\omega)}{2\pi} \hbar\omega \chi^{(CBF)}(q,\omega) \\
&= -\Im m \int_{-\infty}^{\infty} \frac{d(\hbar\omega)}{2\pi} \hbar\omega \chi^{(RPA)}(q,\omega) = t(q)
\end{aligned}
$$

The important point: These sum rules provide a unique definition of a local $V_{p-h}(q)$ from the ground state $S(q)$.

- Feenberg 1969,
  K. N. Pathak and P. Vashishta, Phys. Rev. B **7**, 3649 (1973).

$$
\begin{aligned}
m_3(q) &= -\Im m \int_{-\infty}^{\infty} \frac{d(\hbar\omega)}{2\pi} (\hbar\omega)^3 \chi(k,\omega) \\
&= 2t(k)\left[t^2(k) + 4t(k)\frac{T}{N} + 2t(k)\tilde{v}(k)\right] \\
&+ \left(\frac{\hbar^2}{m}\right)^2 \int \frac{d^d q}{(2\pi)^d \rho} (\mathbf{k}\cdot\mathbf{q})^2 \tilde{v}(q)(S(|\mathbf{k}-\mathbf{q}|) - S(q))\,,
\end{aligned}
$$

- Feenberg 1969,
  K. N. Pathak and P. Vashishta, Phys. Rev. B **7**, 3649 (1973).

$$
\begin{aligned}
m_3(q) &= -\Im m \int_{-\infty}^{\infty} \frac{d(\hbar\omega)}{2\pi} (\hbar\omega)^3 \chi(k,\omega) \\
&= 2t(k)\left[t^2(k) + 4t(k)\frac{T}{N} + 2t(k)\tilde{v}(k)\right] \\
&+ \left(\frac{\hbar^2}{m}\right)^2 \int \frac{d^d q}{(2\pi)^d \rho} (\mathbf{k}\cdot\mathbf{q})^2 \tilde{v}(q)(S(|\mathbf{k}-\mathbf{q}|) - S(q)) \,,
\end{aligned}
$$

- In BW perturbation theory/“uniform limit”
  leading terms for $q \to \infty$ exact;

Sum rules and limits

The m_3 sum rule... A mess, but the only useful one

- Feenberg 1969,
  K. N. Pathak and P. Vashishta, Phys. Rev. B **7**, 3649 (1973).

$$\begin{aligned} m_3(q) &= -\Im m \int_{-\infty}^{\infty} \frac{d(\hbar\omega)}{2\pi} (\hbar\omega)^3 \chi(k,\omega) \\ &= 2t(k)\left[t^2(k) + 4t(k)\frac{T}{N} + 2t(k)\tilde{v}(k)\right] \\ &+ \left(\frac{\hbar^2}{m}\right)^2 \int \frac{d^dq}{(2\pi)^d\rho} (\mathbf{k}\cdot\mathbf{q})^2 \tilde{v}(q)(S(|\mathbf{k}-\mathbf{q}|) - S(q)) \,, \end{aligned}$$

- In BW perturbation theory/“uniform limit”
  leading terms for $q \to \infty$ exact;
- Using full time-dependent pair correlations:
  probably exact (Calculation pretty messy...).

What we are after:

- Zero-energy-large-momentum limit:

$$\lim_{k\to\infty} \Sigma(k,0) = -\frac{4}{3}\frac{T}{N}$$

What we are after:

- Zero-energy-large-momentum limit:

$$\lim_{k\to\infty} \Sigma(k,0) = -\frac{4}{3}\frac{T}{N}$$

- On-shell, high momentum limit. Exact: “impulse approximation” (H. A. Gersch, L. J. Rodriguez and P.N. Smith, Phys. Rev. **A5**, 1547 (1972).

$$\chi(q,\omega) \to \frac{n_c}{t(q) - \hbar\omega + i\Lambda(q)} \qquad \Lambda(q) \to 0 \quad \text{as} \quad q \to \infty$$

as $q \to \infty$, $\hbar\omega \approx t(k)$ n_c: Condensate fraction

Large momentum transfer limit

BW for the sake of discussion:

$$\Sigma_u(q,\omega) = -\sum_n \frac{1}{n!} \sum_{\mathbf{q}_1,\ldots,\mathbf{q}_n} \frac{|\langle \mathbf{q}|\,\delta H\,|\mathbf{q}_1,\ldots,\mathbf{q}_n\rangle|^2}{S(\mathbf{q}_1)\ldots S(\mathbf{q}_n)(\varepsilon(q_1)+\ldots\varepsilon_n - \hbar\omega)}$$

For large q:

$$\langle \mathbf{q}|\,\delta H\,|\mathbf{q}_1,\ldots,\mathbf{q}_n\rangle \to \mathbf{q}\cdot\mathbf{h}(\mathbf{q}_2,\ldots,\mathbf{q}_n)\delta_{\mathbf{q},\mathbf{q}_1} + \text{cycl.}$$

Therefore:

$$\Sigma_u(q,\omega) = -\sum_n \frac{1}{(n-1)!} \sum_{\mathbf{q}_1,\ldots,\mathbf{q}_n} \frac{|\mathbf{q}\cdot\mathbf{h}(\mathbf{q}_2,\ldots,\mathbf{q}_n)|^2}{(t(\mathbf{q}-\mathbf{q}_1)-\hbar\omega)S(\mathbf{q}_2)\ldots S(\mathbf{q}_n)}$$

Full theory messier, correct to order ω^{-2} but basically the same.

$$\Sigma_u(q,0) = -\sum_n \frac{1}{(n-1)!} \sum_{\mathbf{q}_1,\ldots,\mathbf{q}_n} \frac{|\mathbf{q}\cdot\mathbf{h}(\mathbf{q}_2,\ldots,\mathbf{q}_n)|^2}{S(\mathbf{q}_2)\ldots S(\mathbf{q}_n)(t(q) - (\hbar\omega = 0)}$$

- Zero-energy-large-momentum limit given by kinetic energy:

$$\lim_{k\to\infty} \Sigma(k,0) = -\frac{4}{3}\frac{T}{N}$$

- Satisfied by BW in “uniform limit approximation”

$$\sqrt{g(r)} = \sqrt{1+g(r)-1} \approx 1 + \frac{1}{2}(g(r)-1)$$

- Satisfied exactly for correlation functions with full pair fluctuations
- Suggestive: Go to triplet fluctuations for triplet correlations...

$$\Sigma_u(q,0) = -\sum_n \frac{1}{(n-1)!} \sum_{\mathbf{q}_1,\ldots,\mathbf{q}_n} \frac{\delta(\mathbf{q}-\mathbf{q}_1-\ldots\mathbf{q}_n)\,|\mathbf{q}\cdot\mathbf{h}(\mathbf{q}_2,\ldots,\mathbf{q}_n)|^2}{S(\mathbf{q}_2)\ldots S(\mathbf{q}_n)(t(q)-\hbar\omega+\frac{\hbar^2}{m}\mathbf{q}\cdot\mathbf{q}_1)}$$

Recall general limit:

$$\chi(k,\omega) \to \nu_c/(t(q)-\hbar\omega+i\Lambda(q)) \qquad \Lambda(q)\to 0 \quad \text{as} \quad q\to\infty$$

- In RPA/Feynman/Bogoljubov: $\nu_c = 1$

$$\Sigma_u(q,0) = -\sum_n \frac{1}{(n-1)!} \sum_{\mathbf{q}_1,\ldots,\mathbf{q}_n} \frac{\delta(\mathbf{q}-\mathbf{q}_1-\ldots\mathbf{q}_n)\left|\mathbf{q}\cdot\mathbf{h}(\mathbf{q}_2,\ldots,\mathbf{q}_n)\right|^2}{S(\mathbf{q}_2)\ldots S(\mathbf{q}_n)(t(q)-\hbar\omega+\frac{\hbar^2}{m}\mathbf{q}\cdot\mathbf{q}_1)}$$

Recall general limit:

$$\chi(k,\omega) \to \nu_c/(t(q)-\hbar\omega+i\Lambda(q)) \qquad \Lambda(q)\to 0 \quad \text{as} \quad q\to\infty$$

- In RPA/Feynman/Bogoljubov: $\nu_c = 1$
- In 2^{nd} order BW: $\nu_c =$"uniform limit approximation" to n_c.
(H. W. Jackson, Phys. Rev. **185**, 186 (1969).)

$$\Sigma_u(q,0) = -\sum_n \frac{1}{(n-1)!} \sum_{\mathbf{q}_1,\ldots,\mathbf{q}_n} \frac{\delta(\mathbf{q}-\mathbf{q}_1-\ldots\mathbf{q}_n)\left|\mathbf{q}\cdot\mathbf{h}(\mathbf{q}_2,\ldots,\mathbf{q}_n)\right|^2}{S(\mathbf{q}_2)\ldots S(\mathbf{q}_n)(t(q)-\hbar\omega+\frac{\hbar^2}{m}\mathbf{q}\cdot\mathbf{q}_1)}$$

Recall general limit:

$$\chi(k,\omega) \to \nu_c/(t(q)-\hbar\omega+i\Lambda(q)) \qquad \Lambda(q)\to 0 \quad \text{as} \quad q\to\infty$$

- In RPA/Feynman/Bogoljubov: $\nu_c = 1$
- In 2^{nd} order BW: $\nu_c =$"uniform limit approximation" to n_c.
  (H. W. Jackson, Phys. Rev. **185**, 186 (1969).)
- Full time-dependent pair correlations:
  Coefficient ν_c similar but analytically different from Ristig-Clark-Fantoni analysis (See poster by M. Saarela).

$$\Sigma_u(q,0) = -\sum_n \frac{1}{(n-1)!} \sum_{\mathbf{q}_1,\ldots,\mathbf{q}_n} \frac{\delta(\mathbf{q}-\mathbf{q}_1-\ldots\mathbf{q}_n)\,|\mathbf{q}\cdot\mathbf{h}(\mathbf{q}_2,\ldots,\mathbf{q}_n)|^2}{S(\mathbf{q}_2)\ldots S(\mathbf{q}_n)(t(q)-\hbar\omega+\frac{\hbar^2}{m}\mathbf{q}\cdot\mathbf{q}_1)}$$

Recall general limit:

$$\chi(k,\omega) \to \nu_c/(t(q)-\hbar\omega+i\Lambda(q)) \qquad \Lambda(q)\to 0 \quad \text{as} \quad q\to\infty$$

- In RPA/Feynman/Bogoljubov: $\nu_c = 1$
- In 2nd order BW: $\nu_c =$"uniform limit approximation" to n_c.
(H. W. Jackson, Phys. Rev. **185**, 186 (1969).)
- Full time-dependent pair correlations:
Coefficient ν_c similar but analytically different from Ristig-Clark-Fantoni analysis (See poster by M. Saarela).
- Corrections from triplet and likely higher fluctuations.