Dynamic Many-Body Correlations

New developments

with C. E. Campbell, H. M. Böhm, M. Panholzer (Theory)[1]
and H. Godfrin and H. J. Lauter (Experiment)[2]

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Chinfest, March 24-26, 2009

FWF
Der Wissenschaftsfonds.

Outline

Microscopic Hamiltonian

$$H = \sum_i \left[-\frac{\hbar^2}{2m}\nabla_i^2 + U_{ext}(\mathbf{r}_i) \right] + \sum_{i<j} v(|\mathbf{r}_i - \mathbf{r}_j|)$$

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..the way it should be solved for a robust theory

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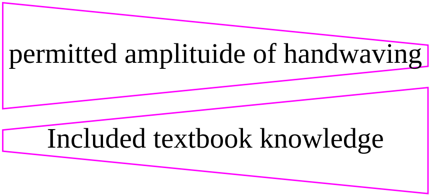

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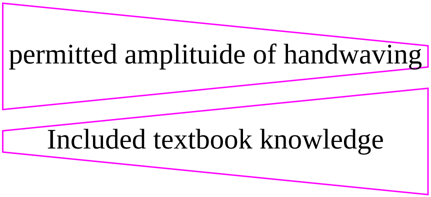

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- Variational methods
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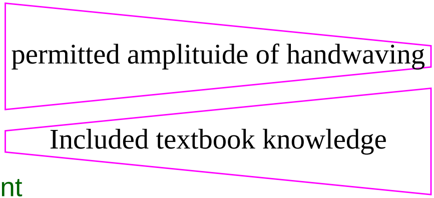
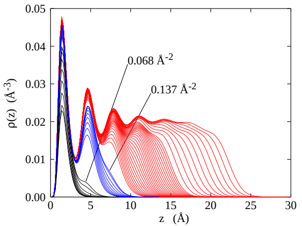


Methods: Correlated wave functions
For those who like it simple..

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

$$\Psi_0(1,\ldots,N) = \exp\frac{1}{2}\left[\sum_i u_1(\mathbf{r}_i) + \sum_{i<j} u_2(\mathbf{r}_i,\mathbf{r}_j) + \ldots\right]\Phi_0(1,\ldots,N)$$
$$\equiv F(1,\ldots,N)\Phi_0(1,\ldots,N)$$

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



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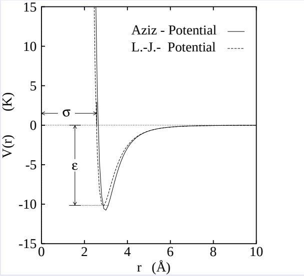

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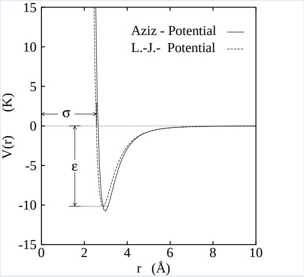

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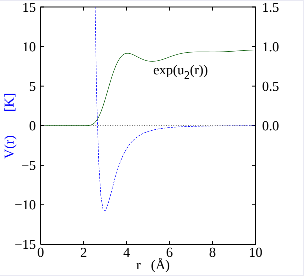

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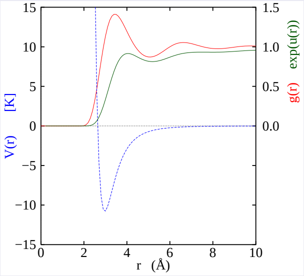

- An intuitive way to include inhomogeneity and core exclusion;
- Diagram summation methods from classical statistics (HNC, PY, BGY);
- Optimization $\delta E/\delta u_n = 0$ makes correlations unique.
- Express everything in terms of physical observables (*i.e.* $g(r)$).

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

Summarizing its two faces

"RPA" face (Campbell, Feenberg 1969)

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

$$S(q) = -\frac{\hbar}{\pi}\int d\omega\, \Im m\, \chi(q,\omega)$$

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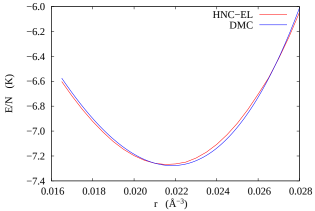
“...it appears that the optimized Jastrow function is capable of summing all rings and ladders, and partially all other diagrams, to infinite order.”

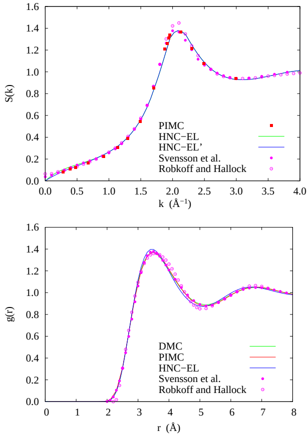
H.-K. Sim, C.-W. Woo and J. R. Buchler, Phys Rev. A2, 2024 (1970).

Application I: How well it works in the bulk
Bragbook :)

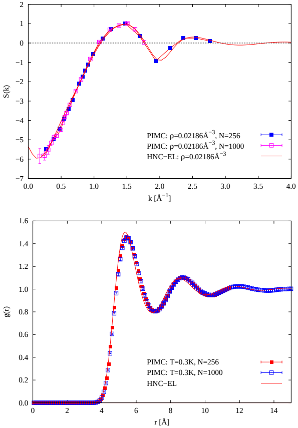
- Equation of state



- Equation of state
- Distribution and structure functions



- Equation of state
- Distribution and structure functions
- Many other quantities, for example impurity properties (Example: Mg impurities, note the huge core)



Application (one of many...)

Aerogels, Gaps (work with Vesa Apaja)

- Two rigid walls at a distance

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Example: a 14 Å wide gap

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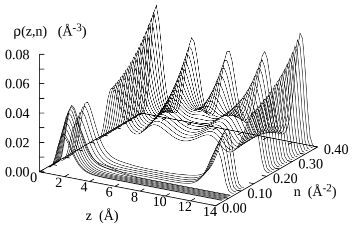

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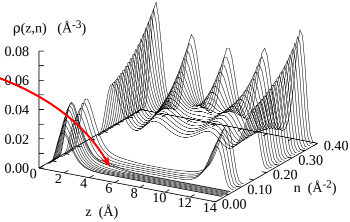
  - Sticking to walls



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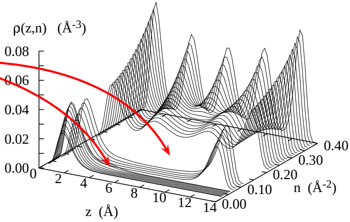

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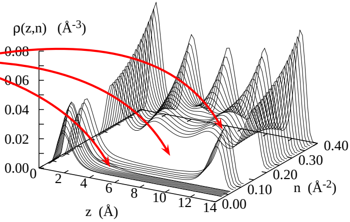

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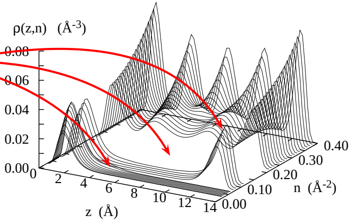

But what could one see experimentally ?

Another example:

- Two rigid walls at double-layer distance
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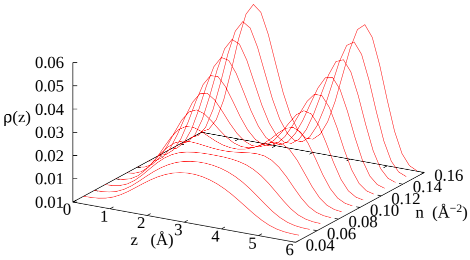

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  - Much larger local density than in bulk
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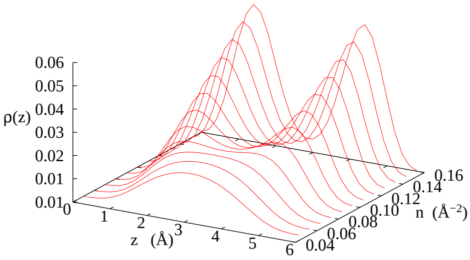

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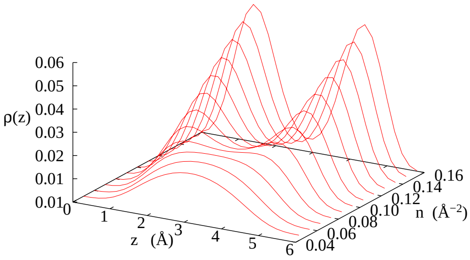

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Wave function for excited states:

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

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

Bosons:

$$\delta U(t) = \sum_i \delta u^{(1)}(\mathbf{r}_i; t) + \sum_{i<j} \delta u^{(2)}(\mathbf{r}_i, \mathbf{r}_j; t) + \ldots$$

Fermions:

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

Action principle:

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

- Linearization:

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

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

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- Dynamic response function:

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

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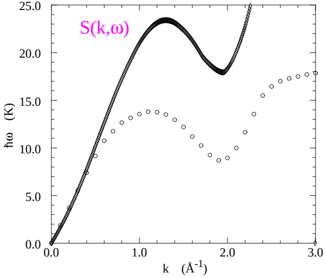
- Dynamic structure function:

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

- "Feynman approximation" $\delta u^{(2)}(\mathbf{r},\mathbf{r}') = 0$ leads to

$$\hbar\omega(k) = \frac{\hbar^2 k^2}{2mS(k)}:$$

off by a factor of two;



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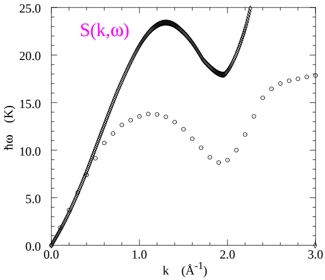

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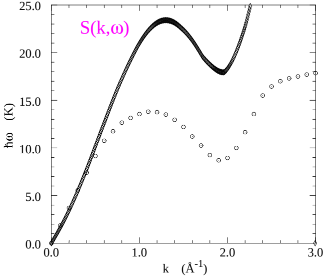

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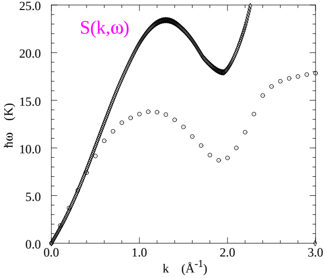
- Expect a similar effect in ^{3}He.



Boson equations of motion

Where the hard work begins – sorry for becoming technical

- Include pair and triplet fluctuations $\delta u^{(n)}(\mathbf{r}_1, \ldots, \mathbf{r}_n), \quad n = 1..3$

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- Calculate density fluctuation:

$$
\begin{aligned}
\delta\rho_1(\mathbf{r};t) &= \int d^3r_1 \frac{\delta\rho_1(\mathbf{r})}{\delta u_1(\mathbf{r}_1)} \delta u_1(\mathbf{r}_1;t) \\
&+ \int d^3r_1 d^3r_2 \frac{\delta\rho_1(\mathbf{r})}{\delta u_2(\mathbf{r}_1,\mathbf{r}_2)} \delta u_2(\mathbf{r}_1,\mathbf{r}_2;t) \\
&+ \int d^3r_1 d^3r_2 d^3r_3 \frac{\delta\rho_1(\mathbf{r})}{\delta u_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)} \delta u_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3;t)\,.
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- The key step:Define $\delta v_1(\mathbf{r};t)$ by

$$\delta\rho_1(\mathbf{r};t) \equiv \int d^3r_1 \frac{\delta\rho_1(\mathbf{r})}{\delta u_1(\mathbf{r}_1)}\,\delta v_1(\mathbf{r}_1;t)$$

- Include pair and triplet fluctuations $\delta u^{(n)}(\mathbf{r}_1, \ldots, \mathbf{r}_n), \quad n = 1..3$
- Calculate density fluctuation:

$$\begin{aligned}\delta\rho_1(\mathbf{r};t) &= \int d^3r_1 \frac{\delta\rho_1(\mathbf{r})}{\delta u_1(\mathbf{r}_1)}\delta u_1(\mathbf{r}_1;t) \\ &+ \int d^3r_1 d^3r_2 \frac{\delta\rho_1(\mathbf{r})}{\delta u_2(\mathbf{r}_1,\mathbf{r}_2)}\delta u_2(\mathbf{r}_1,\mathbf{r}_2;t) \\ &+ \int d^3r_1 d^3r_2 d^3r_3 \frac{\delta\rho_1(\mathbf{r})}{\delta u_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)}\delta u_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3;t)\,.\end{aligned}$$

- The key step:Define $\delta v_1(\mathbf{r};t)$ by

$$\delta\rho_1(\mathbf{r};t) \equiv \int d^3r_1 \frac{\delta\rho_1(\mathbf{r})}{\delta u_1(\mathbf{r}_1)}\,\delta v_1(\mathbf{r}_1;t)$$

- Invert the relationship in terms of “direct correlation functions”.

Same thing for pair fluctuations:

$$\begin{aligned}
\delta g_2(\mathbf{r},\mathbf{r}';t) &= \int d^3r_1 \frac{\delta g_2(\mathbf{r},\mathbf{r}')}{\delta u_1(\mathbf{r}_1)} \delta u_1(\mathbf{r}_1;t) \\
&+ \int d^3r_1 d^3r_2 \frac{\delta g_2(\mathbf{r},\mathbf{r}')}{\delta u_2(\mathbf{r}_1,\mathbf{r}_2)} \delta u_2(\mathbf{r}_1,\mathbf{r}_2;t) \\
&+ \int d^3r_1 d^3r_2 d^3r_3 \frac{\delta g_2(\mathbf{r},\mathbf{r}')}{\delta u_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)} \delta u_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3;t) \\
&\equiv \int d^3r_1 \frac{\delta g_2(\mathbf{r},\mathbf{r}')}{\delta v_1(\mathbf{r}_1)} \delta v_1(\mathbf{r}_1;t) \\
&+ \int d^3r_1 d^3r_2 \frac{\delta g_2(\mathbf{r},\mathbf{r}')}{\delta u_2(\mathbf{r}_1,\mathbf{r}_2)} \delta v_2(\mathbf{r}_1,\mathbf{r}_2;t)\,.
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\end{aligned}$$

Invert the relationship in terms of “direct correlation functions”.

Lagrangian in the new variables:

$$\mathcal{L}(t) = \left\langle \Psi(t) \middle| H + U_{ext}(t) - i\hbar \frac{\partial}{\partial t} \middle| \Psi(t) \right\rangle$$
$$= \mathcal{L}_{ext}(t) + \mathcal{L}_t(t) + \mathcal{L}_{int}(t)$$

Equations of motion:

$$\frac{\delta \mathcal{L}}{\delta v_n^*}(\mathbf{r}_1, \ldots \mathbf{r}_n; t) = 0$$

External Field term:

$$\mathcal{L}_{ext}(t) = \int d^3r U_{ext}(\mathbf{r}) \delta\rho_1(\mathbf{r}; t) = \Re e \left[\int d^3r U_{ext}(\mathbf{r}) \frac{\delta\rho_1(\mathbf{r})}{\delta u_1(\mathbf{r}')} \delta v_1(\mathbf{r}'; t) \right]$$

The external field term contributes only to the one-body equation !

$$\mathcal{L}_t(t) = -\frac{i\hbar}{4}\left[\langle\Psi_0|\,\delta U^*\delta\dot{U}\,|\Psi_0\rangle - \langle\Psi_0|\,\delta U^*\,|\Psi_0\rangle\,\langle\Psi_0|\,\delta\dot{U}\,|\Psi_0\rangle\right]$$

$$\frac{\delta\mathcal{L}_t(t)}{\delta v_n^*(\mathbf{r}_1,\ldots,\mathbf{r}_n;t)} = \frac{i\hbar}{4n!}\int d^3r_1'\ldots d^3r_n'\frac{\delta\rho_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)}{\delta u_n(\mathbf{r}_1',\ldots,\mathbf{r}_n')}\delta\dot{v}_n(\mathbf{r}_1',\ldots,\mathbf{r}_n';t)\,.$$

The time-derivative term is *diagonal* in the new variables

Current: For Jastrow-correlations, $\mathbf{j}(\mathbf{r};t)$ does not depend on $\delta v_3(\mathbf{r}_i;t)$:

$$\frac{\mathbf{j}(\mathbf{r};t)}{\rho_1(\mathbf{r})} = \frac{\hbar}{2mi}\left[\nabla\delta v_1(\mathbf{r};t) - \frac{1}{2}\int d^3r_1 d^3r_2\delta v_2(\mathbf{r}_1,\mathbf{r}_2;t)\nabla_{\mathbf{r}}\frac{\delta\rho_2(\mathbf{r}_1,\mathbf{r}_2)}{\delta\rho_1(\mathbf{r})}\right]$$

even if fluctuating triplet correlations are included.

Lagrangian in the new coordinates:
Interaction term

$$\mathcal{L}_{int}(t) = \frac{m}{2}\int d^3\rho\,|\mathbf{v}(\mathbf{r};t)|^2 + \sum_{i,j=2}^{3}\mathcal{L}_{int}^{(ij)}(t)$$

- Velocity field $\mathbf{v}(\mathbf{r};t) = \mathbf{j}(\mathbf{r};t)/\rho(\mathbf{r})$ does not depend on δv_3.
- $\mathcal{L}_{int}^{(ij)}(t)$ is a symmetric quadratic form of δv_2 and δv_3.
- Two- and three-body equations:

$$\begin{aligned} & \rho_1(\mathbf{r}_1)\rho_1(\mathbf{r}_2)\left[\mathcal{E}_{22}(\omega)*\delta v_2(\omega)+\mathcal{E}_{23}*\delta v_3(\omega)\right](\mathbf{r}_1,\mathbf{r}_2;\omega) \\ = & \; i\hbar\int d^3r_3\,\mathbf{j}(\mathbf{r}_3;\omega)\cdot\nabla_{\mathbf{r}_3}\frac{\delta\rho(\mathbf{r}_1,\mathbf{r}_2)}{\delta\rho_1(\mathbf{r}_3)} \\ 0 = & \; \rho_1(\mathbf{r}_1)\rho_1(\mathbf{r}_2)\left[\mathcal{E}_{32}*\delta v_2(\omega)+\mathcal{E}_{33}(\omega)*\delta v_3(\omega)\right](\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3;\omega) \end{aligned}$$

- $\Rightarrow$ External field appears only in the one-body equation

General pair equation:

$$\begin{aligned}\left[\mathcal{E}(\omega) * \delta v_2(\omega)\right](\mathbf{r}_1, \mathbf{r}_2; \omega) &= \frac{i\hbar}{\rho_1^2} \int d^3 r_3\, \mathbf{j}(\mathbf{r}_3; \omega) \cdot \nabla_{\mathbf{r}_3} \frac{\delta \rho_2(\mathbf{r}_1, \mathbf{r}_2)}{\delta \rho_1(\mathbf{r}_3)} \\ \mathcal{E}(\omega) &= \mathcal{E}_{22}(\omega) - \mathcal{E}_{23} * \mathcal{E}_{33}^{-1}(\omega) * \mathcal{E}_{32} \\ \mathcal{E}_{ii}(\omega) &= \mathcal{T}_{ii} - \hbar\omega\mathcal{G}_{ii} \qquad i = 1, 2\end{aligned}$$

Note: $\mathcal{E}_{23}$ is energy independent due to choice of variables $\delta v_i(\mathbf{r}_1, \ldots; t)$.

General structure of the solution

After lenghty algebra. . .

Response function

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

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Self-energy

$$\Sigma(\mathbf{q},\omega) = \varepsilon(q) - \frac{1}{2}\sum_{\mathbf{q}_i} \langle \mathbf{q}| V^{(3)} |\mathbf{q}_1,\mathbf{q}_2\rangle\, \mathcal{E}^{-1}(\omega) \left\langle \mathbf{q}_1'\mathbf{q}_2' \right| V^{(3)} |\mathbf{q}\rangle$$

The only freedom is how to calculate the ingredients

General structure of the energy denominator:

$$\mathcal{E}(\omega) = \mathcal{E}_{22}(\omega) - \mathcal{E}_{23} * \mathcal{E}_{33}^{-1}(\omega) * \mathcal{E}_{32} = \mathcal{E}_{22}(\omega) + \mathcal{O}(\omega^{-1})$$

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$$\chi^{1-body}(\mathbf{q};\omega) \sim \omega^{-2} \quad \text{as} \quad \omega \to \infty$$
$$\chi^{2-body}(\mathbf{q};\omega) - \chi^{1-body}(\mathbf{q};\omega) \sim \omega^{-4} \quad \text{as} \quad \omega \to \infty$$
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Sum rules up to ω^3 are exactly satisfied already in pair fluctuation approximation.

Sum rules
some rigorous conclusions

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Sum rules up to ω^3 are exactly satisfied already in pair fluctuation approximation.

Note the consequences for the ground state theory !

General structure of the solution
Where it all boins down to

Self-energy

$$\Sigma(\mathbf{q},\omega) = \varepsilon(q) - \frac{1}{2}\sum_{\mathbf{q}_i} \langle \mathbf{q}|\, V^{(3)}\, |\mathbf{q}_1,\mathbf{q}_2\rangle\, \mathcal{E}^{-1}(\omega)\, \langle \mathbf{q}_1'\mathbf{q}_2'|\, V^{(3)}\, |\mathbf{q}\rangle$$

The only freedom is how to calculate the ingredients

Hiearchy of approximations:

- ‘Uniform Limit Approximation”-approximation: $\mathcal{E}(\omega)$ is diagonal im momentum space (not limited to pair fluctuations).
- Pair-Approximation: $\mathcal{E}(\omega) = \mathcal{E}_{22}(\omega) = \mathcal{T}_{22} - \hbar\omega\mathcal{G}_{22}$
- Full HNC+”elementaries”+”triplets” implementation of the pair theory

Note: “Uniform-Limit” + “pair-approximation” = BW-CBF result by Jackson, Feenberg, Campbell

Diagrammatic analysis

General "energy denominator"

$$\mathcal{E}_{22}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2; \hbar\omega) = -\hbar\omega\mathcal{G}_{22}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2)$$
$$-\frac{\hbar^2}{2\rho_1 m}\nabla_1 \cdot \left[\delta(\mathbf{r}_1 - \mathbf{r}'_1)\mathcal{F}_{22}(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}'_2)\right] \nabla'_1 + \ \{1, 1'\} \leftrightarrow \{2, 2'\}$$

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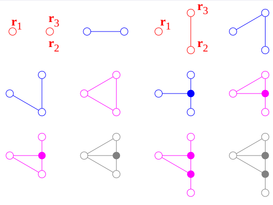
"Kinetic energy"

$$\mathcal{F}_{22}(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) = g_2(\mathbf{r}_1, \mathbf{r}_2)\frac{\delta(\mathbf{r}_2 - \mathbf{r}_3)}{\rho_1} + g_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) - g_2(\mathbf{r}_1, \mathbf{r}_2)g_2(\mathbf{r}_1, \mathbf{r}_3)$$

Long-wavelength property:

$$\rho_1 \int d^3r_2 \mathcal{F}_{22}(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) = 0$$

group like-colored diagrams !



Diagrammatic analysis

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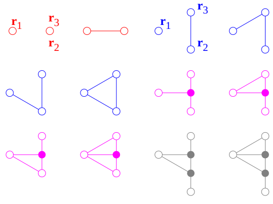
Short-distance property:

$$\mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)\to 0 \text{ as } |\mathbf{r}_1-\mathbf{r}_{\{2,3\}}|\to 0$$

group like-colored diagrams !



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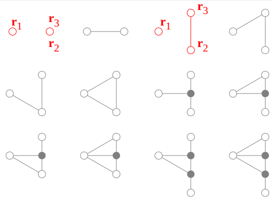
- Must sum infinitely many diagrams !
- "Convolution dapproximation" omits all but two
- Similar analysis for $\mathcal{G}_{22}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}'_1,\mathbf{r}'_2)$



Diagrammatic analysis

The driving term:

$$\frac{1}{\rho_1^2}\frac{\delta\rho_2(\mathbf{r}_1,\mathbf{r}_2)}{\delta\rho_1(\mathbf{r}_3)} = \frac{1}{\rho_1}g(\mathbf{r}_1-\mathbf{r}_2)\left[\delta(\mathbf{r}_1-\mathbf{r}_3)+\delta(\mathbf{r}_1-\mathbf{r}_3)\right] + \frac{\delta g(\mathbf{r}_1,\mathbf{r}_2)}{\delta\rho_1(\mathbf{r}_3)}$$

Defined in terms of multiparticle densities !

Diagrammatic analysis

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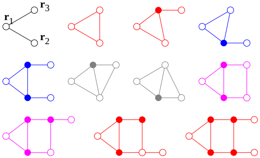
Defined in terms of multiparticle densities !

Long-wavelenth property:

$$\rho_1 \int d^3 r_1 \frac{\delta g(\mathbf{r}_1,\mathbf{r}_2)}{\delta\rho_1(\mathbf{r}_3)} = -\left[g(\mathbf{r}_2,\mathbf{r}_3)-1\right]$$

group like-colored diagrams !



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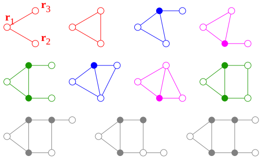

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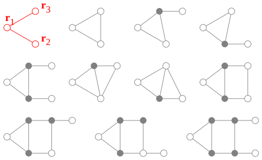
Defined in terms of multiparticle densities !

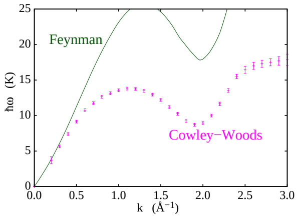
Summarizing:

- Must sum infinitely many diagrams !
- “Convolution approximation” keeps only the first
- Triplets must be added



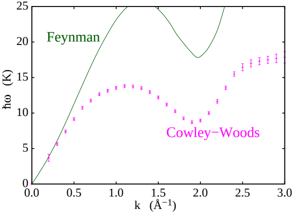
RPA: $\delta u_{2..}(\mathbf{r}_i, \mathbf{r}_j, \ldots; t) = 0$

- Correct long wavelength limit;



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

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



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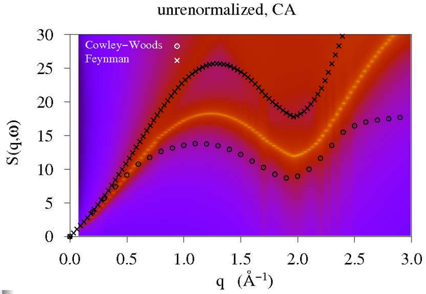
Pair fluctuations:

- Includes "Phonon-splitting";



Bulk ^{4}He
One and two-phonon excitations

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

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Pair fluctuations:

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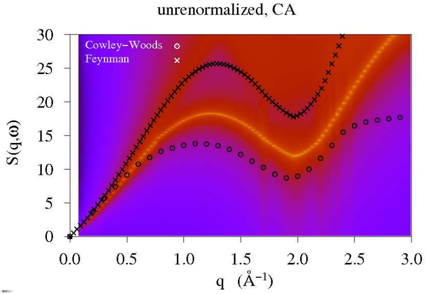
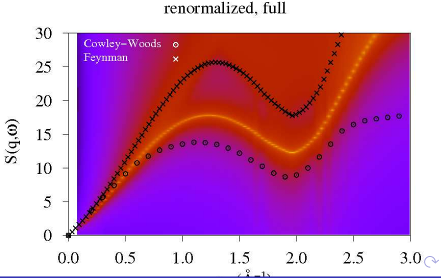
- "All the works" just as good (or bad) as CA !





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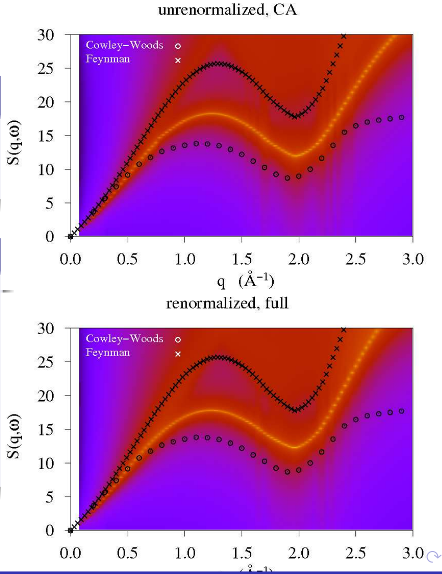
- CA will do for most purposes



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Pair fluctuations:

- Includes "Phonon-splitting";
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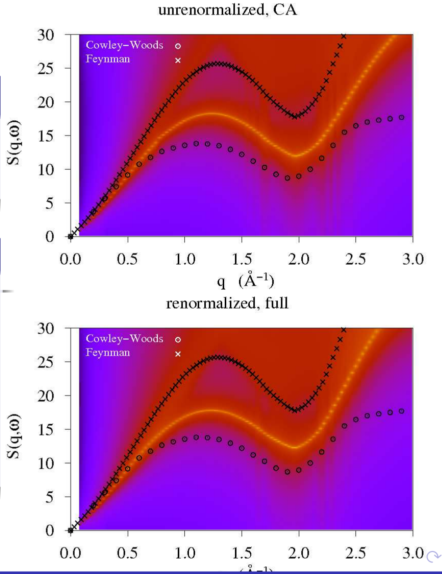
- "Plateau" still missing



- Include triplet fluctuations $\delta u^{(3)}(\mathbf{r}, \mathbf{r}', \mathbf{r}'')$

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- “Uniform limit” is sufficient !
- Technical details complicated and messy, but we get a plausible expression:

$$\Sigma^{(3)}(\mathbf{q},\omega) = \varepsilon(q) - \frac{1}{2}\sum_{\mathbf{q}_1\mathbf{q}_2} \frac{\left|\langle\mathbf{q}|\, V^{(3)}\, |\mathbf{q}_1,\mathbf{q}_2\rangle\right|^2}{\Sigma^{(2)}(q_1,\omega-\varepsilon(q_2)) + \Sigma^{(2)}(q_2,\omega-\varepsilon(q_1)) - \hbar$$

Going beyond:
Three-phonon excitations

- Include triplet fluctuations $\delta u^{(3)}(\mathbf{r},\mathbf{r}',\mathbf{r}'')$
- "Uniform limit" is sufficient !
- Technical details complicated and messy, but we get a plausible expression:

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- Using Feynman energies in the denominator falls back to BW-CBF

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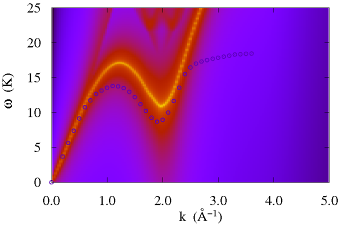
- Using Feynman energies in the denominator falls back to BW-CBF
- With some precognition replace the Feynman energies by full self-energies.

Self-consistent self-energy

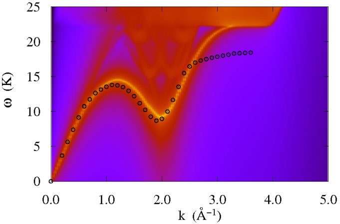
- Convolution approximation (BW-CBF)



Three-phonon excitations
.. and beyond...

Self-consistent self-energy

- Convolution approximation (BW-CBF)
- 1^{st} iteration self-consistency



Self-consistent self-energy

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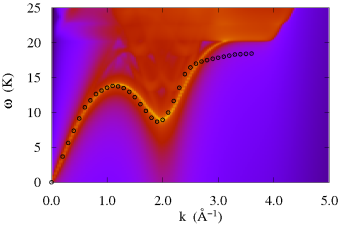

Three-phonon excitations
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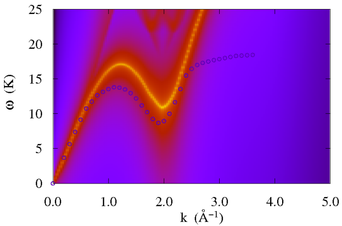
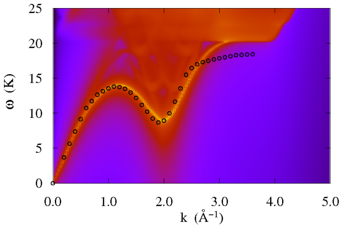
Summarizing:

- Iterations quite easy





Three-phonon excitations
.. and beyond...

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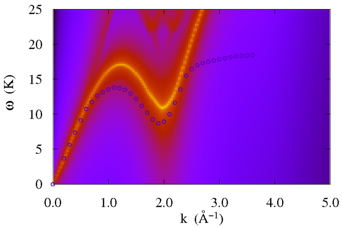
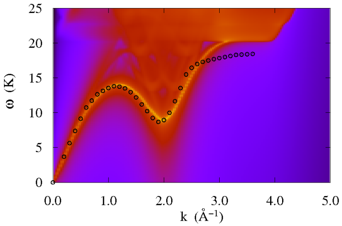
Summarizing:

- Iterations quite easy
- Triplet-Vertex about 10 percent short





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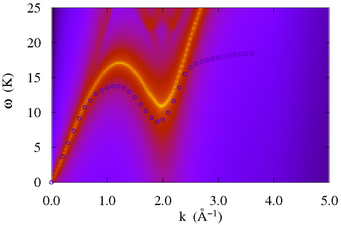

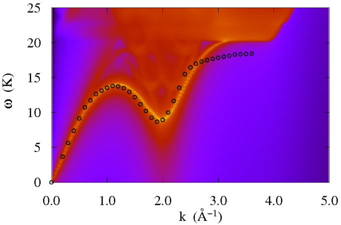

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Summarizing:

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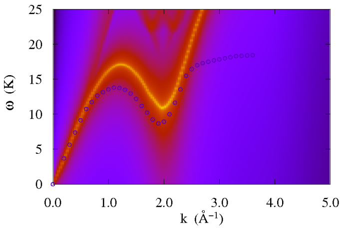
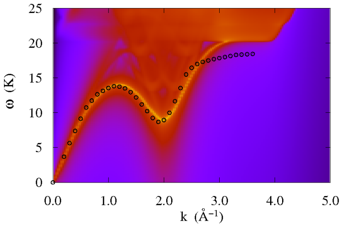
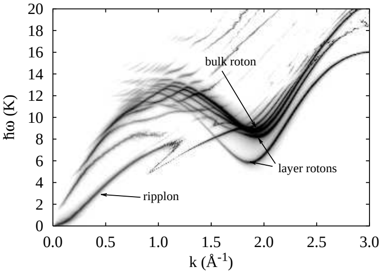
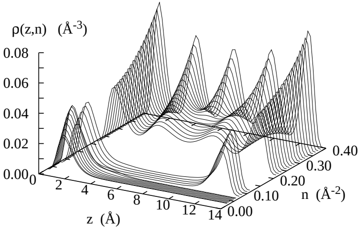
- Converges –expectedly– to plateau
- Inhomogeneous generalization possible





Fully confined fluids:
Layer rotons - 2D rotons ?





"We can identify the layer roton because its energy is like the 2D roton"

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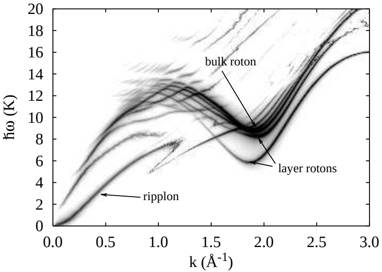
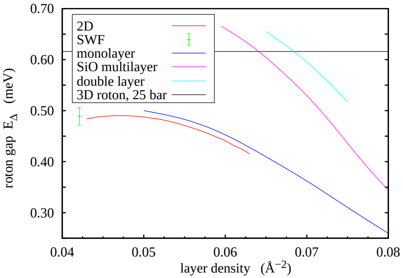




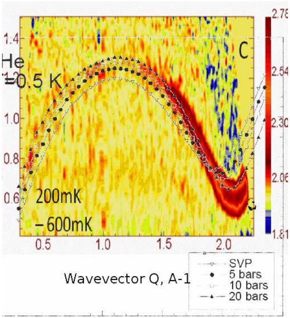
"We can identify the layer roton because its energy is like the 2D roton"

Can we ?

Fully confined fluids:

A bit on solid ^{4}He

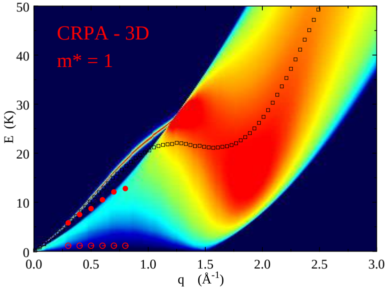
- Neutron scatterin on solid ^{4}He (Lauter and Godfrin, ILL)
- Subtract off Bragg peaks
- Clear presence of *two* rotons below bulk roton
- One of the “rotons” disapppears after annealing
- Comparison with theory: System must contain at least liquid double-layers



What we were told in (some) textbooks:

Dynamic structure function:

$$S(q,\omega) = \frac{1}{\pi}\Im m\,\chi(q,\omega)$$



- interested (for the time being) in *density fluctuations;*

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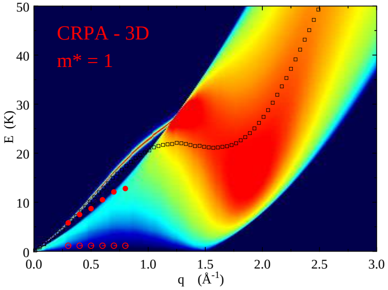

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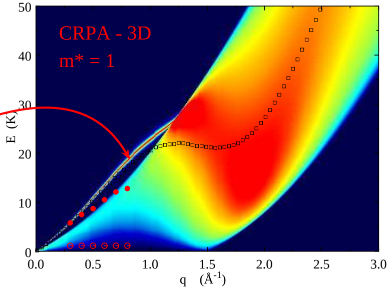

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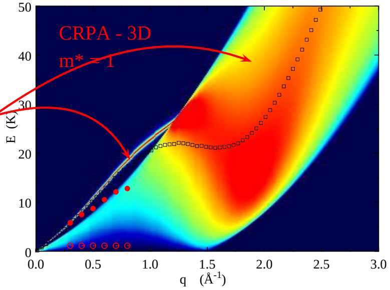
Particle-hole continuum at

$$e(q-k_F) \leq \hbar\omega \leq e(q+k_F)$$



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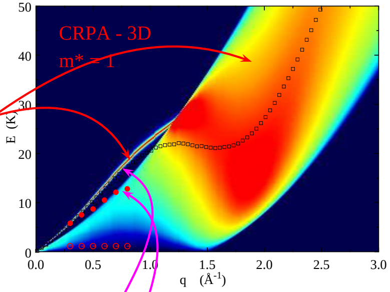
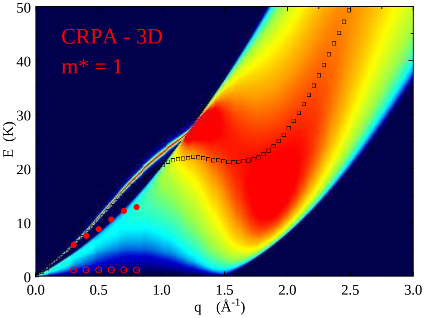


- interested (for the time being) in *density fluctuations;*
- similar effect as for bosons: *RPA is too high compared to experiments.*

- Recall where we started
- An effective mass can (potentially) explain $S(q,\omega)$
- BUT the effective mass is far from constant
- BUT an effective mass messes up sum rules



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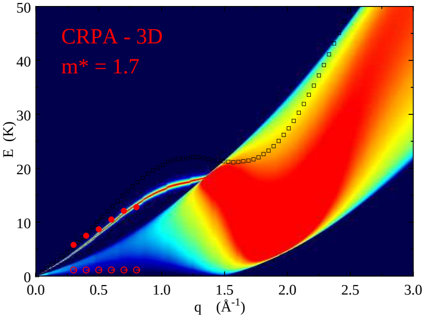

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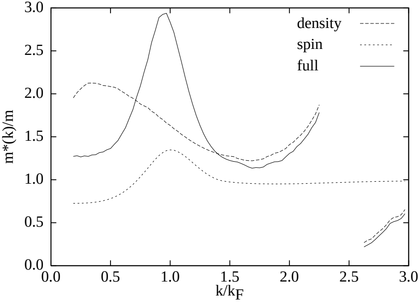

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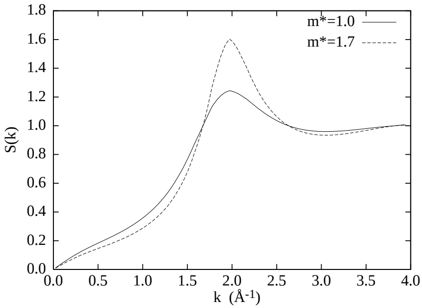
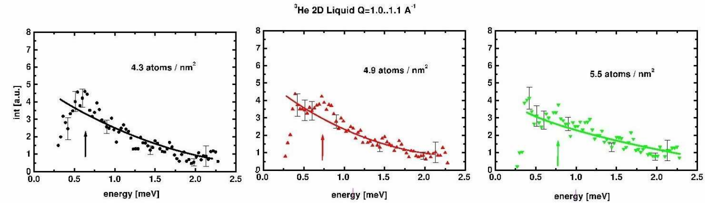


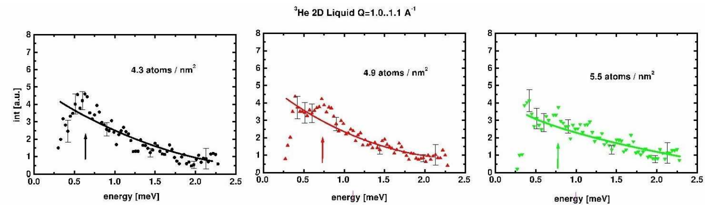
$$m_0(q) \equiv \int_0^\infty d(\hbar\omega) S(q,\omega) = S(q)$$

$$m_1(q) \equiv \int_0^\infty d(\hbar\omega)(\hbar\omega) S(q,\omega) = \frac{\hbar^2 q^2}{2m}$$

$S(k,\omega)$ in two dimensional ^{3}He – the key experiment

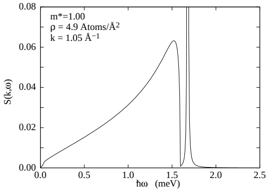
ILL/CNRS measurements: Godfrin, Lauter, Meschke





- RPA gives wrong position of the collective mode relative to the continuum;

$$\frac{m^*}{m} = 1$$



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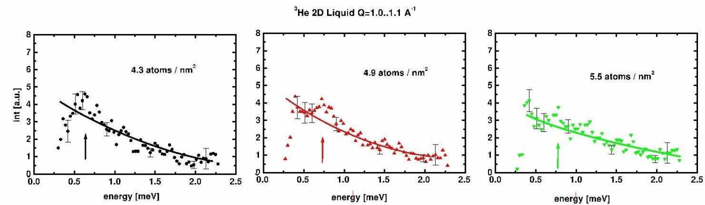
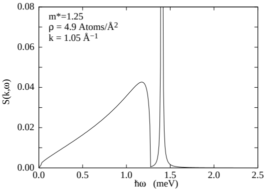


- RPA gives wrong position of the collective mode relative to the continuum;
- Messing with m^* does not help !

$$\frac{m^*}{m} = 1.25$$



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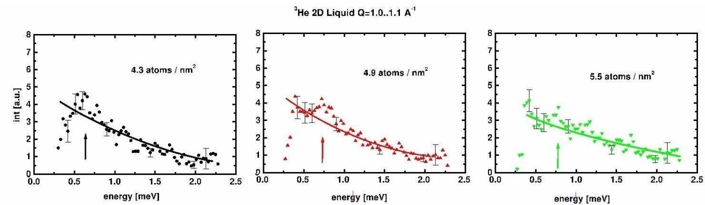

- RPA gives wrong position of the collective mode relative to the continuum;
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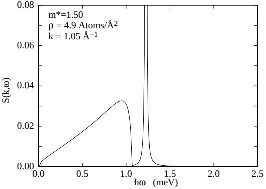
$$\frac{m^*}{m} = 1.50$$



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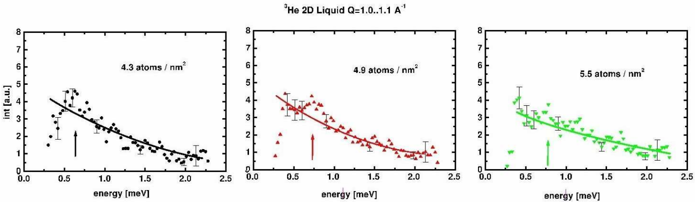

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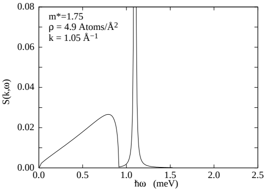
$$\frac{m^*}{m} = 1.75$$



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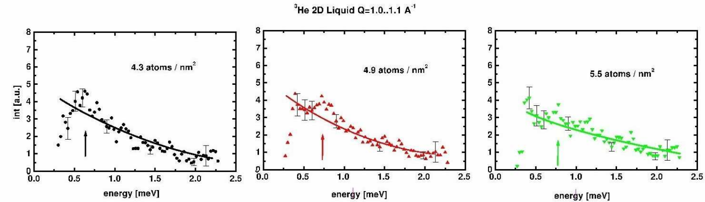

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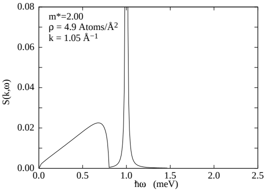
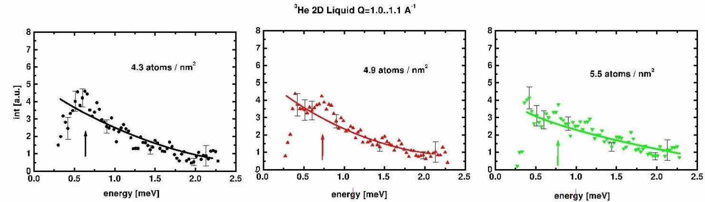
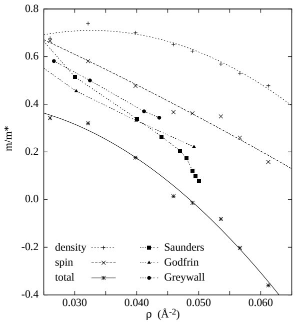
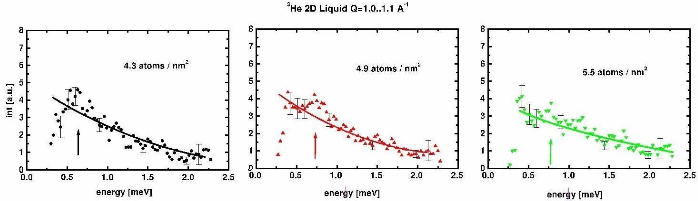
$$\frac{m^*}{m} = 2.00$$





- m^* grows with density – RPA would then predict that the collective mode comes down with density. But the collective mode goes up





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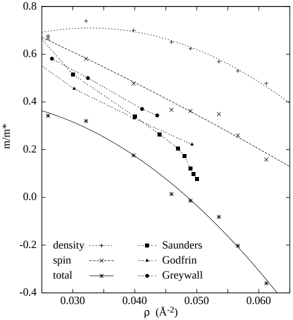
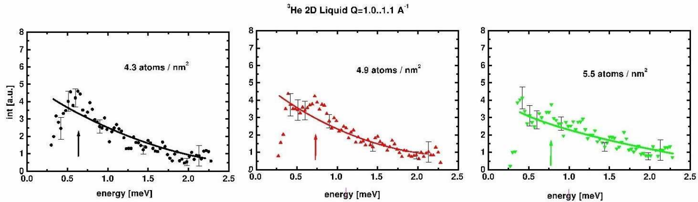
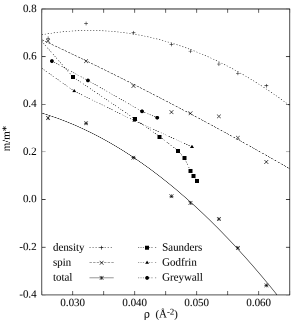
- We must either lower the collective mode through the continuum or demonstrate a significant "pair excitation continuum"





- m^* grows with density – RPA would then predict that the collective mode comes down with density. But the collective mode goes up
- We must either lower the collective mode through the continuum or demonstrate a significant "pair excitation continuum"
- There is every reason to expect that "pair excitations" are in ^{3}He just as important as in ^{4}He.



Recall EOM for bosons:
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:

$$\delta U(t) = \sum_i \delta u^{(1)}(\mathbf{r}_i;t) + \sum_{i<j} \delta u^{(2)}(\mathbf{r}_i,\mathbf{r}_j;t) + \ldots$$

Fermions:

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

• The problem is the sheer number of variables together with exchange diagrams !

- $\delta u^{(2)}_{\mathbf{ph},\mathbf{p'h'}}(t) = 0$, $F = 1$, weakly interacting Hamiltonian:

$$\begin{pmatrix} e_{ph} - \hbar\omega + V^{(A)}_{ph',hp'} & V^{(B)}_{pp',hh'} \\ V^{(B)}_{hh,pp'} & e_{ph} + \hbar\omega + V^{(A)}_{hp',ph'} \end{pmatrix} \begin{pmatrix} \delta u^{(1)}_{ph} \\ \delta u^{*(1)}_{ph} \end{pmatrix} = \begin{pmatrix} U^{(ext)}_{ph} \\ U^{*(ext)}_{ph} \end{pmatrix}$$

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- Set $V^{(A)}_{ph',hp'} = V^{(B)}_{pp',hh'} = V_{ph}(q)$ leads to ordinary RPA.
- $F \neq 1$: Replace bare interaction matrix elements by effective screened matrix elements: Makes theory applicable for strongly interacting systems. Omitting exchanges leads to “correlated” RPA.

- $\delta u^{(2)}_{\mathbf{ph},\mathbf{p'h'}}(t) = 0$, $F = 1$, weakly interacting Hamiltonian:

$$\begin{pmatrix} e_{ph} - \hbar\omega + V^{(A)}_{ph',hp'} & V^{(B)}_{pp',hh'} \\ V^{(B)}_{hh,pp'} & e_{ph} + \hbar\omega + V^{(A)}_{hp',ph'} \end{pmatrix} \begin{pmatrix} \delta u^{(1)}_{ph} \\ \delta u^{*(1)}_{ph} \end{pmatrix} = \begin{pmatrix} U^{(ext)}_{ph} \\ U^{*(ext)}_{ph} \end{pmatrix}$$

- Set $V^{(A)}_{ph',hp'} = V^{(B)}_{pp',hh'} = V_{ph}(q)$ leads to ordinary RPA.
- $F \neq 1$: Replace bare interaction matrix elements by effective screened matrix elements: Makes theory applicable for strongly interacting systems. Omitting exchanges leads to “correlated” RPA.
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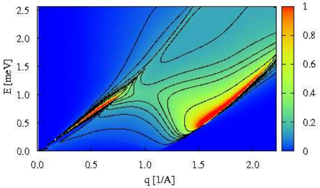
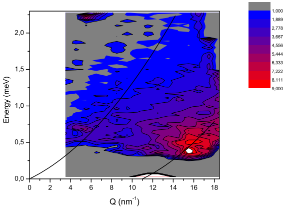
- Knowing how to do triplets was a big help

Pair excitations for Fermions
Results for 2D ^{3}He

Theory

ILL/CNRS experiment





- Pair fluctuations move the zero sound mode to the right energy *without* need to shift the spectrum
- two-particle-two-hole continuum softens single-particle continuum
- We do not claim that proper self-energy inclusions are unimportant;
- Further work is needed to make the connection between G(0)W and CBF more transparent;

Summary

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- Many-Body physics can be quantitative without undue parameter fitting;
- Quantitative microscopic many-body theory can be simple, but sometimes "Mother Nature" wants it complicated;

Thanks to collaborators in this project

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