Variational and Parquet–diagram theory for strongly correlated normal and superfluid systems

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Outline

Postulate:

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Microscopic Many-Body Theory
Hamiltonian, wave functions, observables

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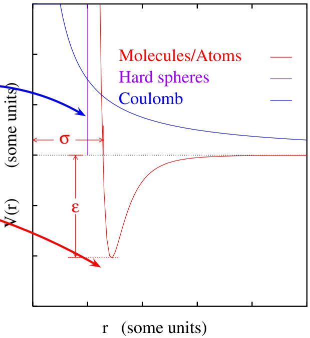
6. Finite-size
7. Phase transitions

A truly microscopic many-body theory should:

- Be robust against the choice of interactions;



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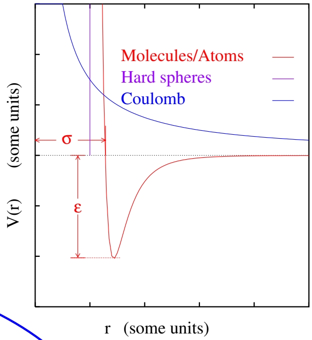

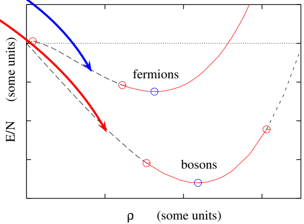

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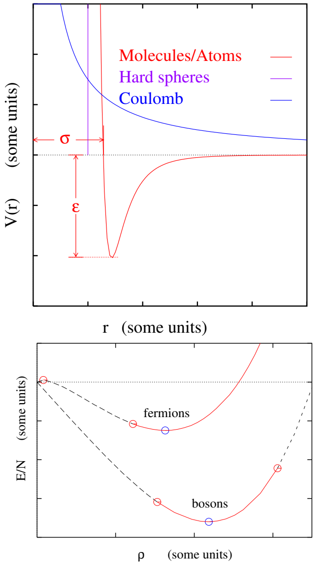
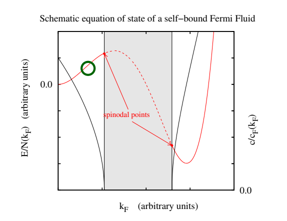
- Not: accept arguments “approximation A *works better* than approximation B”;



- Low densities: Pauli pressure dominates → repulsive Fermi gas



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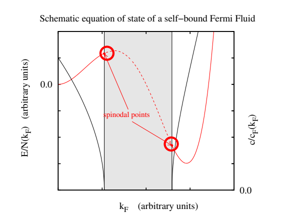
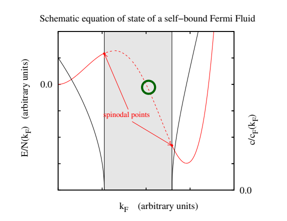


The equation of state
A closer look

- Low densities: Pauli pressure dominates $\rightarrow$ repulsive Fermi gas
- Spinodal instabilities
- No homogeneous solution $\rightarrow$ clustering



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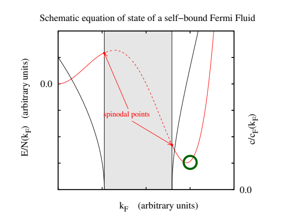

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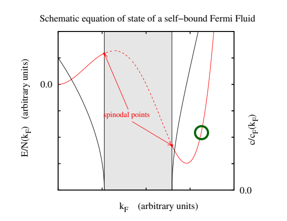

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- No homogeneous solution $\rightarrow$ clustering
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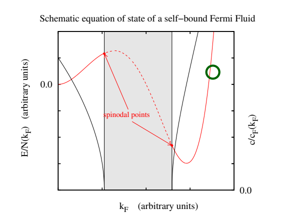
- Saturation
- Other phase transitions ?



What physics tells us:
The argument for parquet diagrams

- Binding and saturation $\Longrightarrow$ short-ranged structure:
  - "bending" of the wave function at small interparticle distances;
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Translate this into the language of perturbation theory:

Short-ranged structure	$\Rightarrow$	Ladder diagrams
Long-ranged structure	$\Rightarrow$	Ring diagrams
Consistency	$\Rightarrow$	parquet diagrams

Correlated wave functions ("Jastrow-Feenberg"):

"Quick and dirty" or "intuitive" ?

What looked like a "simple quick and dirty" method:

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

$$\equiv F(1,\ldots,N)\Phi_0(1,\ldots,N)$$

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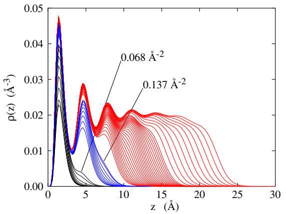
Density profiles of ^{4}He films



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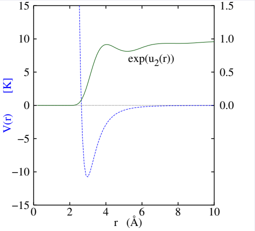
Correlation- and distribution functions



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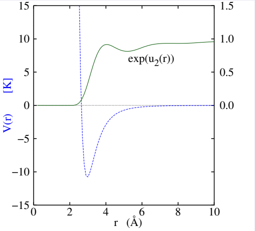

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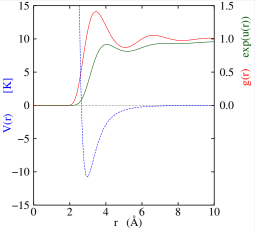

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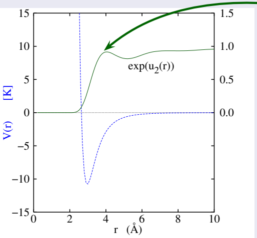

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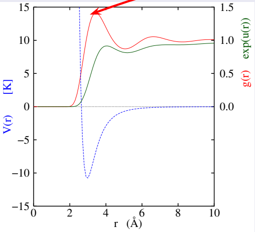

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- Diagram summation methods from classical statistics (HNC, PY, BGY);
- Optimization $\delta E/\delta u_n = 0$ makes correlations unique;
- Express everything in terms of physical observables.

Parquet diagrams:
Summing rings, ladders, and self-energy contributions

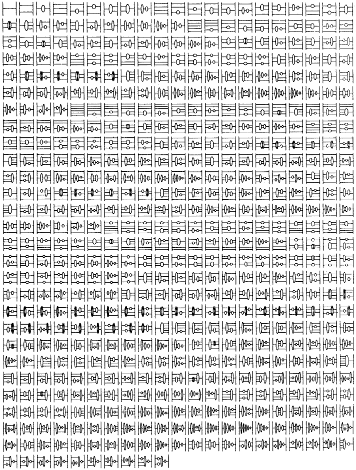

Fig. 8. The parquet contributions to the two-particle vertex, Γ, through sixth order in V. Here, horizontal lines denote the potential. The remaining lines denote propagating particles. Note that self-energy insertions are not indicated.

Local parquet diagrams: making parquet practical

Jackson, Lande, Smith: Physics Reports **86**, 55 (1982)

(100 pages Physics Reports in a nutshell)

- Begin with a local particle-hole interaction, sum the ring diagrams

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- Define an energy-independent particle–hole reducible interaction by demanding that it gives the same observable $S(q)$:

$$\begin{aligned}&\int_0^\infty d\omega \Im m\left[\chi_0(q,\omega)\tilde{w}_{\text{I}}(q,\omega)\chi_0(q,\omega)\right] \\ &= \int_0^\infty d\omega \Im m\left[\chi_0(q,\omega)\tilde{w}_{\text{I}}(q,\bar{\omega}(q))\chi_0(q,\omega)\right]\end{aligned}$$

Parquet diagrams: Ladder diagram summation

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- Sum the ladder diagrams with this local interaction

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- Note that

$$g(r) = |\psi(r)|^2 = 1 + \int \frac{d^3k}{(2\pi)^3\rho}\left[S(k) - 1\right] e^{i\mathbf{r}\cdot\mathbf{k}}$$

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At the end of all of this:

The local parquet-diagram summation leads, for bosons, to equations that are identical to the Euler equations of Jastrow–Feenberg theory.

Two-body Euler or local parquet equations for bosons

Summarizing its two faces

"RPA" face

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

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

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

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"Bethe-Goldstone" face

$$\frac{\hbar^2}{m}\nabla^2\sqrt{g(r)} = V_{\text{p-p}}(r)\sqrt{g(r)}$$

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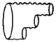
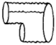
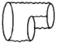
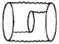
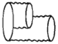
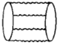
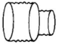
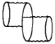
“Parquet” face

Consistency between $S(q)$ and $g(r)$

Parquet diagrams: Self-energy corrections

What is missing beyond rings and ladders ?

approximate parquet equations, and the optimized JHNC scheme. When possible, rows are labelled by the related time-ordered diagrams

Approximate equations	Optimized HNC equations	
$-\frac{5}{2}\rho^3 \int \frac{d^3k}{(2\pi)^3} \frac{V^4(k)}{k^6}$	$-\frac{5}{2}\rho^3 \int \frac{d^3k}{(2\pi)^3} \frac{V^4(k)}{k^6}$	
$-2\rho^2 \int \frac{d^3p}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{V^2(k)V(p)V(p+k)}{k^4p^2}$	$-2\rho^2 \int \frac{d^3p}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{V^2(k)V(p)V(p+k)}{k^4p^2}$	
$-\rho^2 \int \frac{d^3p}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{V^2(k)V(p)V(p+k)}{k^4p^2}$	$-\rho^2 \int \frac{d^3p}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{V^2(k)V(p)V(p+k)}{k^4p^2}$	
$-\rho^2 \int \frac{d^3p}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{V^2(k)V(p)V(p+k)}{p^2(p+k)^2k^2}$	$-\frac{3}{2}\rho^2 \int \frac{d^3p}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{V^2(k)V(p)V(p+k)}{p^2(p+k)^2k^2}$	
-----------------	-----------------	
$-\frac{1}{2}\rho \int \frac{d^3p}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} \frac{V(p)V(q)V(p+k)V(q+k)}{k^2p^2q^2}$	$-\frac{1}{2}\rho \int \frac{d^3p}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} \frac{V(p)V(q)V(p+k)V(q+k)}{k^2p^2q^2}$	
-----------------	-----------------	
-----------------	-----------------	
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- Combining all that is missing at that order is equivalent to including three-body correlations

$$\frac{E_3}{N} = -\frac{1}{24}\int \frac{d^3k d^3p d^3q}{(2\pi)^6 \rho^2} \frac{S(p)S(k)S(q)\,|V_3(\mathbf{p},\mathbf{k},\mathbf{q})|^2}{\varepsilon(k)+\varepsilon(p)+\varepsilon(q)}$$

(PRB **55**, 12925 (1997)).

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Parquet diagrams: Self-energy corrections
Findings:

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Coester's Commandment:

Thou shalt not split small quantities into large pieces !

- RPA

$$S(q) = -\int_0^\infty \frac{d\omega}{\pi} \Im m\, \chi^{(RPA)}(q,\omega) = -\int_0^\infty \frac{d\omega}{\pi} \frac{\chi_0(q,\omega)}{1 - \tilde{V}_{\text{p-h}}(q)\chi_0(q,\omega)}$$

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- Simplify if you care

$$\begin{aligned}
\chi_0(q,\omega) \approx \chi_0^{coll}(q,\omega) &\equiv \frac{2t(q)}{(\hbar\omega + i\eta)^2 - \left(t(q)/S_{\rm F}(q)\right)^2} \\
-\Im m \int_0^\infty \frac{d\omega}{\pi} \chi_0^{coll}(q,\omega) &= -\Im m \int_0^\infty \frac{d\omega}{\pi} \chi_0(q,\omega) = S_{\rm F}(q) \\
-\Im m \int_0^\infty \frac{d\omega}{\pi} \omega \chi_0^{coll}(q,\omega) &= -\Im m \int_0^\infty \frac{d\omega}{\pi} \omega \chi_0(q,\omega) = t(q)\,. \\
S(q) &= S_{\rm F}(q) \left[1 + \frac{2S_{\rm F}^2(q)}{t(q)} \tilde{V}_{\text{p-h}}(q)\right]^{-1/2}
\end{aligned}$$

- Bethe Goldstone equation for the pair correlation function:

$$\left\langle \mathbf{k},\mathbf{k}'\middle|\psi\middle|\mathbf{h},\mathbf{h}'\right\rangle = \left\langle \mathbf{k},\mathbf{k}'\middle|\mathbf{h},\mathbf{h}'\right\rangle - \frac{\bar{n}(k)\bar{n}(k')}{e(\mathbf{k})+e(\mathbf{k}')-e(\mathbf{h})-e(\mathbf{h}')}\left\langle \mathbf{k},\mathbf{k}'\middle|v\psi\middle|\mathbf{h},\mathbf{h}'\right\rangle .$$

Local parquet diagram for fermions
(2) Ladder diagrams

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- Localization: If ψ is a local function $\psi(\mathbf{r})$ then $\left\langle \mathbf{k},\mathbf{k}' \middle| \psi \middle| \mathbf{h},\mathbf{h}' \right\rangle = \tilde{\psi}(\mathbf{k}-\mathbf{h}) \equiv \tilde{\psi}(\mathbf{q})$ and $\left\langle \mathbf{k},\mathbf{k}' \middle| v\psi \middle| \mathbf{h},\mathbf{h}' \right\rangle = [v(\mathbf{r})\psi(\mathbf{r})]^{\mathcal{F}}(\mathbf{q})$

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- ⇒Energy coefficient must be somehow approximated by a function of momentum transfer
- Averaging procedure

$$\langle f(\mathbf{p},\mathbf{h})\rangle(q) = \frac{\sum_{\mathbf{h}} \bar{n}(\mathbf{h}+\mathbf{q})n(\mathbf{h})f(\mathbf{h}+\mathbf{q},\mathbf{h})}{\sum_{\mathbf{h}} \bar{n}(\mathbf{h}+\mathbf{q})n(\mathbf{h})}$$

- As for bosons: Effective interaction

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

Particle-hole reducible part

$$\tilde{w}_I(q,\omega) = \widetilde{W}(q,\omega) - \tilde{V}_{\text{p-h}}(q) = \frac{\tilde{V}_{\text{p-h}}(q)\chi_0(q,\omega)}{1 - \tilde{V}_{\text{p-h}}(q)\chi_0(q,\omega)} .$$

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- Localization procedure

$$\begin{aligned} S(q) &= -\int_0^\infty \frac{d\omega}{\pi} \Im m \left[\chi_0(q,\omega) + \chi_0(q,\omega)\widetilde{W}(q,\bar{\omega}(q))\chi_0(q,\omega)\right] \\ &= S_{\mathrm{F}}(q) - \widetilde{W}(q,\bar{\omega}(q)) \int_0^\infty \frac{d\omega}{\pi} \Im m \chi_0^2(q,\omega)\,. \end{aligned}$$

Local parquet diagram for fermions

(3) Ladder rungs

- As for bosons: Effective interaction

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

Particle-hole reducible part

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- Carry this out for the full or the collective Lindhard function

"Localization" of the energy demoninator

$$e_{\mathbf{q}+\mathbf{h}} - e_{\mathbf{h}} \rightarrow \bar{e}(q) = \frac{\sum_{\mathbf{h}} \bar{n}(\mathbf{h}+\mathbf{q})n(\mathbf{h})(e_{\mathbf{q}+\mathbf{h}} - e_{\mathbf{h}})}{\sum_{\mathbf{h}} \bar{n}(\mathbf{h}+\mathbf{q})n(\mathbf{h})}$$

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- The variational feature makes sure that the approximations are the best one can do for the price.

Summarizing:
..connection of Jastrow-FHNC

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- FHNC-EL or local parquet equations
- Of course, many more fermion diagrams due to exchange structure
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The CBF strategy to do better:

- Sum all parquet diagrams (and, if you care, add fully irreducible) in local approximation
- Correct specific sets of diagrams if needed.

(Collective) “RPA” face

$$S(q) = \frac{S_{\rm F}(q)}{\sqrt{1 + \frac{4mS_{\rm F}^2(q)}{\hbar^2 q^2}\tilde{V}_{\rm p\text{-}h}(q)}}$$

Two-body Euler or local parquet equations for fermions

Summarizing its two faces

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(Collective) "Bethe-Goldstone" face

$$\left[-\frac{\hbar^2 q^2}{mS_{\mathrm{F}}(q)}\right]^{\mathcal{F}}(r)\psi(r) = V_{\mathrm{p\text{-}p}}(r)\psi(r)$$

Two-body Euler or local parquet equations for fermions

Summarizing its two faces

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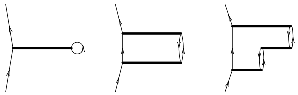
$$\left[-\frac{\hbar^2 q^2}{mS_{\mathrm{F}}(q)}\right]^{\mathcal{F}}(r)\psi(r) = V_{\text{p-p}}(r)\psi(r)$$

"Parquet" face

Consistency between $S(q)$ and $\psi(r)$

- If you care to: Add self–energy diagrams
  They are called "cyclic chain" diagrams in the language of variational theory



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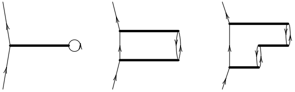
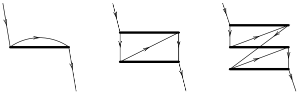


- If so, please include exchange diagrams
  They are included in variational theory



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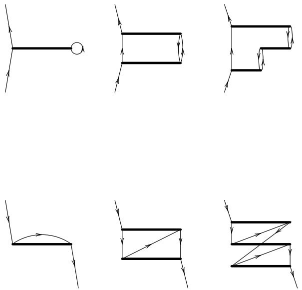
- and mind Coester's commandment !



- A family of Lennard-Jones and square-well interactions

$$V_{\mathrm{LJ}}(r) = 4V_0\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$
$$\equiv \frac{\hbar^2}{2m\sigma^2}4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$
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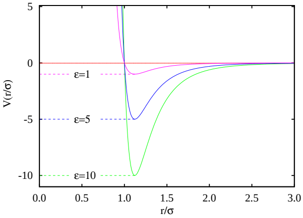

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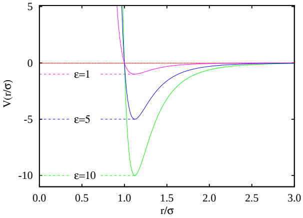
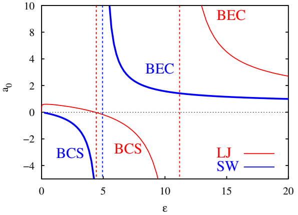
- Adjust ε to obtain the desired scattering lenght a_0 (the cold gas people want it that way);





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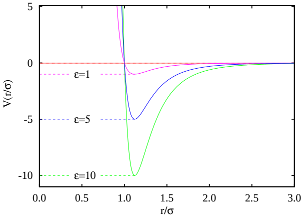
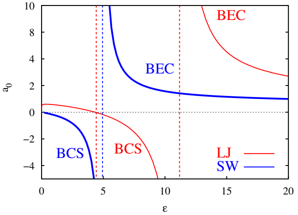
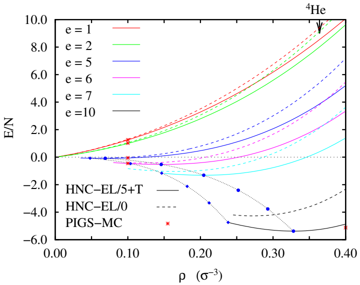




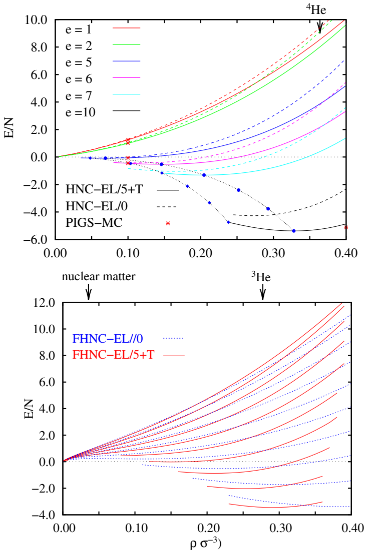
- Adjust ε to obtain the desired scattering lenght a_0 (the cold gas people want it that way);
- First bound state appears at $\varepsilon = 11.18$ (4.33) $\Rightarrow$ Divergence of the vacuum scattering length.

Verification I: The Lennard-Jones liquid
How well it works (Bragbook)

- Equation of state for Bosons



- Equation of state for Bosons
- Equation of state for Fermions



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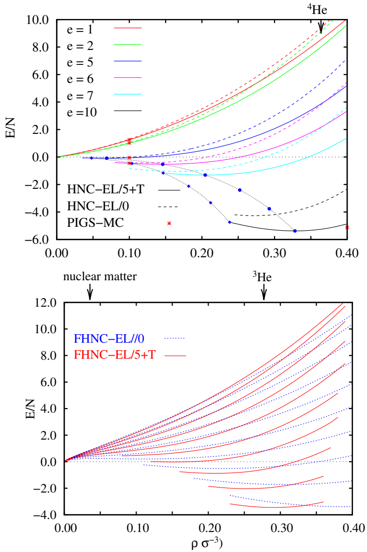

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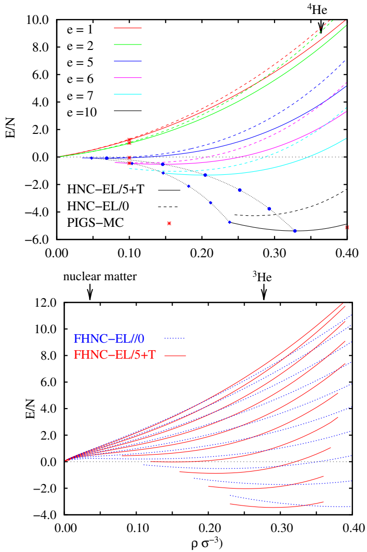

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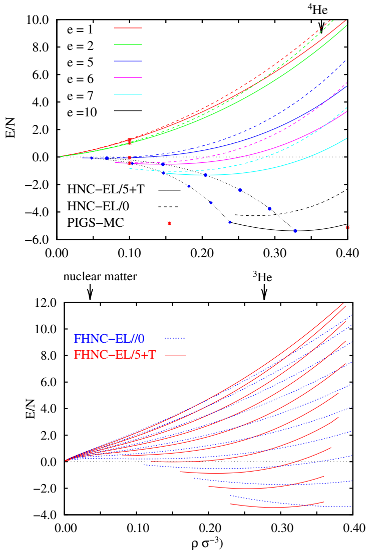
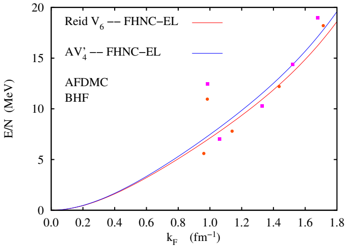
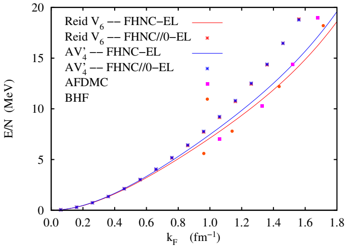
- Works the same in 2D
- FHNC-EL (or parquet) has no solutions if "mother nature" cannot make the system: The equation of state ends at the spinodal points.



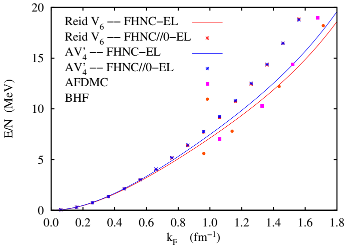
- Equation of state for Neutron matter interacting via Argonne and Reid V_4 potentials



- Equation of state for Neutron matter interacting via Argonne and Reid V_4 potentials
- “Quick and dirty” version has percent accuracy below 0.2*(nuclear matter density)..



- Equation of state for Neutron matter interacting via Argonne and Reid V_4 potentials
- “Quick and dirty” version has percent accuracy below 0.2*(nuclear matter density)..
- This contains only central correlations. “Twisted chain“ diagrams (beyond parquet) may be very important !



- Three (not two) range regimes

Low-density calculations
– the many-body effects

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- Short-ranged correlations
  $0 \le r \le \lambda\sigma$ determined by interaction
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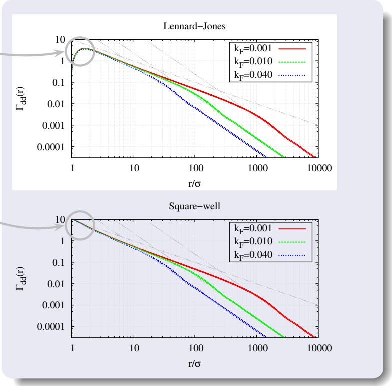

Low-density calculations
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- Three (not two) range regimes
- Short-ranged correlations $0 \le r \le \lambda\sigma$ determined by interaction ($\lambda\sigma$ a typical interaction range)
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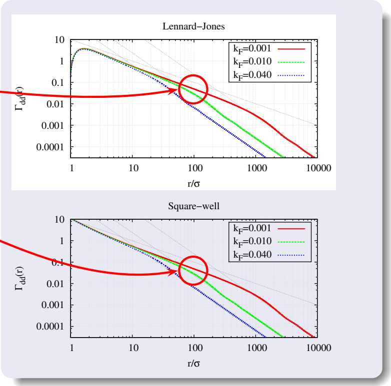

Low-density calculations
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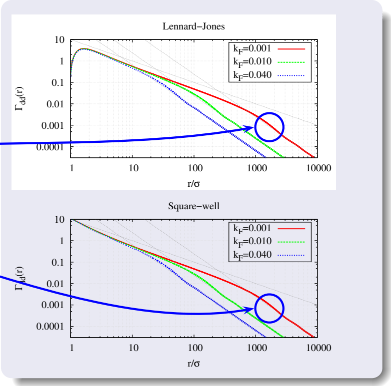
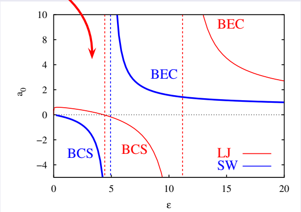
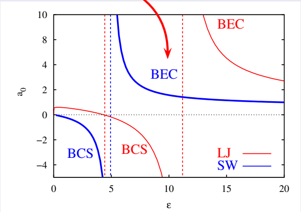
- Long-ranged correlations
  $1/k_\mathrm{F} \le r \le \infty$ determined by many-body properties:
  $\psi(r) \propto F_0^s/(r^2 k_\mathrm{F}^2)$



- For $a_0 > 0$, no bound state
  $\rightarrow$ repulsive Fermi gas;



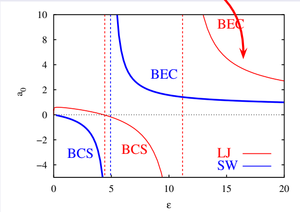
- For $a_0 > 0$, no bound state $\rightarrow$ repulsive Fermi gas;
- For $a_0 < 0$ ("BCS" regime): BCS pairing;



Microscopic ground state calculations

What we expect –

- For $a_0 > 0$, no bound state $\rightarrow$ repulsive Fermi gas;
- For $a_0 < 0$ ("BCS" regime): BCS pairing;
- For $a_0 > 0$ ("BEC" regime): No homogeneous solution ! Dimerization ? Clustering ?



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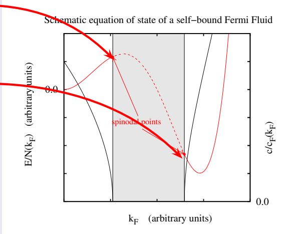

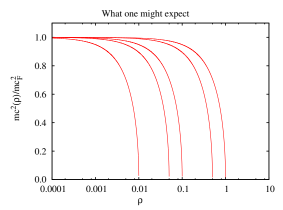

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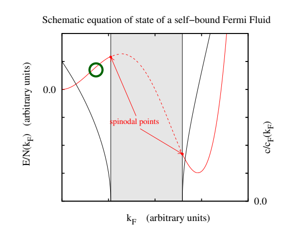

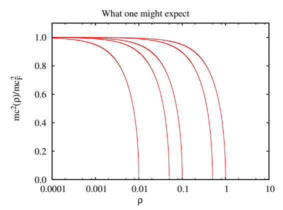

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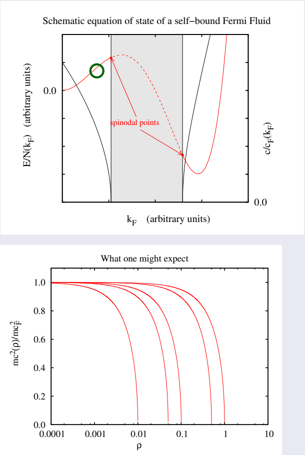

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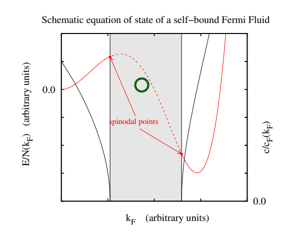

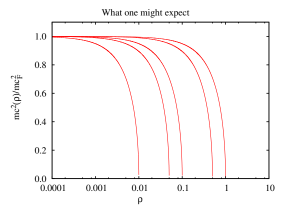

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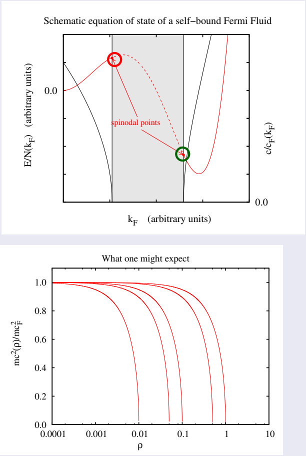
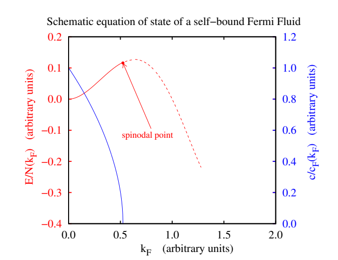


- For SC potentials, there is no high-density homogeneous phase and no upper spinodal point



- For SC potentials, there is no high-density homogeneous phase and no upper spinodal point
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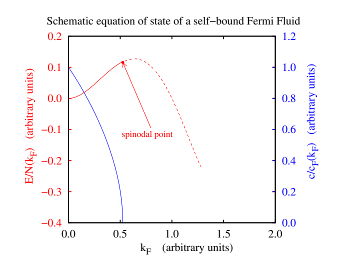

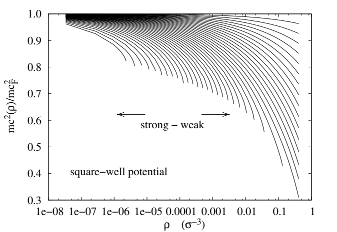

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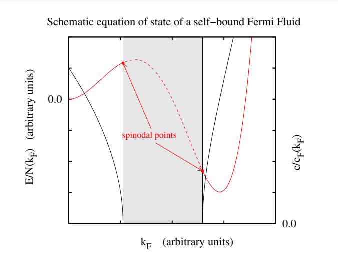

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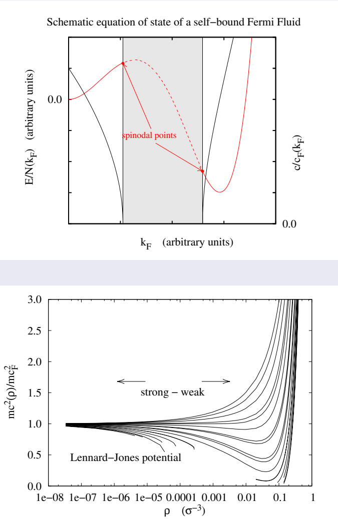
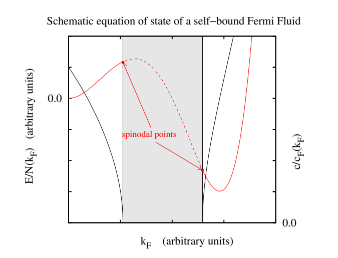
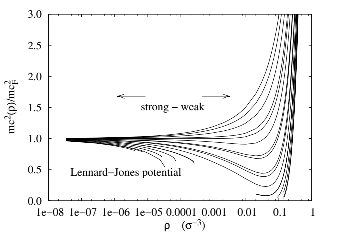


- For SC potentials, there is no high-density homogeneous phase and no upper spinodal point
- It is impossible to get close to the spinodal instability;
- For LJ potentials, we have a repulsive high-density regime and an upper spinodal point;
- It is easy to get close to the upper spinodal instability,
- It is impossible to get close to the lower spinodal instability;



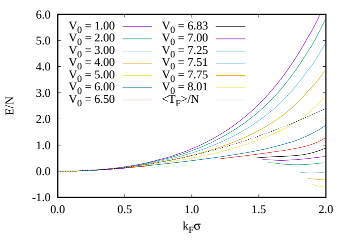


Consistency check:

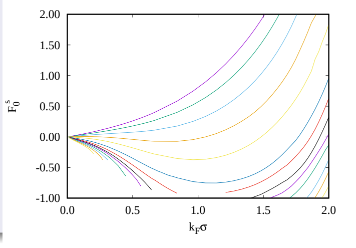
$$mc^2 = mc_F^{*2} + \tilde{V}_{p-h}(0+) \equiv mc_F^{*2}(1 + F_0^S) = \frac{d}{d\rho}\rho^2 \frac{d}{d\rho}\frac{E}{N}$$

$c_F^{*2} = \frac{\hbar^2 k_F^2}{3mm^*}$: speed of sound of the non-interacting Fermi gas with effective mass m^* (Never an exact relationship !)

Equation of state



Fermi liquid paramater



- It is impossible to get close to the low-density spinodal point

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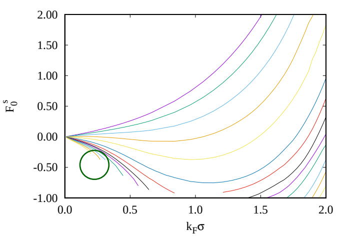
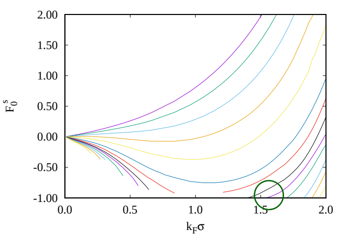


Divergence of parquet-summations
What it means

- It is impossible to get close to the low-density spinodal point
- It is easy to get to the high-density spinodal point

Fermi liquid parameter



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- Improved calculations of F_0^s do not change this

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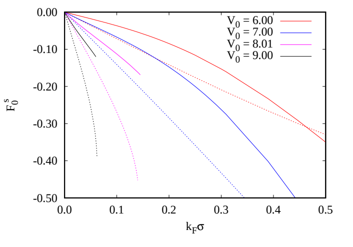

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- It is easy to get to the high-density spinodal point
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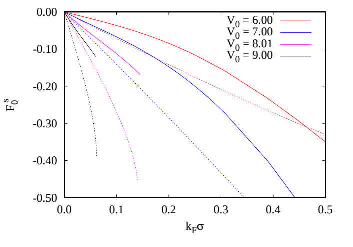
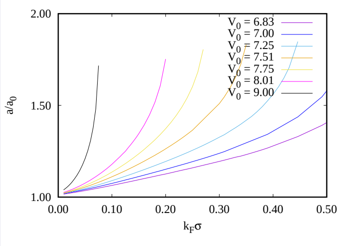
- The in-medium scattering length diverges !

Fermi liquid parameter

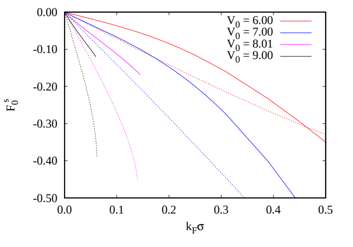


In-medium scattering length



- It is impossible to get close to the low-density spinodal point
- It is easy to get to the high-density spinodal point
- Improved calculations of F_0^s do not change this
- The in-medium scattering length diverges !
- This is a many-body effect (“phonon-exchange driven dimerization”) !

Fermi liquid parameter



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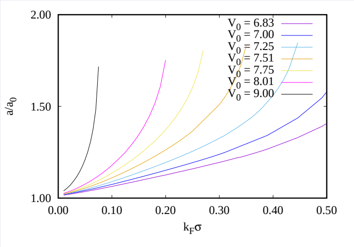

$$\left|\mathrm{BCS}\right\rangle = \prod_{\mathbf{k}} \left[u_{\mathbf{k}} + v_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow} \right] \left|0\right\rangle$$

$$\left|\mathrm{CBCS}\right\rangle = \sum_{N,\mathbf{m}} \frac{}{\sqrt{I_{mm}}} F_N \left|\mathbf{m}^{(N)}\right\rangle \left\langle \mathbf{m}^{(N)} \middle| \mathrm{BCS} \right\rangle$$

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- EK, R. A. Smith and A. D. Jackson: Phys Rev. **B24**, 6404 (1981)
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Strategy: Expand in terms of the *deviation* of the Bogoliubov amplitudes from their normal system values !

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At QFS 2018, Tokyo:, A. J. Leggett

We should not build the superfluid system by creating Cooper pairs from the vacuum,

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BCS Theory with strong correlations

How to derive a BCS wave function with correlations

$$\left|\mathrm{BCS}\right\rangle = \prod_{\mathbf{k}} \left[u_{\mathbf{k}} + v_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow} \right] \left|0\right\rangle$$

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At QFS 2018, Tokyo:, A. J. Leggett

We should not build the superfluid system by creating Cooper pairs from the vacuum, but rather generate Cooper pairs from normal interacting system one at a time.

After lengthy calculations: An (almost) ordinary gap equation

$$\Delta_{\mathbf{k}} = -\frac{1}{2}\sum_{\mathbf{k}'} \mathcal{P}_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{\sqrt{(e_{\mathbf{k}'}-\mu)^2 + \Delta_{\mathbf{k}'}^2}} \,.$$

At low densites, all operators become local

$$\begin{aligned} \mathcal{P}_{\mathbf{k}\mathbf{k}'} &= \left\langle \mathbf{k}\uparrow, -\mathbf{k}\downarrow \middle| \mathcal{W}(1,2) \middle| \mathbf{k}'\uparrow, -\mathbf{k}'\downarrow \right\rangle_a \\ &\quad + (|e_k-\mu| + |e_{k'}-\mu|)\left\langle \mathbf{k}\uparrow, -\mathbf{k}\downarrow \middle| \mathcal{N}(1,2) \middle| \mathbf{k}'\uparrow, -\mathbf{k}'\downarrow \right\rangle_a \\ &\equiv \frac{1}{N}\left[\tilde{\mathcal{W}}(\mathbf{k}-\mathbf{k}') + (|e_k-\mu| + |e_{k'}-\mu|)\tilde{\mathcal{N}}(\mathbf{k}-\mathbf{k}')\right] \,. \end{aligned}$$

- The gap is (mostly) determined by the matrix element $\left\langle \mathbf{k}\uparrow, -\mathbf{k}\downarrow \middle| \mathcal{W}(1,2) \middle| \mathbf{k}'\uparrow, -\mathbf{k}'\downarrow \right\rangle_a$

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- The gap is (mostly) determined by the matrix element $\langle \mathbf{k}\uparrow, -\mathbf{k}\downarrow | \mathcal{W}(1,2) | \mathbf{k}'\uparrow, -\mathbf{k}'\downarrow \rangle_a$
- The “energy numerator” term regularizes the integral for zero-range interactions.

At low density, let

$$a_F = \frac{m}{4\pi\rho\hbar^2}\mathcal{W}_F$$

$$\Delta_F \approx \frac{8}{e^2} e_{\mathrm{F}} \exp\left(\frac{\pi}{2a_F k_{\mathrm{F}}}\right).$$

Corrections: $a_F \to a_0$ for $\rho \to 0+$

If $a_F = a_0\left[1 + \alpha\frac{a_0 k_{\mathrm{F}}}{\pi}\right]$ then

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Questions:

- What influences the pre-factor (Gorkov-corrrections *etc.*):

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Questions:

- What influences the pre-factor (Gorkov-corrrections *etc.*.):
- How accurate is the solution ?
- Are there non-universal effects ?

The gap is determined by a_F

Corrections:

- Interaction corrections ("phonon exchange")

$$\widetilde{\mathcal{W}}(0+) = \frac{4\pi\rho\hbar^2}{m} a = \frac{4\pi\rho\hbar^2}{m} a_0 \left[1 + \alpha' \frac{a_0 k_{\rm F}}{\pi}\right]$$

The gap is determined by a_F

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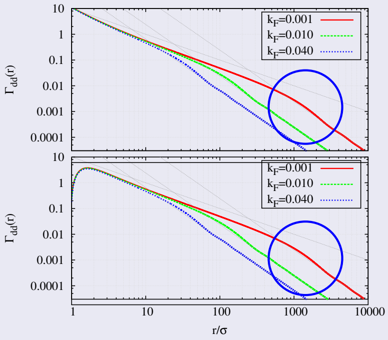
- The value of $\widetilde{\mathcal{W}}_F$ is influenced real space correlations in the interaction regime $r > 1/k_\mathrm{F}$!

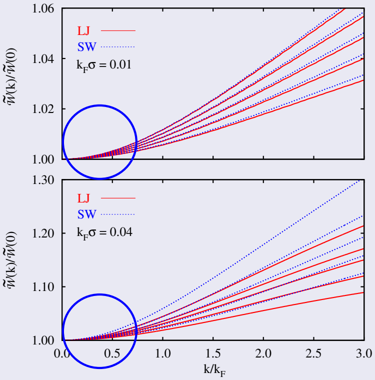
BCS Theory with strong correlations

Finite-range effects

Pair correlations



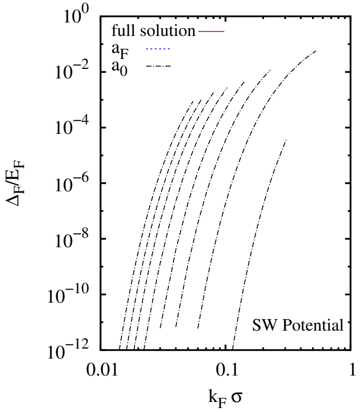
Pairing interaction



Interaction dominated regime

Solution of the gap equation
... and what approximations do

- $\Delta_F = \frac{8}{e^2} e_{\mathrm{F}} \exp\left(\frac{\pi}{2 a_0 k_{\mathrm{F}}}\right)$



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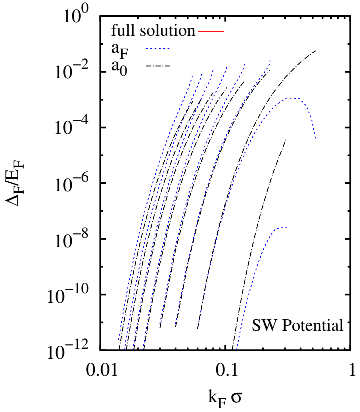

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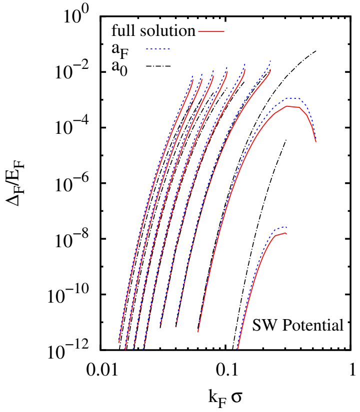
- Full solution



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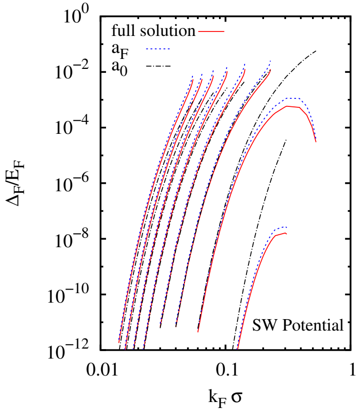

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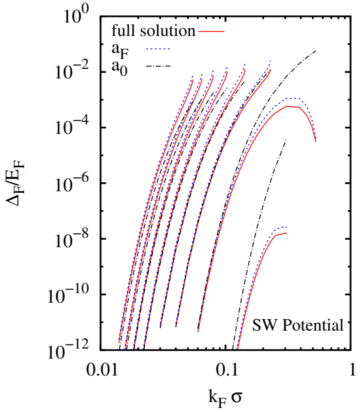
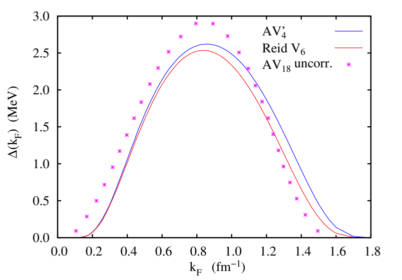


- Exponential behavior becomes universal, prefactor not.
- Low density expansion valid only for physically uninteresting cases.

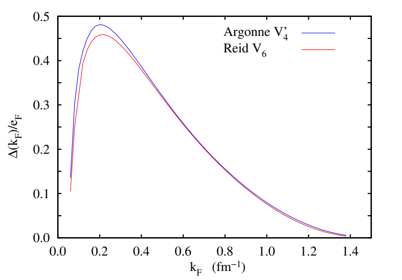
Neutron matter calculations

$^1S_0$ gap for Argonne and Reid V_4

Gap in units of MeV



Gap in units of the Fermi energy



Neutron matter calculations

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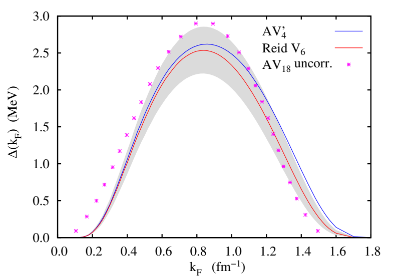

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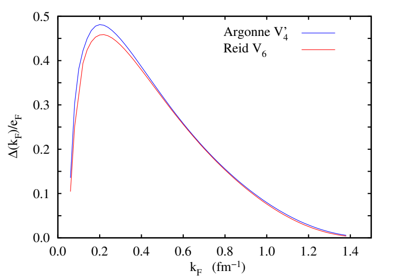

- Weak dependence on the effective mass ($0.9 < m^*/m < 1.1$)

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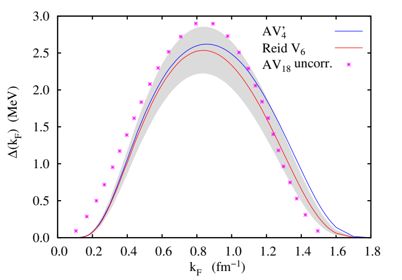

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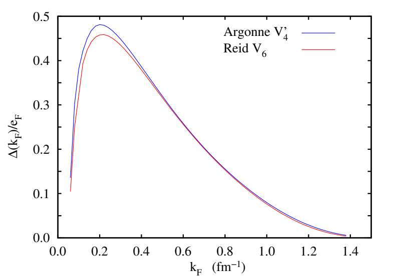

- Weak dependence on the effective mass ($0.9 < m^*/m < 1.1$)
- Is the "weak coupling approximation" justified ?

- Go back to

$$\left|\mathrm{CBCS}\right\rangle = \sum_{N,\mathbf{m}} \left\langle \mathbf{m}^{(N)} \middle| F_N^2 \middle| \mathbf{m}^{(N)} \right\rangle^{-1/2} F_N \left| \mathbf{m}^{(N)} \right\rangle \left\langle \mathbf{m}^{(N)} \middle| \mathrm{BCS} \right\rangle$$

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- Develop diagrammatic expansions at the FHNC or "parquet" level: Looks practically the same as normal system FHNC replacing

$$\ell(r_{ij} k_\mathrm{F}) = \frac{\nu}{\rho\Omega} \sum_{\mathbf{k}} n(\mathbf{k}) e^{i\mathbf{r}_{ij}\cdot\mathbf{k}} =$$ 

by

$$\ell_v(r_{ij}) = \frac{\nu}{\rho\Omega} \sum_{\mathbf{k}} v^2(\mathbf{k}) e^{i\mathbf{r}_{ij}\cdot\mathbf{k}} =$$ 

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What's next ?

Jastrow-HNC and parquet for superfluid systems

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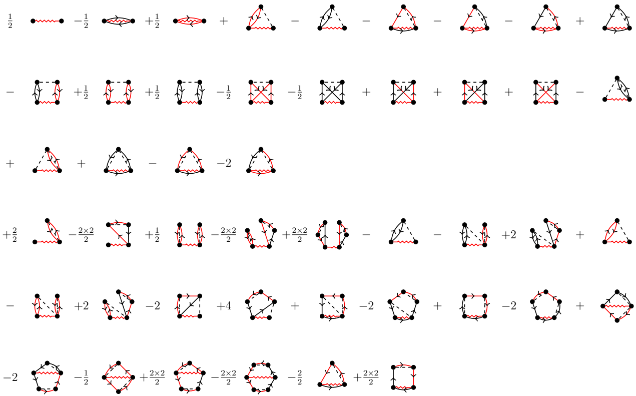
- Derive FHNC and Euler equation

Jastrow-HNC for superfluid systems

..just to impress you



- Recall the “collective RPA”

$$S(q) = \frac{S_{\mathrm{F}}(q)}{\sqrt{1 + \frac{4mS_{\mathrm{F}}^2(q)}{\hbar^2 q^2}\tilde{V}_{\text{p-h}}(q)}}$$

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- FHNC-EL equations have no sensible solution if $\tilde V_{\rm p\text{-}h}(q) > 0$
- This applies to the "fixed-node approximation"

- Recall:

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

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

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- "collective Lindhard function" causes problems

$$\chi_0^{coll}(q,\omega) = \frac{2t(q)}{(\hbar\omega + i\eta)^2 - (t(q)/S_{\rm F}(q))^2}$$

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- Exact Lindhard function(s): $\xi_{\mathbf{k}} = t(k)-\mu$, $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2}$

$$\chi_0^{(\rho,\sigma)}(\mathbf{k},\omega) = -\frac{\nu}{\rho\Omega}\sum_{\mathbf{p},\pm} b_{\mathbf{p},\mathbf{k}}^{(\rho,\sigma)}\left[\pm\frac{1}{E_{\mathbf{k}+\mathbf{p}}-E_{\mathbf{p}}\mp(\omega+i\eta)}\right]$$
$$b_{\mathbf{p},\mathbf{k}}^{(\rho,\sigma)} = v_{\mathbf{p}}^2 u_{\mathbf{k}+\mathbf{p}}^2 \pm u_{\mathbf{p}} v_{\mathbf{p}} u_{\mathbf{k}+\mathbf{p}} v_{\mathbf{k}+\mathbf{p}}\,,$$

- Fixes the spurious problem of Jastrow-Feenberg (fixed node)

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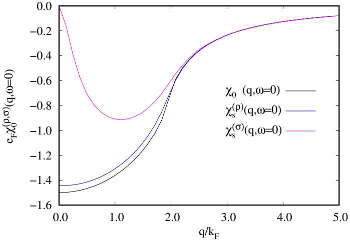
- Suppresses polarization corrections in the spin-channel

$$\widetilde{\mathcal{W}}^{\rho,\sigma}(q,\omega) = \\ = \frac{\tilde{V}^{(\rho,\sigma)}_{\rm p\text{-}h}(q)}{1-\chi_0^{(\rho,\sigma)}(q,\omega)\,\tilde{V}^{(\rho,\sigma)}_{\rm p\text{-}h}(q)}$$



- Fixes the spurious problem of Jastrow-Feenberg (fixed node)
- Suppresses polarization corrections in the spin-channel
- Take effective interaction at $\omega = 0$.

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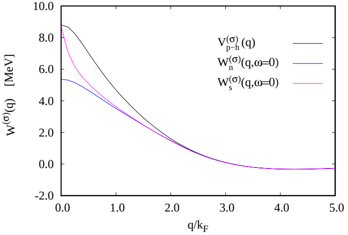
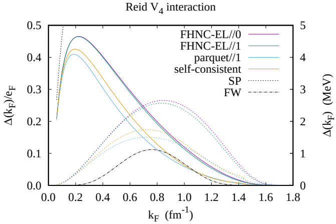
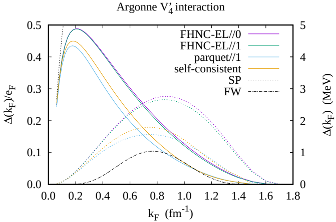


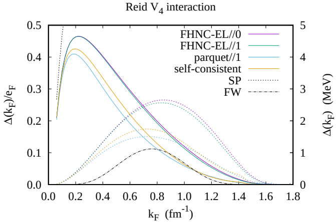
- Calculations of increasing complexity

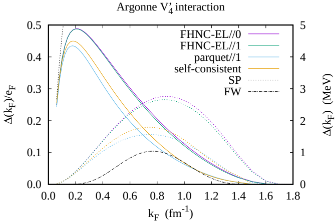




- Calculations of increasing complexity
- Estimate by vacuum scattering lenght is poor

$$\frac{\Delta_{\rm SP}(k_{\rm F})}{e_{\rm F}} = \frac{8}{e^2}\exp\left(\frac{\pi}{2a_0k_{\rm F}}\right)$$





Parquet for superfluid systems
Singlet pairing in neutron matter

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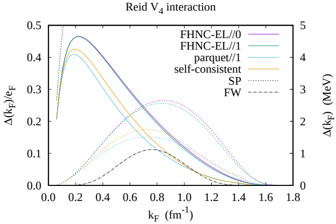
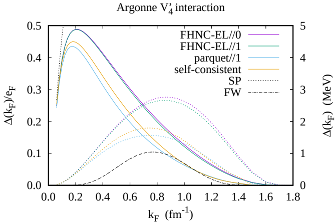
- Estimate by vacuum scattering lenght is poor

$$\frac{\Delta_{\rm SP}(k_{\rm F})}{e_{\rm F}} = \frac{8}{e^2}\exp\left(\frac{\pi}{2a_0 k_{\rm F}}\right)$$

- Estimate by pairig matrix element too small

$$\frac{\Delta_{\rm FW}(k_{\rm F})}{e_{\rm F}} = 8\frac{m}{m^*}\exp\left(\frac{4}{3}\frac{\hbar^2 k_{\rm F}^2}{2m^* W_F}\right)$$





Summary

- Equivalence of Jastrow-Feenberg theory and local parquet
- FHNC-EL diverges for phase transitions:
  in the particle-hole channel for spinodal decomposition,
  in the particle-particle channel for dimer formation
- Long–ranged properties are determined by many-body effects, not by vacuum
- Many-Body effects for *long-ranged* correlations $r > 1/k_{\mathrm{F}}$ imply Many-Body effects for long wavelengths $k < k_{\mathrm{F}}$
- Non-universal behavior of the pairing matrix element.
- The Jastrow-Feenberg wave function is not suitable for superfluid systems
- Superfluid parquet theory fixes the problems
- Operator-dependent correlations are still a wide open field

Thanks to collaborators in this project

Hsuan Hao Fan and Jiawei Wang
University at Buffalo

Thanks for your attention

and thanks to our funding agency:

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Der Wissenschaftsfonds.