Microscopic Many-Body Theory: The long path from the nuclear interaction to neutron matter pairing

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Department of Physics, University at Buffalo SUNY

Karpacz Winter School, Feb. 27, 2020

JOHANNES KEPLER UNIVERSITÄT LINZ

Outline

1. Generica
   - The questions we ask
   - The equation of state of a self-bound system
2. Methods
   - Variational wave functions and optimization
   - Pair density functional theory
   - Parquet diagram summations
3. Testing the method
   - Model quantum fluids
4. Testing the method
   - Model quantum fluids
5. Realistic nuclear interactions
   - The problem of variational wave functions
   - Parquet-diagram summation
   - Where did the problems go ?

Microscopic Many-Body Theory

Hamiltonian, wave functions, observables

Postulate:

1. Hamiltonian $H = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 + \sum_i V_{ext}(i) + \sum_{i<j} V(i,j)$

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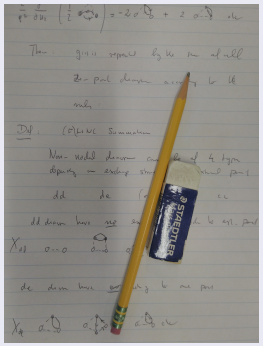

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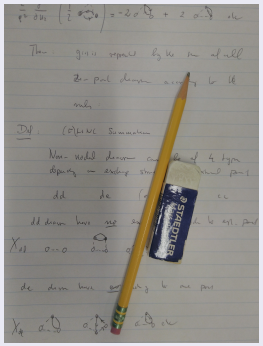

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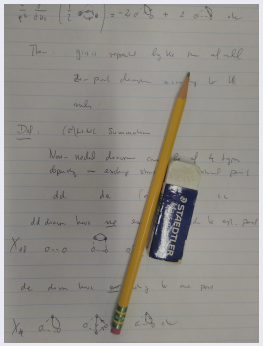

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Calculate from no other information...

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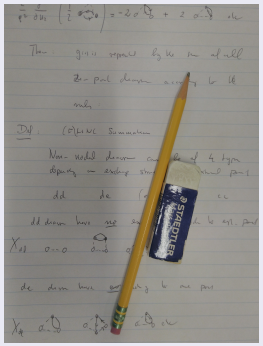

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2. Structure

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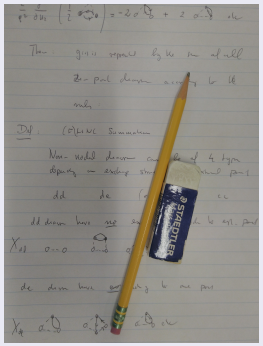

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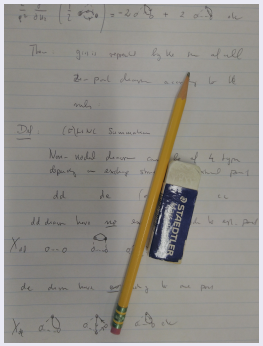

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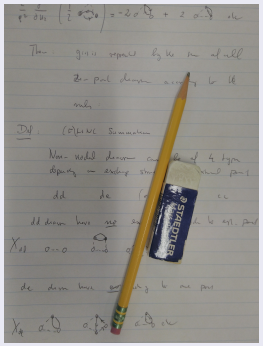

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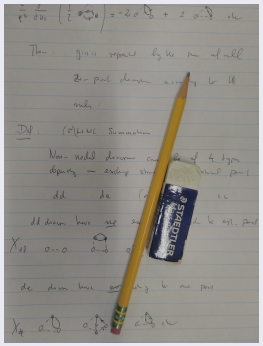

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Calculate from no other information...

1. Energetics
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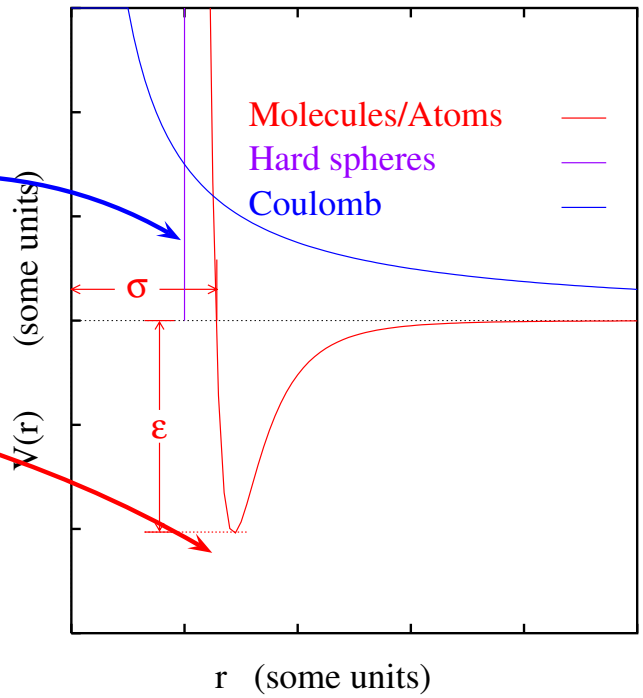
7. Phase transitions

The equation of state

The easy (?) questions ...

A truly microscopic many-body theory should:

- Be robust against the choice of interactions;



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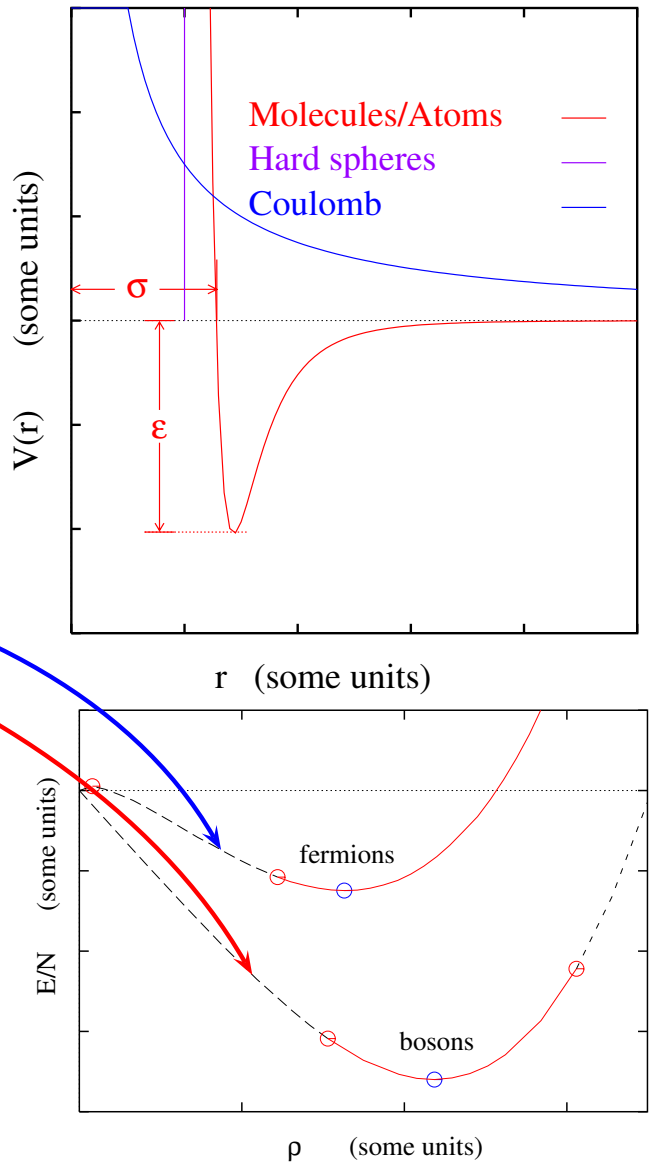

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The easy (?) questions ...

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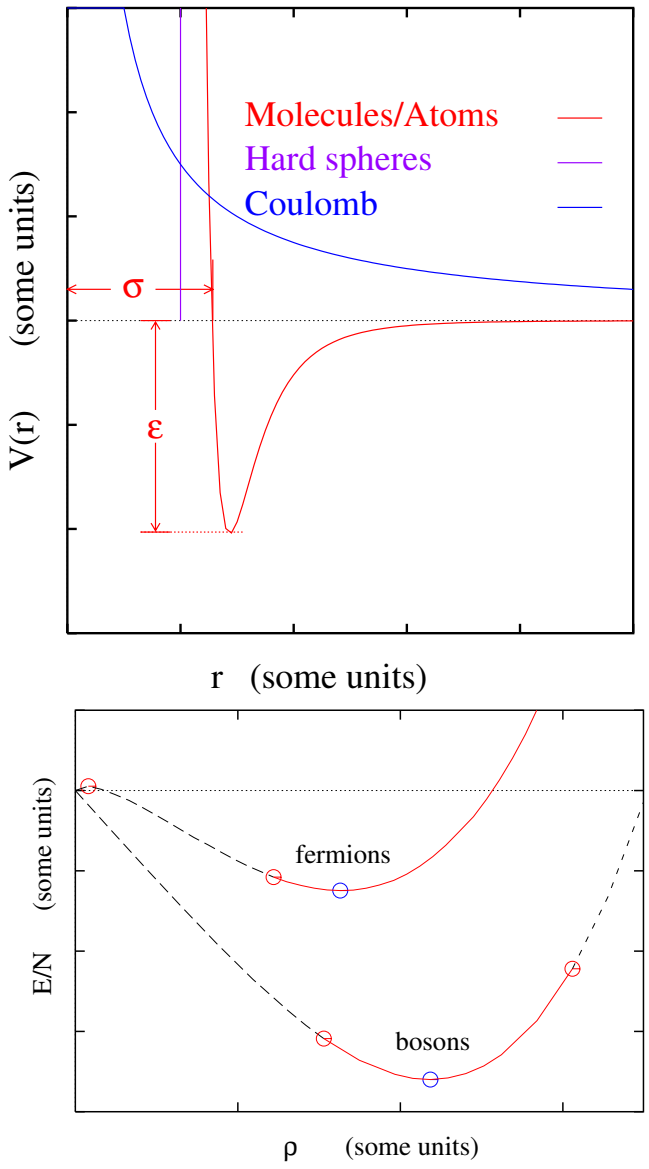
- Be robust against the choice of interactions;
- Have no answers if "mother nature" does not have them;
- Not: accept arguments "approximation A works better than approximation B";



The problem of nuclear systems

... where Pandora's box opens

(Non-relativistic) nuclear Hamiltonian:

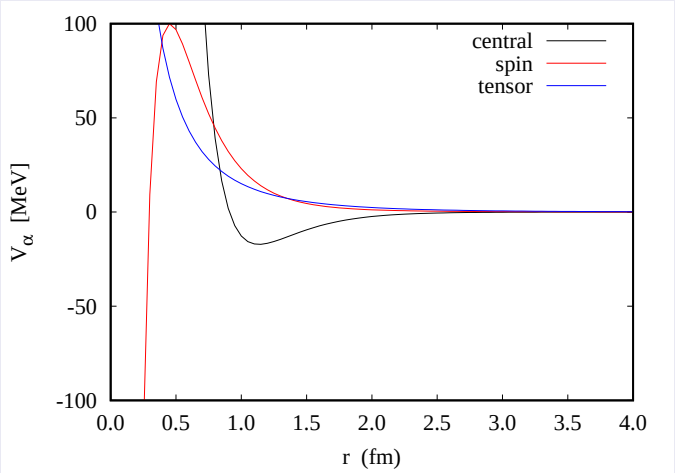
$$H = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 + \sum_i V_{ext}(i) + \sum_{i<j} V(i,j)$$

$$V(i,j) = \sum_\alpha V_\alpha(r) O_\alpha(i,j)$$

Operator Basis

$$\begin{aligned}
O_1(i,j;\hat{r}) &\equiv O_c = \mathbb{1}, \\
O_3(i,j;\hat{r}) &\equiv (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j), \\
O_5(i,j;\hat{r}) &\equiv S(i,j;\hat{r}) \\
&\equiv 3(\boldsymbol{\sigma}_i \cdot \hat{r})(\boldsymbol{\sigma}_j \cdot \hat{r}) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \\
O_{2n}(i,j;\hat{r}) &= O_{2n-1}(i,j;\hat{r})\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j .
\end{aligned}$$

Interactions in operator basis



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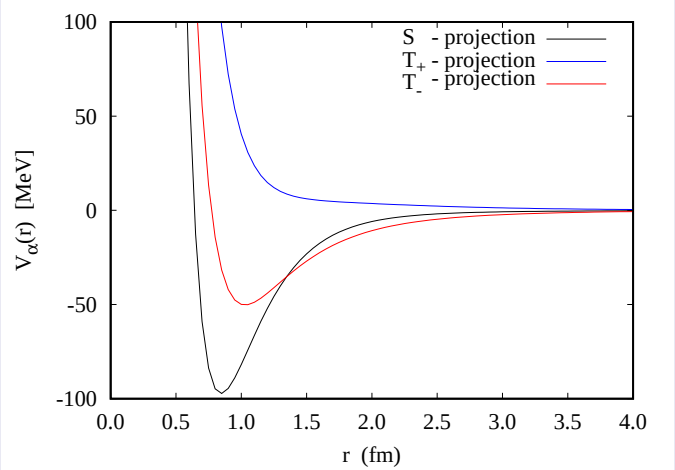
Projector Basis

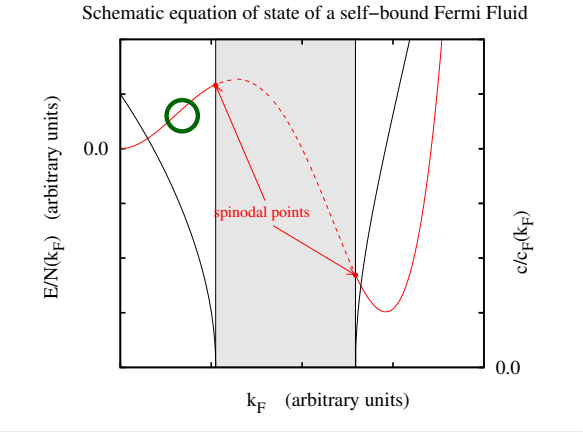
$$\begin{aligned} P_s &= \frac{1}{4}(1 - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \\ P_{t+} &= \frac{1}{6}(3 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + S_{12}(\hat{r})) \\ P_{t-} &= \frac{1}{12}(3 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 - 2S_{12}(\hat{r})) \end{aligned}$$

Interactions in projector basis



The equation of state of a self-bound system
A closer look

- Low densities: Pauli pressure dominates → repulsive Fermi gas



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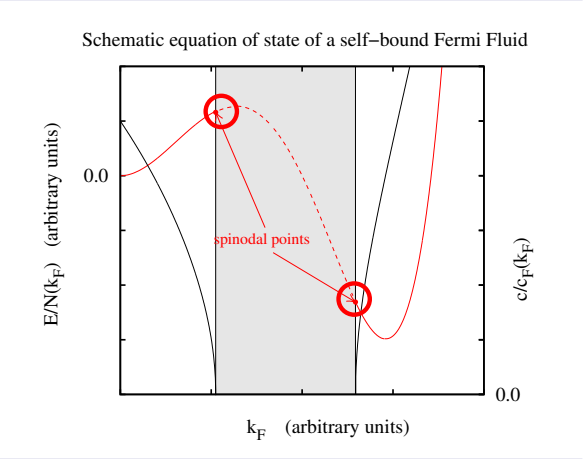

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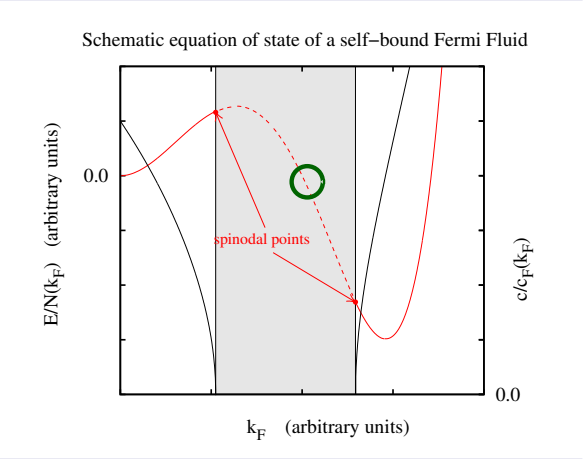

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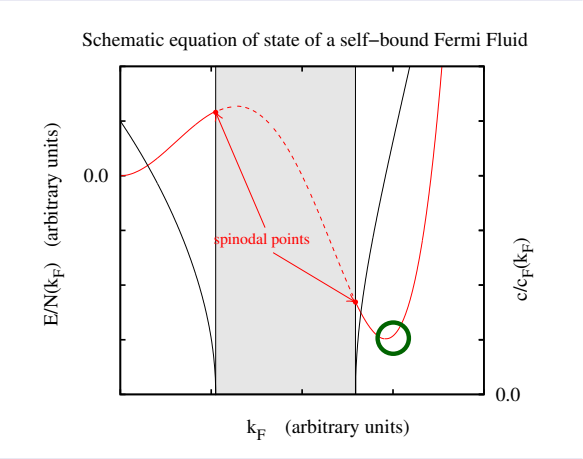
- Many-body binding



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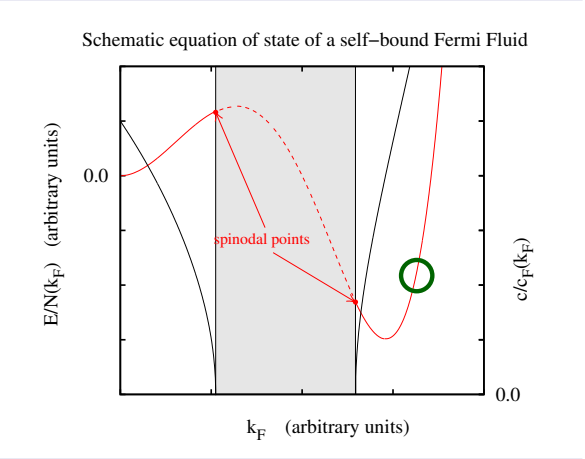
- Saturation



The equation of state of a self-bound system
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- Low densities: Pauli pressure dominates → repulsive Fermi gas
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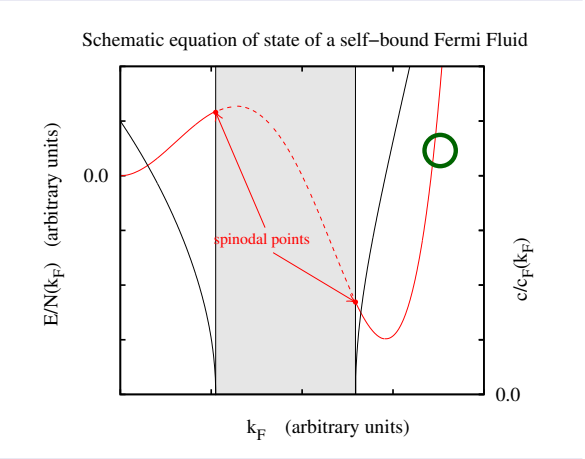
- Many-body binding
- Saturation
- Other phase transitions ?



What physics tells us:

- Binding and saturation
  $\Longrightarrow$ short-ranged structure:
  - "bending" of the wave function at small interparticle distances;
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- Binding and saturation
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  - "local screening" or "local field corrections" in electron systems.
- No answers when mother nature does not have them:
  $\Longrightarrow$ long-ranged structure
  - Show correct instabilities;
  - Deal properly with long-ranged correlations.

Uncorrelated wave functions:
Hartree(-Fock) howto

What we learned in class:

$$\mathrm{H} = \sum_{\mathrm{i}} \mathrm{h}_0(\mathrm{i}) \quad + \quad \sum_{\mathrm{i}<\mathrm{j}} \mathrm{v}(\mathrm{i},\mathrm{j})$$

$$\Psi_0(1,\ldots,\mathrm{N}) \quad = \quad [\mathcal{S}/\mathcal{A}] \prod \phi_{\mathrm{i}}(\mathrm{r}_{\mathrm{j}})$$

$\mathcal{S}$: symmetrized: a "permanent" for bosons
$\mathcal{A}$: antisymmetrized: a determinant for fermions

Determine single particle states:

- Perturbation theory:

$$\mathrm{h}_0 \phi_{\mathrm{n}}(\mathrm{r}_{\mathrm{i}}) = \epsilon_{\mathrm{n}} \phi_{\mathrm{n}}(\mathrm{r}_{\mathrm{i}})$$

- Hartree(-Fock)

$$\frac{\delta}{\delta \phi_{\mathrm{n}}} \langle \Psi_0 | \mathrm{H} - \epsilon_{\mathrm{n}} | \Psi_0 \rangle = 0$$

Uncorrelated wave functions:
The problems

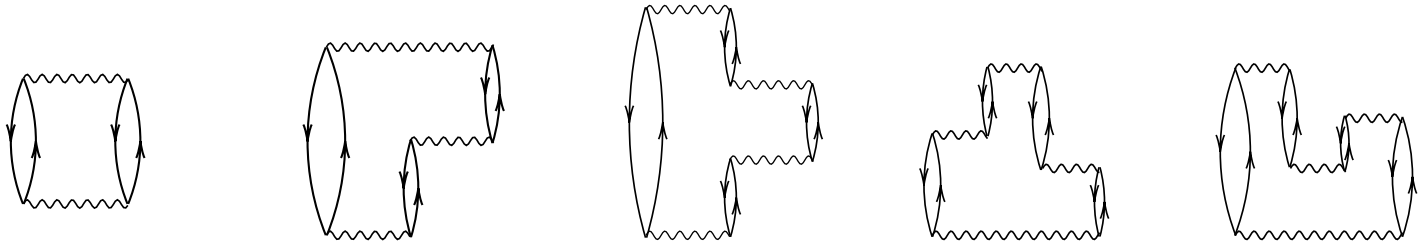
Finite order perturbation theory diverges for long-ranged (Coulomb) interactions

Example: Fetter - Walecka Problem 1.4

Solution: Sum the ring diagrams (RPA equation)

W. Macke,
Über die Wechselwirkungen im Fermi-Gas. Z. Naturf. 5a, 192 (1950).

M. Gell-Mann and K. A. Brueckner,
Correlation Energy of an Electron Gas at High Density.
Phys. Rev. 106, 364 (1957).



Uncorrelated wave functions:
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Finite order perturbation theory diverges for short-ranged (nuclear and atomic) interactions

Solution: Sum the ladder diagrams (Bethe-Goldstone equation)

K. A. Brueckner: Many-Body Problem for Strongly Interacting Particles. Phys. Rev. 100, 36 (195).

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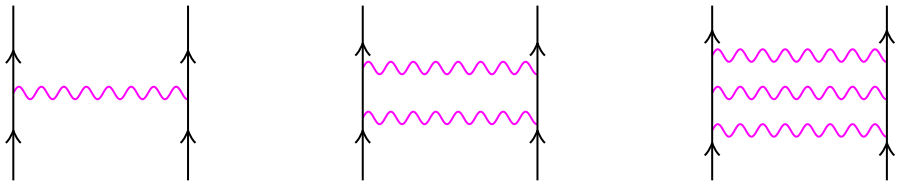

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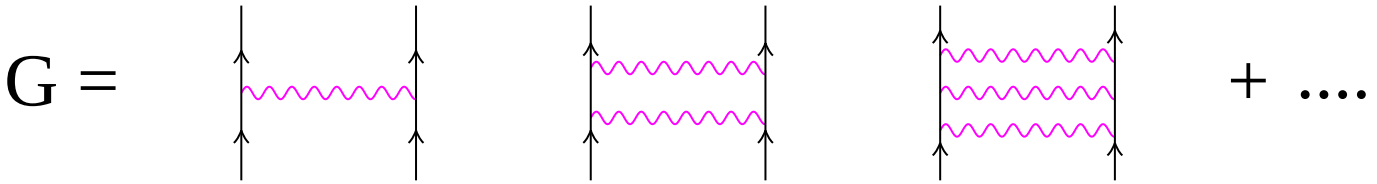
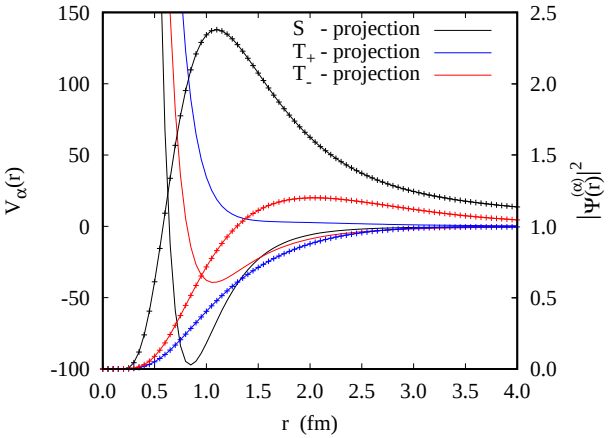
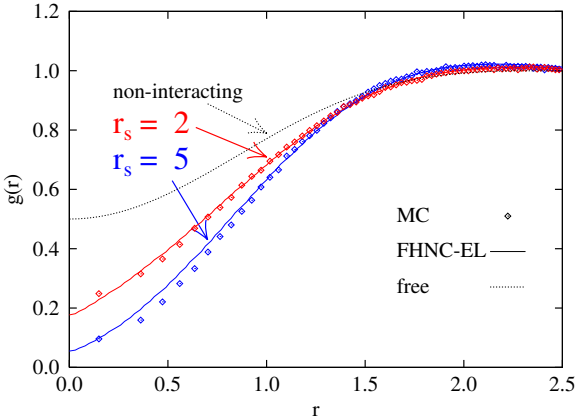


Neutron matter



Electrons



Correlated wave functions

A "simple quick and dirty (?)" method:

$$\Psi_0(1,\ldots,N) = F(1,\ldots,N)\Phi_0(1,\ldots,N) = \prod_{i<j} f(r_i,r_j)\Phi_0(1,\ldots,N)$$

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

$F(1,\ldots,N)$ "Correlation operator" (symmetric in $1,\ldots,N$)

Determine the pair correlations (here: for homogeneous systems)

- The poor man's way:
  "Low order constrained variation" (LOCV)

$$-\frac{\hbar^2}{m}\nabla^2 f(r) + v(r)f(r) = \lambda f(r)$$

and $f(r) = 1$ for $r > r_c$

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- Better: Unconstrained functional minimization:

$$\frac{\delta}{\delta f(r)} \frac{\langle \Psi_0 | H | \Psi_0 \rangle}{\langle \Psi_0 \mid \Psi_0 \rangle} = 0$$

Correlated wave functions:
What correlations do

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

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- An intuitive way to include

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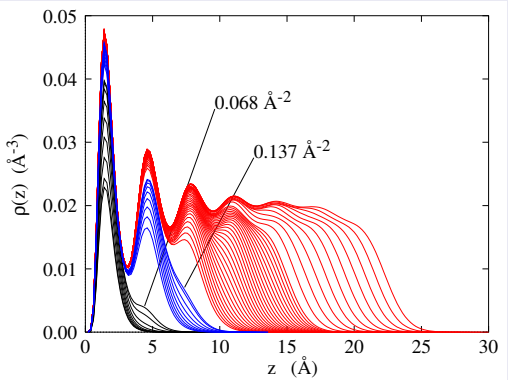
Density profiles of ^{4}He films



- An intuitive way to include inhomogeneity,

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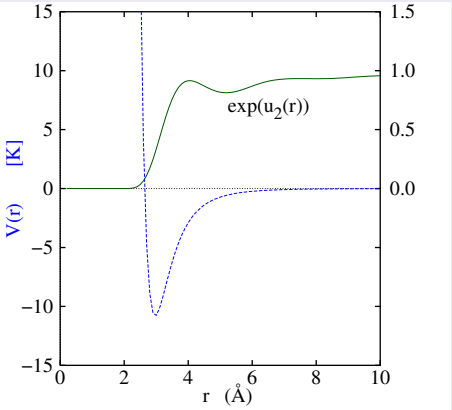
Correlation- and distribution functions



- An intuitive way to include inhomogeneity, core exclusion

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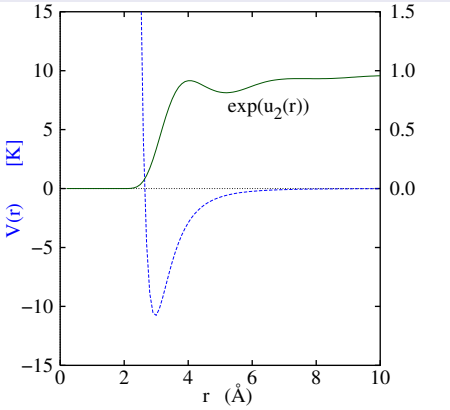

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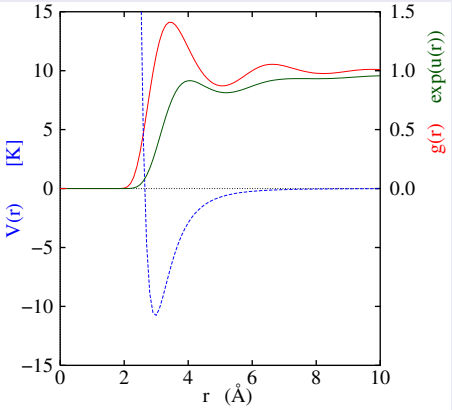

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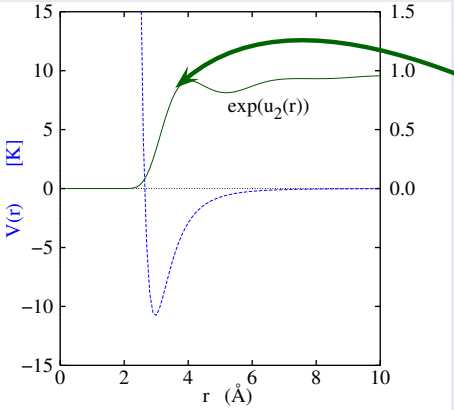

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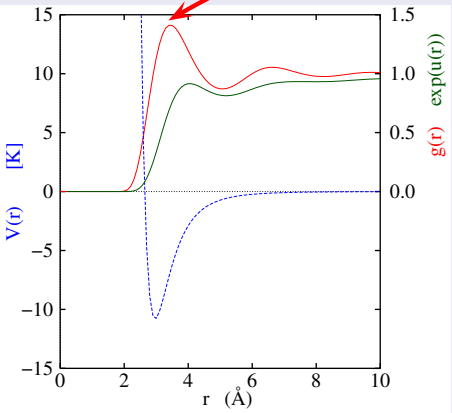

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- Optimization $\delta E/\delta u_n = 0$ makes correlations unique;
- Express everything in terms of physical observables;

Techniques: Diagram expansions

Techniques from statistical physics of non-ideal classical gases:

- "Generating functional": Identify $u_2(r_{ij}) \leftrightarrow -\beta v(r_{ij})$

$$G \equiv \ln \langle \Psi_0 \mid \Psi_0 \rangle = \ln \int d^3r_1, \ldots d^3r_N \, \exp\left[u_2(r_{ij})\right]$$

- "Power-series expansion method":
  Let $\eta(r) = e^{u_2(r)} - 1 \to 0 \quad \text{for} \quad r \to \infty$

$$\begin{aligned} G &= \ln \int d^3r_1, \ldots d^3r_N \prod_{i<j} \left[1 + \eta(r_{ij})\right] \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n}{d\alpha^n} \ln \int d^3r_1, \ldots d^3r_N \prod_{i<j} \left[1 + \alpha\eta(r_{ij})\right] \Bigg|_{\alpha=0} \\ &= \sum_{n=0}^{\infty} (\Delta G)_n \end{aligned}$$

Cluster expansions coming from statistical physics

...Diagrammatics makes life easier ...(Ursell-Mayer expansions)

- Circles depict particle coordinates ("external points"),

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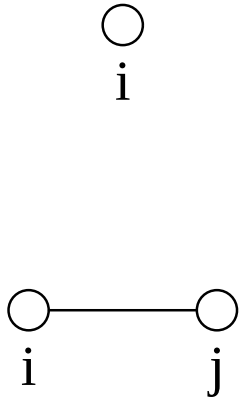

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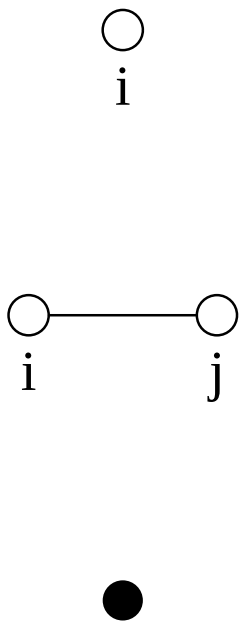

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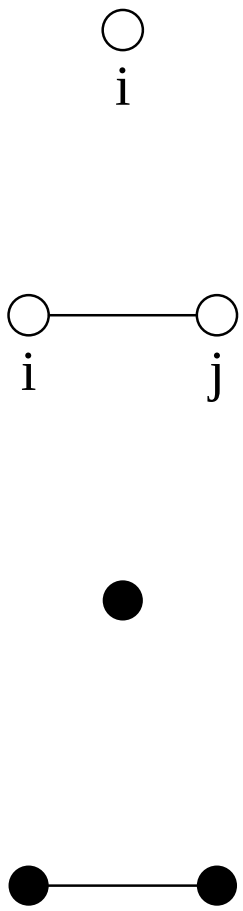
- Example: This diagram represents the integral $\rho^2 \int \mathrm{d^3 r_1 d^3 r_2} \eta(\mathrm{r_{12}})$



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...More Diagrammatics ...

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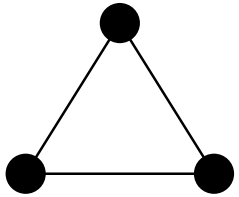

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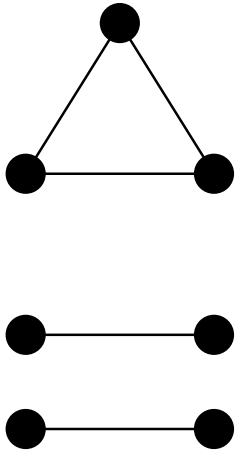

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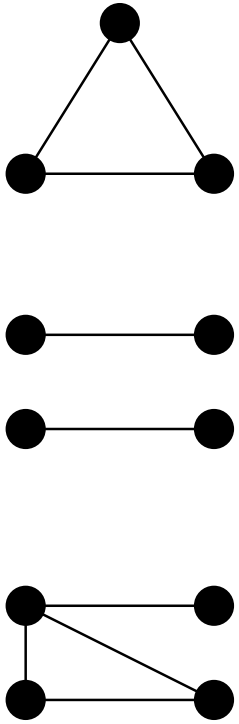

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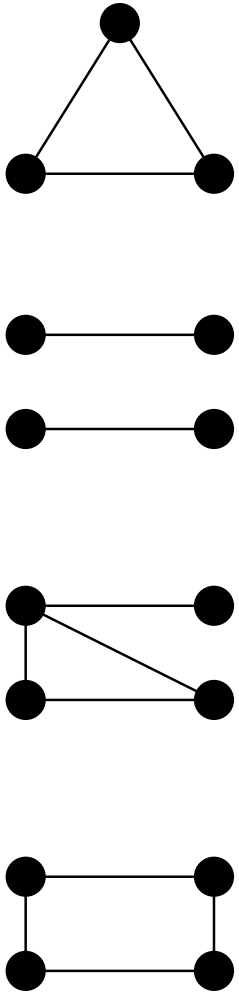
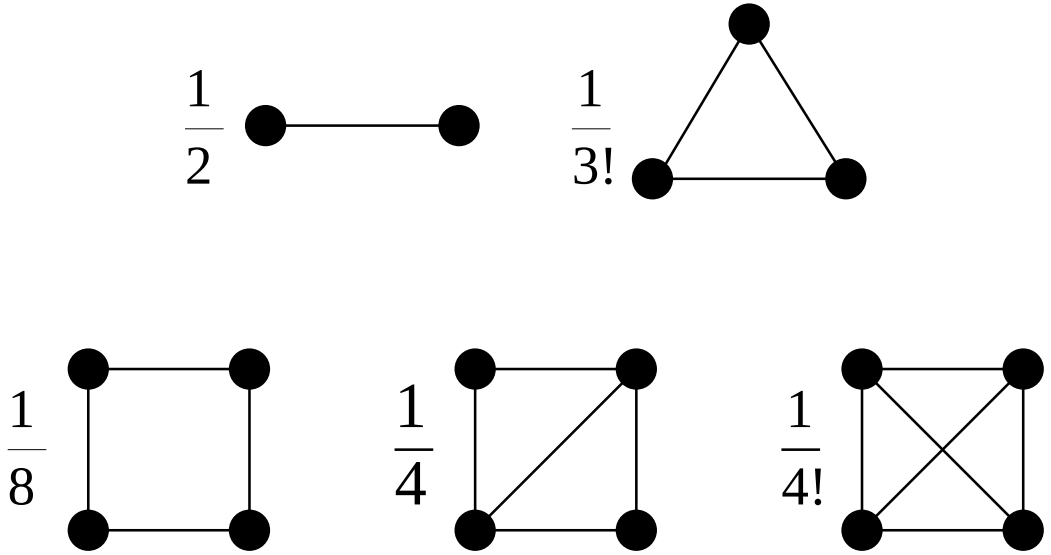


Back to the generating functional

Diagrammatic representation



Theorem (Morita)

$$(\Delta G)_n = \frac{1}{n!} \times \left\{ \begin{array}{l} \text{The sum of all topologically} \\ \text{distinct irreducible n-point dia-} \\ \text{grams without external points.} \end{array} \right\}$$

Pair distribution function:
Diagrammatic representation

Recall the generating functional

$$G = \ln \int d^3r_1 \ldots d^3r_N \exp\left[\sum_{i<j} u_2(r_{ij})\right]$$

Then: 2-body density

$$\begin{aligned}
\rho_2(r_1, r_2; \beta) &= N(N-1) \int d^3r_3 \ldots d^3r_N \left|\psi_0^2(r_1, \ldots, r_N)\right|^2 \equiv \\
\rho^2 g(|r_1 - r_2|) &= 2\frac{\delta G}{\delta u_2(r_1, r_2)}
\end{aligned}$$

Doing this is practice: Let

$$\begin{aligned}
(\Delta G)_1 &= \frac{\rho^2}{2} \int d^3r_1 d^3r_2 \left[e^{u_2(r_1, r_2)} - 1\right] \\
\frac{\delta (\Delta G)_1}{\delta u_2(r_1, r_2)} &= \frac{\rho^2}{2} e^{u_2(r_1, r_2)}
\end{aligned}$$

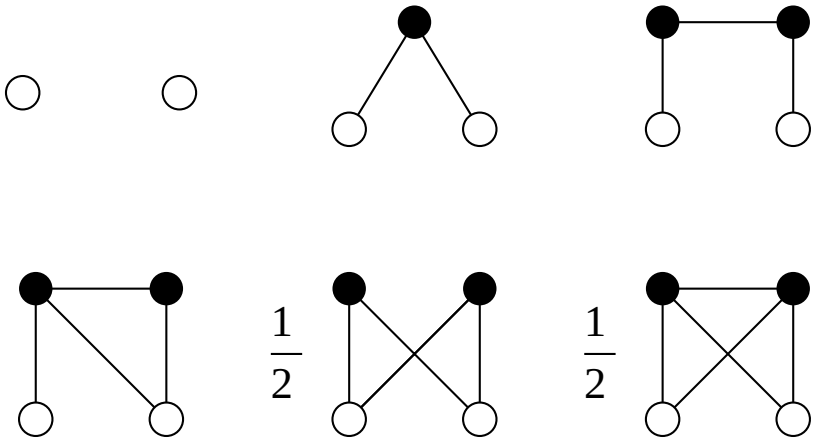
Pair distribution function:
Diagrammatic expansion

Write

$$g(r) = e^{u_2(r)} C(r)\,, \quad C(r) = 1 + \sum_{n=3}^{\infty} (\Delta C)_n(r)$$

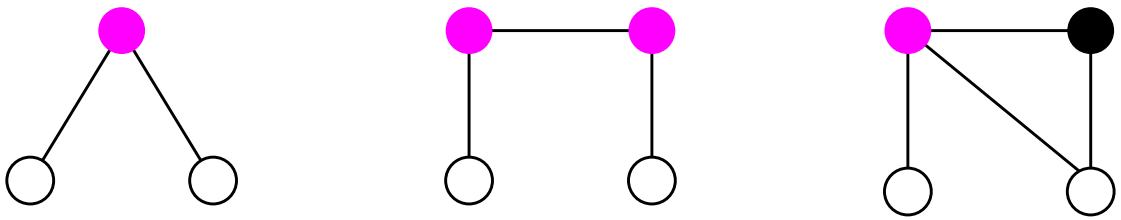
and derive a diagrammatic expansion of $C(r)$.

$$(\Delta C)_n(r) \quad = \quad \frac{1}{(n-2)!} \times \left\{ \begin{array}{l} \text{The sum of all topologically} \\ \text{distinct irreducible n-point} \\ \text{diagrams with two external} \\ \text{points.} \end{array} \right\}$$



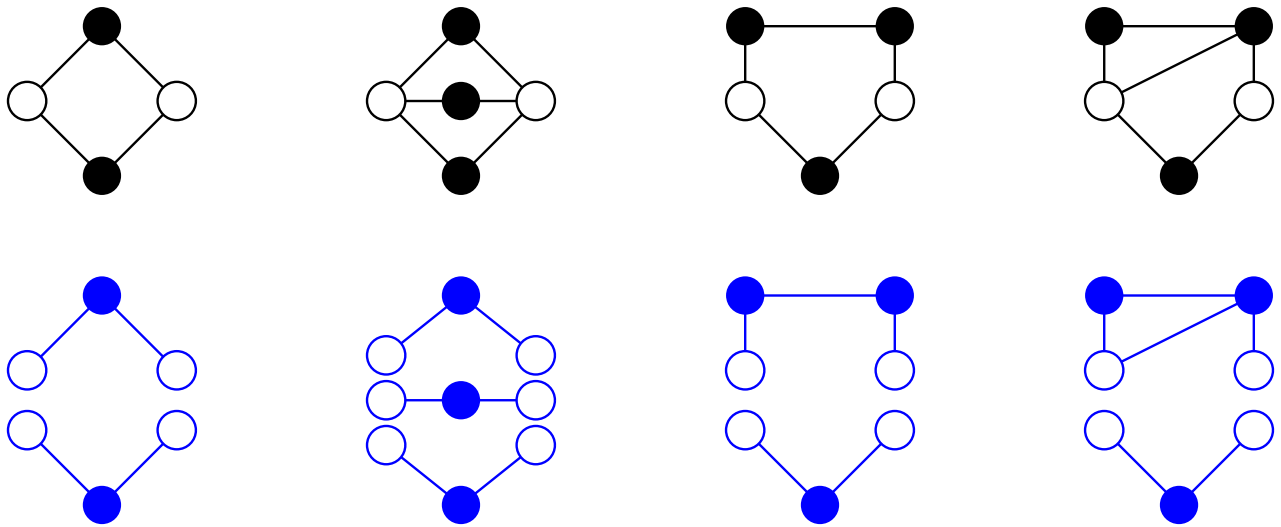
Diagrams:
Establishing order ("Nodal diagrams")

A 1-2 diagram is said to be nodal if it contains one or more nodes, a node being an internal point through which all paths from point 1 to point 2 must pass.



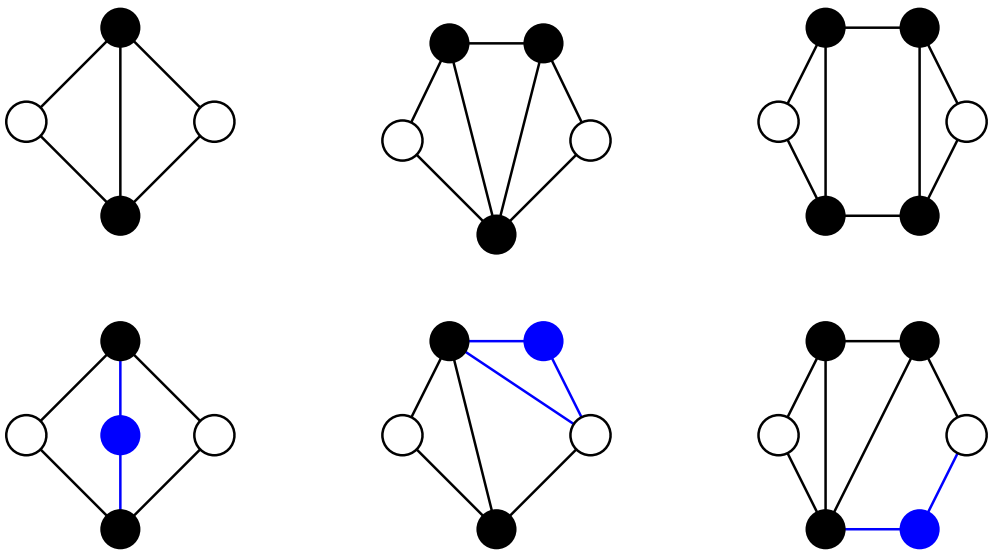
Diagrams:
Establishing order ("Composite diagrams")

A 1-2 diagram is called composite if its contribution can be factored into two or more independent functions of r_1 and r_2.



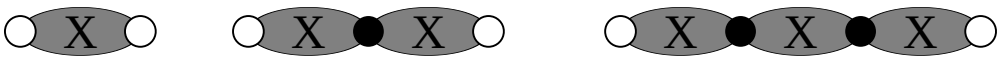
Diagrams:
Establishing order ("Elementary diagrams")

A 1-2 diagram is called elementary if it is neither nodal nor composite. A 1-2 diagram is called basic if its only 1-2 subdiagram is the single bond.



Diagrams:
Summing nodal diagrams

Let X(r) be any (or the sum of all) non-nodal diagrams. Sum the series:



$$\begin{aligned} N(r_1, r_2) &= \rho \int d^3r_2 X(r_1 - r_3) X(r_3 - r_2) \\ &+ \rho^2 \int d^3r_3 d^3r_4 X(r_1 - r_3) X(r_3 - r_4) X(r_3 - r_2) + \ldots \end{aligned}$$

Let

$$\tilde{f}(k) \equiv \rho \int d^3r \, e^{ik\cdot r} f(r)$$

Then

$$\tilde{N}(k) = \tilde{X}^2(k) + \tilde{X}^3(k) + \ldots = \frac{\tilde{X}^2(k)}{1 - \tilde{X}(k)}$$

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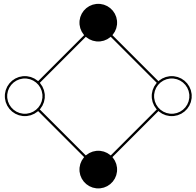
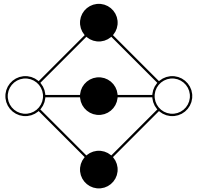
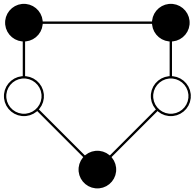
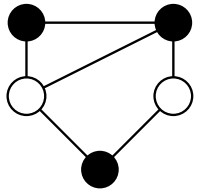
Let N(r) be some (or the sum of all) nodal diagrams. Sum the series:

$\frac{1}{2!}$  $\frac{1}{3!}$   

$$
\begin{aligned}
S(r_1 - r_2) &= \frac{1}{2!}N^2(r_1 - r_2) + \frac{1}{3!}N^3(r_1 - r_2) + \ldots \\
&= \exp\left[N(r_1 - r_2)\right] - N(r_1 - r_2) - 1
\end{aligned}
$$

The "Hypernetted Chain" equations:
Summing all diagrams

$$
\begin{aligned}
g(r) &= \exp\left[u_2(r) + N(r) + E(r)\right] \\
X(r) &= \exp\left[u_2(r) + N(r) + E(r)\right] - N(r) - 1 \\
\tilde{N}(k) &= \frac{\tilde{X}^2(k)}{1 - \tilde{X}(k)} \\
S(k) &= 1 + \rho \int d^3r\, e^{ik\cdot r}\left[g(r) - 1\right] = \frac{1}{1 - \tilde{X}(k)}
\end{aligned}
$$

• $E(r)$ is the sum of all "elementary" diagrams in terms of the bond $\eta(r)$, or the sum of all "basic" diagrams in terms of the bond $h(r) \equiv g(r) - 1$.

• The equations can used to eliminate the correlation function $u_2(r)$ and express the energy in terms of the physical observable $g(r)$.

$$u_2(r) = \ln g(r) - N(r) - E(r)$$

Energy:
An explicit functional of g(r):

- We have an explicit relationship between $u_2(r)$ and $g(r)$;

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- Question 3: Is the variational problem generic ?

The two-body Euler equation: $[\delta E/\delta g])r) = 0$

The "Bethe-Goldstone face"

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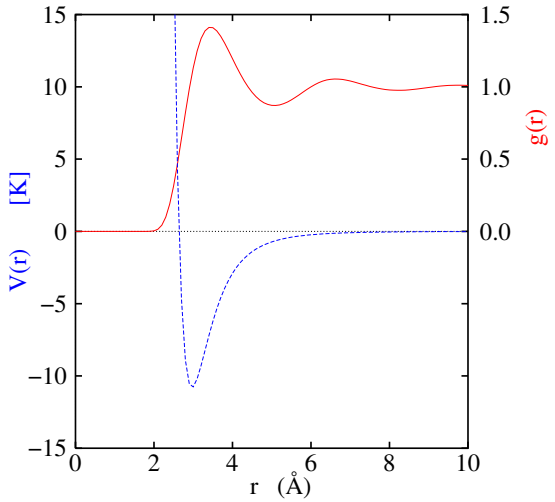
  L. J. Lantto and P. J. Siemens,
  Phys. Lett. B 68, 308 (1977)
  The short-ranged structure is determined by a 2-body Schrödinger equation.

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



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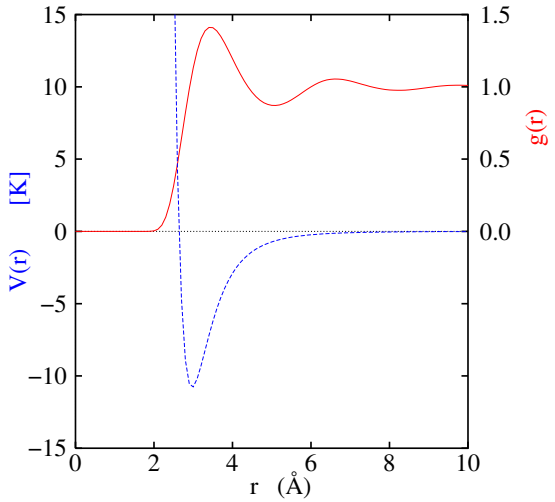

- $w(r)$"induced interaction": Guarantees that $g(r) \to 1 + \mathcal{O}(r^{-4})$ as $r \to \infty$

Two-body Euler equation: $\delta E/\delta g = 0$

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

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- To remember:

$$\begin{aligned} \chi^{(RPA)}(q,\omega) &= \frac{\chi_0(q,\omega)}{1 - \tilde{V}_{p\text{-}h}(q)\chi_0(q,\omega)}, \\ S(q,\omega) &= -\frac{1}{\pi}\Im m\,\chi(q,\omega), \qquad S(q) = \int d(\hbar\omega) S(q,\omega) \end{aligned}$$

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$$\begin{aligned} \chi^{(RPA)}(q,\omega) &= \frac{\chi_0(q,\omega)}{1 - \tilde{V}_{p\text{-}h}(q)\chi_0(q,\omega)}, \\ S(q,\omega) &= -\frac{1}{\pi}\Im m\,\chi(q,\omega), \qquad S(q) = \int d(\hbar\omega) S(q,\omega) \end{aligned}$$

- For bosons: Free response function

$$\chi_0(q,\omega) = \frac{2t(q)}{\hbar^2\omega^2 - t^2(q)}, \qquad t(q) = \frac{\hbar^2 q^2}{2m}$$

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

Summarizing its two faces:

- "RPA" view:

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

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

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$$\tilde{w}(k) = \frac{\hbar^2 k^2}{4m}\left[1 - S^{-1}(k)\right]^2 [2S(k) + 1]$$

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

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A pair–density–functional theory

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- The proof is identical to that of the Hohenberg-Kohn theorem.

Constructing the functional
A formal argument

Assume we have some prescription

$$g_\lambda(r) = g(r; \lambda v(r)) \qquad 0 \leq \lambda \leq 1$$

Then (Feynman–Hellman):

$$E = E_0 + \frac{\rho}{2} \int d^3r v(r) \int_0^1 d\lambda g_\lambda(r)$$

Because

- $g_{\lambda=1}(r) = g(r, v(r))$
- HK-II $\Rightarrow$ the mapping can be inverted
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and hence for the exact ground state:

$$\boxed{E = E[v(r), g(r)] = T[g(r)] + \tfrac{\rho}{2} \int d^3r\, v(r) g(r).}$$

Reverse statement: Assume we have a variational principle

$$\frac{\delta E[v(r), g(r)]}{\delta g(r)} = 0$$

Then

$$\begin{aligned} \frac{dE}{d\lambda} &= \frac{\rho}{2}\int d^3r v(r) g_\lambda(r) + \int d^3r \frac{\delta E}{\delta g_\lambda(r)} \frac{dg_\lambda(r)}{d\lambda} \\ &= \frac{\rho}{2}\int d^3r v(r) g_\lambda(r). \end{aligned}$$

and hence

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- The Feynman-Hellman-Theorem leads to a $E[v(r), g(r)]$;
- Any variational principle leads to a Feynman-Hellman-Theorem;
- The Feynman-Hellman-Theorem is more general than originally formulated.

Constructing the functional

"Small amplitude hand-waving"

- In coordinate space, a Bethe-Goldstone equation:

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

$V_{p-p}(r)$ is some"particle–particle" interaction, $V_{p-p}(r) \approx v(r)$ as $r \to 0+$.

- In momentum space, a "linear response" equation

$$\begin{aligned}\chi(q,\omega) &= \frac{\chi_0(q,\omega)}{1-\tilde{V}_{p-h}(q)\chi_0(q,\omega)} \\ S(q) &= \int \frac{d\omega}{2\pi}\Im m\chi(q,\omega)\end{aligned}$$

$V_{p-h}(r)$ is some"particle–hole" interaction,

- Demand consistency

$$g(r) = 1 + \int \frac{d^3q}{(2\pi)^3\rho}e^{-iq\cdot r}\left[S(q)-1\right]$$

Result

The equations of the variational theory ! ... with $v(r) \to v(r) + V_I(r)$.

$$E = K + V + E_Q + E_I = E_{HNC} + E_I.$$

Kinetic energy due to the curvature of the wave function at short distances:

$$K = \rho \frac{\hbar^2}{2m} \int d^3r \left| \nabla \sqrt{g(r)} \right|^2 .$$

"Ring–diagrams":

$$E_Q = -\frac{\hbar^2}{8m} \int \frac{d^3q}{(2\pi)^3 \rho} q^2 \frac{(S(q)-1)^3}{S(q)}$$

E_I is a functional of the pair distribution function $g(r)$ which generates the irreducible interaction through

$$V_I(r) = \frac{2}{\rho} \frac{\delta E_I}{\delta g(r)}.$$

Analog of the "exchange-correlation energy", but at most a 15% effect !

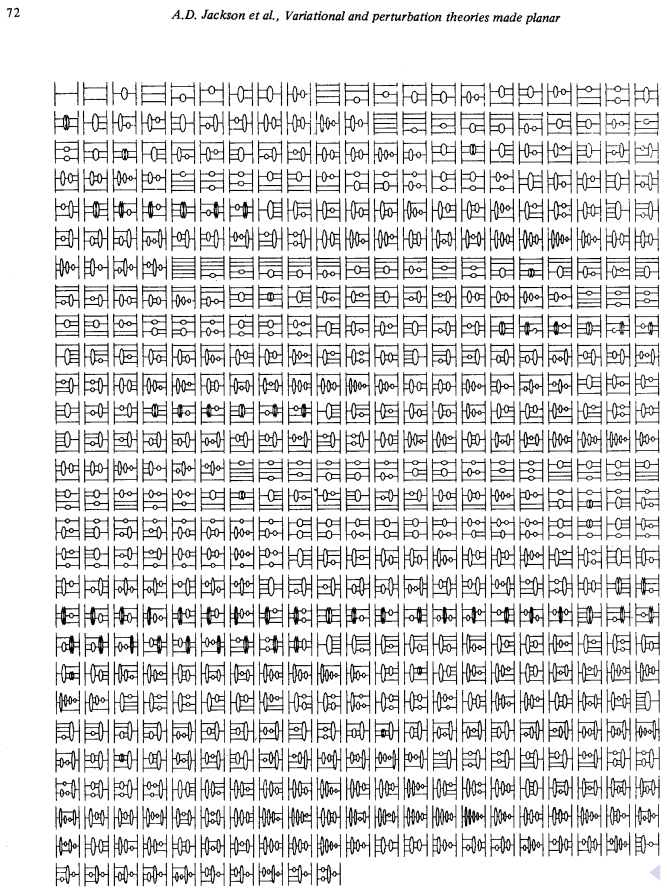
Local parquet diagrams

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

Recall this conjecture:

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

... and make it quantitative:



Local parquet diagrams: making parquet practical

Summarizing 100 pages Physics Reports

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

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

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- Define an energy–dependent particle–hole reducible interaction

$$\begin{aligned} \tilde{\mathrm{w}}_{\mathrm{I}}(\mathrm{q},\omega) &= \tilde{\mathrm{V}}_{\text{p-h}}(\mathrm{q})/(1 - \tilde{\mathrm{V}}_{\text{p-h}}(\mathrm{q})\chi_0(\mathrm{q},\omega)) \\ \chi(\mathrm{q},\omega) &= \chi_0(\mathrm{q},\omega) + \chi_0(\mathrm{q},\omega)\tilde{\mathrm{w}}_{\mathrm{I}}(\mathrm{q},\omega)\chi_0(\mathrm{q},\omega) \end{aligned}$$

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

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

Parquet diagrams: Ladder diagram summation

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

- Sum the ladder diagrams with this local interaction

$$\frac{\hbar^2}{\mathrm{m}}\nabla^2\psi(\mathrm{r}) = (\mathrm{v}(\mathrm{r}) + \mathrm{w_I}(\mathrm{r}, \bar{\omega}(\mathrm{q})))\psi(\mathrm{r})$$

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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.

Summarizing
Boson theory

- There are by now 4 different ways to derive the same equations:
  - Variational method
  - Local parquet
  - Pair-DFT
  - "Super-SUB2" version of Coupled Cluster theory

> It appears that the development of the many-body problem has reached a point where different version differ in language but not in substance. (A. D. Jackson)

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- If HNC-EL is not enough, include triplets
  - 3-body Jastrow-Feenberg correlations $u_3(r_i, r_j, r_k)$
    Chang and Campbell, PRB 15, 4238 (1977)
  - Parquet: Include leading totally irreducible diagrams and relax the local approximation
    Jackson, Lande, Guitink, Smith PRB 31, 403 (1985)
  - Lead again to the same equations.

The Fermion problem:
Back to cluster expansions and HNC equations

$$
\begin{aligned}
\Psi_0(1,\ldots,N) &= F(r_1,\ldots,r_N)\Phi_0(1,\ldots,N) \\
F(r_1,\ldots,r_N) &= \exp\frac{1}{2}\left[\sum_{i<j}^{N} u_2(r_i,r_j)+\ldots\right] \\
\Phi_0(1,\ldots,N) &= \det\left[\phi_i(r_j)\chi(i)\right]
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$\Phi_0(1,\ldots,N)$: Slater–determinant of model orbitals

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Strategy:

- Identify the approximation leading from Jastrow-Feenberg to parquet. Justify, as far as possible, by Monte Carlo.
- Jastrow-Feenberg may be too tedious or even wrong, then use parquet diagrams with the same approximations.

The Fermion problem:
Back to cluster expansions and HNC equations

Requirements:

- Must contain right physics,
- Must be optimizable,
- Must be efficient.

Need:

- Diagram expansions,
- (Hierarchy of) Euler–equation(s),
- Identify connection to parquet

Cluster expansions of the generating functional
Diagrammatic elements

$$G = \ln \left\langle \Phi_0 \left| \exp \left[\sum_{i<j} u_2(r_i, r_j) \right] \right| \Phi_0 \right\rangle = \sum_{n=0}^{\infty} (\Delta G)_n \, .$$

Graphical elements:

Cluster expansions of the generating functional

Diagrammatic elements

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- Open and filled circles

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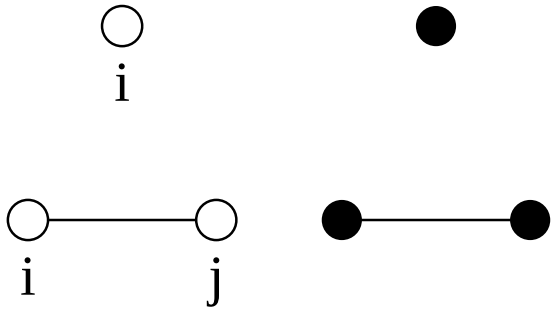

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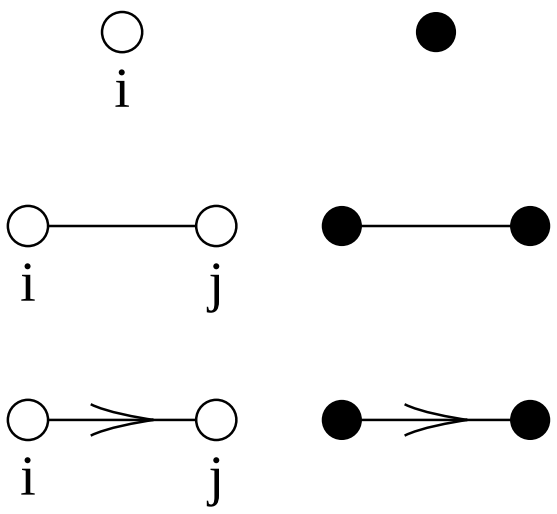
- NEW: "exchange lines" connectig circles i and j depict $\ell(r_{ij}) = \frac{1}{N} \sum_{k \le k_F} e^{ik \cdot (r_i - r_j)}$.

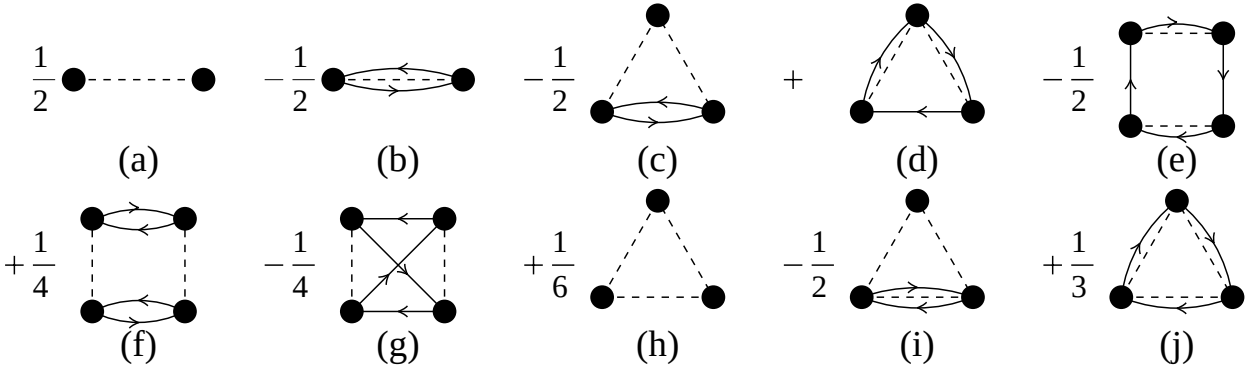


Cluster expansions of the generating functional

Diagrammatic rules

- Each n–body diagram has a counting factor $1/n!$.
- Each point is attached by at least one correlation line $\eta(r_i, r_j)$. Two different points may be connected by at most one correlation factor.
- Each point is attached by exactly one incoming and one outgoing exchange line (Don't display exchanges lines returning into themselves).
- Exchange lines occur always in closed polygons and carry a factor $(-\nu)^{1-n}$, where n is the number of points connected by the exchange loop and ν is the degree of degeneracy of the single particle states.

Expansion for G



Local parquet diagram for fermions
(1) Ring diagrams

- RPA

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

Local parquet diagram for fermions
(1) Ring diagrams

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- Simplify if you care (this leads to JF)

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

Local parquet diagram for fermions
(2) Ladder diagrams

- Bethe-Goldstone equation for the pair correlation function:

$$\begin{aligned}\langle \mathrm{k}, \mathrm{k}' | \psi | \mathrm{h}, \mathrm{h}' \rangle &= \langle \mathrm{k}, \mathrm{k}' | \mathrm{h}, \mathrm{h}' \rangle \\ &\quad - \frac{\bar{\mathrm{n}}(\mathrm{k})\bar{\mathrm{n}}(\mathrm{k}')}{\mathrm{e}(\mathrm{k}) + \mathrm{e}(\mathrm{k}') - \mathrm{e}(\mathrm{h}) - \mathrm{e}(\mathrm{h}')} \langle \mathrm{k}, \mathrm{k}' | \mathrm{v}\psi | \mathrm{h}, \mathrm{h}' \rangle \,.\end{aligned}$$

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- $\Rightarrow$Energy coefficient must be somehow approximated by a function of momentum transfer
- Averaging procedure leading to JF:

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

Local parquet diagram for fermions
(3) Ladder rungs

- Just like for bosons: Effective interaction

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

Particle-hole reducible part

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- Localization procedure

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

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

Summarizing:
..connection of Jastrow-FHNC

"Localization" of the energy demoninator

$$e_{q+h} - e_h \to \bar{e}(q) = \frac{\sum_h \bar{n}(h+q)n(h)(e_{q+h} - e_h)}{\sum_h \bar{n}(h+q)n(h)}$$

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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.

Two-body Euler or local parquet equations for fermions

Summarizing its two faces

(Collective) "RPA" face

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

Two-body Euler or local parquet equations for fermions

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

Two-body Euler or local parquet equations for fermions

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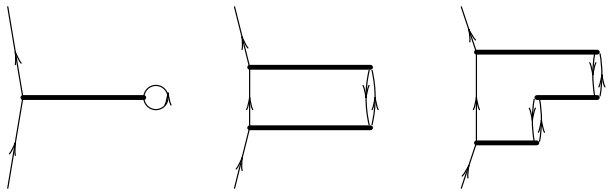
"Parquet" face

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

Self-energy diagram summation
..for fermions

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



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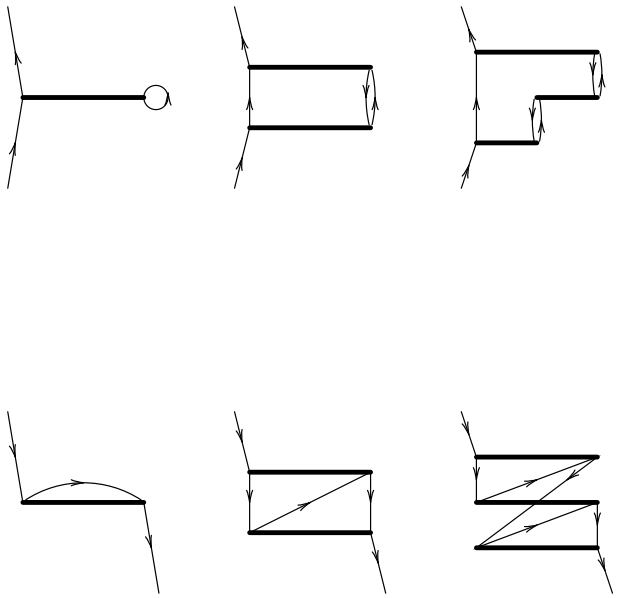

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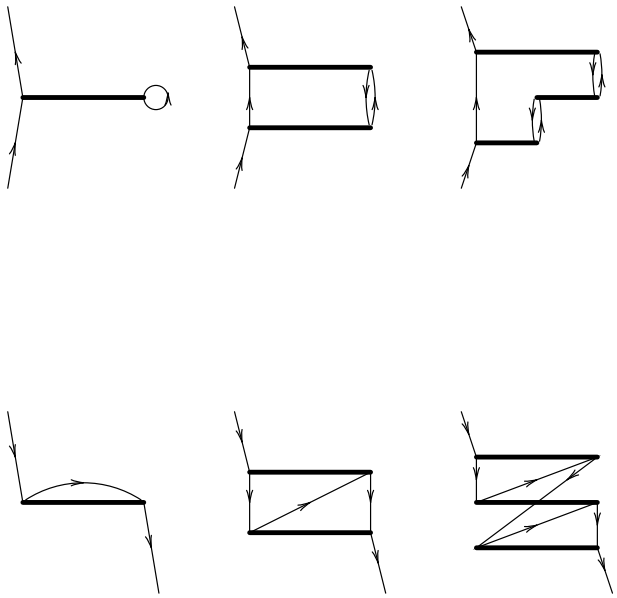

Coester's Commandment:

Thou shalt not split small quantities into large pieces !

Verification: Why look at the helium liquids ?

Worst case scenario

- ^{3}He at saturation:
  Saturation density: $k_F = 0.78\,\text{Å}^{-1}$, $\rho_0 = 0.0166\,\text{Å}^{-3}$.
  core size $\sigma = 2.556$Å.
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- Nuclear matter at saturation:
  Saturation density: $k_F = 1.4\,\text{fm}^{-1}$, $\rho_0 = 0.185\,\text{fm}^{-3}$.
  Core size $\sigma = 0.7\ldots1.0\,\text{fm}$.
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- Low density neutron matter:
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  Core size $\sigma = 0.7\ldots1.0\,\text{fm}$.
  $\rho_0 = 0.011\ldots0.034\,\sigma^{-3}$.

Verification I: Lennard-Jones and square-well fluids

How well it works (Bragbook)

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

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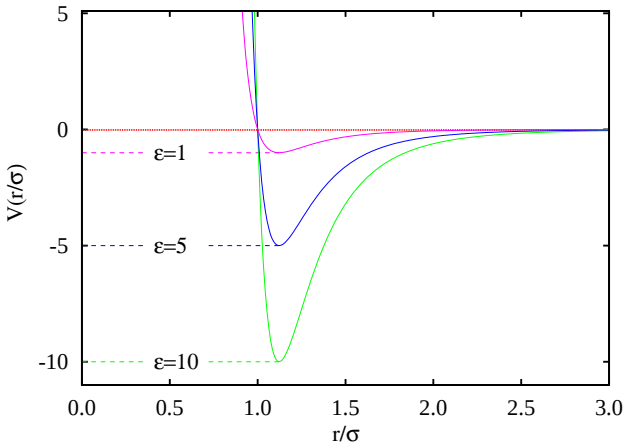

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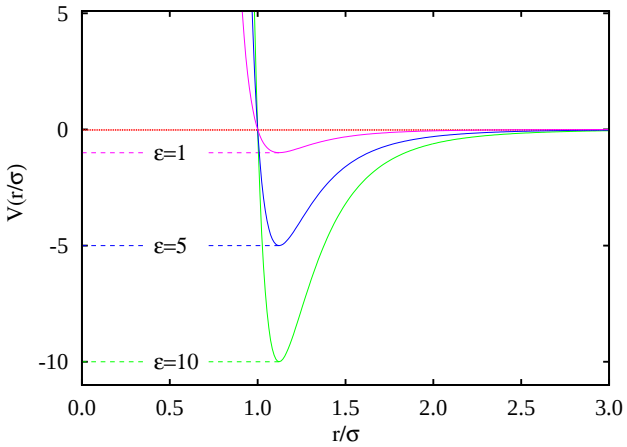
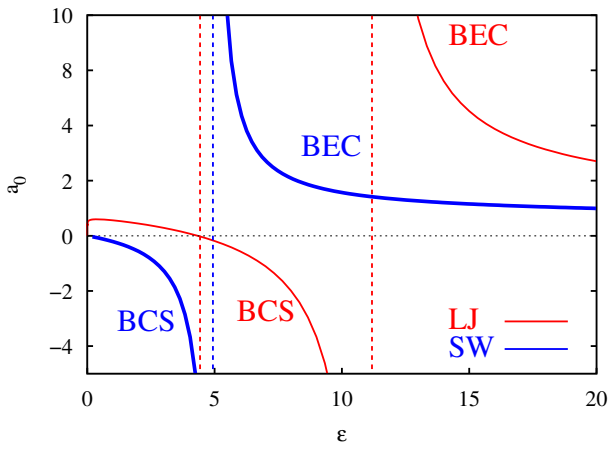
- Adjust ε to obtain the desired scattering lenght a_0 (the cold gas people want it that way);





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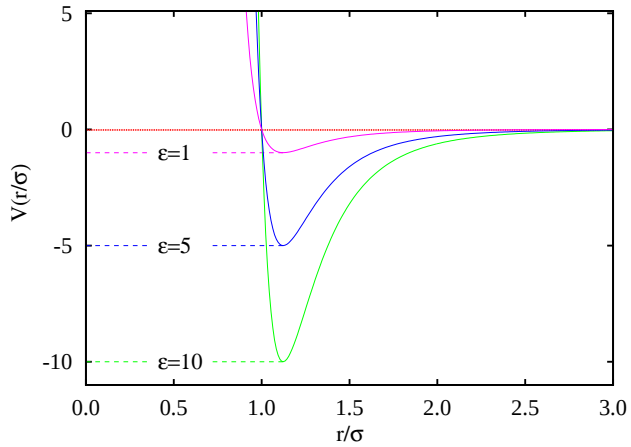
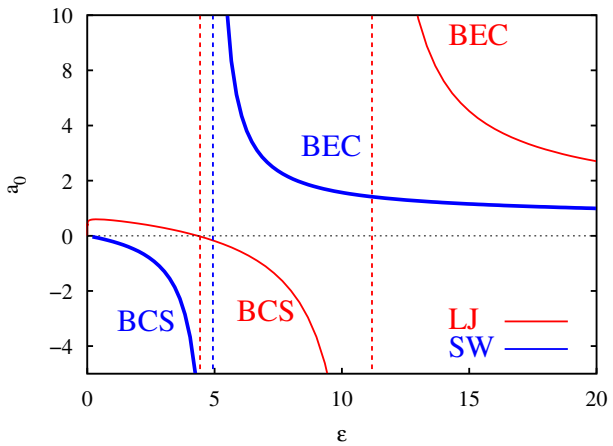
- Adjust ε to obtain the desired scattering lenght a_0 (the cold gas people want it that way);
- First bound state appears at $\varepsilon = 11.18$ (4.33) $\Rightarrow$ Divergence of the vacuum scattering length.





Verification I: The Lennard-Jones liquid

How well it works (Bragbook)

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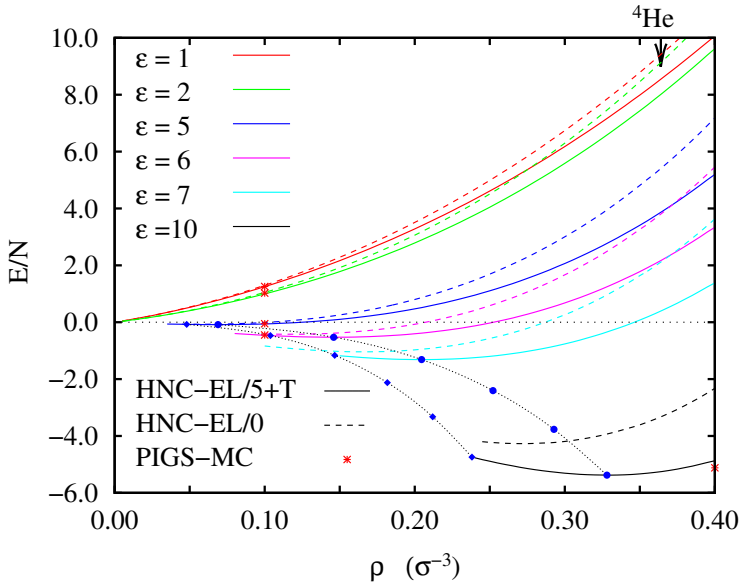
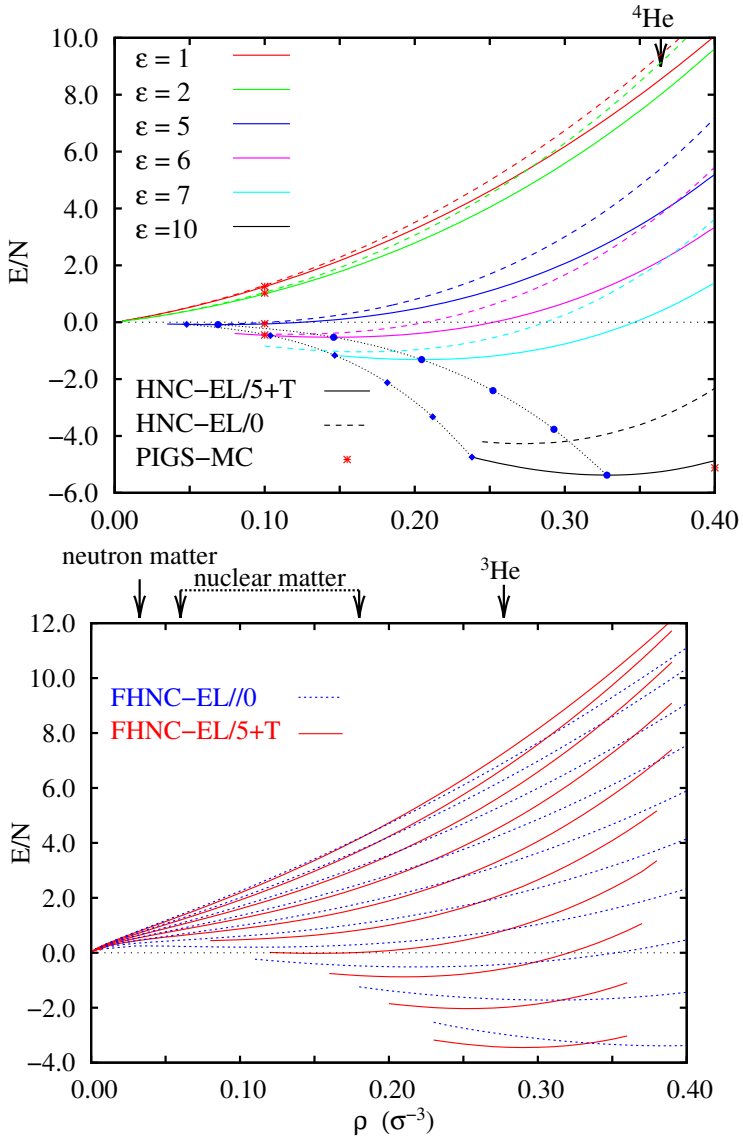


Verification I: The Lennard-Jones liquid

How well it works (Bragbook)

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



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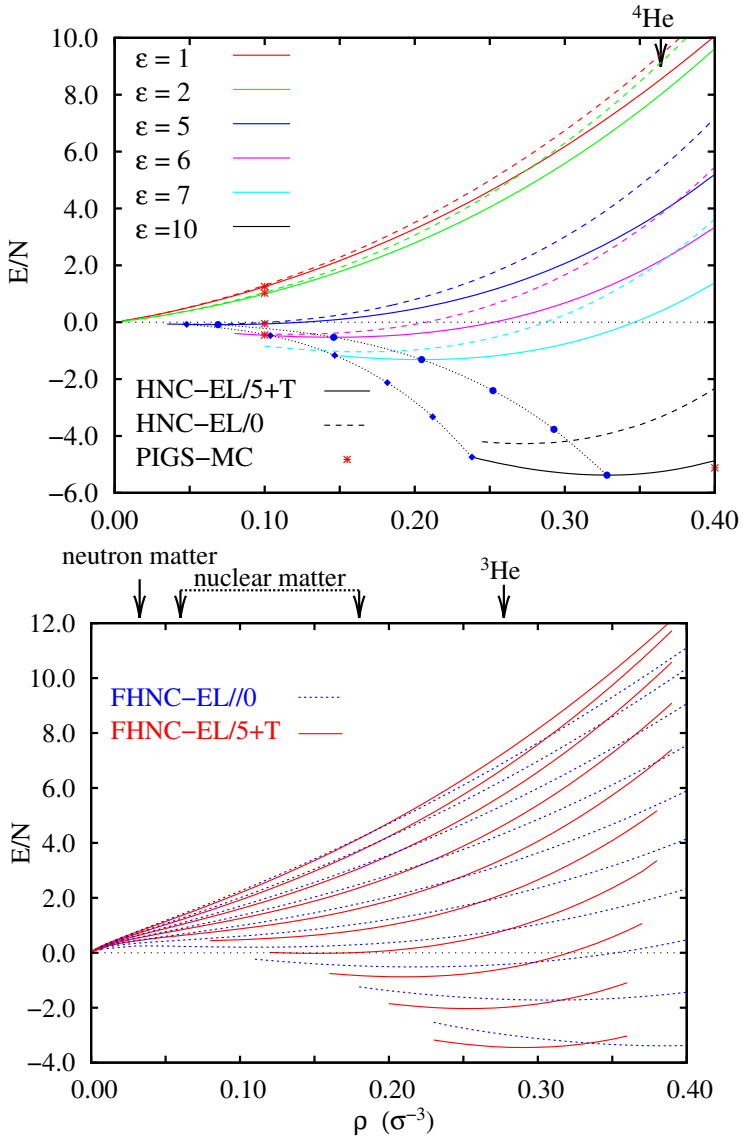

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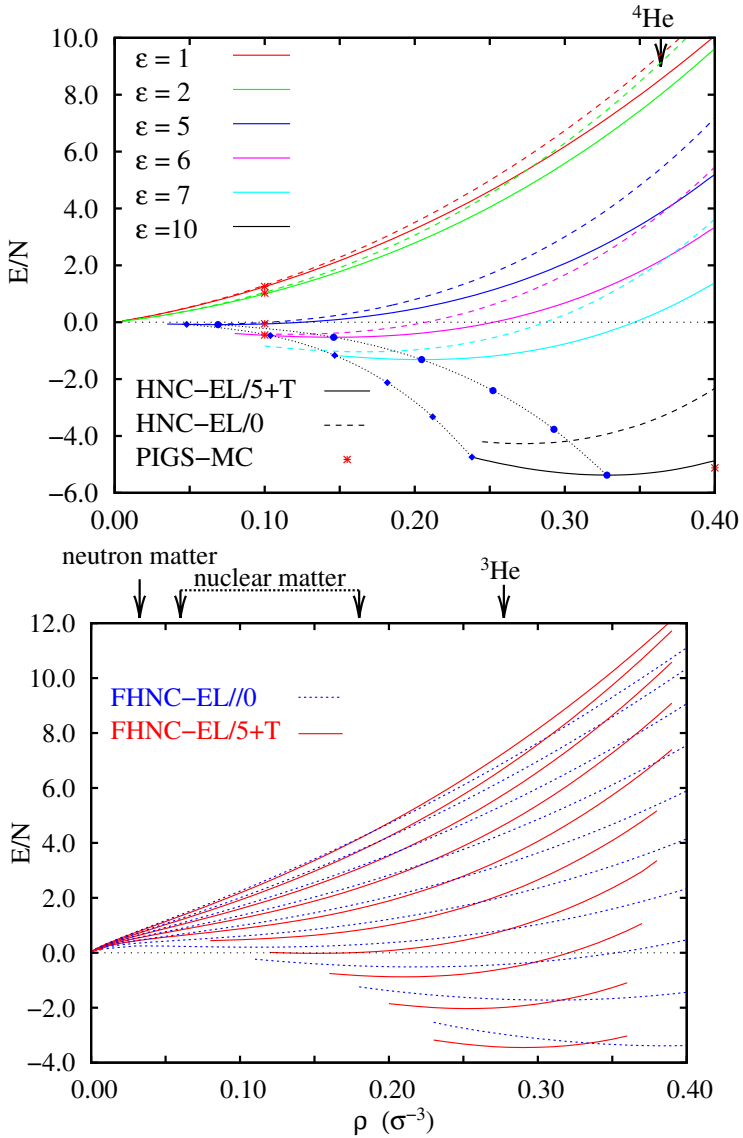

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- Equation of state for Bosons
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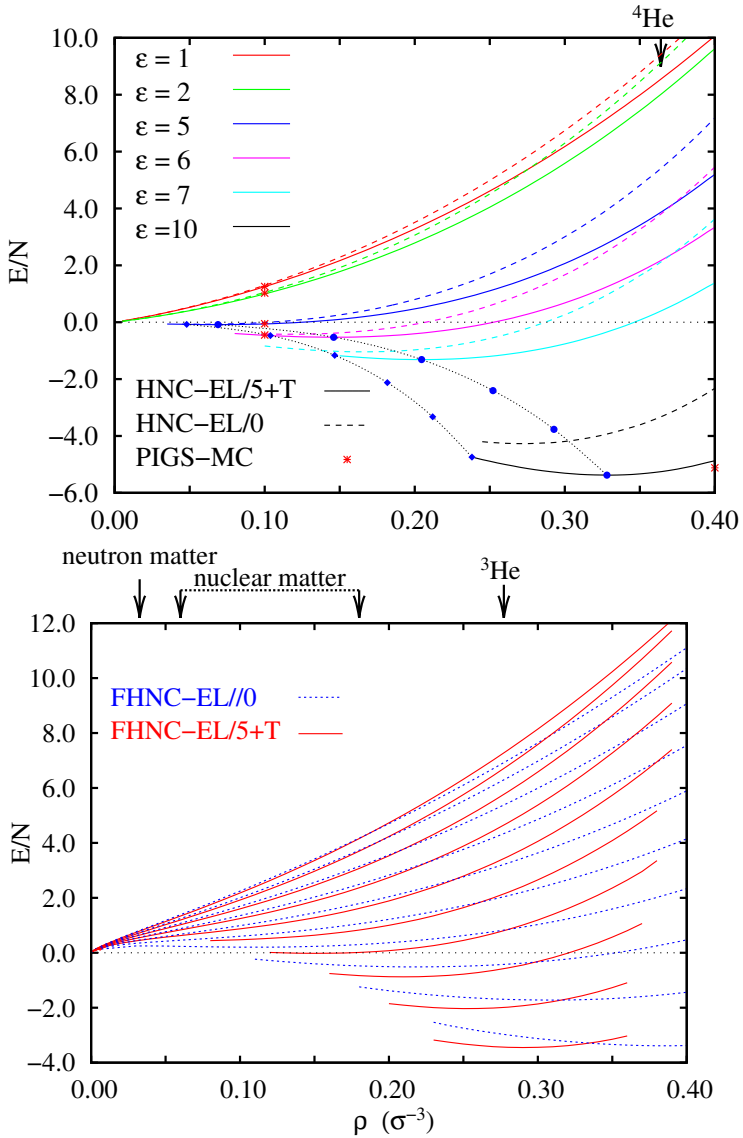
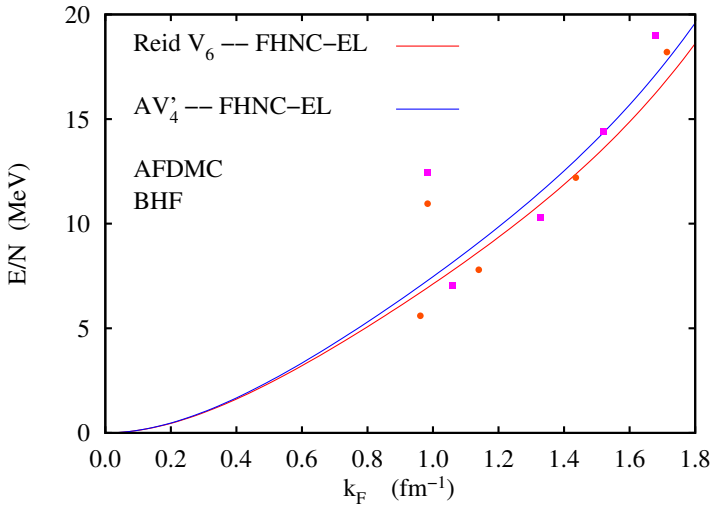
- Works the same in 2D
- FHNC-EL (or parquet) has no solutions if "mother nature" cannot make the system: The equation of state ends at the spinodal points.



Verification II: Nuclear interactions
Argonne and Reid V_4

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



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Argonne and Reid V_4

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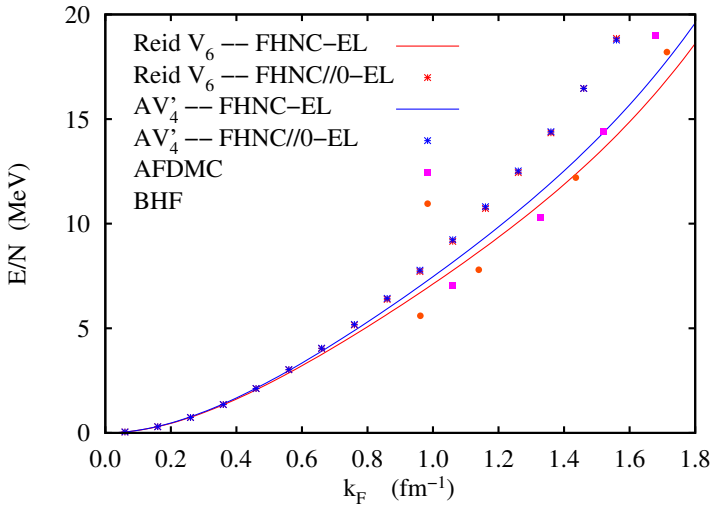
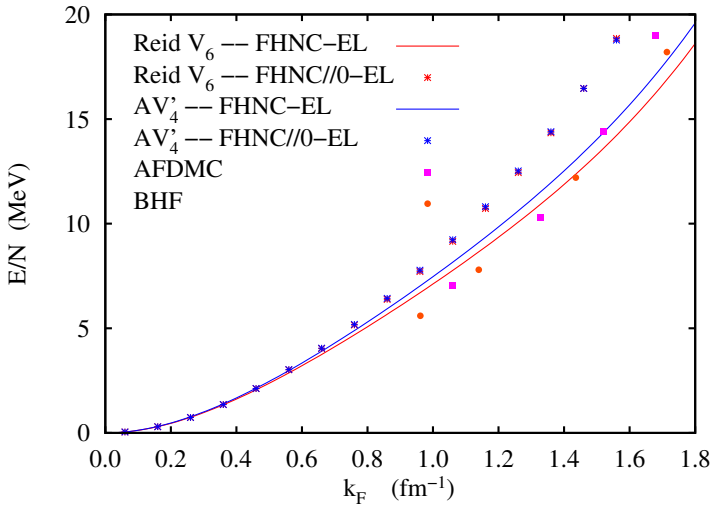


Verification II: Nuclear interactions
Argonne and Reid V_4

- 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 !



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– the many-body effects

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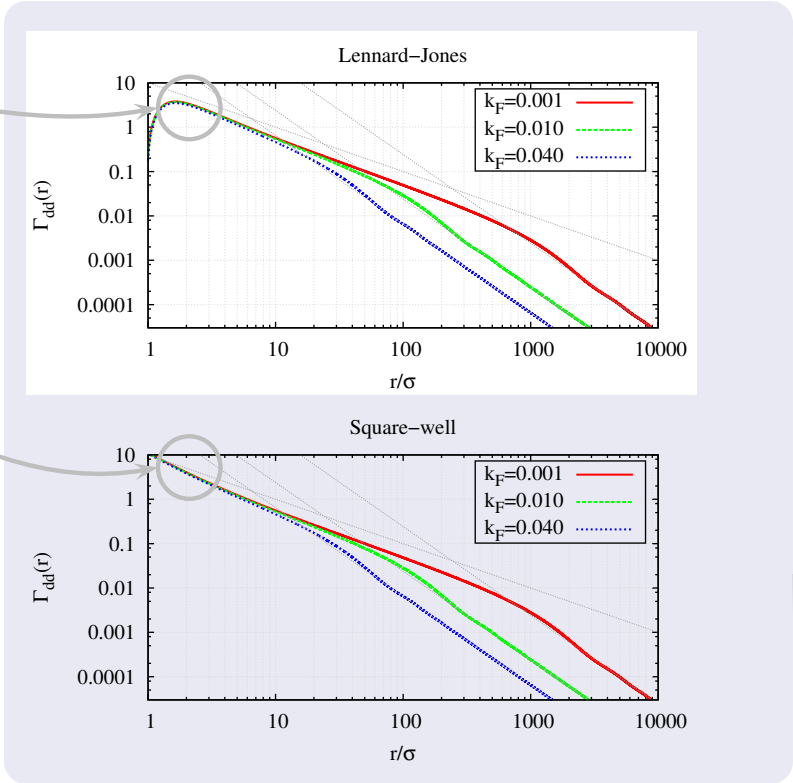

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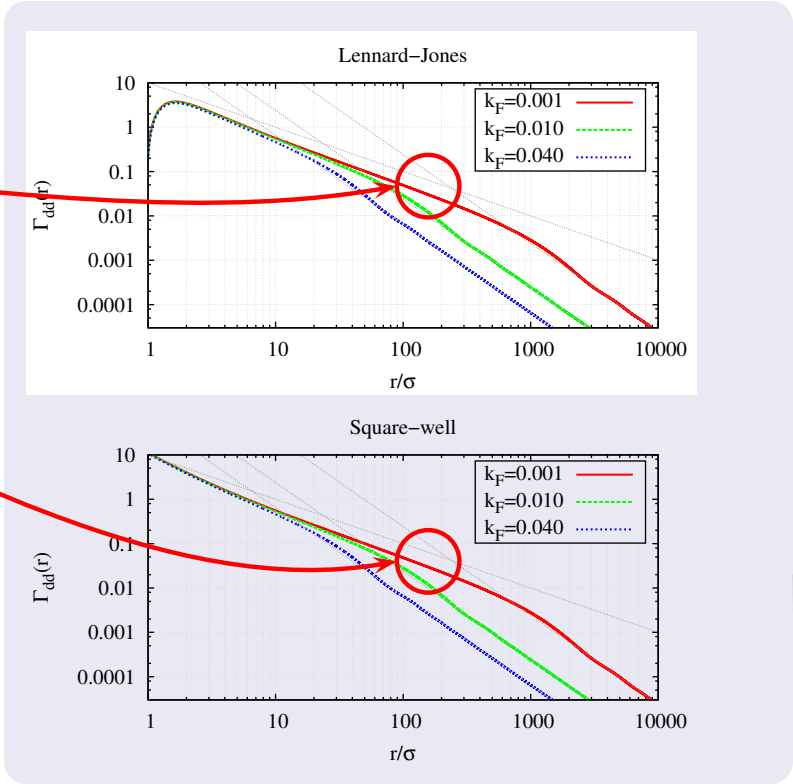

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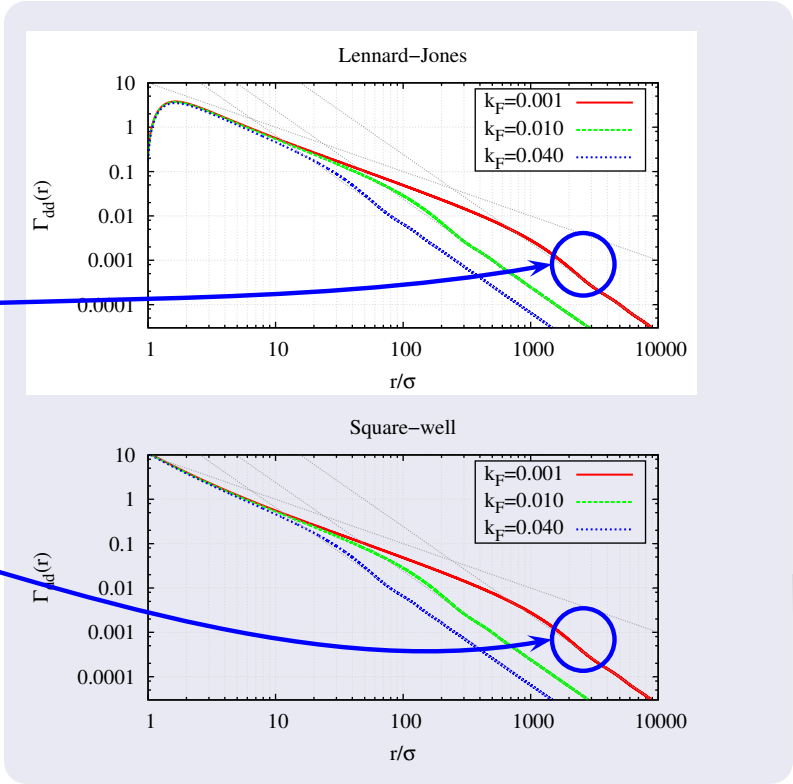


Summarizing the Lennard-Jones Liquid

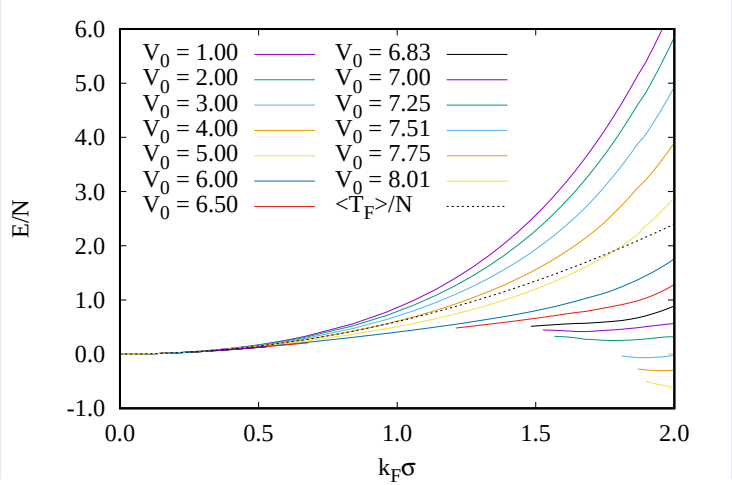
Include exchanges and parquet

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



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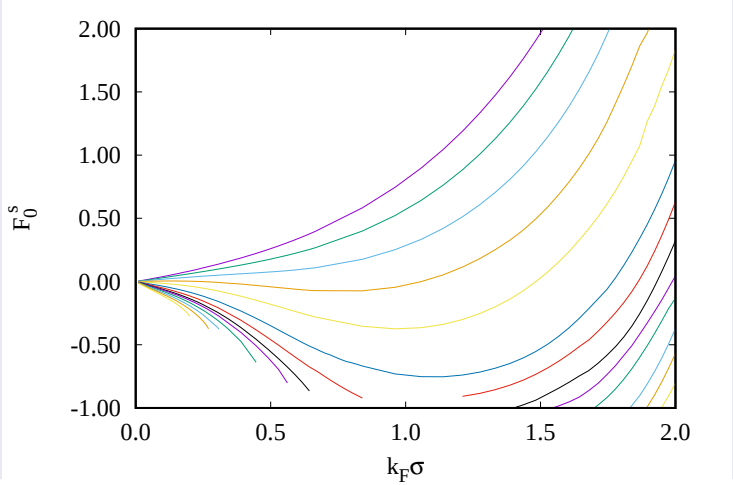

Divergence of parquet-summations
What it means

- We get the low-density spinodal point

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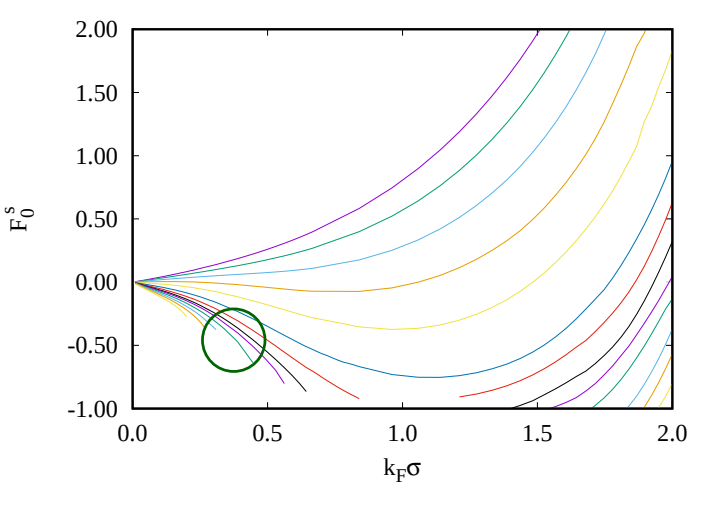

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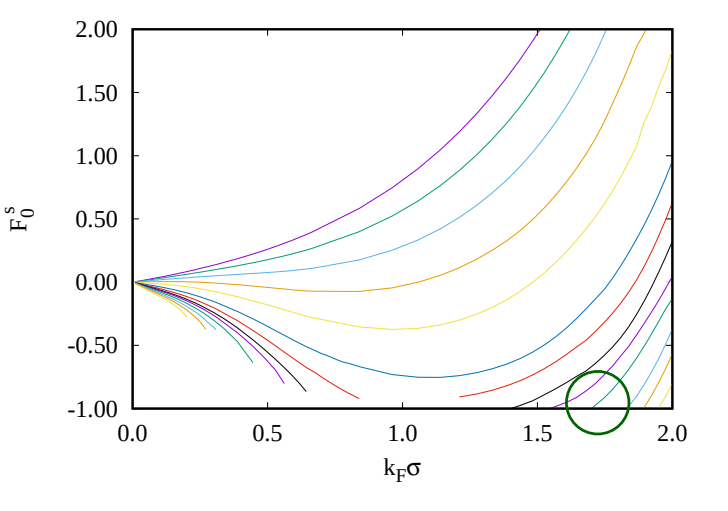

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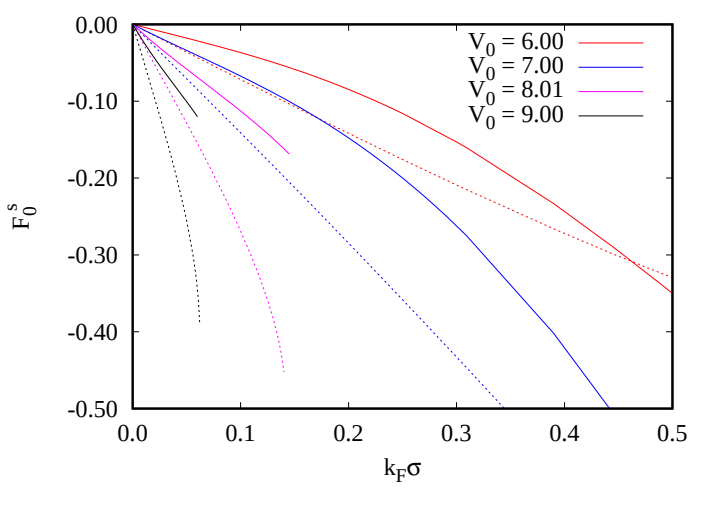

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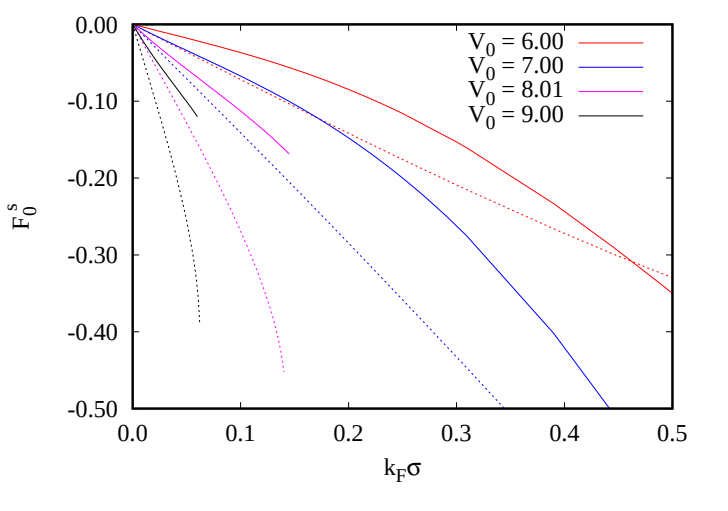
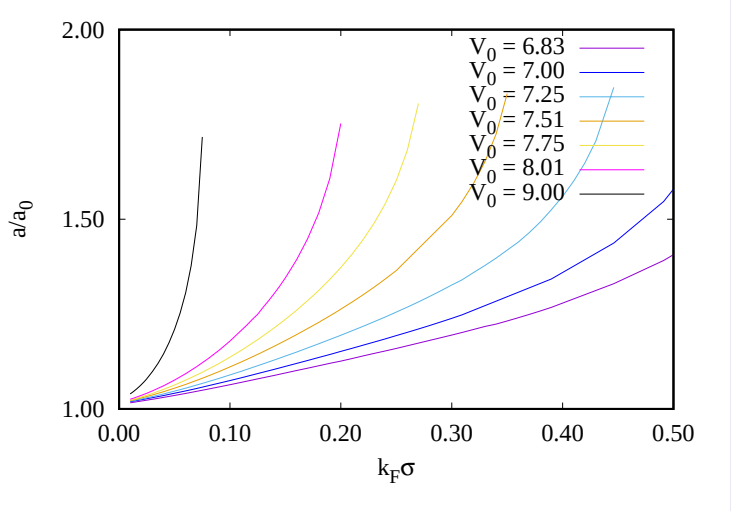


In-medium scattering length



Realistic nucleon-nucleon Interactions

...and variational wave functions

Recall the non-relativistic nuclear Hamiltonian:

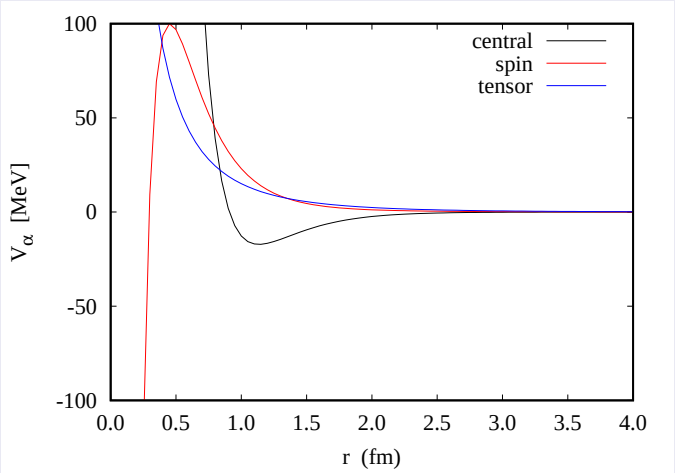
$$H = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 + \sum_i V_{ext}(i) + \sum_{i<j} V(i,j)$$

$$V(i,j) = \sum_\alpha V_\alpha(r) O_\alpha(i,j)$$

Operator Basis

$$\begin{aligned}
O_1(i,j;\hat{r}) &\equiv O_c = \mathbb{1}, \\
O_3(i,j;\hat{r}) &\equiv (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j), \\
O_5(i,j;\hat{r}) &\equiv S(i,j;\hat{r}) \\
&\equiv 3(\boldsymbol{\sigma}_i \cdot \hat{r})(\boldsymbol{\sigma}_j \cdot \hat{r}) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \\
O_{2n}(i,j;\hat{r}) &= O_{2n-1}(i,j;\hat{r})\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j .
\end{aligned}$$

Interactions in operator basis



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Projector Basis

$$\begin{aligned} P_s &= \frac{1}{4}(1 - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \\ P_{t+} &= \frac{1}{6}(3 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + S_{12}(\hat{r})) \\ P_{t-} &= \frac{1}{12}(3 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 - 2S_{12}(\hat{r})) \end{aligned}$$

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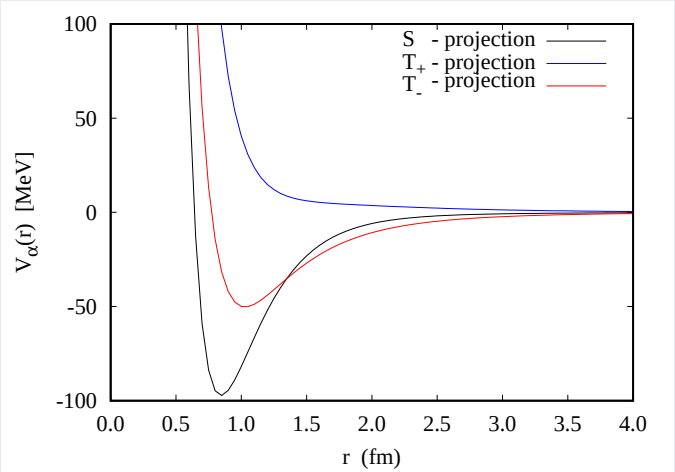

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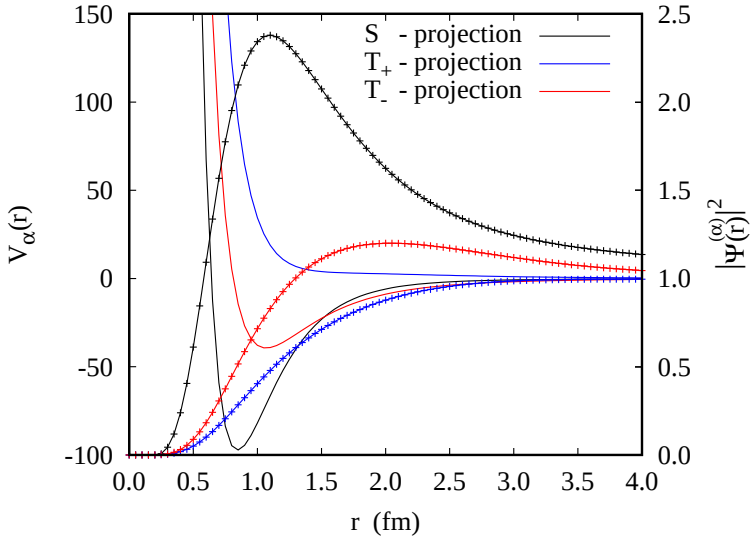
...Try to formulate a variational wave function

Correlated wave function

$$\Psi_0(1,\ldots,N) = F(1,\ldots,N)\Phi_0(1,\ldots,N) =$$

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

$F(1,\ldots,N)$ "Correlation operator" (symmetric in $1,\ldots,N$)



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$$-\frac{\hbar^2}{m}\nabla^2\psi^{(\alpha)}(r)+v_\alpha(r)\psi^{(\alpha)}(r) = \lambda_\alpha\psi^{(\alpha)}(r)$$

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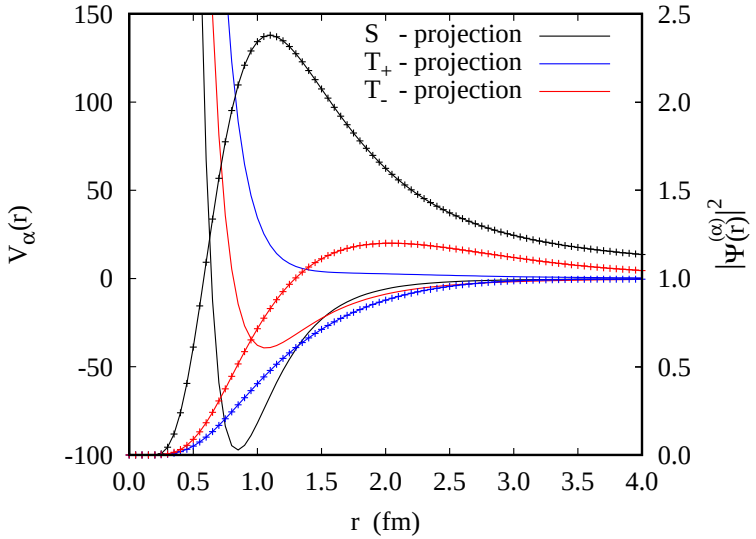

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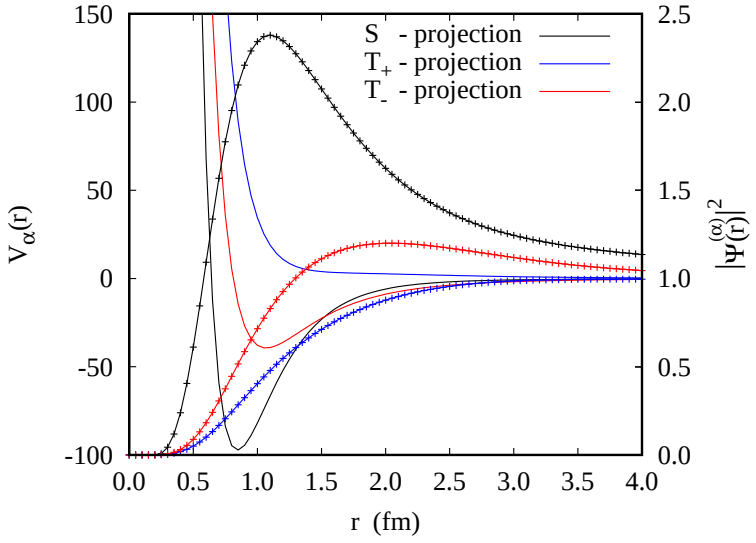

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$$g_k(r-r') = \frac{1}{\rho^2\left\langle\Psi_0\middle|\Psi_0\right\rangle}\left\langle\Psi_0\middle|\sum_{i\neq j}\delta(r-r_i)P_k(i,j)\delta(r'-r_j)\middle|\Psi_0\right\rangle$$

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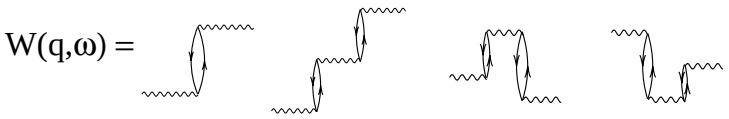

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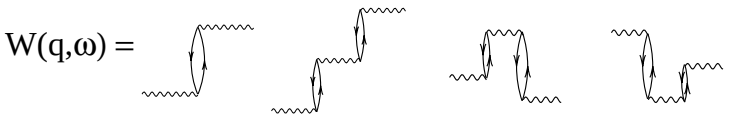

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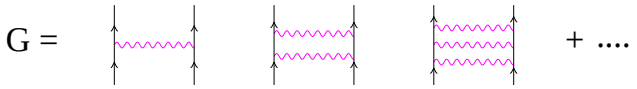

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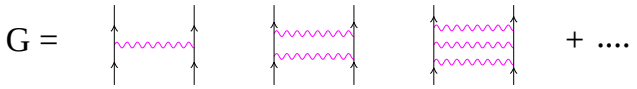

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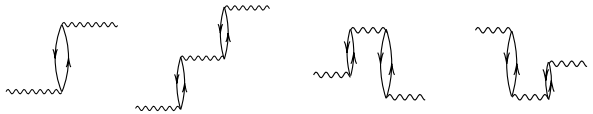

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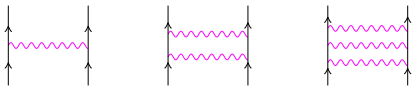

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- Where did the commutators go ?

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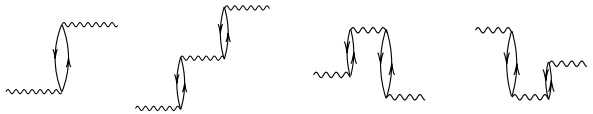

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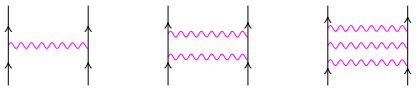
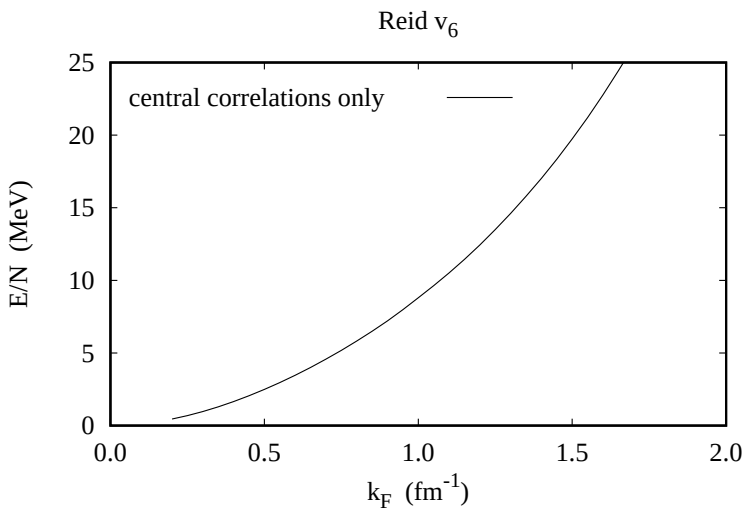


+ ....

Rungs are $v(q) + W(q,\bar{\omega}(q))$

Local parquet for fermions
Energetics and effective interactions

- Energetics:
  - Central correlations only



Local parquet for fermions
Energetics and effective interactions

- Energetics:
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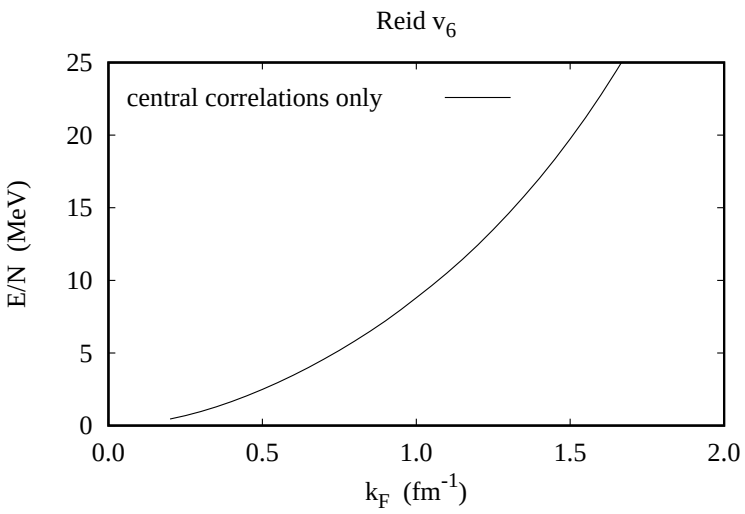
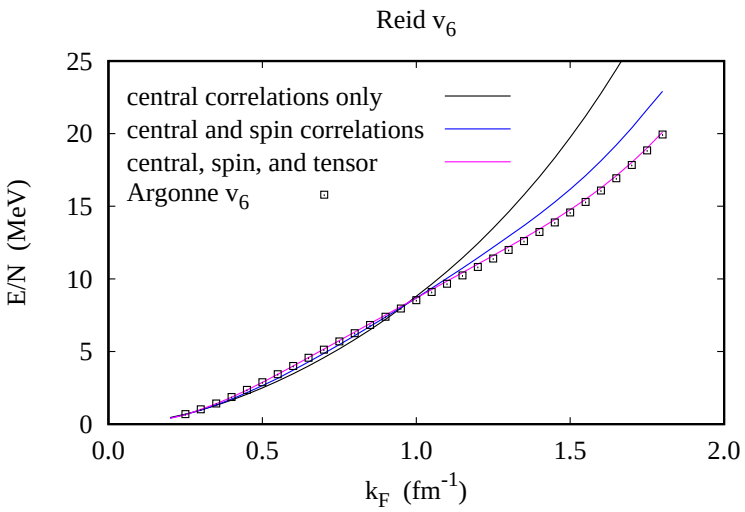
  - Parquet makes not much change





Local parquet for fermions
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- Particle-hole interactions:
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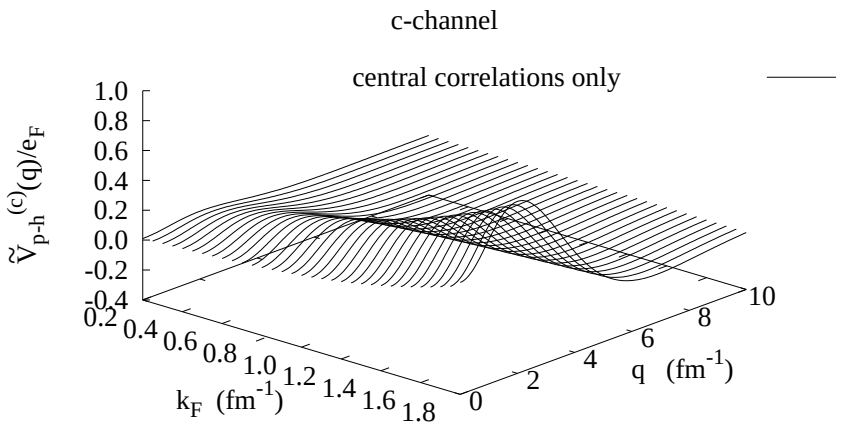

Local parquet for fermions
Energetics and effective interactions

- Energetics:
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- Particle-hole interactions:
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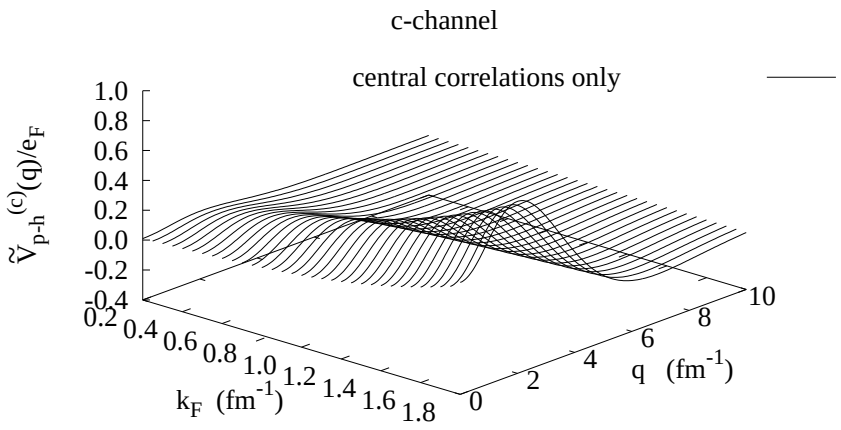
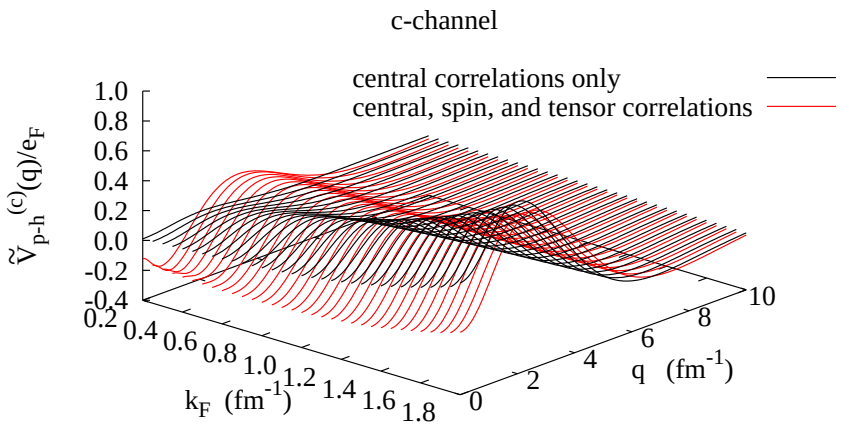
  - Parquet makes drastic change





Local parquet for fermions
Energetics and effective interactions

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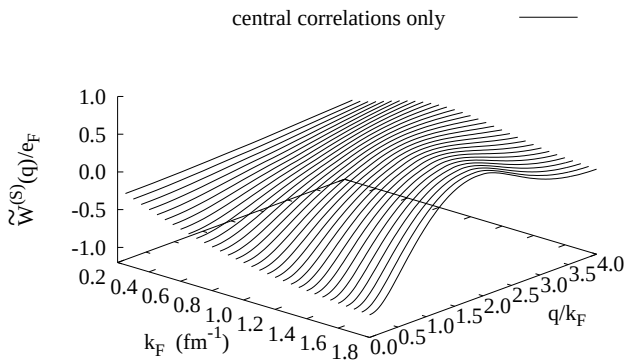

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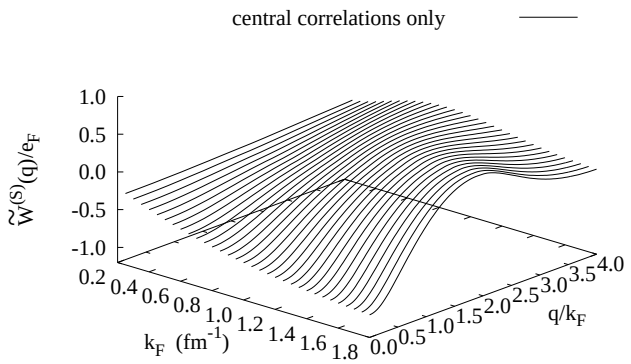
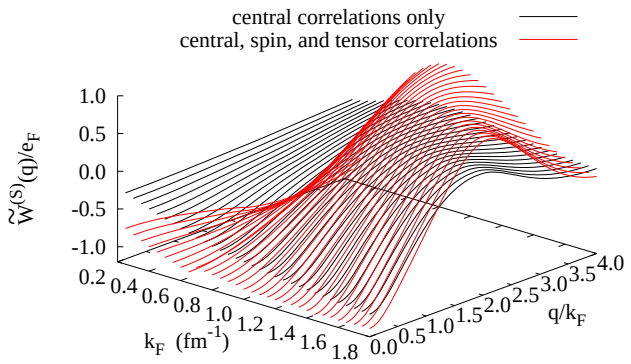
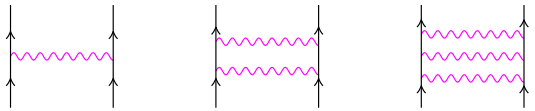




Local parquet for fermions
Where did the commutators go ?

- These are the ladders we have kept

G =



+ ....

Local parquet for fermions
Where did the commutators go ?

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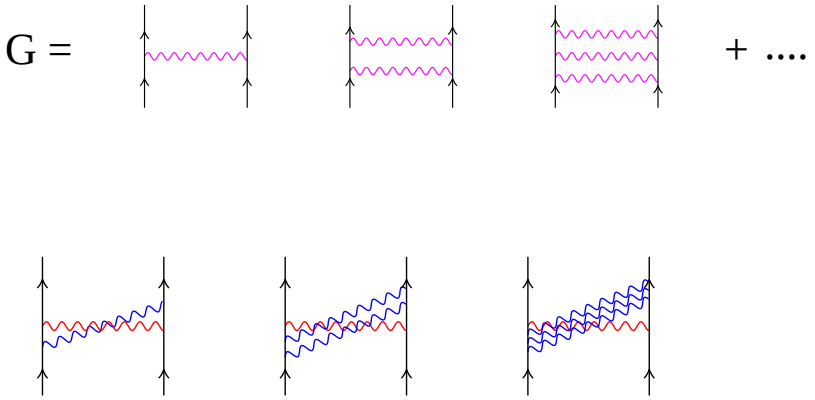
- These are the ladders we have ignored !



Local parquet for fermions
Where did the commutators go ?

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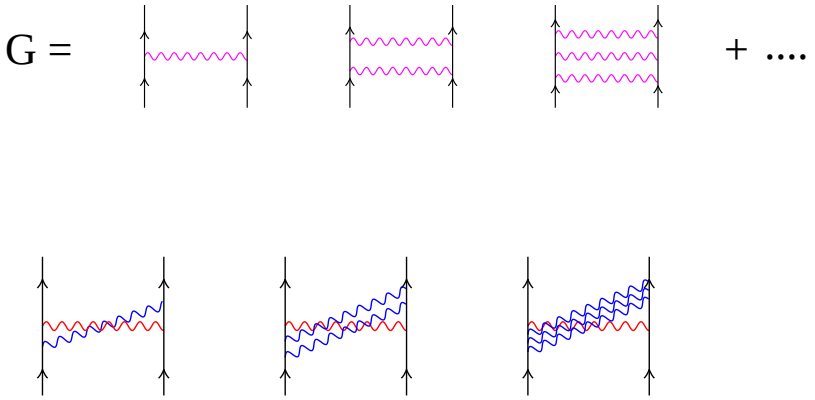
- Crossing excitation may carry spin/isospin !



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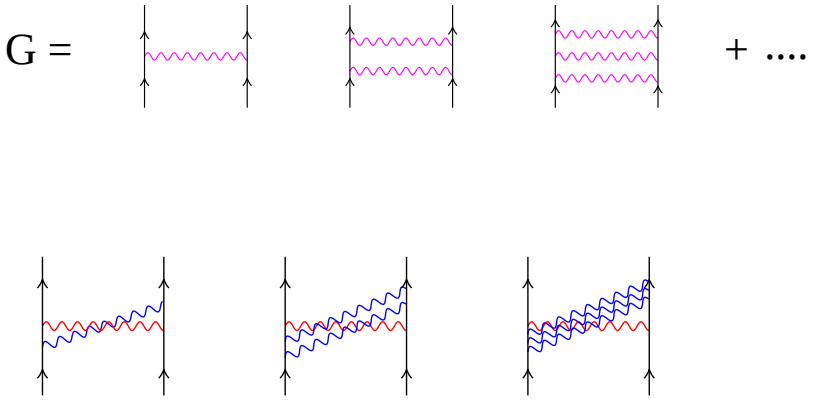

Much work needs to be done !