Variational Theory and Parquet Diagrams for Nuclear Systems
A Comprehensive Study of Neutron Matter

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Outline

Postulate:

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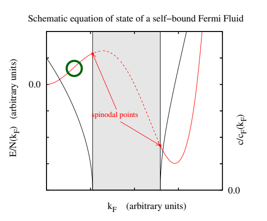
We want a "robust" method that is independent of the interactions
We not only want the right answer but also the underlying physical mechanisms

- Low densities: Pauli pressure dominates → repulsive Fermi gas



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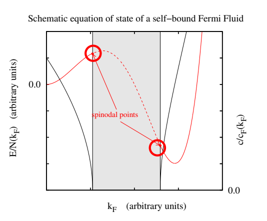

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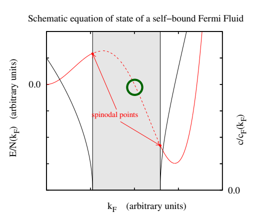

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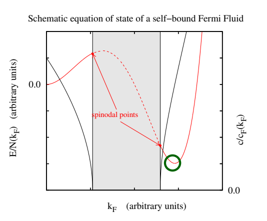

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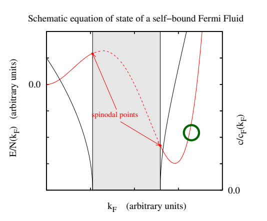
- Saturation



The equation of state of a self-bound Fermi system
A close look

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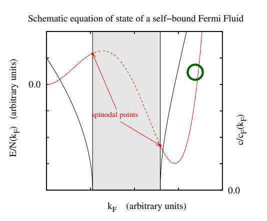

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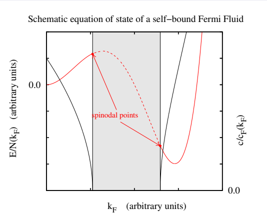

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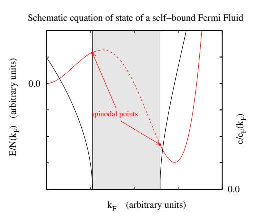

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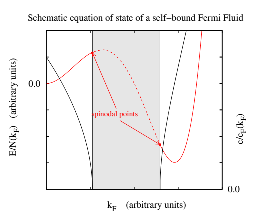

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The equation of state is a non-analytic function of the density

Order-by-order perturbation theory does not work !

$$V = \sum_{i<j} V(|r_i - r_j|)$$

Optimized Variational Method (Feenberg 1969)

- Wave function $\Psi_0(1, \ldots N) = \prod_{i<j} f(|r_i - r_j|)$.
- Hypernetted Chain summations
- Optimization $\frac{\delta}{\delta f(r)} \frac{\langle \Psi_0 | H | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = 0$

Local Parquet Diagram Summations (Jackson Lande Smith 1983)

- Sum all rings and ladders self-consistently
- Local Approximations

These meet the above requirements.
and lead to the same set of equations !

Simple interactions for Fermions
^{3}He, electrons

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Optimized Variational Method (Feenberg 1969)

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Local Parquet Diagram Summations (Jackson Lande Smith 1983)

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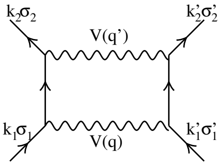
These meet the above requirements.
Equivalence established for ladders, rings, and self-energy insertions

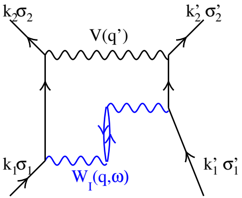
Localizing parquet diagrams

- Bethe Goldstone ladders



Localizing parquet diagrams

- Bethe Goldstone ladders
- Add induced interaction $\hat{W}(q,\omega)$



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

Localizing parquet diagrams

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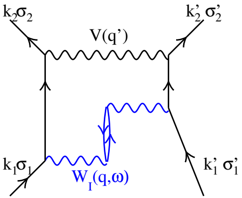

$$\widetilde{W}_I(q, \omega) = \frac{\tilde{V}_{p-h}(q)}{1 - \chi_0(q, \omega) V_{p-h}(q)}$$

$$S(q) = -\int_0^\infty \frac{d\hbar\omega}{\pi} \Im m \left[\chi_0(q, \omega) + \chi_0^2(q, \omega) \widetilde{W}_I(q, \omega) \right]$$

Localizing parquet diagrams

- Bethe Goldstone ladders
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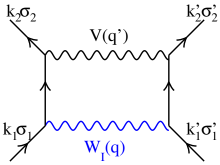
- Energy independent induced interaction



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(Non-relativistic) nuclear Hamiltonian:

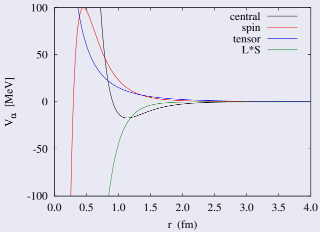
$$H = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 + \sum_i V_{ext}(i) + \sum_{i<j} \hat{V}(i,j)$$

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

Operator Basis

$$\begin{aligned}
O_1(i,j;\hat{r}) &\equiv O_c = \mathbb{1}, \\
O_3(i,j;\hat{r}) &\equiv \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\,, \\
O_5(i,j;\hat{r}) &\equiv S(i,j;\hat{r}) \\
&\equiv 3(\boldsymbol{\sigma}_i \cdot \hat{r})(\boldsymbol{\sigma}_j \cdot \hat{r}) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \\
O_7(i,j;\hat{r}) &\equiv L \cdot S \\
O_{2n}(i,j;\hat{r}) &= O_{2n-1}(i,j;\hat{r})\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j\,.
\end{aligned}$$

Interactions in operator basis



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Projector Basis

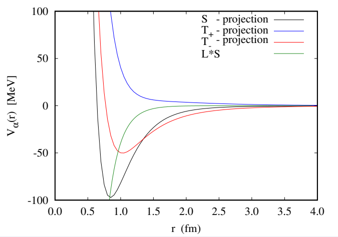
$$P_s = \frac{1}{4}(1 - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)$$

$$P_{t+} = \frac{1}{6}(3 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + S_{12}(\hat{r}))$$

$$P_{t-} = \frac{1}{12}(3 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 - 2S_{12}(\hat{r}))$$

$$O_7 = L \cdot S$$

Interactions in projector basis



"Symmetrized operator product wave function"

$$\Psi_0^{\mathrm{SOP}} = \mathcal{S}\Big[\prod_{\substack{i,j=1 \\ i<j}}^{N} \hat{f}(i,j)\Big]\Phi_0 \equiv F_N \Phi_0 \,,$$

Correlation functions:

$$\hat{f}(i,j) = \sum_{\alpha=1}^{n} f_\alpha(r_{ij})\,\hat{O}_\alpha(i,j)\,,$$

Pair distribution functions:

$$\hat{g}(i,j) = \sum_{\alpha=1}^{n} g_\alpha(r_{ij})\,\hat{O}_\alpha(i,j)\,,$$

With

$$\rho^2 g_\alpha(|r-r'|) = \frac{\left\langle \Psi_0^{\mathrm{SOP}} \middle| \sum_{i<j} \delta(r-r_i)\delta(r'-r_j)\hat{O}_\alpha(i,j) \middle| \Psi_0^{\mathrm{SOP}} \right\rangle}{\frac{1}{\nu^2}\mathcal{T}r_{12}\,\hat{O}_\alpha^2(1,2)\left\langle \Psi_0^{\mathrm{SOP}} \middle| \Psi_0^{\mathrm{SOP}} \right\rangle}\,.$$

The problem of variational wave functions
A technical nuiscance ?

With symmetrization, the pair distribution functions have the form

$$g_\alpha(r) = \sum_{\beta\gamma} f_\beta(r) f_\gamma(r) F^{(\alpha)}_{\beta\gamma}(r) \,. \qquad \{\alpha,\beta,\gamma\} \in \{S, T_+, T_t\}$$

The coefficients $F^{(\alpha)}_{\beta\gamma}(r)$ are not diagonal in the indices α, β, γ.
There is no systematic way to calculate these to infinite order.

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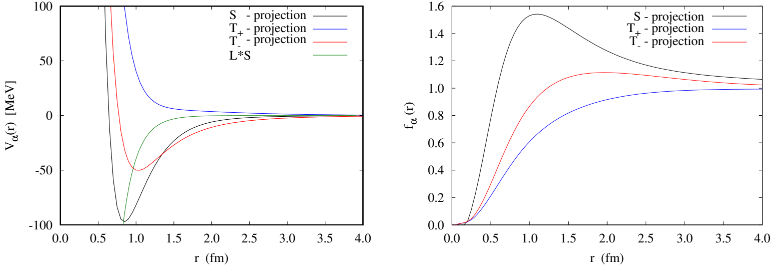

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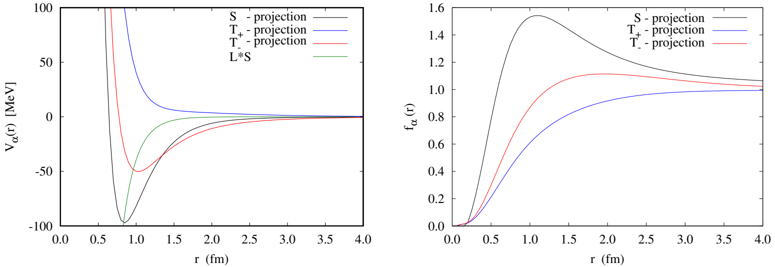

Spin-singlet correlation functions $f_{singlet}(r_{ij})$ contribute to the spin-triplet distribution function $g_{triplet}(r_{ij})$ and vice versa !

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  > If the effect is real then it must be represented by non-parquet diagrams !

Assume a simple interaction

$$\begin{aligned}\hat{\mathrm{v}}(\mathrm{q}) &= \tilde{\mathrm{v}}_{\mathrm{c}}(\mathrm{q}) + \tilde{\mathrm{v}}_{\sigma}(\mathrm{q})\boldsymbol{\sigma}_{\mathrm{i}}\cdot\boldsymbol{\sigma}_{\mathrm{j}} \\ &= \tilde{\mathrm{v}}_{\mathrm{S}}(\mathrm{q})\mathrm{P}_{\mathrm{S}} + \tilde{\mathrm{v}}_{\mathrm{T}}(\mathrm{q})\mathrm{P}_{\mathrm{T}}\end{aligned}$$

Calculate Goldstone Ladder diagrams

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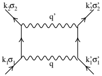

- First diagram: Ordinary Bethe-Goldstone ladder

$$= \int \frac{d^3q}{(2\pi)^3\rho} \frac{1}{E(k,q)} \underbrace{\left[V_S(q)V_s(k-q)P_S + V_T(q)V_T(k-q)P_T\right]}_{\text{direct term}}$$

Beyond Parquet

Beyond the Bethe Goldstone equation

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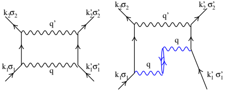

- First diagram: Ordinary Bethe-Goldstone ladder
- Second diagram: Ladder with an induced interaction

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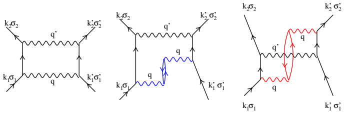
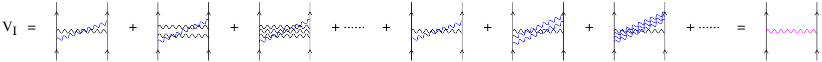


- First diagram: Ordinary Bethe-Goldstone ladder
- Second diagram: Ladder with an induced interaction
- Not parquet but the same ingredients

$$= \int \frac{d^3q}{(2\pi)^3\rho}\frac{1}{E(k,q)} \underbrace{[V_S(q)W_s(k-q)P_S + V_T(q)W_T(k-q)P_T]}_{\text{direct term}}$$

$$\underbrace{+4\int \frac{d^3q}{(2\pi)^3\rho}\frac{1}{E(k,q)} V_\sigma(q)W_\sigma(k-q)(P_T - 3P_S)}_{\text{commutator}}$$

Sum these:



Beyond Parquet
Instead of equations

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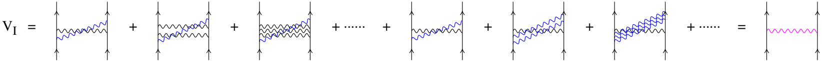
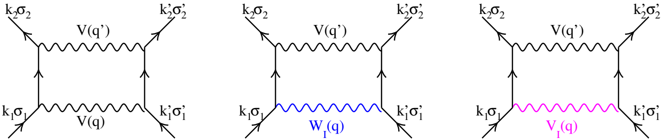


Parquet: Supplement in Bethe-Goldstone equation

$$V(r) \rightarrow V(r) + V_I(r) + W_I(r)$$



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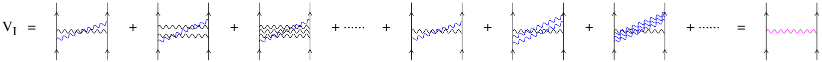

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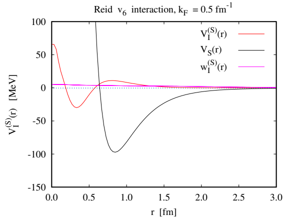

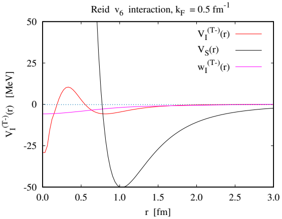

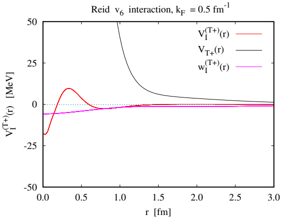

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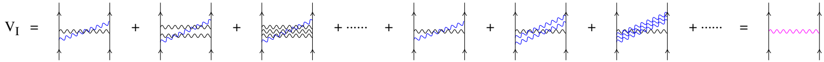

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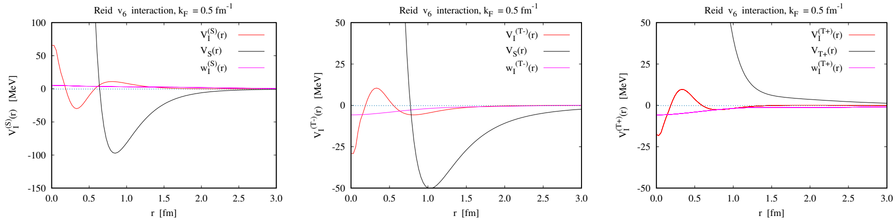

Non-parquet contributions are larger than all other many-body effects

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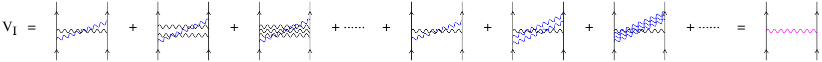

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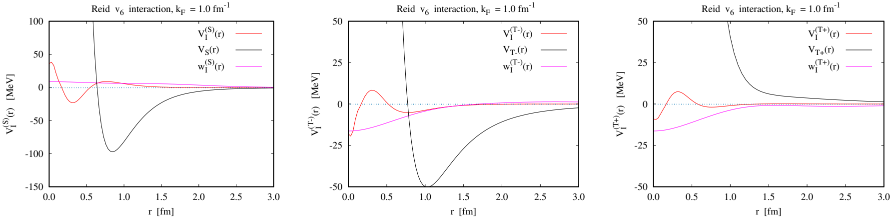

Non-parquet contributions are larger than all other many-body effects

Unit $\hat{\mathrm{Q}}_1 = \mathbb{1}$, "Longitudinal" $\hat{\mathrm{Q}}_3 = (\boldsymbol{\sigma}_1 \cdot \hat{\mathrm{q}})(\boldsymbol{\sigma}_2 \cdot \hat{\mathrm{q}})$ and "Transverse" operators $\hat{\mathrm{Q}}_5 = \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2 - (\boldsymbol{\sigma}_1 \cdot \hat{\mathrm{q}})(\boldsymbol{\sigma}_2 \cdot \hat{\mathrm{q}})$
Effective interactions:

$$\hat{\mathrm{W}}^{(\alpha)}(\mathrm{q};\omega) = \sum_{\alpha\,\mathrm{odd}} \frac{\tilde{\mathrm{V}}^{(\alpha)}_{\mathrm{p-h}}(\mathrm{q})}{1 - \chi_0(\mathrm{q};\omega)\tilde{\mathrm{V}}^{(\alpha)}_{\mathrm{p-h}}(\mathrm{q})} \hat{\mathrm{Q}}_\alpha$$

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$$\tilde{\mathrm{V}}^{(\mathrm{c})}_{\mathrm{p-h}}(\mathrm{q};\omega) \equiv \tilde{\mathrm{V}}^{(\mathrm{c})}_{\mathrm{p-h}}(\mathrm{q}) + \frac{1}{4}\chi_0^{(\perp)}(\mathrm{q};\omega)\left[\tilde{\mathrm{V}}^{(\mathrm{LS})}_{\mathrm{p-h}}(\mathrm{q})\right]^2,$$

$$\tilde{\mathrm{V}}^{(\mathrm{T})}_{\mathrm{p-h}}(\mathrm{q};\omega) \equiv \tilde{\mathrm{V}}^{(\mathrm{T})}_{\mathrm{p-h}}(\mathrm{q}) + \frac{1}{8}\chi_0^{(\perp)}(\mathrm{q};\omega)\left[\tilde{\mathrm{V}}^{(\mathrm{LS})}_{\mathrm{p-h}}(\mathrm{q})\right]^2.$$

$$\chi_0^{(\perp)}(\mathrm{q};\omega) = \frac{1}{\mathrm{N}}\mathcal{T}\mathrm{r}_{\boldsymbol{\sigma}}\sum_{\mathrm{h}}\frac{|\hat{\mathrm{q}}\times\mathrm{h}|^2}{\mathrm{k}_\mathrm{F}^2}\frac{2(\mathrm{t(p)}-\mathrm{t(h)})}{(\hbar\omega - \mathrm{i}\eta)^2 - (\mathrm{t(p)}-\mathrm{t(h)})^2}$$

$$\hat{\mathrm{W}}^{(\mathrm{odd})}_{\mathrm{LS}}(\mathrm{q};\omega) = \mathrm{W}^{(\mathrm{LS})}(\mathrm{q},\omega)\widetilde{\mathrm{L}\cdot\mathrm{S}}$$

$$\mathrm{W}^{(\mathrm{LS})}(\mathrm{q},\omega) = \frac{1}{2}\frac{\tilde{\mathrm{V}}^{(\mathrm{LS})}_{\mathrm{p-h}}(\mathrm{q})}{1-\chi_0(\mathrm{q};\omega)\tilde{\mathrm{V}}^{(\mathrm{c})}_{\mathrm{p-h}}(\mathrm{q};\omega)} + \frac{1}{2}\frac{\tilde{\mathrm{V}}^{(\mathrm{LS})}_{\mathrm{p-h}}(\mathrm{q})}{1-\chi_0(\mathrm{q};\omega)\tilde{\mathrm{V}}^{(\mathrm{T})}_{\mathrm{p-h}}(\mathrm{q};\omega)},$$

Some small terms have been omitted.

Key takeaways from spin-orbit potentials

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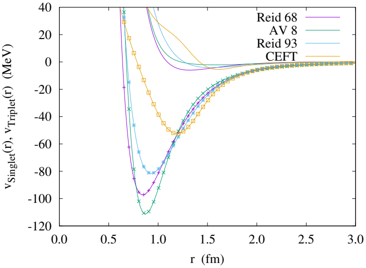

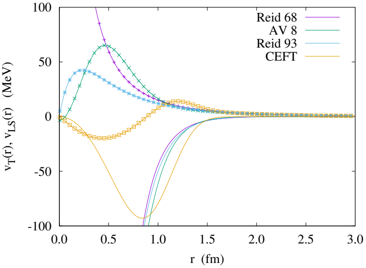

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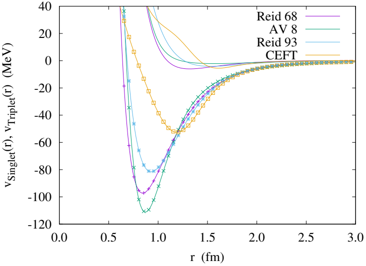
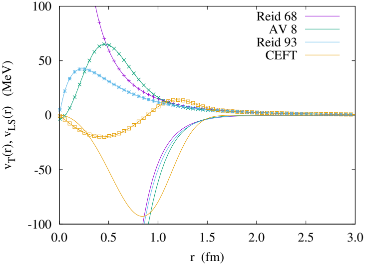


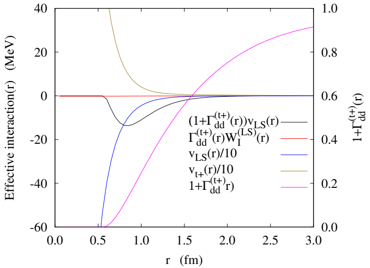


- Effective interactions contain the spin-orbit force in the form

$$V^{(LS)}_{eff}(r) \approx \psi_T(r) \left[V_{LS}(r) + W_{LS}(r) \right] \psi_T(r)$$

where $\psi_T(r)$ triplet pair wave function of the Bethe-Goldstone equation $= \sqrt{1 + \Gamma^{(T)}_{dd}(r)}$ "direct correlation function".

Key takeaways from spin-orbit potentials



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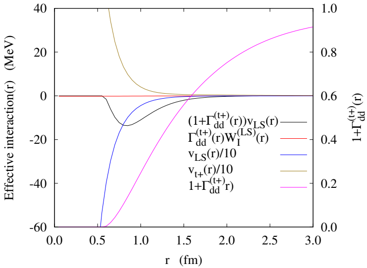

The spin-orbit potential is suppressed by the short-ranged repulsive spin-triplet correlations

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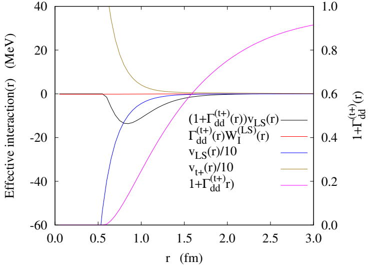

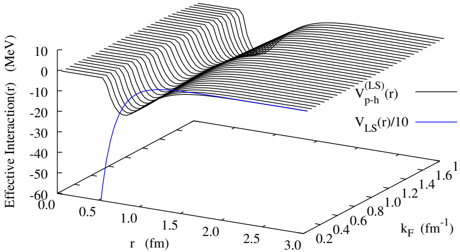

The spin-orbit potential is suppressed by the short-ranged repulsive spin-triplet correlations

Textbook knowledge: BCS gap-equation for the pairing function $\Delta(\mathrm{k})$

$$\Delta(\mathrm{k}) = -\frac{1}{2}\sum_{\mathrm{k}'}\langle \mathrm{k}|\mathrm{V}|\mathrm{k}'\rangle \frac{\Delta(\mathrm{k}')}{\mathrm{E}(\mathrm{k}')}$$

Single-particle spectrum

$$\mathrm{E}(\mathrm{k}) = \sqrt{(\epsilon(\mathrm{k}) - \mu)^2 + |\Delta(\mathrm{k})|^2}$$

$\langle \mathrm{k}|\mathrm{V}|\mathrm{k}'\rangle$: (effective) pairing interaction
Multicomponent version

$$\Delta^{(\ell)}(\mathrm{k}) = -\frac{1}{2}\sum_{\ell'}\int \frac{d^3\mathrm{k}'}{(2\pi)^3} \frac{\mathrm{V}_{\ell\ell'}(\mathrm{k},\mathrm{k}')\Delta^{(\ell')}(\mathrm{k}')}{\sqrt{(\epsilon(\mathrm{k}') - \mu)^2 + \mathrm{D}^2(\mathrm{k}')}} .$$

$$\mathrm{E}(\mathrm{k}) \approx \sqrt{(\epsilon(\mathrm{k}) - \mu)^2 + \mathrm{D}^2(\mathrm{k})} \qquad \mathrm{D}^2(\mathrm{k}) = \frac{1}{4\pi}\int d\Omega_{\mathrm{k}}\, |\Delta(\mathrm{k})|^2$$

- correlated BCS state

$$\left|\mathrm{CBCS}\right\rangle = \sum_{\mathrm{m,N}} \frac{1}{\mathrm{I}_{\mathrm{m}}^{(\mathrm{N})}} \mathrm{F}_{\mathrm{N}} \left|\mathrm{m}^{(\mathrm{N})}\right\rangle \left\langle \mathrm{m}^{(\mathrm{N})} \right|\mathrm{BCS}\rangle$$

Landau potential

$$\langle \mathrm{H} - \mu \mathrm{N} \rangle_{\mathrm{c}} = \frac{\left\langle \mathrm{CBCS} \middle| \mathrm{H} - \mu \mathrm{N} \middle| \mathrm{CBCS} \right\rangle}{\left\langle \mathrm{CBCS} \middle| \mathrm{CBCS} \right\rangle} \, .$$

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- Expansions in correlated wave functions

Strongly interacting systems

- correlated BCS state

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- Expansions in correlated wave functions
- Identify Jastrow-diagrams with parquet-diagrams

Strongly interacting systems

- correlated BCS state

$$\left|\mathrm{CBCS}\right\rangle = \sum_{m,N} \frac{1}{I_m^{(N)}} F_N \left|m^{(N)}\right\rangle\left\langle m^{(N)}\middle|\mathrm{BCS}\right\rangle$$

  Landau potential

$$\left\langle H - \mu N\right\rangle_c = \frac{\left\langle \mathrm{CBCS}\middle|H - \mu N\middle|\mathrm{CBCS}\right\rangle}{\left\langle \mathrm{CBCS}\middle|\mathrm{CBCS}\right\rangle}\,.$$

- Expansions in correlated wave functions
- Identify Jastrow-diagrams with parquet-diagrams
- Minimize with respect to the Bogoliubov amplitudes

Summary without technicalities

- The gap equation remains the same but

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- The interaction matrix elements and the single particle spectrum become dependent on the gap function

$$\langle \mathrm{k} | \mathrm{V} | \mathrm{k} \rangle \rightarrow \langle \mathrm{k} | \mathrm{V}[\Delta] | \mathrm{k} \rangle$$

$$\epsilon(\mathrm{k}) \rightarrow \epsilon(\mathrm{k}, \Delta)$$

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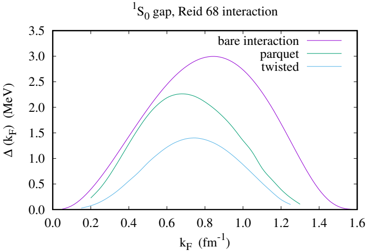
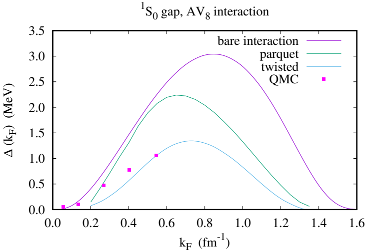
- In the weakly coupled limit, these can be obtained from ground state properties
- Contain, among others, medium polarization and self-energy corrections.

S wave pairing:
The importance of "beyond parquet"





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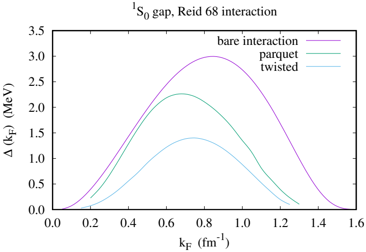
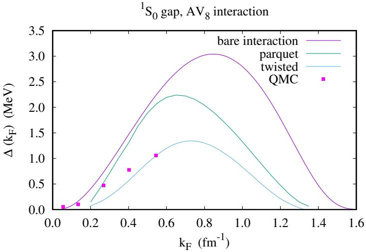
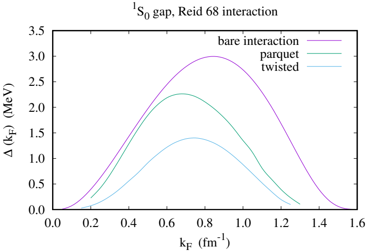
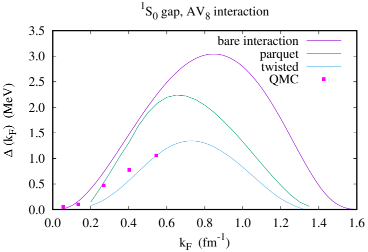




key takeaways:

- Results for Reid 68 and Argonne are quite similar





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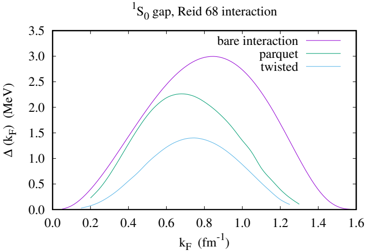

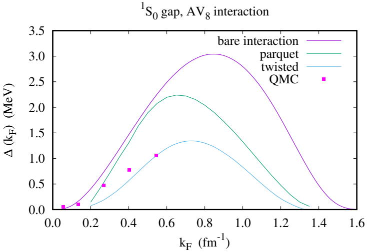

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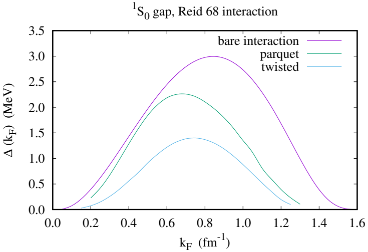
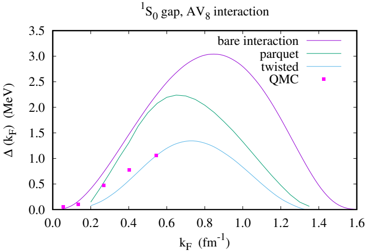


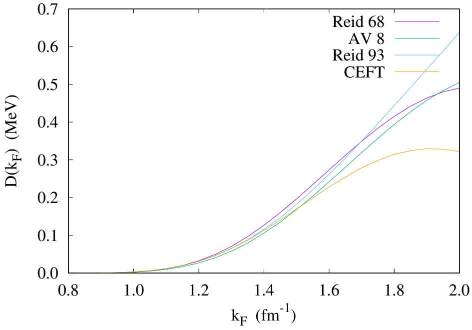


key takeaways:

- Results for Reid 68 and Argonne are quite similar
- Parquet-type many-body corrections reduce gap
- Additional repulsion from non-parquet diagrams reduces the gap by another factor of 2 !
- Good agreement with QMC should be taken with a grain of salt.

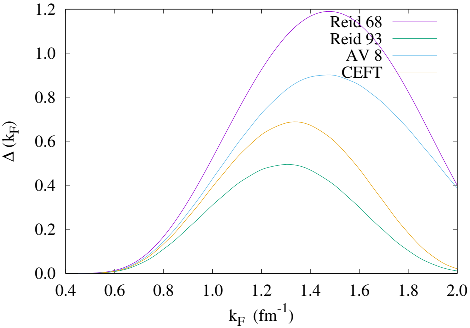
Bare interaction results: Some history
(Tamagaki, Takatsuka 1970-1972)

$^3P_2$-$^3F_2$ gap with bare interactions



Bare interaction results: Some history (Tamagaki, Takatsuka 1970-1972)

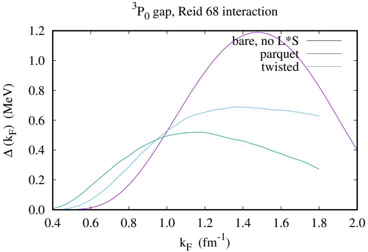
$^3P_0$ gap with bare interactions and spin-orbit force turned off

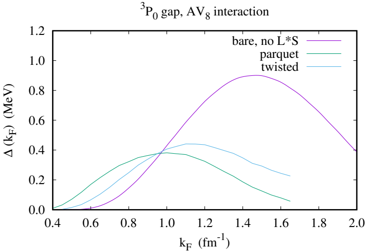


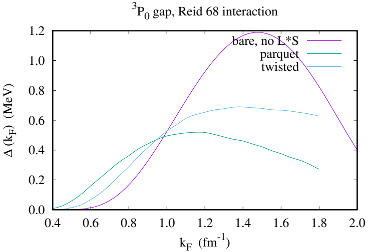
However: "Without an attractive spin-orbit interaction, neutrons would form a $^3P_0$ superfluid, in which the spin and orbital angular momenta are anti-aligned, rather than the $^3P_2$ state, in which they are aligned." (Gezerlis et al. in "Pairing and superfluidity of nucleons in neutron star")

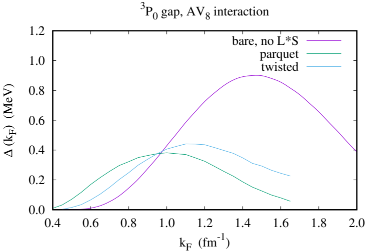
P wave superfluidity

The importance of many-body effects









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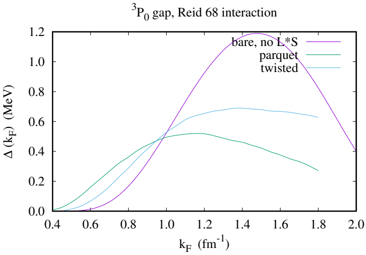
- Results for Reid 68 and Argonne are reasonably different



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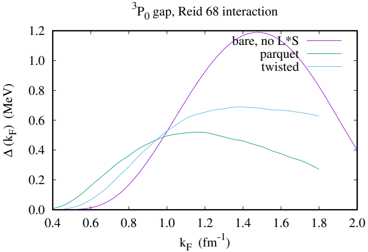

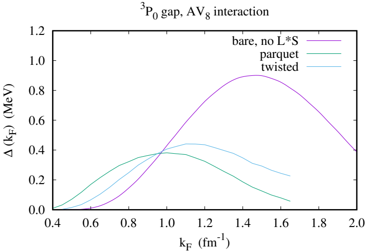

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Make the correlated wave function time dependent !

$$|\Psi(t)\rangle = e^{-iE_0 t/\hbar} \frac{F e^{\frac{1}{2}\delta U} |\Phi_0\rangle}{\langle \Phi_0 | e^{\frac{1}{2}\delta U^\dagger} F^\dagger F e^{\frac{1}{2}\delta U} | \Phi_0 \rangle]^{1/2}} \equiv e^{-iE_0 t/\hbar} |\Phi(t)\rangle$$

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

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Bosons:

$$\delta U(t) = \sum_i \underbrace{\delta u^{(1)}(r_i;t)}_{\text{long wavelength excitations}} + \sum_{i<j} \underbrace{\delta u^{(2)}(r_i,r_j;t)}_{\text{short wavelength excitations}} + \dots$$

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Fermions: (a correlated version of "second"(S)RPA)

$$\delta U(t) = \sum_{p,h} \underbrace{\delta u^{(1)}_{p,h}(t) a^\dagger_p a_h}_{\text{long wavelength excitations}} + \sum_{p,h,p',h'} \underbrace{\delta u^{(2)}_{p,h,p',h'}(t) a^\dagger_p a^\dagger_{p'} a_h a_{h'}}_{\text{short wavelength excitations}}$$

Dynamic Many-Body Theory (DMBT)

(Multi-)particle fluctuations for bosons and fermions

Make the correlated wave function time dependent !

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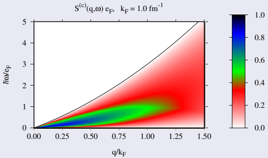
Action principle: Assume a weak external potential $U_{ext}(r;t)$:

$$\delta\int_{t_0}^{t_1}\left\langle\Psi(t)\left|\hat{H} - i\hbar\frac{\partial}{\partial t} + U_{ext}(t)\right|\Psi(t)\right\rangle dt$$

$$= \delta\int_{t_0}^{t_1}\left\langle\Phi(t)\left|\hat{H} - E_o - i\hbar\frac{\partial}{\partial t} + U_{ext}(t)\right|\Phi(t)\right\rangle dt = 0\,.$$

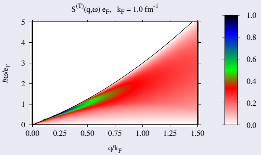
Neutron matter response
....at the 1p-1h level

Density channel



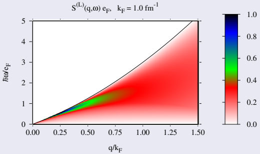
Phonon strongly Landau damped

Transverse spin mode



Strength close to continnum

Longitudinal spin mode



Very similar to longitudinal mode

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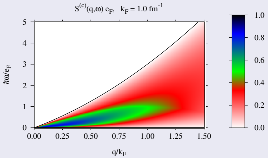

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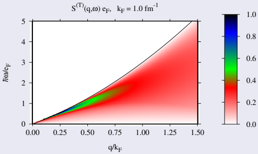

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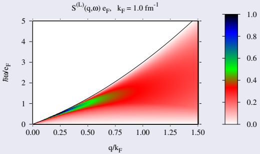
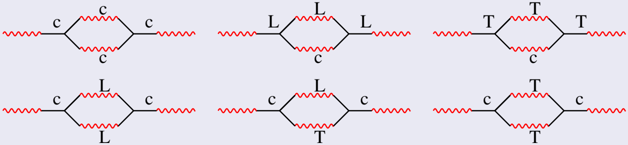


Very similar to longitudinal mode

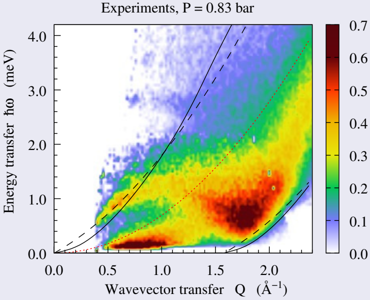
Phonon/magnon splitting processes:

Included in DMBT



Experiments:

$$S(Q,\omega) = S_c(Q,\omega) + \frac{\sigma_i}{\sigma_c} S_I(Q,\omega)$$



DMBT:

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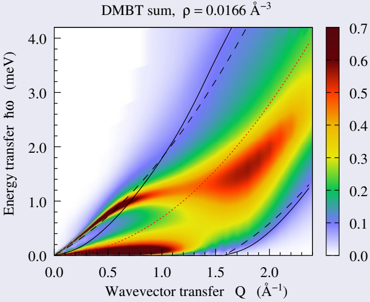

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- Dynamic response and single-particle spectrum is still in the works.