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

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JOHANNES KEPLER UNIVERSITÄT LINZ

Outline

Postulate:

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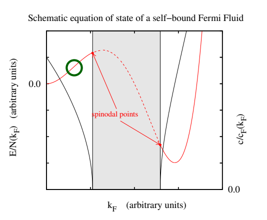
We want a "robust" method that is independent of the interactions
We not only want the right answer but also the underlying physical mechanisms

- Low densities: Pauli pressure dominates $\rightarrow$ repulsive Fermi gas



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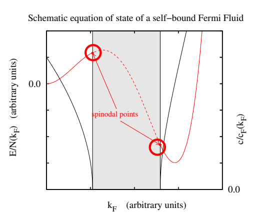

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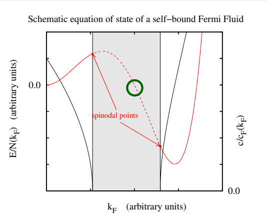

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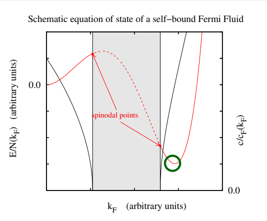

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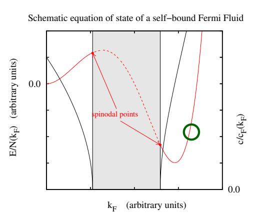

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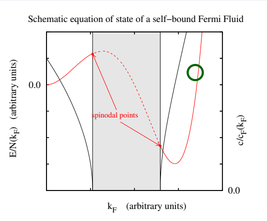

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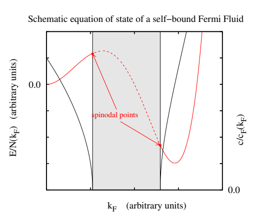

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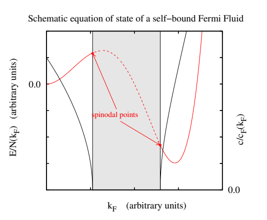

$\boxed{\text{The equation of state is a non-analytic function of the coupling constant in the grey-shaded area}}$

$\boxed{\text{Order-by-order perturbation theory does not work !}}$

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

Optimized Variational Method (Feenberg 1969)

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

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 !

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Local Parquet Diagram Summations (Jackson Lande Smith 1983)

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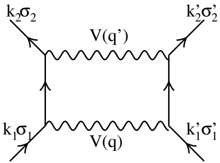
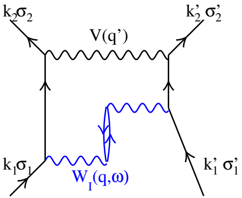
These meet the above requirements
Equivalence established for ladders, rings, and self-energy insertions

Localization procedure

- Bethe Goldstone ladders



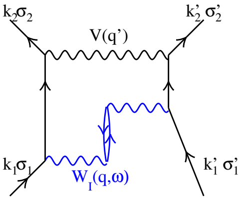
- Bethe Goldstone ladders
- Add induced interaction $\hat{W}(q, \omega)$



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

Localization procedure

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



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

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

Localization procedure

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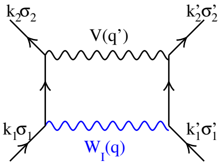
- Add induced interaction $\hat{\mathrm{W}}(\mathrm{q},\omega)$, calculate $\mathrm{S}(\mathrm{q})$
- Energy independent induced interaction



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(Non-relativistic) nuclear Hamiltonian:

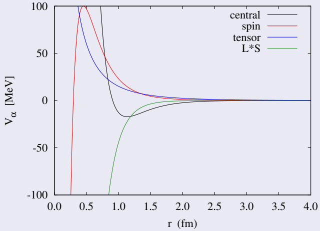
$$\mathrm{H} = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 + \sum_i \mathrm{V}_{\mathrm{ext}}(i) + \sum_{i<j} \hat{\mathrm{V}}(i,j)$$

$$\hat{\mathrm{V}}(i,j) = \sum_\alpha \mathrm{V}_\alpha(r)\mathrm{O}_\alpha(i,j)$$

Operator Basis

$$\begin{aligned}
\mathrm{O}_1(i,j;\hat{r}) &\equiv \mathrm{O}_c = \mathbb{1}, \\
\mathrm{O}_3(i,j;\hat{r}) &\equiv \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\,, \\
\mathrm{O}_5(i,j;\hat{r}) &\equiv \mathrm{S}(i,j;\hat{r}) \\
&\equiv 3(\boldsymbol{\sigma}_i \cdot \hat{r})(\boldsymbol{\sigma}_j \cdot \hat{r}) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \\
\mathrm{O}_7(i,j;\hat{r}) &\equiv \mathrm{L} \cdot \mathrm{S} \\
\mathrm{O}_{2n}(i,j;\hat{r}) &= \mathrm{O}_{2n-1}(i,j;\hat{r})\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j\,.
\end{aligned}$$

Interactions in operator basis



(Non-relativistic) nuclear Hamiltonian:

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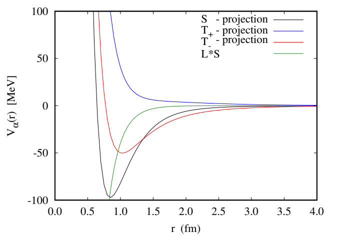
$$\hat{V}(i,j) = \sum_\alpha V_\alpha(r) P_\alpha(i,j)$$

Projector Basis

$$\begin{aligned} P_s &= \frac{1}{4}(1 - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \\ P_{t+} &= \frac{1}{6}(3 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + S_{12}(\hat{r})) \\ P_{t-} &= \frac{1}{12}(3 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 - 2S_{12}(\hat{r})) \\ O_7 &= L \cdot S \end{aligned}$$

Interactions in projector basis



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

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

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

With symmetrization, the pair distribution functions have the form

$$\mathrm{g}_\alpha(\mathrm{r}) = \sum_{\beta\gamma} \mathrm{f}_\beta(\mathrm{r})\mathrm{f}_\gamma(\mathrm{r})\mathrm{F}^{(\alpha)}_{\beta\gamma}(\mathrm{r})\,. \qquad \{\alpha,\beta,\gamma\} \in \{\mathrm{S},\mathrm{T}_+,\mathrm{T}_\mathrm{t}\}$$

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

The problem of variational wave functions
A technical nuiscance ?

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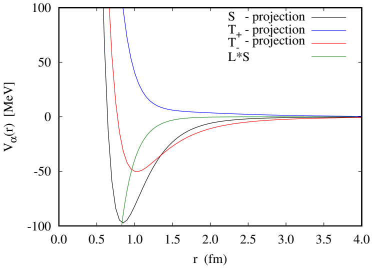

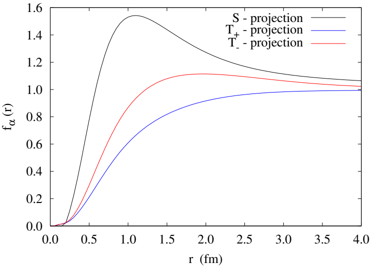

With symmetrization, the pair distribution functions have the form

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

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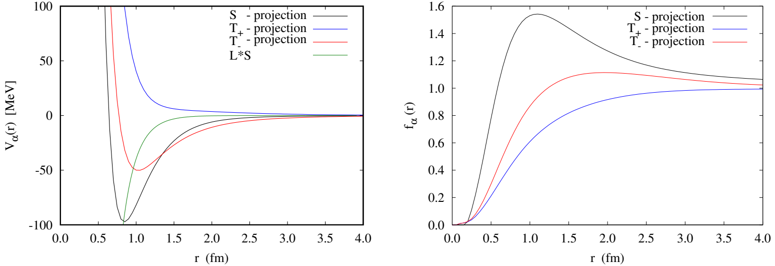

Spin-singlet correlation functions $f_{singlet}(r_{ij})$ contribute to the spin-triplet distribution function $g_{triplet}(r_{ij})$ and vice versa !

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- The problem is an artefact of the “Symmetrized Operator Product” wave function:
  Parquet diagram summations (Smith & Jackson 1988) do not lead to such effects.
- There is physics to be learned !

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 diagrams

Beyond Parquet
Beyond the Bethe Goldstone equation

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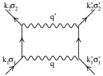
Calculate Goldstone diagrams



- First diagram: Ordinary Bethe-Goldstone ladder

$$
= \int \frac{\mathrm{d}^3\mathrm{q}}{(2\pi)^3\rho} \frac{1}{\mathrm{E}(\mathrm{k},\mathrm{q})} \underbrace{[\mathrm{V}_{\mathrm{S}}(\mathrm{q})\mathrm{V}_{\mathrm{s}}(\mathrm{k}-\mathrm{q})\mathrm{P}_{\mathrm{S}} + \mathrm{V}_{\mathrm{T}}(\mathrm{q})\mathrm{V}_{\mathrm{T}}(\mathrm{k}-\mathrm{q})\mathrm{P}_{\mathrm{T}}]}_{\text{direct term}}
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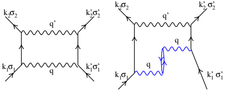

- First diagram: Ordinary Bethe-Goldstone ladder
- Second diagram: Ladder with an induced interaction

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

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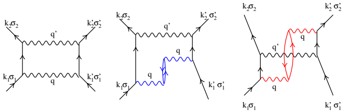

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- Not parquet but the same ingredients

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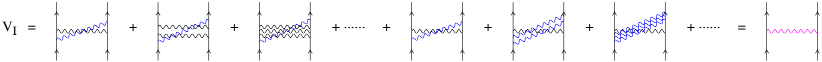
$$\underbrace{+4\int \frac{d^3q}{(2\pi)^3\rho}\frac{1}{E(k,q)} V_\sigma(q)W_\sigma(k-q)(P_T - 3P_S)}_{\text{commutator}}$$

Beyond Parquet
Instead of equations

Sum these:



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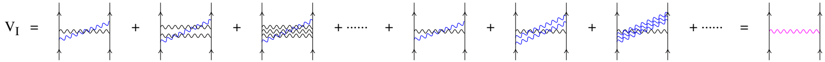
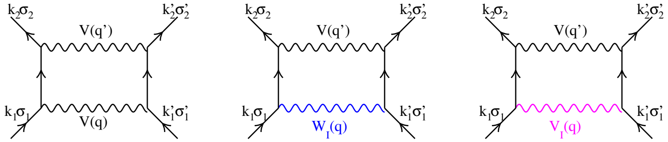


Parquet: Supplement in Bethe-Goldstone equation

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



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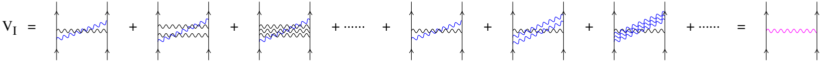

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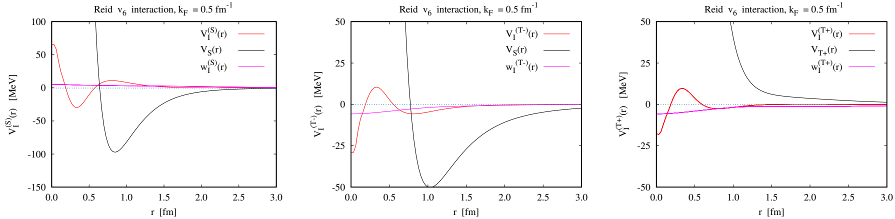

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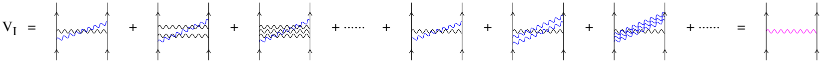

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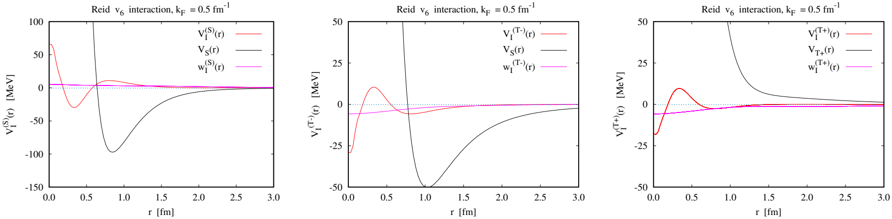

Non-parquet contributions are larger than all other many-body effects

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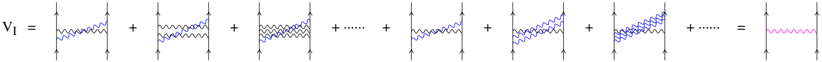

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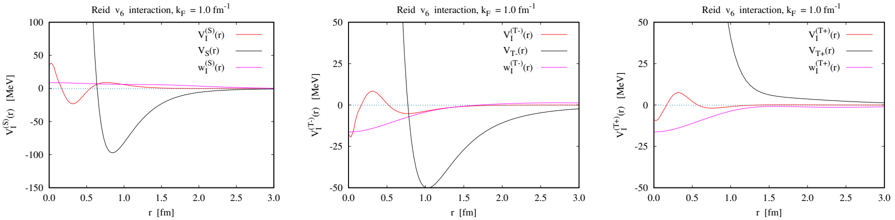

Non-parquet contributions are larger than all other many-body effects

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:

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

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 $\hat{\mathrm{Q}}_5 = \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2 - (\boldsymbol{\sigma}_1 \cdot \hat{\mathrm{q}})(\boldsymbol{\sigma}_2 \cdot \hat{\mathrm{q}})$
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$$\begin{aligned}
\tilde{\mathrm{V}}^{(\mathrm{c})}_{\mathrm{p-h}}(\mathrm{q};\omega) &\equiv \tilde{\mathrm{V}}^{(\mathrm{c})}_{\mathrm{p-h}}(\mathrm{q}) + \frac{1}{4}\chi_0^{(\perp)}(\mathrm{q};\omega)\left[\tilde{\mathrm{V}}^{(\mathrm{LS})}_{\mathrm{p-h}}(\mathrm{q})\right]^2 \\
&, \\
\tilde{\mathrm{V}}^{(\mathrm{T})}_{\mathrm{p-h}}(\mathrm{q};\omega) &\equiv \tilde{\mathrm{V}}^{(\mathrm{T})}_{\mathrm{p-h}}(\mathrm{q}) + \frac{1}{8}\chi_0^{(\perp)}(\mathrm{q};\omega)\left[\tilde{\mathrm{V}}^{(\mathrm{LS})}_{\mathrm{p-h}}(\mathrm{q})\right]^2 \\
&.
\end{aligned}$$

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

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

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

Some small terms have been omitted.

Key takeaways from spin-orbit potentials

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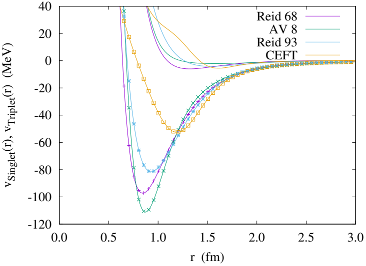

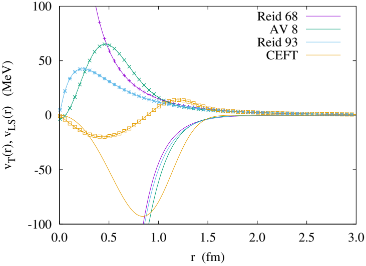

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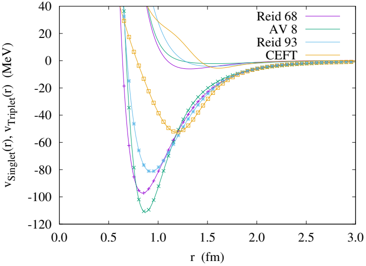
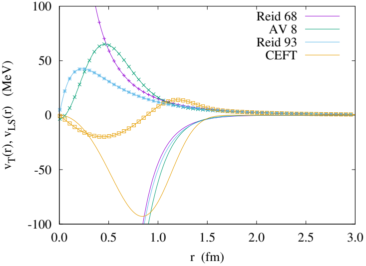


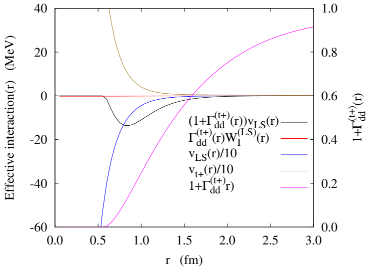


- Effective interactions contain the spin-orbit force in the form

$$V_{\rm eff}^{(LS)}(r) \approx \psi_T(r)\,[V_{LS}(r) + W_{LS}(r)]\,\psi_T(r)$$

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

Key takeaways from spin-orbit potentials



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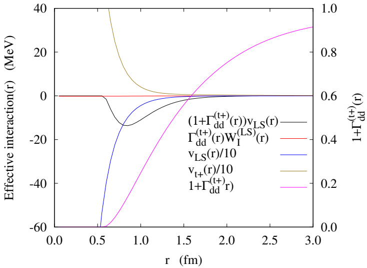

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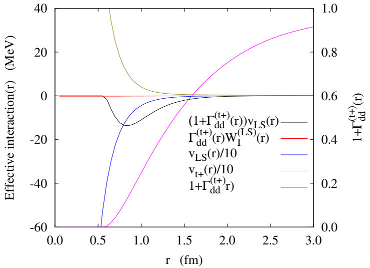

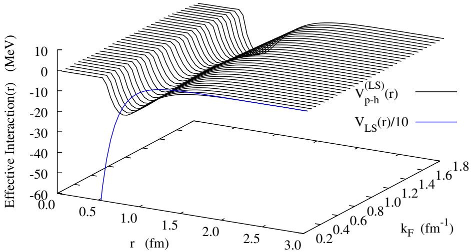

The spin-orbit potential is suppressed by the short-ranged repulsive spin-triplet correlations

Applications: Singlet and Triplet pairing neutron matter

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

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

Landau potential

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

Strongly interacting systems

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- Expansions in correlated wave functions
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- Expansions in correlated wave functions
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- Minimize with respect to the Bogoliubov amplitudes

Summary without technicalities

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

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

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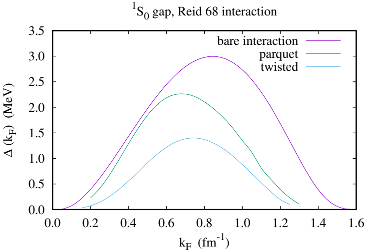
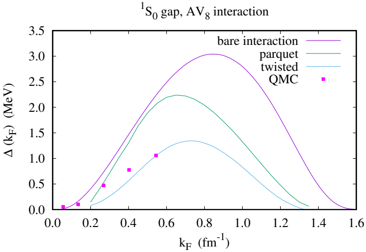
- In the weakly coupled limit, these can be obtained from ground state properties
- Contain, among others, medium polarization and self-energy corrections.

S wave pairing:
The importance of “beyond parquet”





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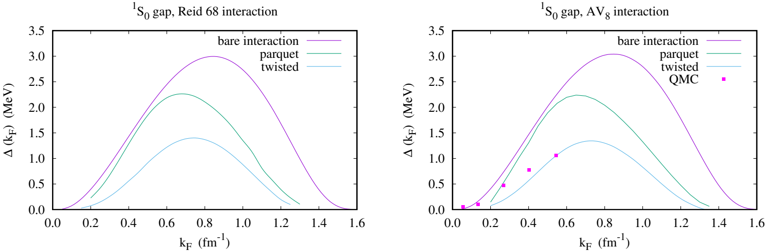

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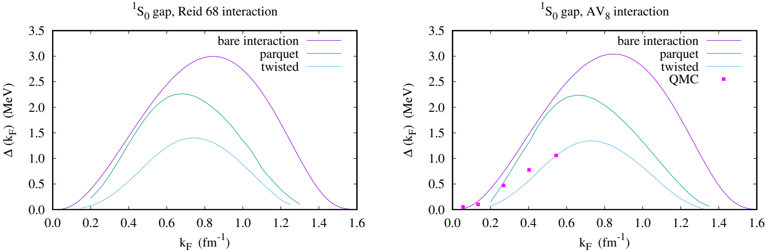
- Results for Reid 68 and Argonne are quite similar



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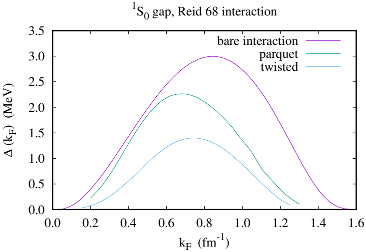

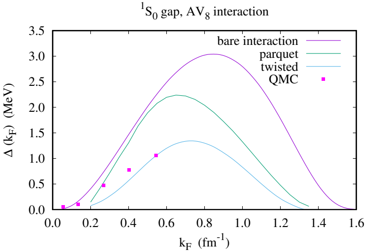

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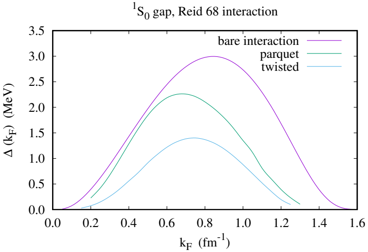

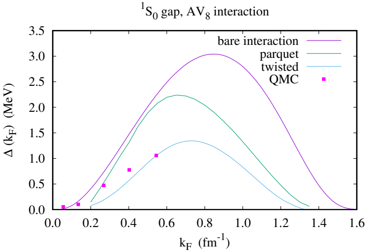

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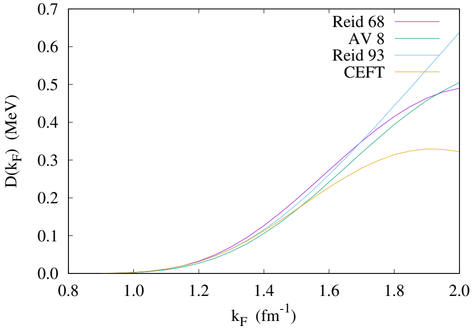
- Additional repulsion from non-parquet diagrams reduces the gap by another factor of 2 !
- Good agreement with QMC should be taken with a grain of salt.

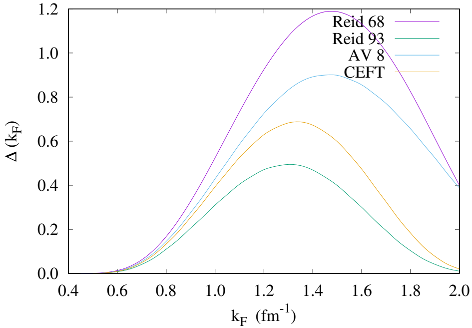
Bare interaction results: Some history
(Tamagaki, Takatsuka 1970-1972)

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



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

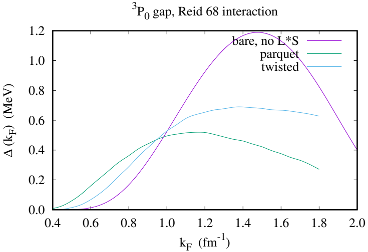
$^3P_0$ gap with bare interactions and spin-orbit force turned off

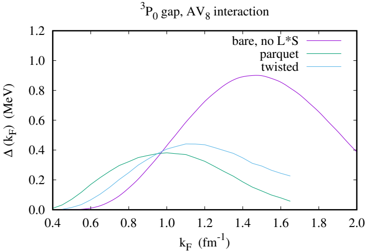


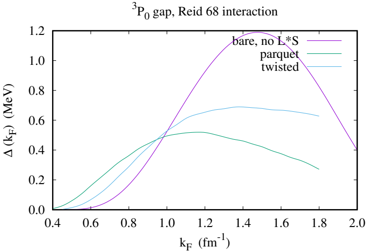
However: "Without an attractive spin-orbit interaction, neutrons would form a $^3P_0$ superfluid, in which the spin and orbital angular momenta are anti-aligned, rather than the $^3P_2$ state, in which they are aligned." (Gezerlis et al. in "Pairing and superfluidity of nucleons in neutron star")

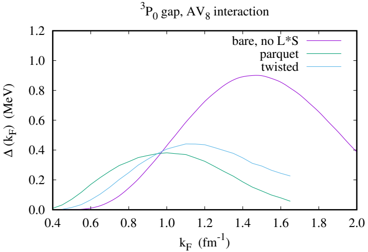
P wave superfluidity

The importance of many-body effects









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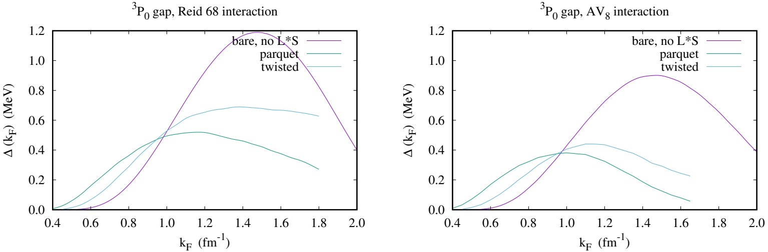

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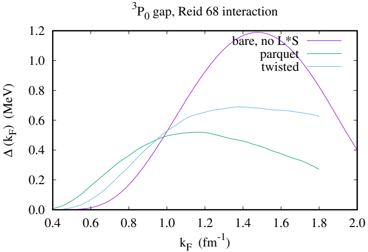

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Make the correlated wave function time dependent !

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

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

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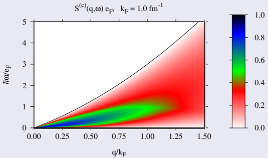
Action principle: Assume a weak external potential $U_{ext}(r;t)$:

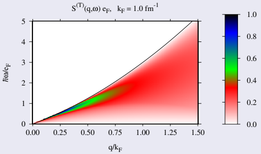
$$\begin{aligned} &\delta \int_{t_0}^{t_1} \left\langle \Psi(t) \left| \hat{H} - i\hbar \frac{\partial}{\partial t} + U_{ext}(t) \right| \Psi(t) \right\rangle dt \\ = \;\; &\delta \int_{t_0}^{t_1} \left\langle \Phi(t) \left| \hat{H} - H_{oo} - i\hbar \frac{\partial}{\partial t} + U_{ext}(t) \right| \Phi(t) \right\rangle dt = 0\,. \end{aligned}$$

Density channel



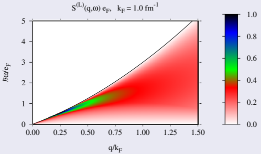
Phonon strongly Landau damped

Transverse spin mode



Strength close to continnum

Longitudinal spin mode

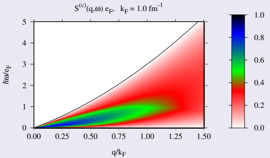


Very similar to longitudinal mode

Neutron matter response

....at the 1p-1h level

Density channel



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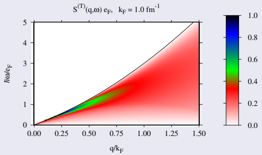

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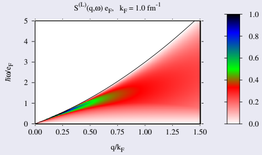

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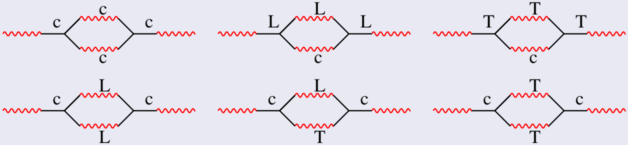
Phonon/magnon splitting processes:

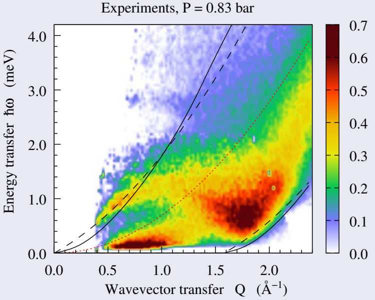
Included in DMBT



Example
^{3}He in 3D

Experiments:

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



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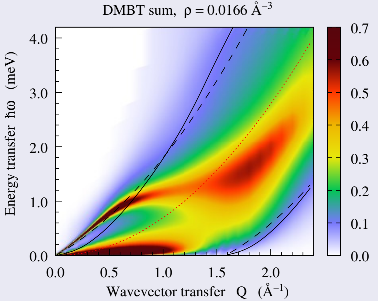

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- Diagrammatic many-body methods give access to energetics, dynamics, and phase transitions;
- S-wave pairing gets suppressed by the repusive triplet interaction in intermediate states;
- $^3P_2$-$^3F_2$ is suppressed by the suppression of the spin-orbit interaction by short ranged correlations;
- $^3P_0$ is enhanced by the suppression of the spin-orbit interaction by short ranged correlations.
- Dynamic response is still in the works.