Correlated Basis Function theory of the fermion hard-sphere fluid

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Otranto, May 30-June 4, 2011

Outline

- ⋆ Fermi gas radial distribution function
- ⋆ Diagrammatic expansion for Fermi systems
- ⋆ FHNC equations for the radial distribution function
- ⋆ Calculation of the ground state energy
- ⋆ The CBF effective interaction. Shear viscosity of the Fermi hard sphere fluid
- ⋆ Extension to neutron star matter

Ditribution function of the free Fermi gas

- Consider (dx_i denotes $\mathbf{r}_i$ integration and sum over discrete degrees of freedom)

$$g_{FG}(r_{12}) == \frac{N(N-1)}{\rho^2} \frac{\int dx_3 \ldots dx_N |\Phi_0(x_1,\ldots,x_N)|^2}{\int dx_1 \ldots dx_N |\Phi_0(x_1,\ldots,x_N)|^2}$$

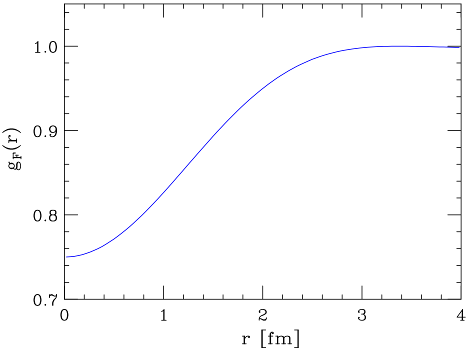
- Exploiting the properties of determinants the above equation can be rewritten (recall: $|\mathbf{k}_i|$, $|\mathbf{k}_j| < k_F$)

$$\rho^2 g_{FG}(r_{12}) = \sum_{i,j} \phi_i^\dagger(\mathbf{r}_1)\phi_j^\dagger(\mathbf{r}_2)\left[\phi_i(\mathbf{r}_1)\phi_j(\mathbf{r}_2) - \phi_j(\mathbf{r}_1)\phi_i(\mathbf{r}_2)\right]$$

$$= \frac{\nu^2}{(2\pi)^6} \left[\left(\frac{4\pi k_F^3}{3}\right)^2 - \frac{1}{\nu}\left| \int_{|\mathbf{k}|<k_F} d^3k \, e^{i\mathbf{k}\cdot\mathbf{r}_{12}} \right|^2 \right] = \rho^2 \left[1 - \frac{1}{\nu}\ell^2(k_F r_{12}) \right]$$

$$\ell(x) = \frac{3}{x^3}\left[\sin x - x\cos x\right]$$

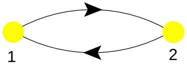
$g_{FG}(r)$ in symmetric nuclear matter at equilibrium density



Diagrammatic representation of g_{FG}

$$g_{FG}(r_{12}) = 1 - \frac{1}{\nu}\ell^2(k_F r_{12}) =$$

+



- ⋆ Diagrammatic rules
  - ▷ statistical correlations between particles 1 and 2, corresponding to

$$-\frac{1}{\nu}\int_{|\mathbf{k}|<k_F} d^3k\, \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_{12}} = -\frac{1}{\nu}\ell(k_F r_{12})$$

    are represented by oriented solid lines
  - ▷ oriented lines form loops that do not touch one another
  - ▷ each loop contributes a factor $-\nu$
  - ▷ in the cluster expansion of $g(r)$ the statistical correlation lines can be superimposed to dynamical correlation lines
- ⋆ only connected and irreducible diagrams contribute

Effect of statistical correlation

- As an exmple, consider the term of order ρ in the expansion of the radial distribution function. In the case of Fermi statistics

$$\int d^3 r_3 \ h(r_{13}) h(r_{32}) \Rightarrow \int d^3 r_3 \ h(r_{13}) h(r_{32}) \Delta(1,2,3)$$

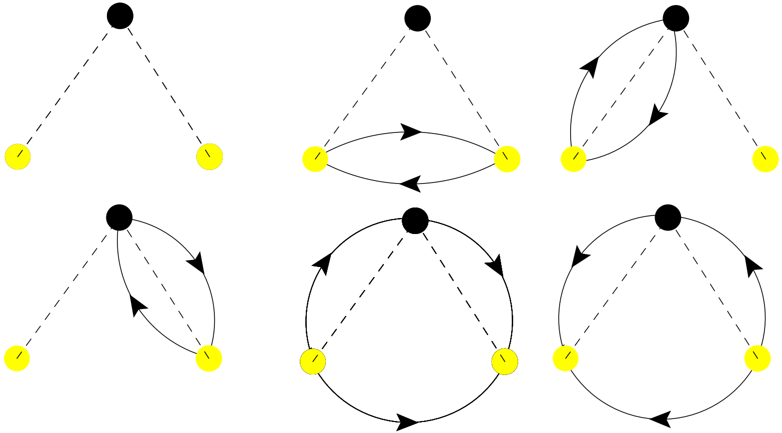
$$\Delta(1,2,3) = \int dx_4 \dots dx_N |\Phi_0(1,\dots,N)|^2$$

$$= 1 - \frac{1}{\nu} \ell^2(k_F r_{12}) - \frac{1}{\nu} \ell^2(k_F r_{13}) - - \frac{1}{\nu} \ell^2(k_F r_{32})$$

$$- \frac{1}{\nu^2} \ell(k_F r_{12}) \ell(k_F r_{23}) \ell(k_F r_{32}) - \frac{1}{\nu^2} \ell(k_F r_{13}) \ell(k_F r_{32}) \ell(k_F r_{21})$$

- Antisymmetrization of the grond state leads to the appearance of five additional contributions.

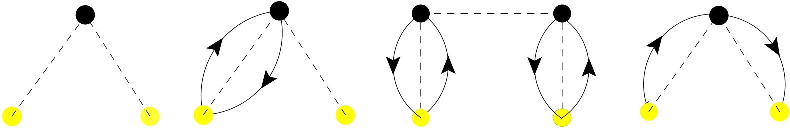
Diagrams contributing to $g_1(r)$



★ The diagrams can be classified according to the pattern of statistical correlation lines reaching the external points

Classification of nodal diagrams

- In Fermi systems nodal diagrams $N(r_{12})$ can be classified in four different classes
  - $N_{dd}(r_{12})$ nodal diagrams having no statistical correlation lines reaching the external points
  - $N_{de}(r_{12})$ $N_{de}(r_{21})$ nodal diagrams in which either of the external points belongs to a *binary* exchange loop involving one internal point
  - $N_{ee}(r_{12})$ nodal diagrams in which both external points belong to a *binary* exchange loops, involving internal points
  - $N_{cc}(r_{12})$ nodal diagrams in which both external points belong to a *circular* exchange loop involving internal points



Parallel connection of nodal diagrams

- Define:

$$F(r_{12}) = f^2(r_{12}) e^{N_{dd}(r_{12})}$$

- Composite diagrams can be generated through parallel connections of the nodal diagrams $N_{xy}(r_{12})$ according to

$$X_{dd}(r_{12}) = F(r_{12}) - N_{dd}(r_{12}) - 1$$

$$X_{de}(r_{12}) = F(r_{12}) N_{de} - N_{de}(r_{12})$$

$$\begin{aligned} X_{ee}(r_{12}) &= F(r_{12})[N_{ee}(r_{12}) + N_{de}^2(r_{12}) - \nu N_{cc}^2(r_{12}) \\ &+ 2\ell(k_F r_{12}) N_{cc}(r_{12}) - \frac{1}{\nu}\ell^2(k_F r_{12})] \end{aligned} \tag{1}$$

$$X_{cc}(r_{12}) = F(r_{12})[N_{cc}(r_{12}) - \frac{1}{\nu}\ell(k_F r_{12})] - \frac{1}{\nu}\ell(k_F r_{12}) - N_{cc}(r_{12})$$

FHNC equations (Fantoni & Rosati, AD 1975)

- Define:

$$W_{xy}(r_{12}) = X_{xy}(r_{12}) + N_{xy}(r_{12})$$

- The integral equations for the $N_{xy}(r_{12})$ are

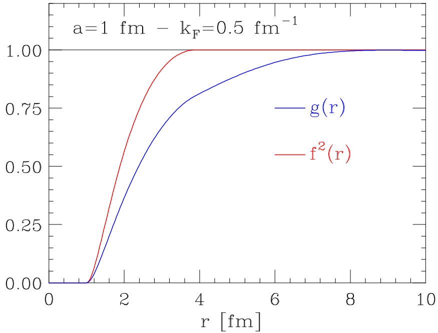
$$N_{dd}(r_{12}) = \rho \int d^3 r_3 \{[X_{dd}(r_{13}) + X_{de}(r_{13})] W_{dd}(r_{32}) + X_{dd}(r_{13}) W_{de}(r_{32})\}$$

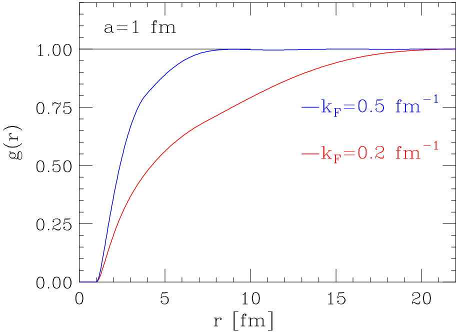
$$N_{de}(r_{12}) = \rho \int d^3 r_3 \{[X_{dd}(r_{13}) + X_{de}(r_{13})] W_{dd}(r_{32}) + X_{dd}(r_{13}) W_{ee}(r_{32})\}$$

$$N_{ee}(r_{12}) = \rho \int d^3 r_3 \{X_{ed}(r_{13}) W_{ee}(r_{32}) + [X_{dd}(r_{13}) + x_{ee}(r_{13}) W_{de}(r_{32})\}$$

$$N_{cc}(r_{12}) = \rho \int d^3 r_3 \{X_{cc}(r_{13}) [W_{cc}(r_{32}) - \frac{1}{\nu} \ell(k_F r_{32})]$$

FHNC results: $g(r)$ of the fermion hard sphere liquid





$$g(r) = 1 + W_{dd}(r) + 2W_{de}(r) + W_{ee}(r)$$

Calculation of the ground state energy

- Use the variational principle to determine the shape of the correlation function and the ground state energy

$$\Psi_0 = F\,\Phi_0 = \Pi_{j>i=1}^{N} f(r_{ij})\Phi_0$$

$$f(r) = \begin{cases} 0 & r < a \\ \frac{d}{r}\,\frac{\sin[k_0(r-a)]}{\sin[k_0(d-a)]} & r > a \end{cases}$$

$$\min_d \frac{\langle 0|F\,H\,F|0\rangle}{\langle 0|F^2|0\rangle} \geq E_0$$

- k_0 determined in such a way as to have

$$\left(\frac{df}{dr}\right)_{r=d} = 0$$

Kinetic energy

- Ambiguity involved in the calculation of the kinetic energy

$$\frac{\langle \Phi_0 | F \left(\sum_{i=1}^{N} - \frac{\nabla_i^2}{2m} \right) F | \Phi_0 \rangle}{\langle \Phi_0 | F^2 | \Phi_0 \rangle}$$

- From

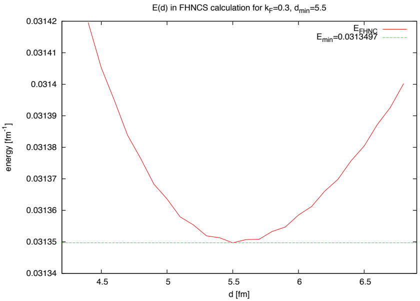
$$\langle \Phi_0 F \, \nabla_i^2 \, F \Phi_0 \rangle = \langle \Phi_0 [F^2 (\nabla_i^2 \Phi_0) + F(\nabla_i^2 F) \Phi_0 + 2F(\boldsymbol{\nabla} F) \cdot (\boldsymbol{\nabla} \Phi_0)] \rangle$$

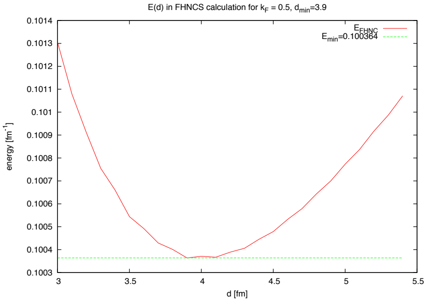
integrating by parts we obtain

$$\langle \Phi_0 F^2 (\nabla_i^2 \Phi_0) \rangle - \langle \Phi_0 (\boldsymbol{\nabla} F)^2 \Phi_0 \rangle - \langle (\boldsymbol{\nabla} \Phi_0) F \cdot (\nabla F) \Phi_0 \rangle + \langle \Phi_0 (\boldsymbol{\nabla} \Phi_0) \cdot F(\nabla F) \rangle$$

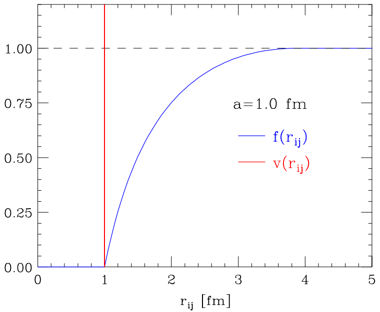
- Note that, as the FHNC calculation of the expectation value does not include all diagrams, the above expressions do not yield the same result. The small (typically less than few percent) difference between the two results provides an estimate of the accuracy of the calculation

Minimization of the ground state expectation value $\langle H \rangle$





Shape of the correlation function at $k_F = 0.5 \text{ fm}^{-1}$



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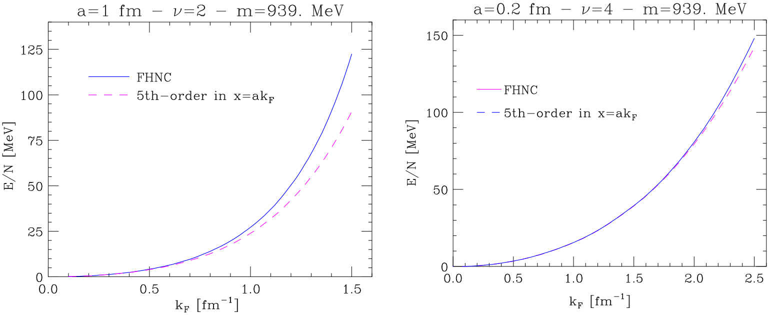
Comparison between FHNC and perturbation theory



- ⋆ The requirement that the FNHC results provide an upper bound to the ground state energy ia always fulfilled

To the equation of state and beyond

- ⋆ The formalism of correlated basis functions (CBF) and the FHNC equations provides a viable computational scheme to obtain the ground state energy per particle, thus allowing to determine the EOS

$$e(\rho) = \frac{E}{N} \Rightarrow \epsilon(\rho) = \rho e\,,\ P(\rho) = \rho^2 \left(\frac{\partial e}{\partial \rho} \right) \Rightarrow P = P(\epsilon)$$

- ⋆ The $P(\epsilon)$ relation is needed to obtain M and R of non rotating stars from the solution of the Tolmann-Oppenheimer-Volkoff equations (see Ignazio Bombaci's lectures)

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- ⋆ The $P(\epsilon)$ relation is needed to obtain M and R of non rotating stars from the solution of the Tolmann-Oppenheimer-Volkoff equations (see Ignazio Bombaci's lectures)
- ⋆ Can the theoretical approach used to compute the EOS be exploited to consistently obtain other properties of astrphysical interest?

Transport properties of neutron matter

- ⋆ Abrikosov & Khalatnikov (AK) formalism (AD 1957). Starting point: Boltzman equation

$$\frac{\partial n}{\partial t} + \frac{\partial n}{\partial \mathbf{r}}\frac{\partial \epsilon_{\mathbf{p}}}{\partial \mathbf{p}} - \frac{\partial n}{\partial \mathbf{p}}\frac{\partial \epsilon_{\mathbf{p}}}{\partial \mathbf{r}} = I(n)$$

$$n = n_0 + \delta n \quad , \quad n_0 = \{1 + \exp[\beta(\epsilon - \mu)]\}^{-1}$$

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- The collision integral $I(n)$ depends on the probability of the scattering process $1 + 2 \longrightarrow 1' + 2'$
- Consider *shear viscosity* as an example. Using Landau theory of Fermi liquids AK obtain the *approximate* (although rather accurate) result

$$\eta_{AK} = \frac{1}{5} \rho m^* v_F^2 \tau \frac{2}{\pi^2 (1 - \lambda_\eta)}$$

★ quasiparticle lifetime and angle-averaged scattering probability $\langle W \rangle$

$$\tau T^2 = \frac{8\pi^4}{m^{*3}} \frac{1}{\langle W \rangle} \qquad \langle W \rangle = \int \frac{d\Omega}{2\pi} \frac{W(\theta,\phi)}{\cos\theta/2}$$

$$\lambda_\eta = \frac{\langle W(1-3\sin^4\theta/2\sin^2\phi)\rangle}{\langle W \rangle}$$

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★ exact solution by Brooker & Sykes (AD 1968)

$$\eta = \eta_{AK} C(\lambda_\eta)$$

$$C(\lambda_\eta) = \frac{1-\lambda_\eta}{4} \sum_{k=0}^{\infty} \frac{4k+3}{(k+1)(2k+1)[(k+1)(2k+1)-\lambda_\eta]}$$

$$-2 < \lambda_\eta < 1 \quad , \quad 0.750 < C(\lambda_\eta) < 0.925$$

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★ Similar expressions can be obtained for the other transport coefficients

Calculations of transport coefficients

- Calculation of the transport coefficients within the AK approach requires
  - The quasiparticle spectrum $\epsilon_{\mathbf{p}}$, needed to calculate the effective mass from

$$\frac{1}{m^\star} = \frac{1}{p}\frac{d\epsilon_{\mathbf{p}}}{dp}$$

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  - The scattering probability, related to the scattering cross section in the nuclear medium through

$$\frac{d\sigma}{d\Omega} = \frac{{m^\star}^2}{16\pi^2} W(\theta,\phi) \ ,$$

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- ⋆ Strategy: use the CBF formalism to obtain an *effective interaction*, derived from the bare potentials, allowing for a consistent calculation of all relevant quantities.

The CBF effective interaction

- The effective interaction is defined through

$$\langle H \rangle = \frac{\langle 0 | T + V | 0 \rangle}{\langle 0 | 0 \rangle} = \langle 0_{FG} | T + V_{\rm eff} | 0_{FG} \rangle$$

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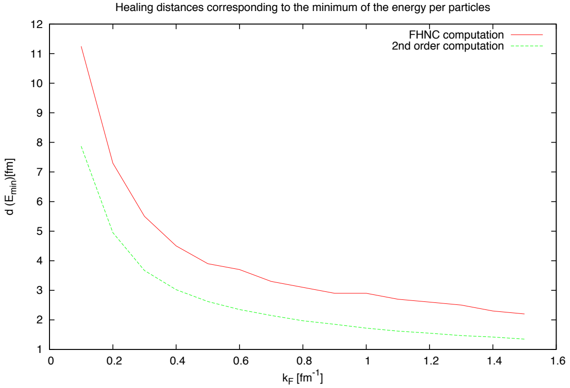
- At two-body cluster level (recall: $\langle 0_{FG}|F\ V\ F|0_{FG}\rangle = 0$)

$$V_{\rm eff} = \sum_{j>i} v_{\rm eff}(r_{ij})$$

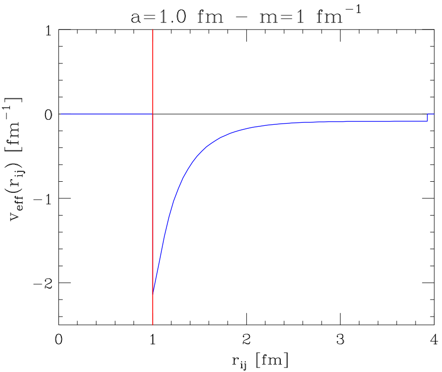
$$v_{\rm eff}(r_{ij}) = f(r_{ij})\left\{-\frac{1}{m}[\nabla^2 f(r_{ij}] - \frac{2}{m}[\nabla f(r_{ij})]\cdot\nabla\right\} \approx -\frac{1}{m} f(r_{12})\nabla^2 f(r_{ij})$$

- Correlation range determined requiring that the FHNC energy be reproduced in the two-body cluster approximation

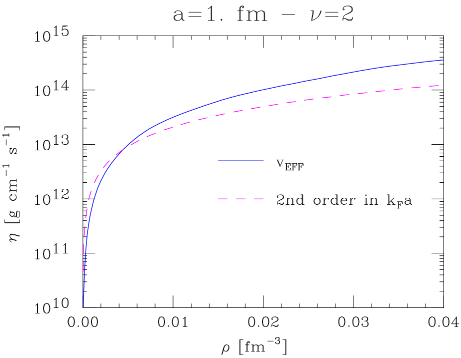
Effective interaction range



Shape of the CBF effective interaction at $k_F = 0.5\ \text{fm}^{-1}$



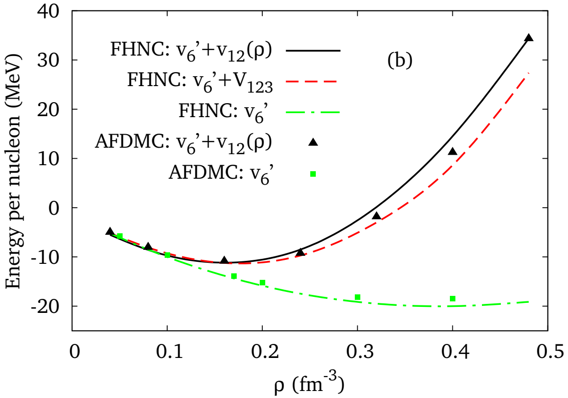
Density dependence of the shear viscosity coefficient



Extension to neutron star matter

- ⋆ NN interactions have a complex operatorial structure
- ⋆ Many-nucleon forces are known to be important (in fact critical at large density)
- ⋆ Correlation functions reflect the operatorial structure of the NN interaction, implying that $[f_{ij}, f_{jk}] \neq 0$
- ⋆ Cluster diagrams classification and FHNC equations become much more complicated. Further approximations needed. Comparison with Monte Carlo simulations suggest that the extended FHNC scheme provides accurate results.
- ⋆ The CBF based effective interaction approach appears to be a viable option to circumvent some of the above difficulties. In adition, it allows for a unified description of structure and dynamics of neutron star matter based on “realistic” NN potential.

FHNC energy per particle of symmetric nuclear matter



In medium NN cross section

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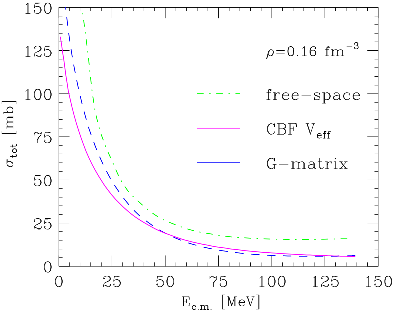
In medium NN cross section

- The matrix elements of G and V_{eff} can be used to obtain the in medium neutron neutron cross section
- Total neutron-neutron x-section. Argonne v_6' potential



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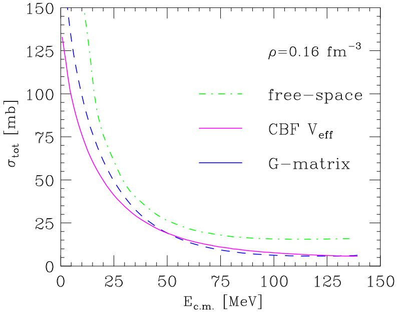
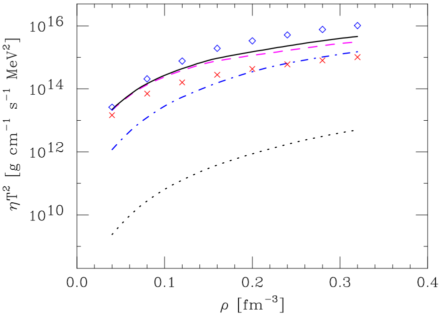
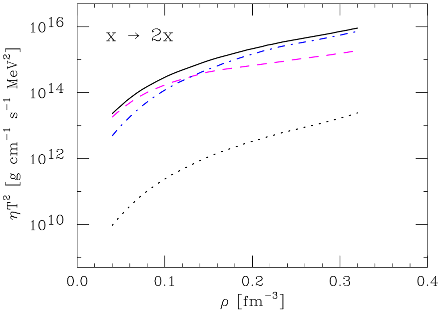


- ⋆ The effects of the three-nucleon force can be included in the CBF effective interaction, through a density-dependent two-nucleon interaction

Shear viscosity of β-stable *npe* matter

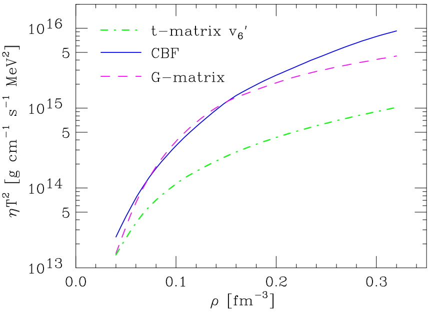
- ⋆ Required inputs [proton (and electron) fraction, effective masses & scattering rates] obtained from the CBF effective interaction

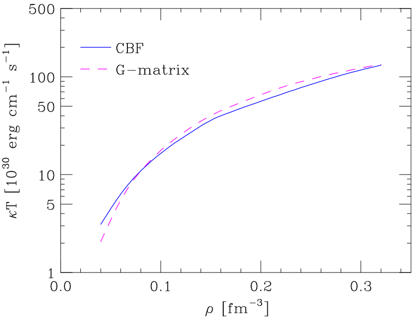




- ⋆ Increasing the electron fraction leads to a significant modification of the balance between the different contributions to the viscosity.
- ⋆ consistency is a critical issue

- Results obtained using the Argonne v_6' potential

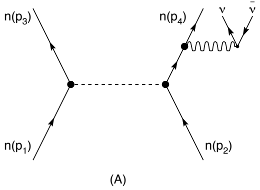




- Medium effects are large. The model dependence is not critical, although it can be clearly seen in the case of viscosity at supranuclear density.

Emissivity due to bremsstrahlung of $\nu - \bar{\nu}$ pairs

★ In Born approximation, the emission rate of the process

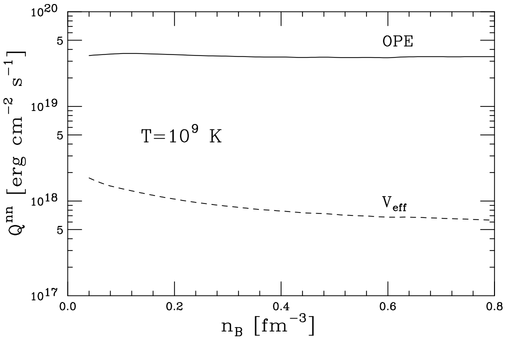


is driven by the trace

$$H^{ii} = 16 \, \frac{1}{\omega^2} \sum_{M_S M_{S'}} \left| \langle 1 M_{S'} | \left[S_i, v_{eff}(\mathbf{q}) \right] | 1 M_S \rangle \right|^2 \; .$$

where S denotes the total spin

One Pion Exchange (OPEP) vs CBF effective interaction



- ⋆ Nuclear dynamics beyond OPEP: factor $\sim 4 \div 5$ (Reddy *et al*, AD 2001)
- ⋆ Screening due to neutron-neutron correlations: factor $\sim 6 \div 7$