Nuclear Effective Interaction From Correlated Basis Functions

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Bridging nuclear *ab-initio* and energy-density-functional theories

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OUTLINE

- ⋆ Motivation
- ⋆ The paradigm of Nuclear Many-Body Theory
- ⋆ Derivation of the CBF effective interaction
- ⋆ Applications: the nuclear matter equation of state and beyond
- ⋆ Perspectives & Open Questions

Motivation

- ⋆ Astrophysical applications require theoretical approaches capable to provide a *consistent* description of properties of nuclear matter other than the equation of state at zero temperature, including the neutrino emission and absorption rates, the transport coefficients as well as the superfluid and superconducting gaps
- ⋆ Effective interactions obtained from a *microscopic nuclear dynamics*—strongly constrained by phenomenology—combine the flexibility of the effective interaction approach with the ability to provide a realistic description of a variety of equilibrium and non equilibrium properties.

THE PARADIGM OF *ab initio* NUCLEAR MANY-BODY THEORY

- Nuclear systems can be described as a collection of pointlike protons and neutrons interacting through the hamiltonian

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{j>i} \mathrm{v}_{ij} + \sum_{k>j>i} \mathrm{V}_{\mathrm{ijk}} = H_0 + H_I$$

- The Hamiltonian is determined from the properties of exacltly ($A = 2, 3$)—or nearly exactly ($A \to \infty$)—systems. In principle, describing the properties of more complex systems should not require additional adjustable parameters.
- The matrix elements of H_I between eigenstates of H_0, are generally large, and cannot be used to do *standard* perturbation theory
- Effective interactions are designed to obtain accurate estimates of nuclear properties at lowest order perturbation theory
- Ideally, effective interactions should be derived from the bare Hamiltonian

Introducing the Effective Interaction

- Consider nuclear matter. The eigenstates of H_0 are Fermi gas states $\{|n_{FG}\rangle\}$
- Taming the matrix element of the Hamiltonian

$$\langle m_{FG}|H|n_{FG}\rangle \Rightarrow \begin{cases} \langle m_{FG}|H_{\rm eff}|n_{FG}\rangle & (H \Rightarrow H_{\rm eff}) \\ \langle m|H|n\rangle & (\{|n_{FG}\rangle\} \Rightarrow \{|n\rangle\}) \end{cases}$$

  - Use the *effective* Hamiltonian $H_{\rm eff}$ in standard perturbation theory with Fermi gas basis states, as in the G-matrix approach
  - Use the *bare* Hamiltonian to do perturbative calculations in the new basis, as in the approach based on Correlated Basis Functions (CBF)
- The effective interaction must be designed in such a way as to provide accurate estimates of nuclear matter properties at lowest order of standard perturbation theory

- In principle, the two approaches may be merged defining the new basis states through the transformation

$$|n\rangle = F|n_{FG}\rangle$$

leading to

$$H_{\rm eff} = F^\dagger H F$$

- Implementing this simple prescription requires qualifications, associated with the definition and determination of F
- In the *generalised* Jastrow *ansatz*

$$F = \prod_{j>i} F_{ij} \quad , \quad F_{ij} = \sum_n f^{(n)}(r_{ij}) O^{(n)}_{ij}$$

with the operator structure of F_{ij} reflecting the one of the nucleon-nucleon (NN) potential. As $r_{ij} \to \infty$, $F_{ij} \to \mathbb{1}$

DETERMINATION OF THE CORRELATION FUNCTION

- The shape of the $f^{(n)}(r_{ij})$ is determined variationally, minimising the expectation value of the Hamiltonian in the *correlated* ground state, evaluated using the cluster expansion techinque

$$\langle H \rangle = \frac{\langle 0|H|0\rangle}{\langle 0|0\rangle} \geq E_0$$

- Accurate nuclear calculations can be carried out exploiting the cluster expansion formalism

$$\langle H \rangle = E_{FG} + \frac{\partial}{\partial\beta} \ln\langle 0|\mathrm{e}^{\beta(H-E_{FG})}|0\rangle\Big|_{\beta=0} = E_{FG} + \sum_{\ell\geq 2} \Delta E_\ell[F]$$

where $\Delta E_\ell[F]$ is the contribution arising from clusters of ℓ *correlated* particles, and summing up all relevant contributions solving the FHNC/SOC integral equations

- $\langle H \rangle$ is minimized with respect to a set of variational parameters determining the range of the correlation functions

FROM $\langle H \rangle$ TO $\langle H_{\text{eff}} \rangle$

- The effective interaction is *defined* through the equation

$$\begin{aligned} \langle H \rangle_{\text{FHNC/SOC}} &= E_{FG} + \sum_{\ell \leq \ell_{\max}} \Delta_\ell[\tilde{F}] \\ &= E_{FG} + \langle 0_{FG} | V_{\text{eff}} | 0_{FG} \rangle \end{aligned}$$

with

$$\begin{aligned} V_{\text{eff}} &= \sum_{j>i} v_{\text{eff}}^{ij} \quad , \quad v_{\text{eff}}^{ij} = \sum_n v_{\text{eff}}^{(n)}(r_{ij}) O_{ij}^{(n)} \\ O_{ij}^{(n \leq 6)} &= [1, (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j), S_{ij}] \otimes [1, (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)] \\ S_{ij} &= \frac{3}{r_{ij}^2} (\boldsymbol{\sigma}_i \cdot \mathbf{r}_{ij})(\boldsymbol{\sigma}_j \cdot \mathbf{r}_{ij}) - (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) \end{aligned}$$

and the range of $\tilde{F}$ is adjusted in such a way as to obtain the FHNC/SOC results at low order of the cluster expansion

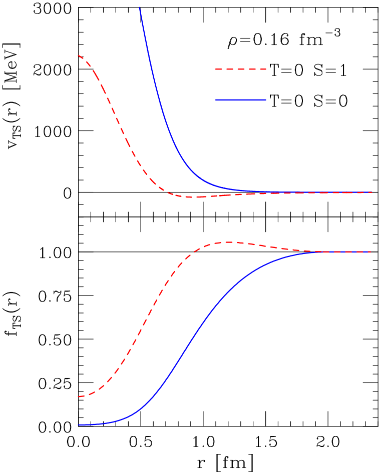
- Pedagogical example: neglecting three-nucleon forces, one may set $\ell_{\rm max} = 2$, and obtain

$$v_{\rm eff}^{ij} = \frac{1}{m}\left(\nabla \tilde{F}_{ij}\right)^2 + \tilde{F}_{ij} v_{ij} \tilde{F}_{ij}$$

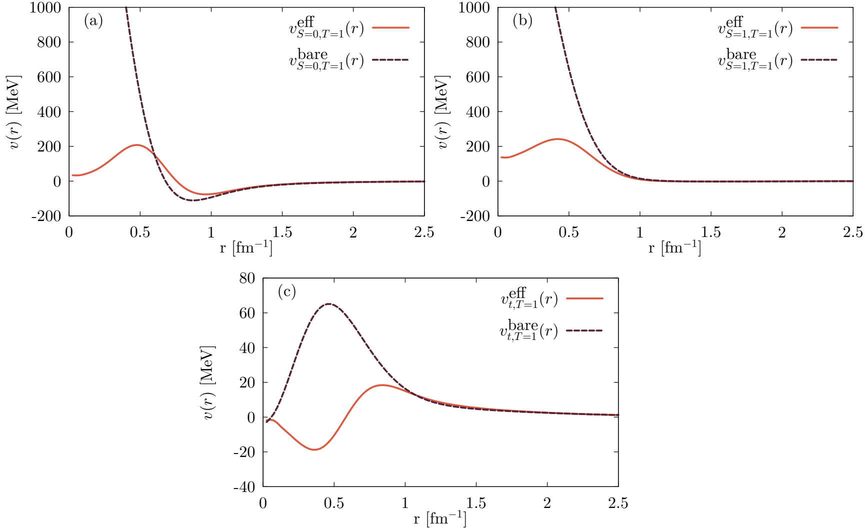
- Note that the correlation function $\tilde{F}_{ij}$ depends on density, and so does the effective interaction
- Adding three-body cluster terms allows to take into account the leading contributions arising from the three-nucleon potential, the inclusion of which is essential to obtain saturation in isospin-symmetric nuclear matter
- The resulting effective interaction reproduces the FHNC/SOC ground-state energies of *both* isospin-symmetric nuclear matter (SNM) and pure neutron matter (PNM). It can be used to describe matter at fixed baryon density and arbitrary proton fraction

NN Potential and Correlation Functions

⋆ ANL v_6' potential

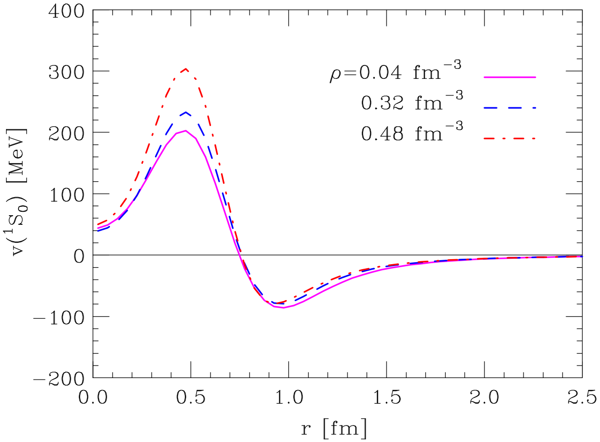


- CBF effective interaction in the $T = 1$ channel at nuclear matter equilibrium density, obtained from the Argonne $v_6' + UIX$ nuclear Hamiltonian



DENSITY DEPENDENCE OF THE EFFECTIVE INTERACTION

⋆ $^1S_0$ channel



Ground state energy and single-particle spectrum

- The ground state energy per baryon can be computed at first order in the effective interaction —that is, in Hartree–Fock approximation—for fixed baryon density and arbitrary proton fraction and polarizartions

$$\frac{E}{N_B} = \sum_{\mathbf{k}\lambda} \frac{\mathbf{k}^2}{2m} n_\lambda(\mathbf{k}) + \frac{1}{2} \sum_{\mathbf{k}\lambda\ ,\mathbf{k}'\lambda'} \langle \mathbf{k}\lambda\ \mathbf{k}'\lambda' | v^{\rm eff} | \mathbf{k}\lambda\ \mathbf{k}'\lambda' \rangle_A \ n_\lambda(\mathbf{k}) n_{\lambda'}(\mathbf{k}')$$

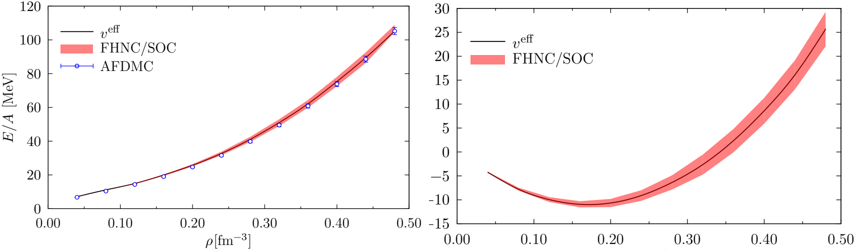
where $\lambda = 1, 2, 3, 4$ corresponds to $p\uparrow$, $p\downarrow$, $n\uparrow$, $n\downarrow$, and

$$n_\lambda(\mathbf{k}) = \theta(k_{F_\lambda} - |\mathbf{k}|) \quad , \quad k_{F_\lambda} = (3\pi^2\rho_\lambda)^{1/3}$$

- The same approximation can be employed to obtain the single-nucleon spectrum and the effective masses

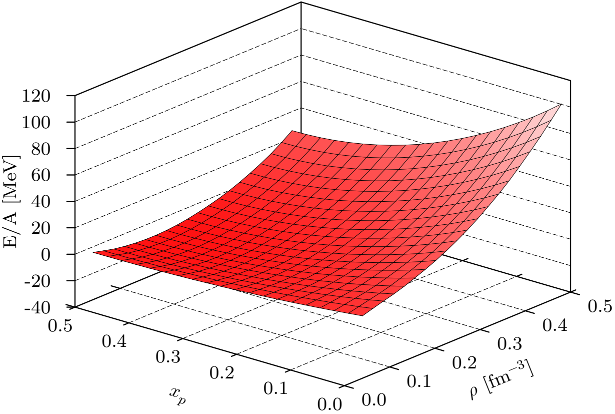
$$e_\lambda(\mathbf{k}) = \frac{\mathbf{k}^2}{2m} + \sum_{\mathbf{k}'\lambda'} \langle \mathbf{k}\lambda\ \mathbf{k}'\lambda' | v^{\rm eff} | \mathbf{k}\lambda\ \mathbf{k}'\lambda' \rangle_A \ n_\lambda(\mathbf{k}) \quad , \quad \frac{1}{m^\star} = \frac{1}{|\mathbf{k}|} \frac{de_\lambda(\mathbf{k})}{d|\mathbf{k}|}$$

- Density dependence of the ground state energy per nucleon of unpolarized pure neutron matter (PNM) and isopspin-symmetric nuclear matter (SNM) obtained from the Argonne $v_6' + UIX$ nuclear Hamiltonian



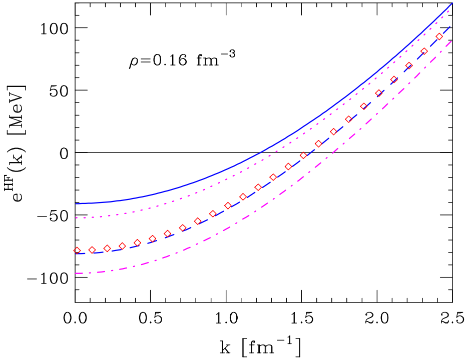
- Note that the $v_6' + UIX$ Hamiltonian, while yielding saturation at $\rho \approx \rho_0 = 0.16 \text{ fm}^{-3}$, underestimates the equilibrium energy of SNM by ~ 5 MeV, corresponding to a $\sim 15\%$ underestimate of the interaction energy

⋆ Energy of unpolarized nuclear matter as a function of baryon density and proton fraction $0 \leq x_p \leq 0.5$



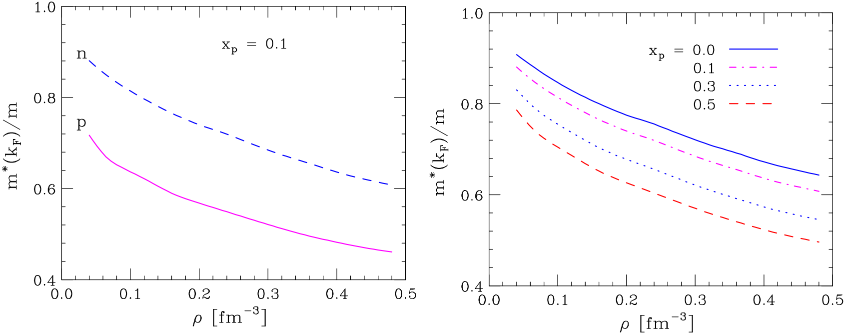
Single-nucleon spectrum

- Momentum dependence of proton and neutron spectra at nuclear matter equilibrium density and different proton fraction



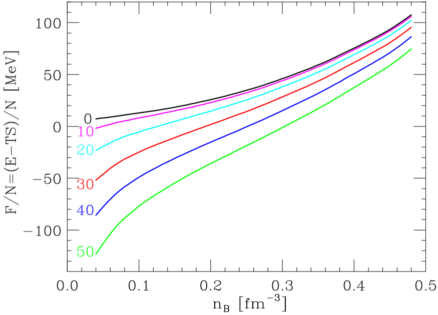
EFFECTIVE MASS (HARTEE-FOCK)

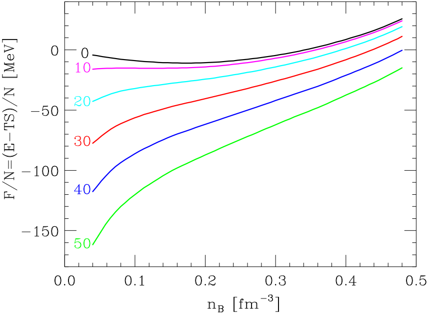
⋆ Density dependence of $m^\star(k_F)/m$



EXTENSION TO $T > 0$

- Assuminhg that thermal effect do not significantly affect the dynamics of strong interactions, the effective interaciotns can be used to obtain the properties of nuclear matter at $T > 0$
- Replace $\theta(k_F - k) \rightarrow \{1 + \exp[e(k) - \mu]/T\}^{-1}$





Perspectives & Open Questions

- ⋆ The effective interaction based on the CBF formalism and the cluster expansion technique can be used to carry out consistent calculations of a variety of nuclear matter properties relevant to astrophysical processes.
- ⋆ Improving the accuracy using more realistic bare Hamiltonian, including chirally inspired potentials, does not involve any conceptual difficulties
- ⋆ In a way, the CBF effective interaction can be seen as belonging to the family of Skyrme-like interaction, as it is defined in terms of its ground-state expectation value. However, it has the most important property of reducing to the bare NN interaction in the zero-density limit
- ⋆ The ability to carry out accurate calculations of quantities other than the ground-state energy at zero temperature cannot be taken for granted. It is an assumption that needs to be thoroughly tested at numerical level

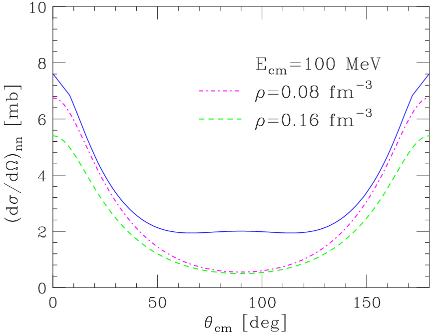
Additional Slides

In-Medium Cross Section

⋆ Neutron-Neutron Channel

$$W(\mathbf{p},\mathbf{p}') = 2\pi \left|\hat{V}_{eff}(\mathbf{p}-\mathbf{p}')\right|^2 \rho(\mathbf{p}')$$

$$\frac{d\sigma}{d\Omega_{\mathbf{p}'}} = \frac{m^{\star 2}}{16\pi^2} \left|\hat{V}_{eff}(\mathbf{p}-\mathbf{p}')\right|^2$$

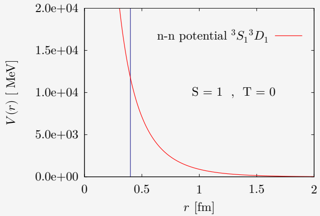


THE HARD-SPHERE MODEL

The Fermi hard-sphere model: point-like spin one-half particles

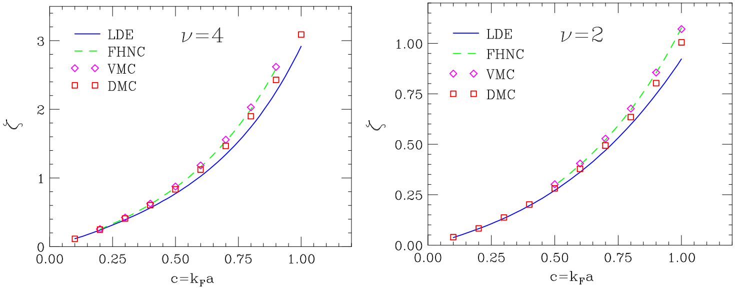
$$v(r) = \begin{cases} \infty & r < a \\ 0 & r > a \end{cases}$$

- ⋆ Valuable model to study properties of nuclear matter.
- ⋆ Purely repulsive potential to prevent the possibility of Cooper pairs formation.
- ⋆ A simple many-body system to investigate the validity and robustness of the assumptions of CBF effective interaction approach.



THE GROUND-STATE ENERGY

$$E_0 = \frac{3k_F^2}{10m}(1+\zeta)$$

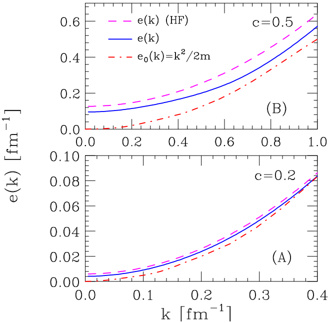


- The accuracy of the variational results depends on the quality of the trial wave function.
- Long-range statistical correlations effects in $f(r)$ much larger for $\nu = 2$ than for $\nu = 4$.
- DMC overcomes the limitations of the variational approach by using a projection technique on the trial wave function.

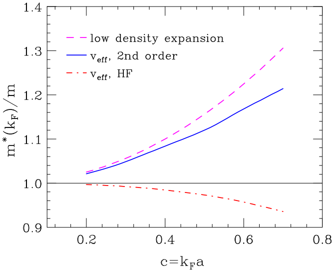
Effective Mass

- ⋆ Second order, energy-dependent, contributions included

Quasiparticle spectrum



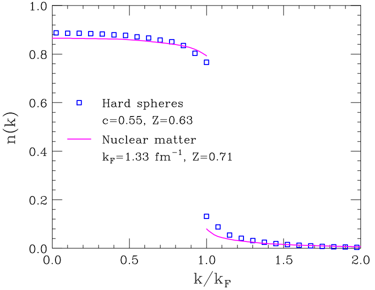
$$m^\star = \left[\frac{1}{k}\frac{de(k)}{dk}\right]^{-1}$$



$$\frac{de(k)}{dk} = \left[\frac{k}{m} + \frac{\partial}{\partial k}\mathrm{Re}\Sigma(k,E)\right]\left[1 - \frac{\partial}{\partial E}\mathrm{Re}\Sigma(k,E)\right]^{-1}_{E=e(k)}$$

MOMENTUM DISTRIBUTION $\nu = 4$

In comparison with non orthogonal CBF perturbation theory



S. Fantoni and V. R. Pandharipande, Nucl. Phys. A **427**(1984)

Momentum distribution of HS

$$c \equiv k_F a = 0.55$$

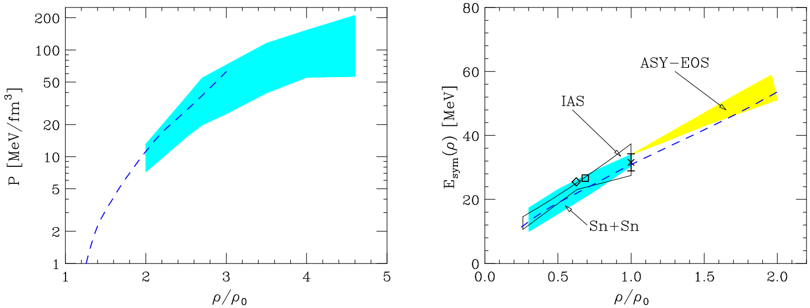
corresponds to $n(k)$ of nuclear matter

$$\rho_{NM} = 0.16 \text{ fm}^{-3}$$
$$k_F = 1.33 \text{ fm}^{-1}$$

Nucleons in nuclear matter $\sim$ HS of radius $a = 0.55/1.33 \sim 0.4$ fm.

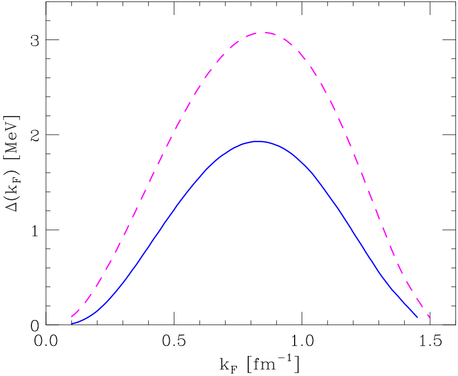
Virtual scattering processes between strongly correlated particles are mainly driven by the short-range repulsive core of the nucleon-nucleon interaction.

Pressure of SNM and Symmetry Energy



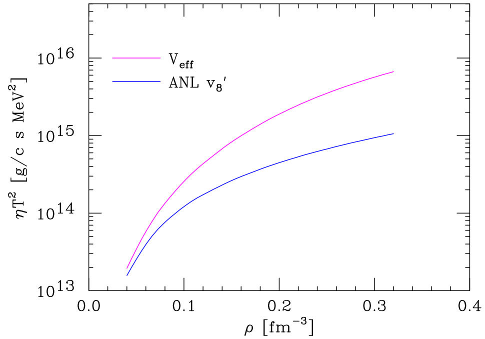
DENSITY DEPENDENCE OF Δ_F

- Gap function obtained using the bare v_6' potential (dashed line) with kinetic energy spectrum (dashed line) and the CBF effective interaction with Hartee-Fock spectrum (solid line)



Shear Viscosity of PNM

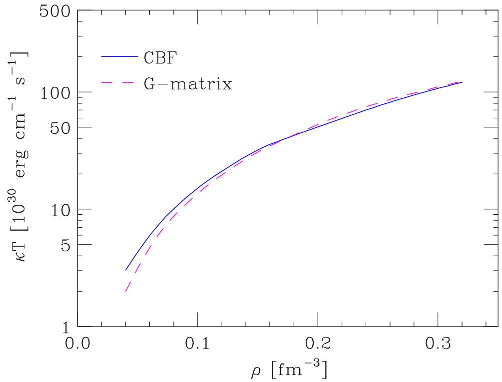
- ⋆ Density dependence of ηT^2 of PNM



- ⋆ Medium modifications of the scattering cross section increase ηT^2 by a factor $\sim 3 - 7$ @ $\rho/\rho_0 \sim 1 - 2$

Thermal Conductivity of PNM

- ⋆ Results from PRC 81, 024305 (2009). Three-nucleon interactions not taken into account.



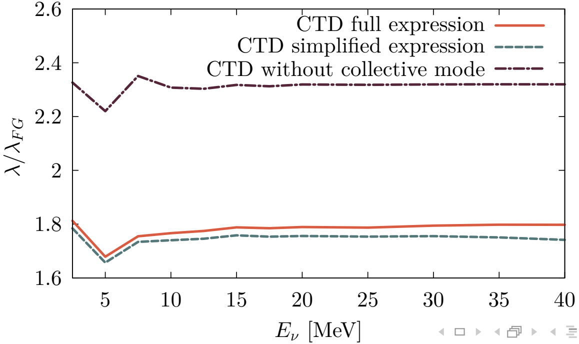
- ⋆ The transport coefficients computed using the CBF effective interaction is remarkably close to the result obtained within the G-matrix approach using the same bare NN potential.

Neutrino Mean Free Path in Cold Neutron Matter

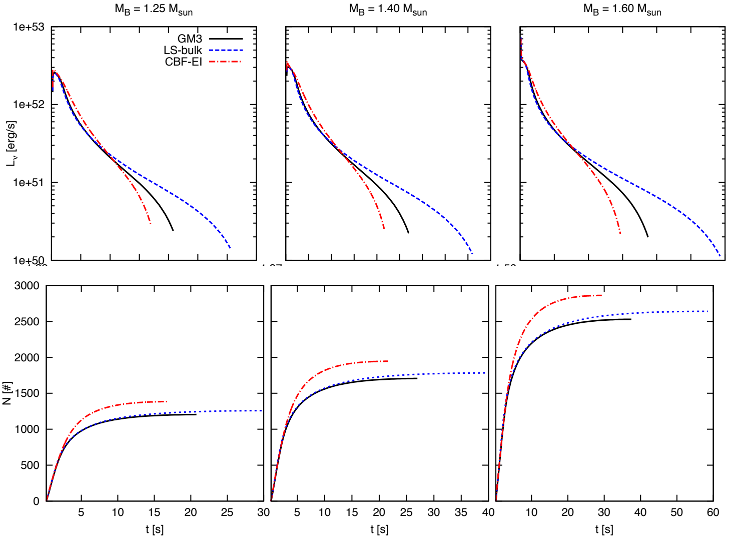
- The mean free path of non degenerate neutrinos at zero temperature is obtained from

$$\frac{1}{\lambda} = \frac{G_F^2}{4}\rho \int \frac{d^3q}{(2\pi)^3} \left[(1+\cos\theta)S(\mathbf{q},\omega) + \mathbf{C_A^2}(\mathbf{3}-\cos\theta)\mathcal{S}(\mathbf{q},\omega)\right]$$

where S and $\mathcal{S}$ are the density (Fermi) and spin (Gamow Teller) response, respectively [A. Lovato et al, NPA 89, 025804 (2013); PRC 89, 025804 (2013)]



NEUTRINO LUNINOSITY OF PROTO NEUTRON STARS (PNS)



Frequencies of Quasi Normal Modes of PNS