Chiral EFT Equation of State Module

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muses

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Overview

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Background

Chiral Effective Field Theory (EFT) for Nuclear Forces

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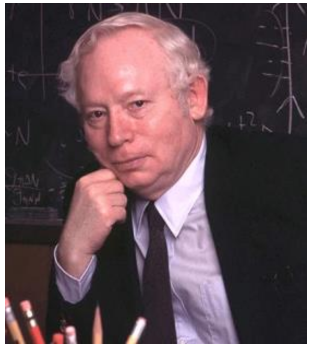
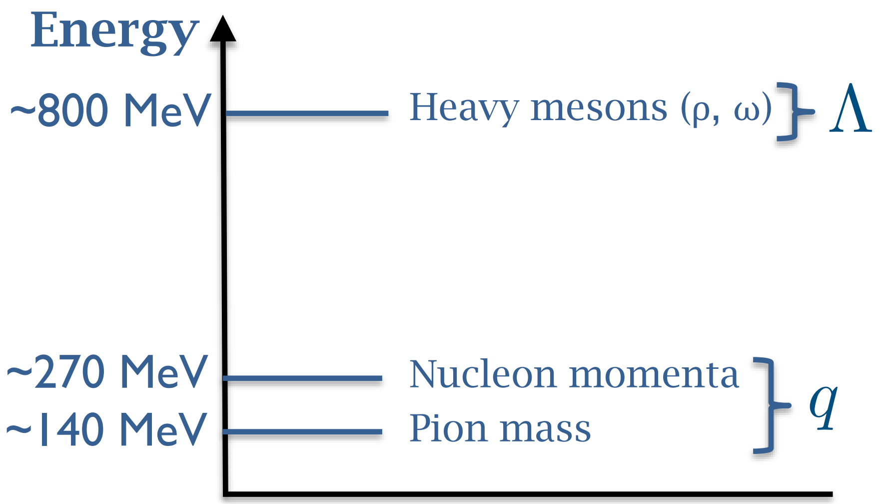


Steven Weinberg, 1979:
"one writes down the *most general possible Lagrangian*, including all terms consistent with *assumed symmetry principles…*"

1. Natural Separation of Scales



2. Goldstone bosons (pions) weakly-coupled at low momenta

$$\mathcal{L}^{(2)}_{\pi\pi} = \frac{1}{2}\partial_\mu\vec{\pi}\cdot\partial^\mu\vec{\pi} + \frac{1}{2f_\pi^2}(\partial_\mu\vec{\pi}\cdot\vec{\pi})^2$$

$$\mathcal{L}^{(1)}_{\pi N} = \bar{N}\left(i\gamma^\mu D_\mu - m - \frac{g_A}{2f_\pi}\gamma^\mu\gamma_5\vec{\tau}\cdot\partial_\mu\vec{\pi}\right)N$$

$$\mathcal{L}_{QCD} = -\frac{1}{4}G^a_{\mu\nu}G^{\mu\nu}_a + \bar{q}_L i\gamma_\mu D^\mu q_L + \bar{q}_R i\gamma_\mu D^\mu q_R - \bar{q}\mathcal{M}q$$

Quarks & gluons

Nucleons & pions

$$\mathcal{L}_{\text{eff}} = \mathcal{L}^{(2)}_{\pi\pi} + \mathcal{L}^{(1)}_{\pi N} + \mathcal{L}^{(2)}_{\pi N} + \mathcal{L}^{(0)}_{NN} + \mathcal{L}^{(2)}_{NN}$$

Constraints on Equation of State

- **Free energy** ($F(\rho, T, Y_p)$)
  + 1st and 2nd derivatives

- **Baryon Density**:

$$0 < n < 2 \text{ - } 3\, n_0$$

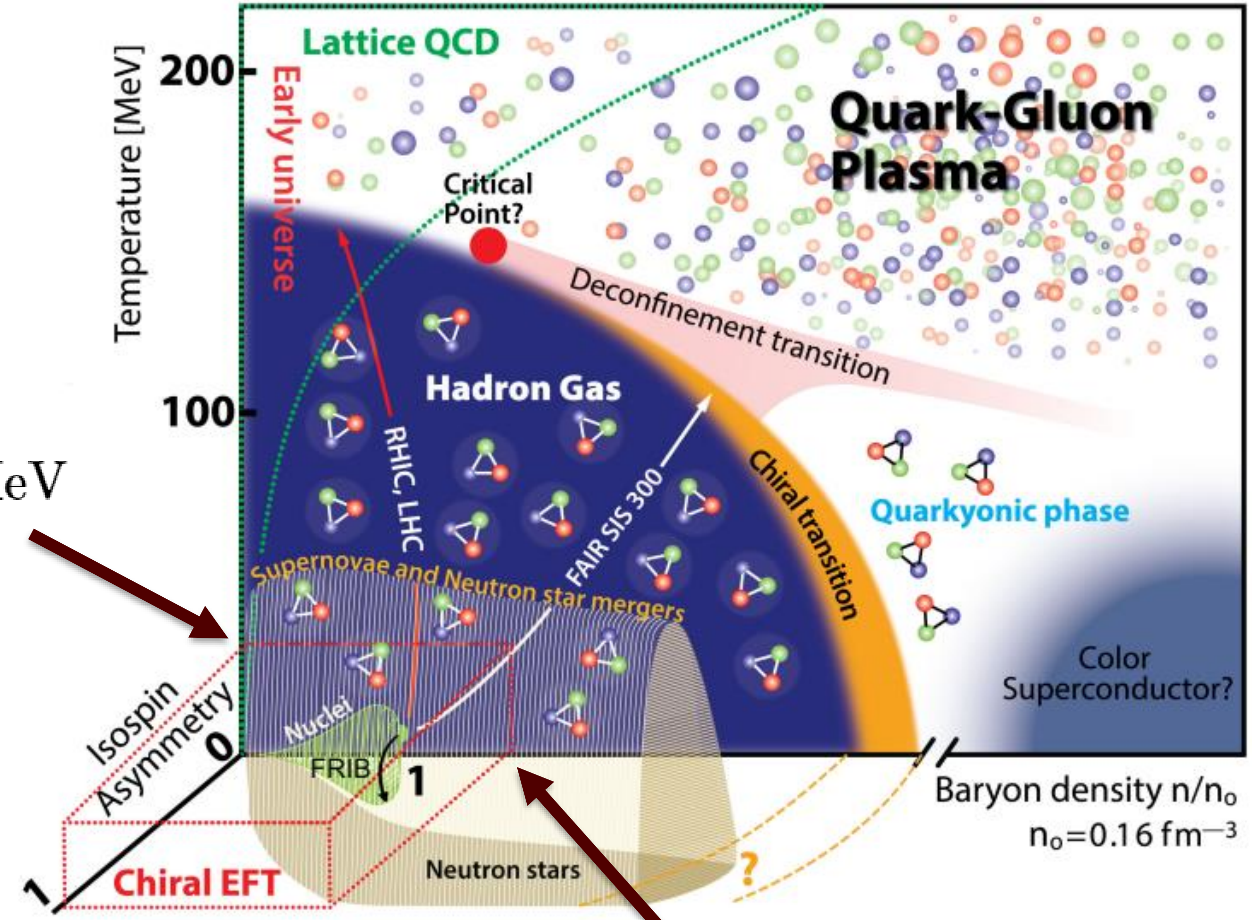
- **Temperature**:

$$0 < T < 30\,\text{MeV}$$

- **Proton fraction**:

$$0 < Y_p < 0.6$$

$\sim 30\,\text{MeV}$



$\sim 2 \text{ - } 3\, n_0$

Similar scales to **core-collapse supernovae** & **neutron star mergers** (e.g. GW170817)

$10^5 < \rho < 10^{15}\,\text{g/cm}^3$ $0 < T < 50\,\text{MeV}$

Microscopic Modeling: Many-Body Perturbation Theory

normal + **anomalous** contribution

- Finite-Temperature MBPT: **Matsubara formalism**

$$\Omega(\mu, T) = -P(\mu, T) = \Omega_0(\mu, T) + \lambda\Omega_1(\mu, T) + \lambda^2\Omega_2(\mu, T) + \mathcal{O}(\lambda^3).$$

- Expansion of Grand Can. Pot. in orders of **NN potential** (derived from Chiral EFT at **N^{3}LO**)

- **Kohn-Luttinger-Ward** method: Expand $\mu = \mu_0 + \lambda\,\mu_1 + \lambda^2\mu_2 + \mathcal{O}(\lambda^3)$

cancels anomalous term

$$\boxed{F(\mu_0, T) = F_0(\mu_0, T) + \lambda\Omega_1(\mu_0, T) + \lambda^2\left(\Omega_2(\mu_0, T) - \frac{1}{2}\frac{(\partial\Omega_1/\partial\mu_0)^2}{\partial^2\Omega_0/\partial\mu_0^2}\right) + \mathcal{O}(\lambda^3).}$$

- Expansion of **Free Energy** in order of **NN Potential** evaluated at **non-interacting chem. pot**.

Satisfies the $T \to 0$ limits

$$\rho(\mu_0, T) = -\frac{\partial\Omega_0}{\partial\mu_0}$$

Microscopic Modeling: Many-Body Perturbation Theory ($T > 0$)

- Kohn-Luttinger-Ward perturbation series for F in terms of the grand canonical potential Ω

normal + **anomalous** contribution

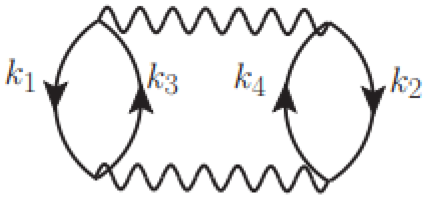
Cancels with anomalous term

$$F(\mu_0, T) = F_0(\mu_0, T) + \lambda \Omega_1(\mu_0, T) + \lambda^2 \left(\Omega_2(\mu_0, T) - \frac{1}{2} \frac{(\partial \Omega_1 / \partial \mu_0)^2}{\partial^2 \Omega_0 / \partial \mu_0^2} \right) + \mathcal{O}(\lambda^3).$$

Isospin symmetric

(a) (1,NN)

$$\Omega_{1,\mathrm{NN}}(\mu_0, T) = \frac{1}{2} \operatorname{tr}_{\sigma_1,\tau_1} \operatorname{tr}_{\sigma_2,\tau_2} \int \frac{\mathrm{d}^3 k_1}{(2\pi)^3} \int \frac{\mathrm{d}^3 k_2}{(2\pi)^3} \, n_{k_1} n_{k_2} \; \langle \mathbf{12} \, | (1 - P_{12}) V_{\mathrm{NN}} | \, \mathbf{12} \rangle$$



(c) (2,normal)

$$\Omega_{2,\mathrm{normal}}(\mu_0, T) = -\frac{1}{8} \left(\prod_{i=1}^{4} \operatorname{tr}_{\sigma_i,\tau_i} \int \frac{\mathrm{d}^3 k_i}{(2\pi)^3} \right) (2\pi)^3 \, \delta(\vec{k}_1 + \vec{k}_2 - \vec{k}_3 - \vec{k}_4)$$
$$\times \frac{n_{k_1} n_{k_2} \bar{n}_{k_3} \bar{n}_{k_4} - \bar{n}_{k_1} \bar{n}_{k_2} n_{k_3} n_{k_4}}{\varepsilon_3 + \varepsilon_4 - \varepsilon_1 - \varepsilon_2} \, |\langle \mathbf{12} \, | (1 - P_{12}) V_{\mathrm{NN}} | \, \mathbf{34} \rangle|^2$$

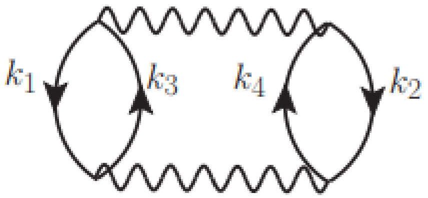
Chiral EFT Module

Module Goal

- Calculate the **First** and **Second** order contributions to the free energy at arbitrary density and temperature

(a) (1,NN)

$$\Omega_{1,\mathrm{NN}}(\mu_0,T)=\frac{1}{2}\,\mathrm{tr}_{\sigma_1,\tau_1}\,\mathrm{tr}_{\sigma_2,\tau_2}\int\frac{\mathrm{d}^3k_1}{(2\pi)^3}\int\frac{\mathrm{d}^3k_2}{(2\pi)^3}\;n_{k_1}n_{k_2}\;\langle\mathbf{12}\,|(1-P_{12})V_{\mathrm{NN}}|\,\mathbf{12}\rangle$$



(c) (2,normal)

$$\Omega_{2,\mathrm{normal}}(\mu_0,T)=-\frac{1}{8}\left(\prod_{i=1}^{4}\mathrm{tr}_{\sigma_i,\tau_i}\int\frac{\mathrm{d}^3k_i}{(2\pi)^3}\right)(2\pi)^3\,\delta(\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}_4)$$
$$\times\frac{n_{k_1}n_{k_2}\bar{n}_{k_3}\bar{n}_{k_4}-\bar{n}_{k_1}\bar{n}_{k_2}n_{k_3}n_{k_4}}{\varepsilon_3+\varepsilon_4-\varepsilon_1-\varepsilon_2}\;|\langle\mathbf{12}\,|(1-P_{12})V_{\mathrm{NN}}|\,\mathbf{34}\rangle|^2$$

Fermi-Dirac dist. n_{k_1}

NN potential matrix V_{NN}

Isospin symmetric

Computational Methods

Partial-Wave expansion of Nuclear potential

Obtained from **Chiral EFT** potential matrix table (**N³LO**)

$$\tilde{V}_{\mathrm{NN}}^{J,\ell,\ell',S,\mathcal{T}}$$

Lagrange Poly. Interpolation

$$L(x) = \sum_{j=0}^{k} y_j \ell_j(x).$$

Arbitrary **single-particle energy** spectrum

Self-Energy

$$\varepsilon(k;\rho,T) = \frac{k^2}{2M} + \Sigma(k;\rho,T)$$

Gauss-Legendre Quadrature

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

First-Order Normal contribution (HF)

Two momentum integrations, **One** angular integration

$$\Omega_{1,\mathrm{NN}}(\mu_0,T)$$

Second-Order Normal contribution

Three momentum integrations, **Two** angular integrations

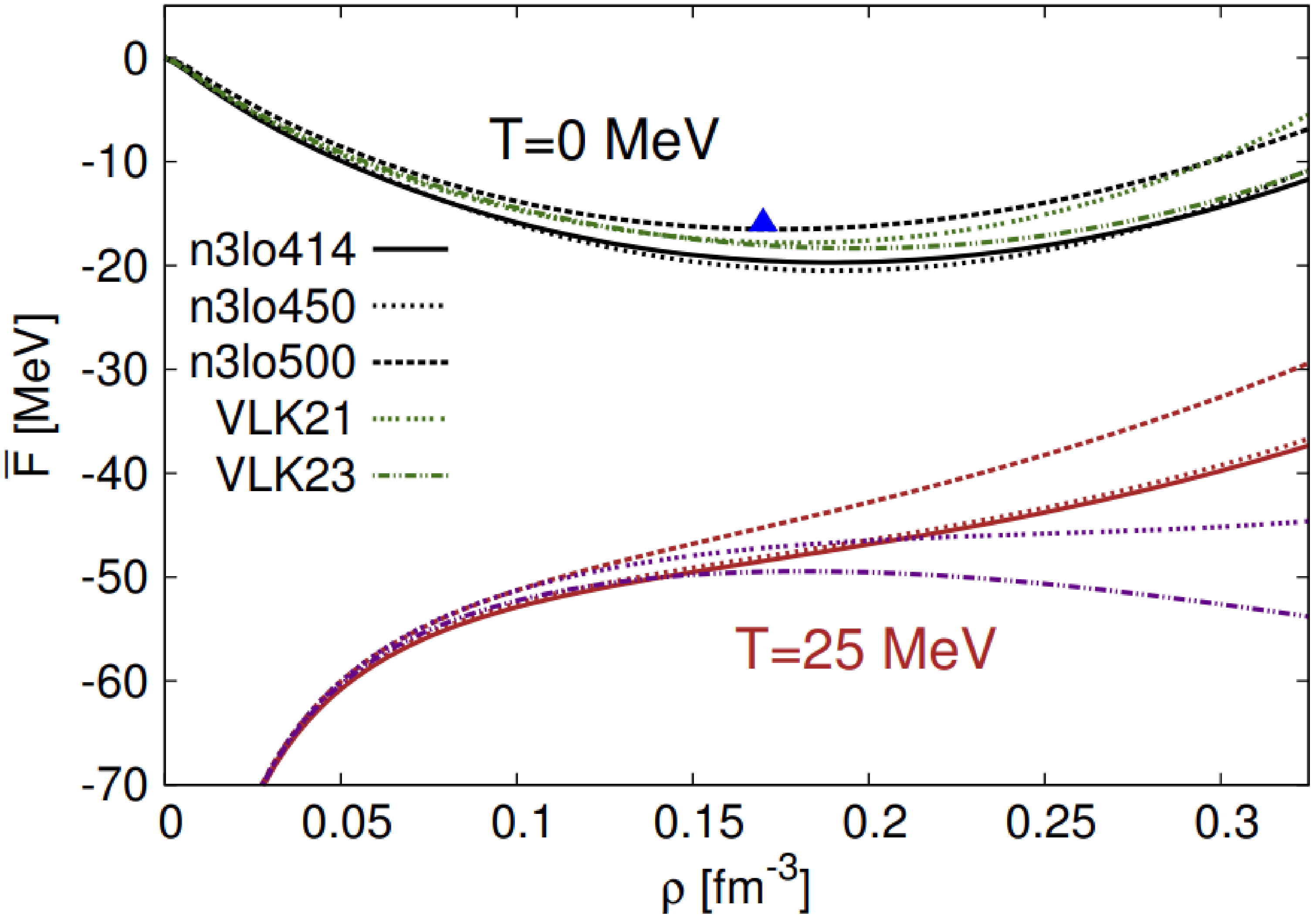
$$\Omega_{2,\mathrm{normal}}(\mu_0,T)$$

VEGAS Adaptive Monte Carlo

Importance sampling

Complicated integration region

Computational Methods



Lagrange Poly. Interpolation

$$L(x) = \sum_{j=0}^{k} y_j \ell_j(x).$$

Gauss-Legendre Quadrature

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

VEGAS Adaptive Monte Carlo

Importance sampling

Complicated integration region

Module Summary

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Environment Inputs

- Density ρ
- Temperature T
- Proton fraction Y_p

Interaction Inputs

- NN partial wave matrix elements $\tilde{V}_{\mathrm{NN}}^{J,\ell_1,\ell_2,S,T}$
- Nucleon Self-Energy correction $\Sigma(k;\rho,T)$

(Standardized table format)

1st-order code (Gauss-Legendre quadrature)

- Chemical potentials μ_p , μ_n obtained iteratively
- Grand canonical potential: $\Omega^{(1)}(\mu_p^0,\mu_n^0,T)$
- Free energy: $F^{(1)}(\mu_p^0,\mu_n^0,T)=F^{(0)}(\mu_p^0,\mu_n^0,T)+\Omega^{(1)}(\mu_p^0,\mu_n^0,T)$

2nd-order code (VEGAS Monte Carlo)

- Same chemical potentials μ_p μ_n
- Grand canonical potential: $\Omega^{(2)}(\mu_p^0,\,\mu_n^0,\,T)$
- Free energy: $F^{(1)}(\mu_p^0,\mu_n^0,T)=F^{(0)}(\mu_p^0,\mu_n^0,T)+\Omega^{(1)}(\mu_p^0,\mu_n^0,T)+\Omega^{(2)}(\mu_p^0,\,\mu_n^0,\,T)$

Interface with MUSES cyberinfrastructure: Docker container, Calculation Engine, etc.

Module Summary

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Current Progress

- Rewritten legacy Fortran code in modern C++
- Python **yaml adaptors** to support interfacing with Cyberinfrastructure
- Parallelization using C++ standard library (**ctpl stl**)
- Produces fast, accurate results at **First Order**

Necessary Improvements

- Refactor code organization (better workflow structure)
- Update **integration** and **interpolation** codes
- Improve parallelization technique
- Speed improvements at **Second Order**
- Containerize with Docker and interface with Calculation Engine

Next Steps

Isospin Asymmetry

- Extend QCD phase space into third dimension

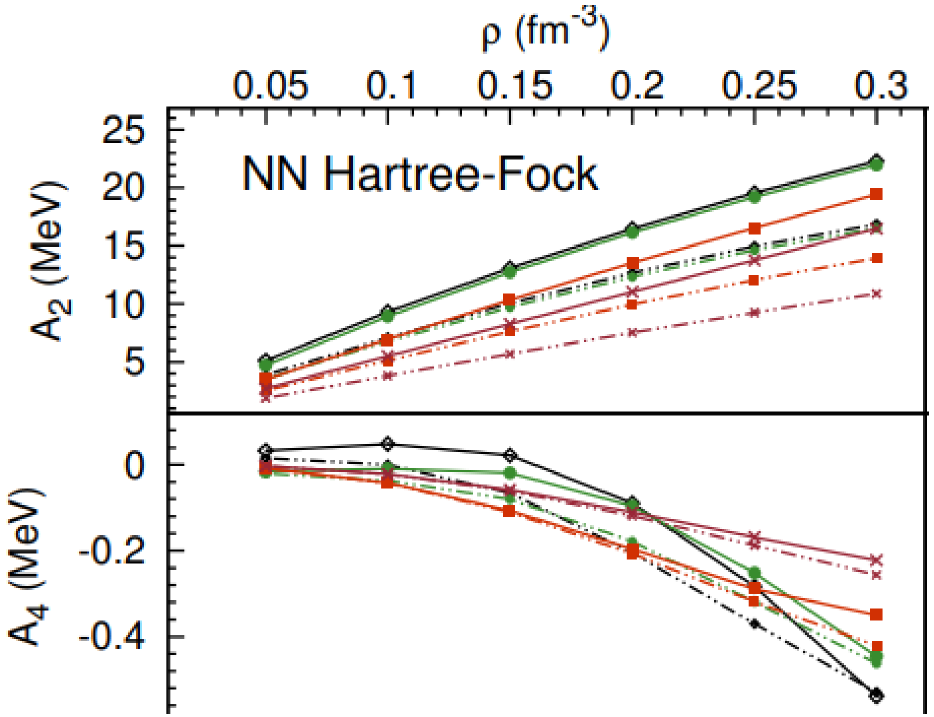
$$\delta = \frac{\rho_n - \rho_p}{\rho_n + \rho_p} = 1 - 2Y_p$$

- **Symmetry Free Energy Approach** (quadratic interpolation):

$$\overline{F}(T,\rho,\delta) = \overline{F}(T,\rho,\delta=0) + \overline{F}_{\rm sym}(T,\rho)\,\delta^2$$

PNM

SNM - PNM



- **Direct Approach** (when computationally feasible):

Sum over all isospin configurations of NN Potential

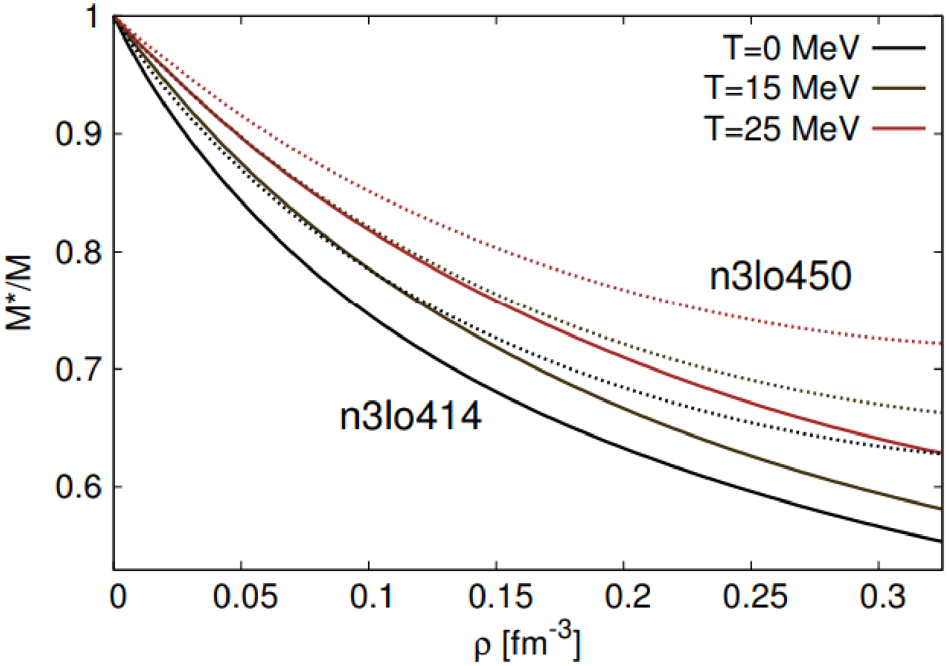
Nucleon Self-Energy Corrections

- MBPT **Self-Energy** contribution appears in n_k and explicitly at second order

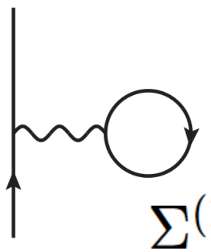
$$\varepsilon(k;\rho,T) = \frac{k^2}{2M} + \Sigma(k;\rho,T) \simeq \frac{k^2}{2M^*(\rho,T)} + U_0(\rho,T),$$

Effective mass approximation

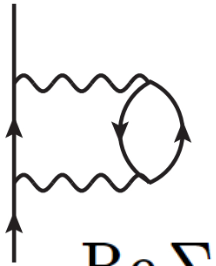
$$\frac{M^*(\rho,T)}{M} \leq 1$$



- Effective mass controls **density of states** and therefore aspects of thermal excitations
- **Equation of state**, optical potentials, scattering cross-sections



$\Sigma^{(1)}(k)$



$\mathrm{Re}\,\Sigma^{(2)}(k,\omega)$

Summary

- **Chiral EFT** allows for **Equation of State** calculations at **low temperatures near nuclear saturation density**, with clear quantification of uncertainties

- The **Chiral EFT Module for MUSES** can now calculate the Equation of State in region of phase space up to **second-order in perturbation theory**

- The module can be extended to include **isospin asymmetry** and **self-energy corrections** up to second-order

Thank You!

References

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