Neutron Matter from non–local Chiral forces and Quantum Monte Carlo

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INT - 31 Jul, 2014 The r-process: status and challanges

- Quantum Monte Carlo methods
- Low–density Pure Neutron matter with χ -EFT
 - Equation of State
 - Nucleon chemical potential (self-energies)
- Impurities in neutron-matter and constraints for DFT functionals

Collaborators:

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- Lorenzo Contessi UNITN
- Abhishek Mukherjee ECT*

Central objects are random walks :

$$X^{k+1} = T[X^k] \quad \xrightarrow{\text{choose basis}} \quad X_j^{k+1} = \sum_i T_{ji} X_i^k$$

Under general conditions the asymptotic distribution depends on $\ensuremath{\mathcal{T}}$ in a predictable way

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To sample ground–state $|\Phi_0\rangle$ of Schroedinger equation you can use the propagator in imaginary–time $(it \rightarrow \tau)$

$$e^{- au\hat{H}}|\Psi_k
angle = |\Psi_{k+1}
angle \quad \lim_{n o\infty} e^{-n au\hat{H}}|\Psi_{in}
angle \propto |\Phi_0
angle$$

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Figure: S. Pieper, R. Wiringa et. al (ANL)

Monte Carlo in Slater-Determinant space

Our basis are A-body slater determinants constructed from a single particle space $S \longrightarrow$ we can use χ -EFT in this basis!!



• single-particle space $S = \{ \text{ plane waves } | k^2 <= k_{max}^2 \} \otimes \{S, I\}$

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• single-particle space $S = \{ \text{ plane waves } | k^2 <= k_{max}^2 \} \otimes \{S, I\}$ Coulomb gas \longrightarrow good agreement with R-space QMC calculations [A. R., A. Mukherjee and F. Pederiva, Phys. Rev. B 88,115138 (2013)]

Neutron Matter with χ -EFT interactions



Neutron Matter with χ -EFT interactions

Nucleon chemical potential (\sim self-energy at zero momentum)



[A. R., A. Mukherjee and F. Pederiva, PRL 112, 221103 (2014)]

Constrining Nuclear Energy Density Functionals

Energy density functional for uniform matter:

$$\mathcal{E} = \mathcal{E}_{\mathrm{kin}} + \sum_{t=0,1} \left(C_t^{\rho} \rho_t^2 + C_t^{\tau} \rho_t \tau_t + C_t^{s} s_t^2 + C_t^{\tau} s_t T_t \right).$$

contributions from both time-even and time-odd components.

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Idea: [M. M. Forbes et al. PRC 89, 041301(R) (2014)]

Calculate binding energy of an impurity in polarized neutron matter

$$\varepsilon_{\tau\sigma} = \left. \frac{\partial \mathcal{E}}{\partial \rho_{\tau\sigma}} \right|_{\rho_{\tau\sigma} \to 0} \quad \to \quad \text{eg} \quad \varepsilon_{n\downarrow} \propto (C_0^s + C_1^s), (C_0^T + C_1^T)$$

The neutron impurity [arXiv:1406.1631]



• Green pts from: M. M. Forbes et al. PRC 89, 041301(R) (2014)

The proton impurities I [arXiv:1406.1631]



The proton impurities II [arXiv:1406.1631]





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- we have developed a MC method that works for general interactions (non-local too!) providing rigourus upper-bounds on energy
- low density neutron-matter from many-body calculations and realistic forces to constrain Mean-Field theories
- proton impurities in polarized neutron matter as tight constraint on time-odd part of nuclear EDF

Goals and needs for the future:

- extend to three-body forces (coming soon) and finite nuclei
- symmetric matter (also soon)
- estimate uncertaintes coming from interaction (soon)
- Finite-temperature? (not so soon with χ -EFT)

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Neutron Matter with χ -EFT interactions



[A. R., A. Mukherjee and F. Pederiva, PRL 112, 221103 (2014)]