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

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Three-Body Forces: From Matter to Nuclei

Outline & Acknowledgements

- Monte Carlo in Configuration Interaction space
- Low–density Pure Neutron matter with χ-EFT at NNLO
  - Equation Of State
  - Momentum Distributions
  - Nucleon chemical potential
- Impurities in neutron–matter and constraints for DFT functionals

Collaborators:

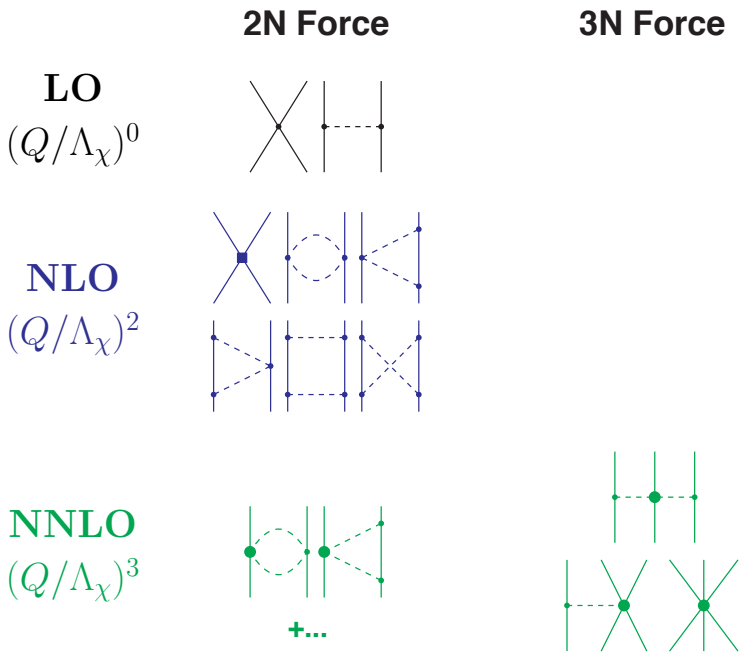
- Francesco Pederiva - UNITN
- Lorenzo Contessi - UNITN
- Abhishek Mukherjee - ECT*

Chiral Effective Field Theory (χ-EFT) interactions

- pions interact weakly at small energies (Goldstone bosons)

low-scales Q, m_π high-scales m_ρ,$\Lambda_\chi = m_\Delta - m_N$

- expand the interaction in powers of Q/Λ_χ, m_π/Λ_χ



- short range contact–interaction + pions
- many–body forces treated in a systematic way

R. Machleidt, D. R. Entem,
Phys.Rept 503,1 (2011)

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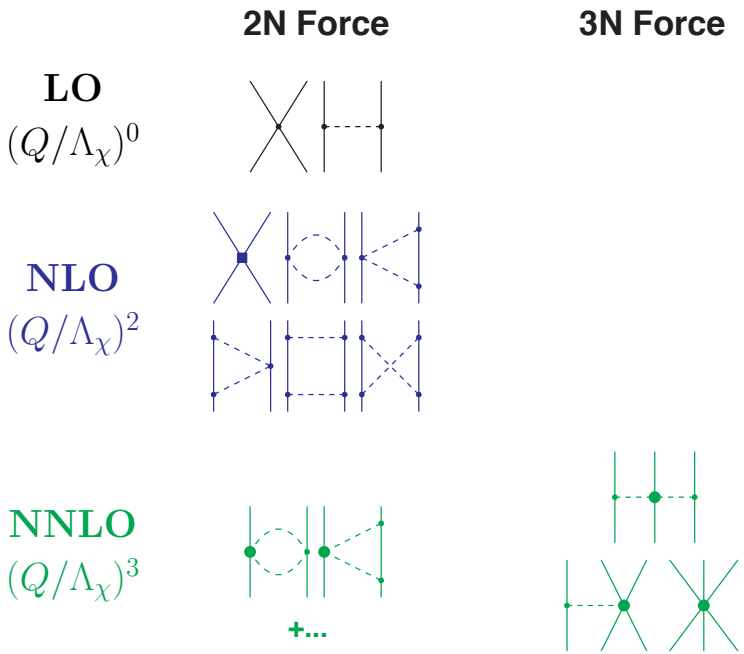

- short range contact–interaction + pions
- many–body forces treated in a systematic way
- non–local in coordinate–space ($\geq$NLO)

$$V(x,y) \neq V(x)\delta(x-y)$$

Locality is needed for conventional QMC

Gezerlis et al., PRL 111, 032501 (2013)

R. Machleidt, D. R. Entem, Phys.Rept 503,1 (2011)

Monte Carlo methods

Use a projection operator to filter the ground–state

$$P[\hat{H}]|\Psi_n\rangle = |\Psi_{n+1}\rangle \quad | \quad \lim_{n\to\infty} P[\hat{H}]^n|\Phi_T\rangle = |0\rangle$$

$$\text{eg.} \quad P_a[\hat{H}] = 1 - \Delta\tau\hat{H} \quad \text{or} \quad P_b[\hat{H}] = e^{-\Delta\tau\hat{H}}$$

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The Standard Way

- work in coordinate–space
- for local interactions the projector factors in

$$\langle Y|e^{-\Delta\tau\hat{H}}|X\rangle = \langle Y|e^{-\Delta\tau\hat{T}}|X\rangle e^{-\Delta\tau V(X)} + O(\Delta\tau^2)$$

$$\approx G_0(Y,X)B(X)$$

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The Standard Way

- work in coordinate–space
- for non–local interactions the projector doesn't factor

$$\langle Y|e^{-\Delta\tau\hat{H}}|X\rangle = \int dZ\langle Y|e^{-\Delta\tau\hat{T}}|Z\rangle\langle Z|e^{-\Delta\tau\hat{V}}|X\rangle + O(\Delta\tau^2)$$

$$\approx \int dZ G_0(Y,Z)G_V(Z,X)$$

Monte Carlo in Configuration Interaction space

Idea: in a finite basis non–locality is not an issue anymore

work in occupation number basis: $|\mathbf{n}\rangle = |\ldots 01100010\ldots\rangle$

We now need a projector $\hat{P}$ in this space such that

$$\langle \mathbf{m}|\hat{P}^M|\mathbf{n}\rangle\langle \mathbf{n}|\Phi\rangle \xrightarrow{M\to\infty} \langle \mathbf{m}|\Psi_0\rangle$$

- example: $\langle \mathbf{m}|\hat{P}|\mathbf{n}\rangle = \Lambda\delta_{\mathbf{m},\mathbf{n}} - \Delta\langle \mathbf{m}|\hat{H}|\mathbf{n}\rangle$ with $\Delta \ll 1$

Problem:

for the probability interpretation to hold we need $\langle \mathbf{m}|\hat{P}|\mathbf{n}\rangle \geq 0$ but that's not true in general $\longrightarrow$ sign problem

Dealing with the sign problem I

- cancellation methods [FCIQMC (Alavi et al.),SQMC(Umrigar et al.)]
  - exponential computational cost with growing system-size BUT with much smaller exponent than full diagonalization
- fixed–node methods
  [van Bemmel et.al PRL 72 2442, Mukerjee et al. PRA 88 053622]

$$\langle \mathbf{m}|\hat{P}|\mathbf{n}\rangle \;\rightarrow\; \langle \mathbf{m}|\hat{P}|\mathbf{n}\rangle_{FN} = \Psi_T(\mathbf{m})\langle \mathbf{m}|\hat{P}|\mathbf{n}\rangle\Psi_T^{-1}(\mathbf{n})$$

  - biased, BUT gets better by improving the trial wave–function (complementar to coordinate space FN)
  - polynomial growth of computational cost

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Coupled–Cluster ansatz: [A.R. et al. PRB 88,115138]

$$|\Psi_T\rangle = e^{-\hat{T}}|\Phi_{ref}\rangle \quad \text{with} \quad \hat{T} = \hat{T}_1 + \hat{T}_2 + \dots$$

Here we will restrict to CCD case: $\hat{T} = \hat{T}_2 = \frac{1}{2}\sum_{ij,ab} t_{ij}^{ab}\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i.$

Dealing with the sign problem II

Solving CC equations can be costly, can we avoid that?

	E-E$_{HF}$ [a.u.]
ccd	-0.58303(6)
pt2	-0.5829(5)
quad pt2	-0.582(2)
dble pt2	-0.576(2)

Table: 3DHEG at $r_s = 1$

$$|\Psi_T\rangle = e^{-\frac{1}{2}\sum_{ij,ab} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i} |\Phi_{HF}\rangle$$
$$= \left(1 - \hat{T}_2 + \frac{1}{2}\hat{T}_2^2 + \dots\right) |\Phi_{HF}\rangle$$

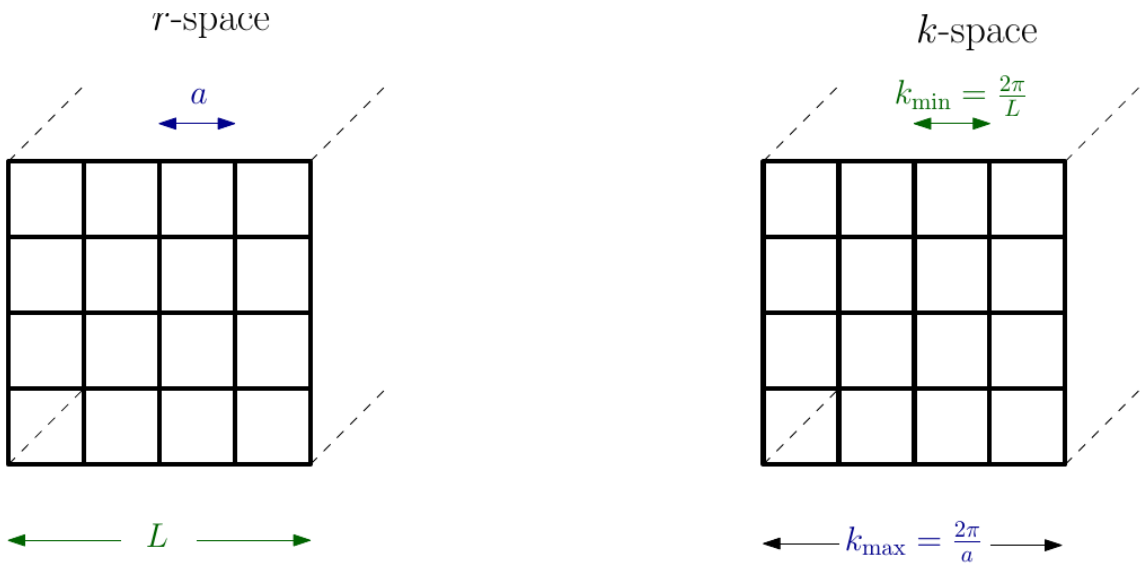
Coefficients t_{ij}^{ab} obtained from

- solution of CCD equations [ccd]
- perturbation–theory [pt2]

Truncating expansion at

- quadruple excitations [quad pt2]
- double excitations [dble pt2]

Single–particle basis for bulk systems



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

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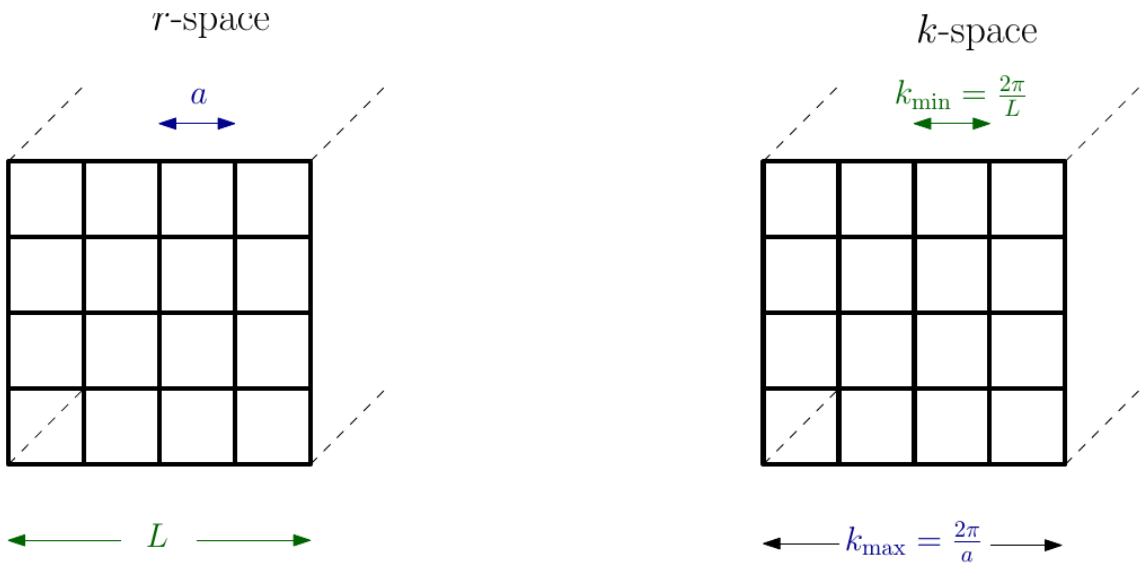

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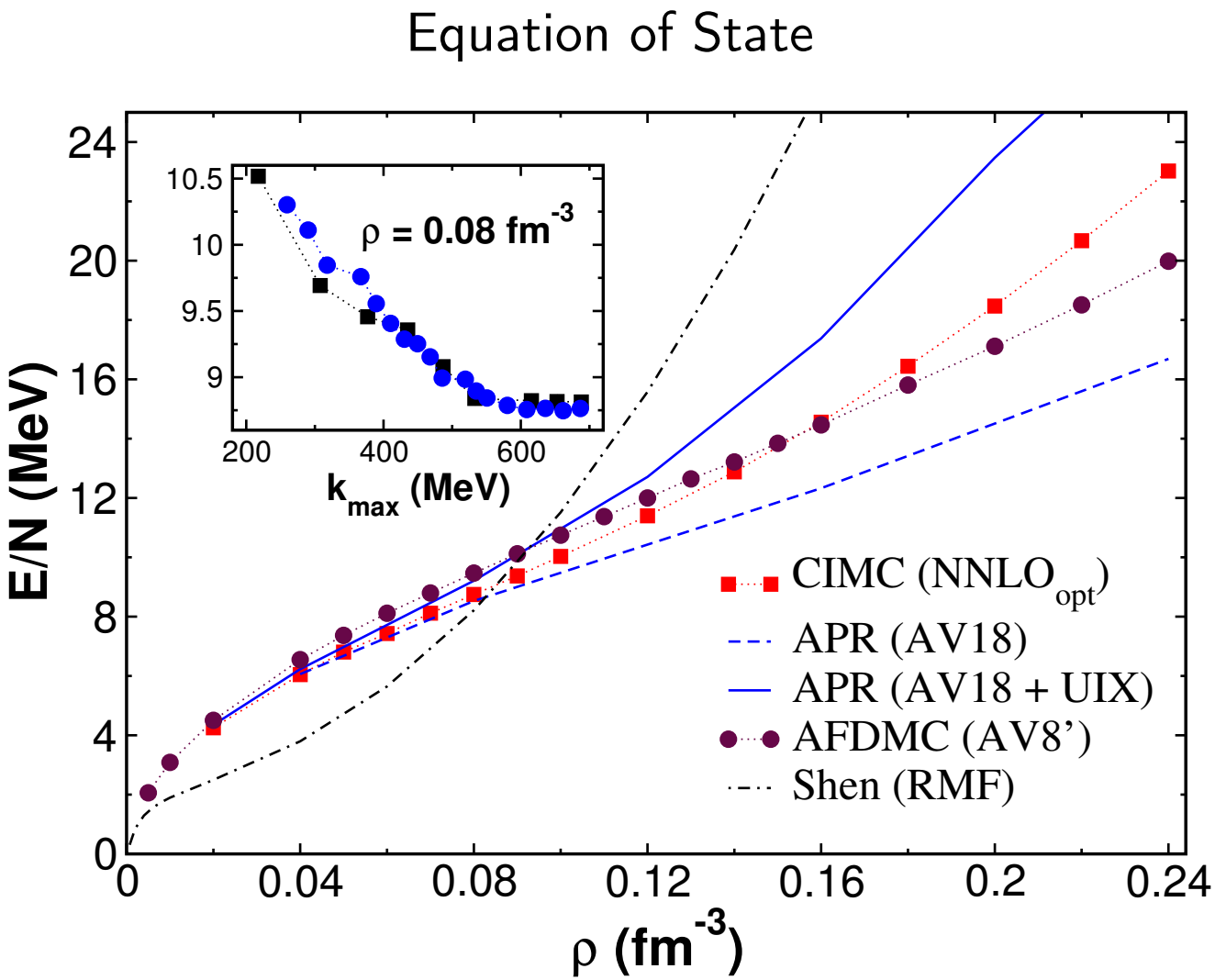
Coulomb gas $\longrightarrow$ good agreement with R–space QMC calculations

[A. R., A. Mukherjee and F. Pederiva, Phys. Rev. B 88,115138 (2013)]

Neutron Matter with χ-EFT interactions at N2LO



[A. R., A. Mukherjee and F. Pederiva, arXiv:1402.1576 (2014)]

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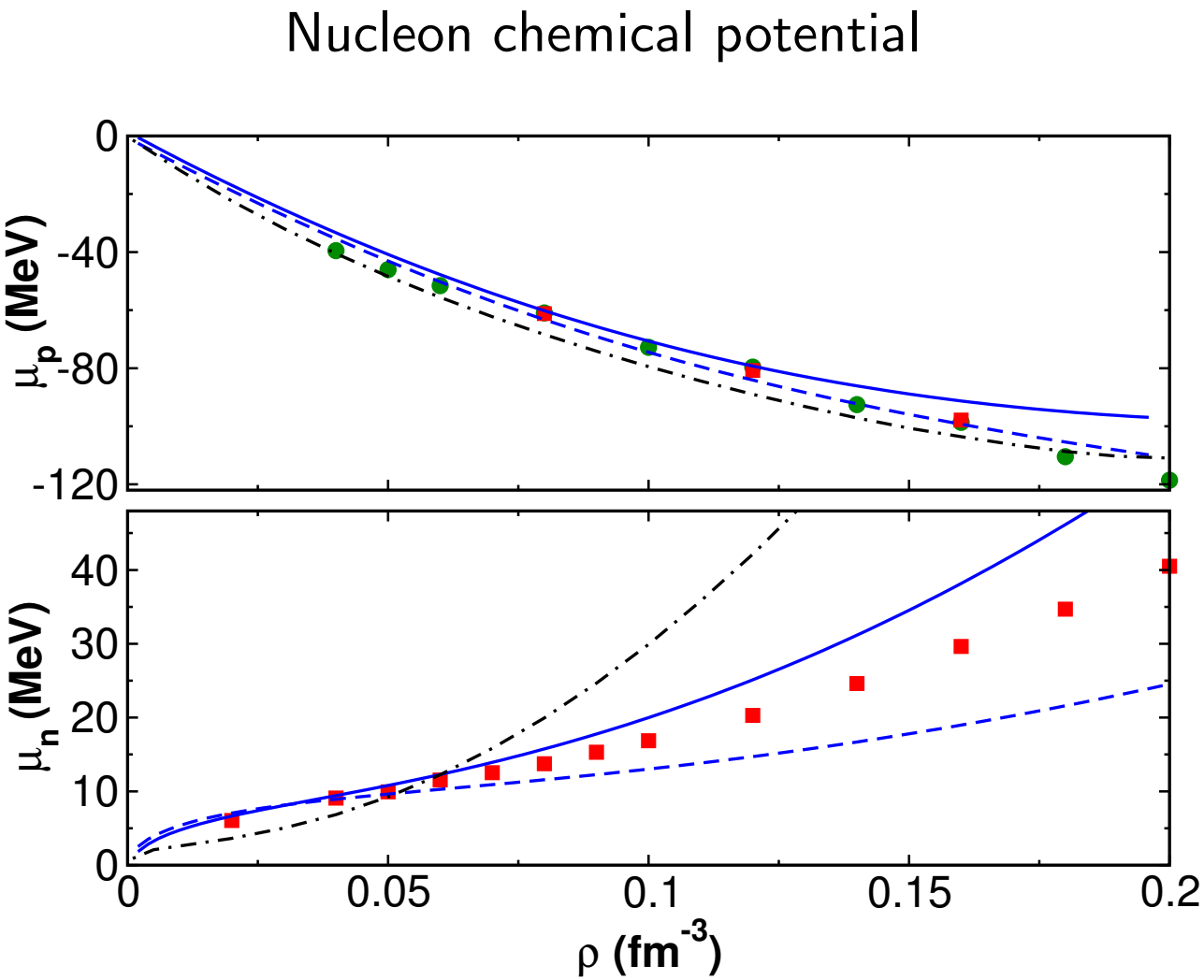

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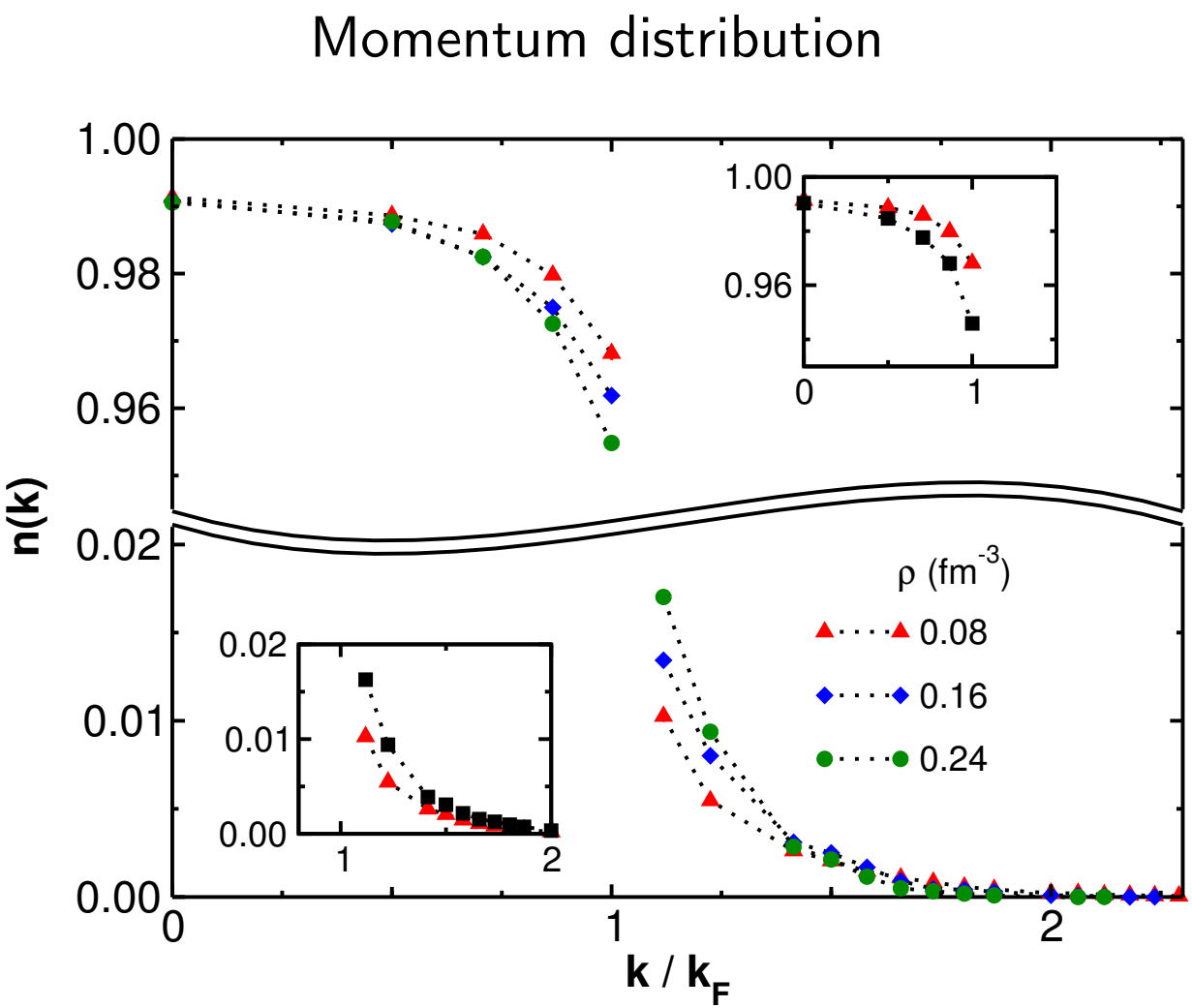

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Constrining Nuclear Energy Density Functionals

Energy density functional for uniform matter:

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

- contributions from both time–even and time–odd components.
- time–even part constrained eg. by even–even nuclei
- no effective way to constrain time–odd part

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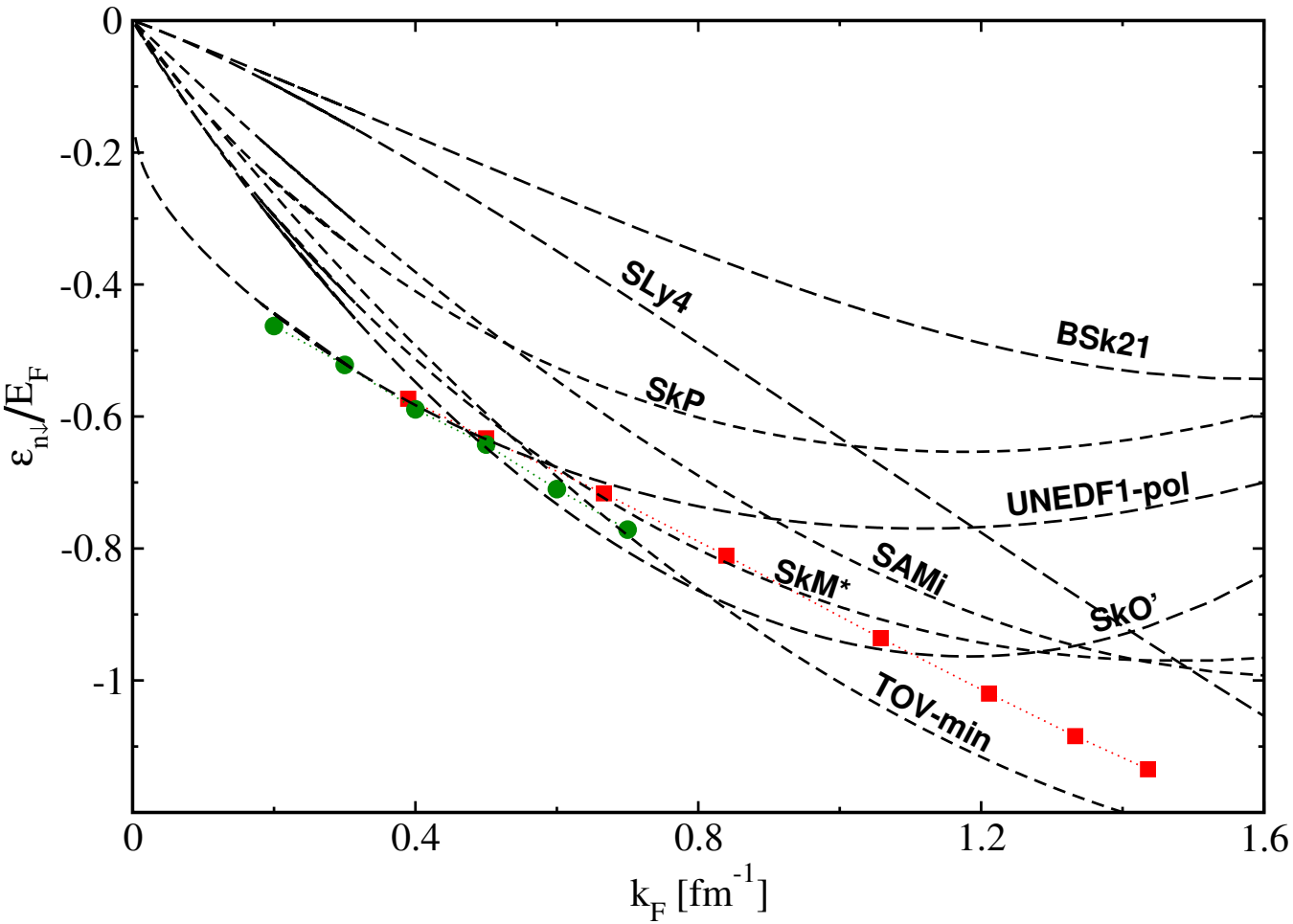
Idea: [M. M. Forbes et al. PRC 89, 041301(R) (2014)]

Calculate binding energy of an impurity in polarized neutron matter

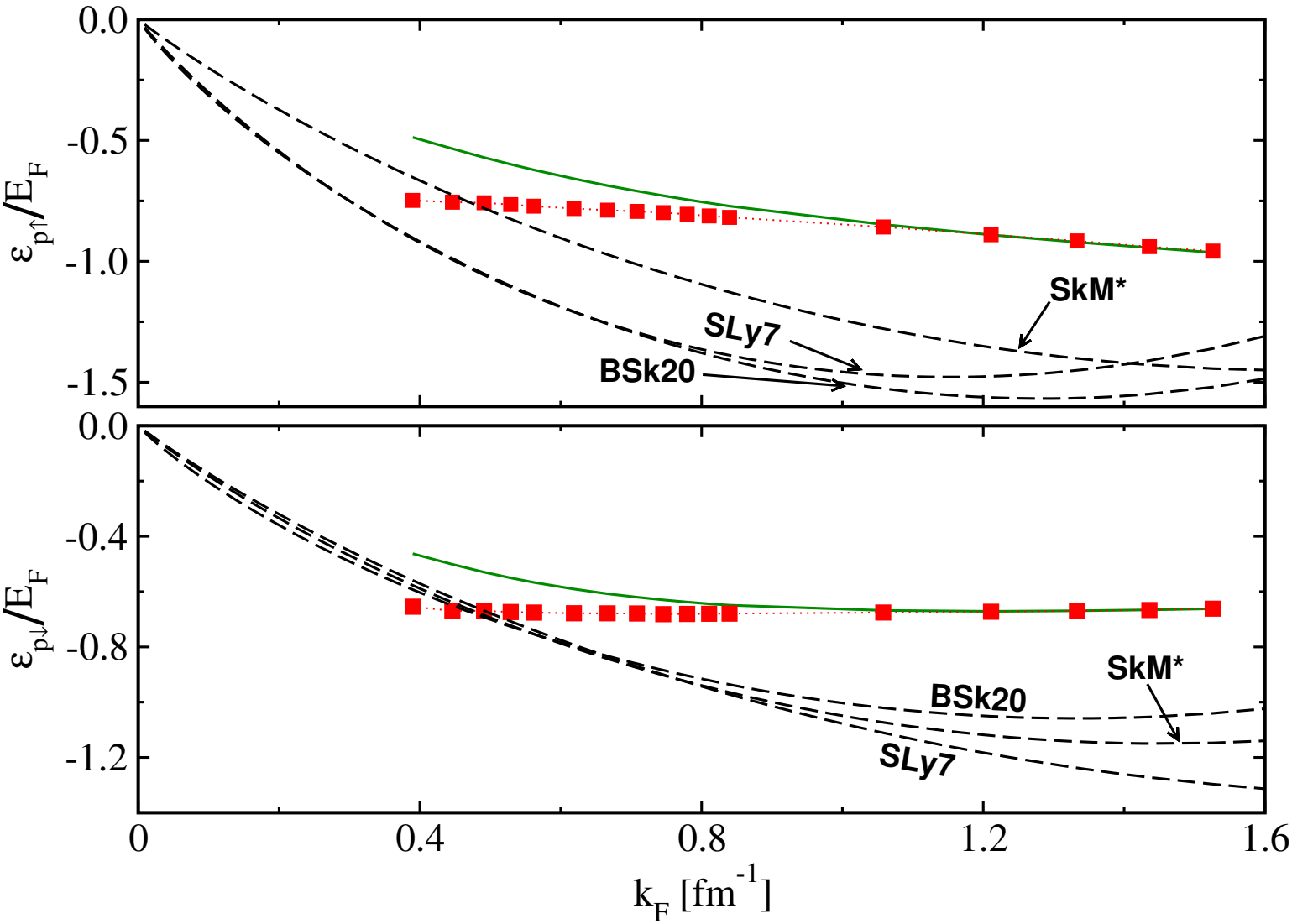
$$\varepsilon_{\tau\sigma} = \left. \frac{\partial \mathcal{E}}{\partial \rho_{\tau\sigma}} \right|_{\rho_{\tau\sigma} \to 0} \quad \to \quad \text{eg} \quad \varepsilon_{n\downarrow} \propto (C_0^s + C_1^s), (C_0^T + C_1^T)$$

The neutron impurity



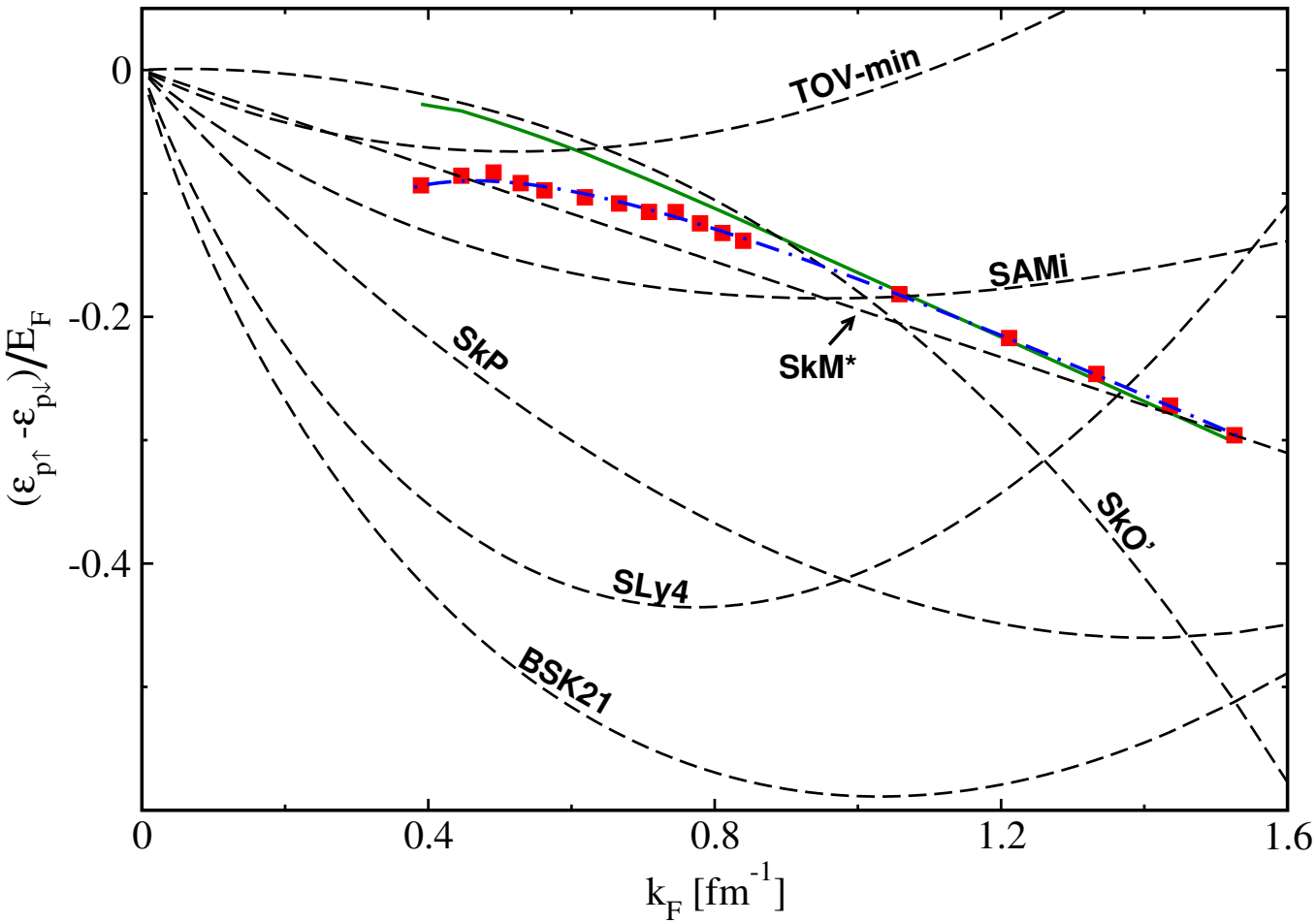
- Green pts from: M. M. Forbes et al. PRC 89, 041301(R) (2014)

The proton impurities I



The proton impurities II

$$\frac{\varepsilon_{p\uparrow} - \varepsilon_{p\downarrow}}{E_F} = \frac{4m(C_0^s - C_1^s)}{3\pi^2\hbar^2} k_F - \frac{2m(C_0^T - C_1^T)}{5\pi^2\hbar^2} k_F^3.$$



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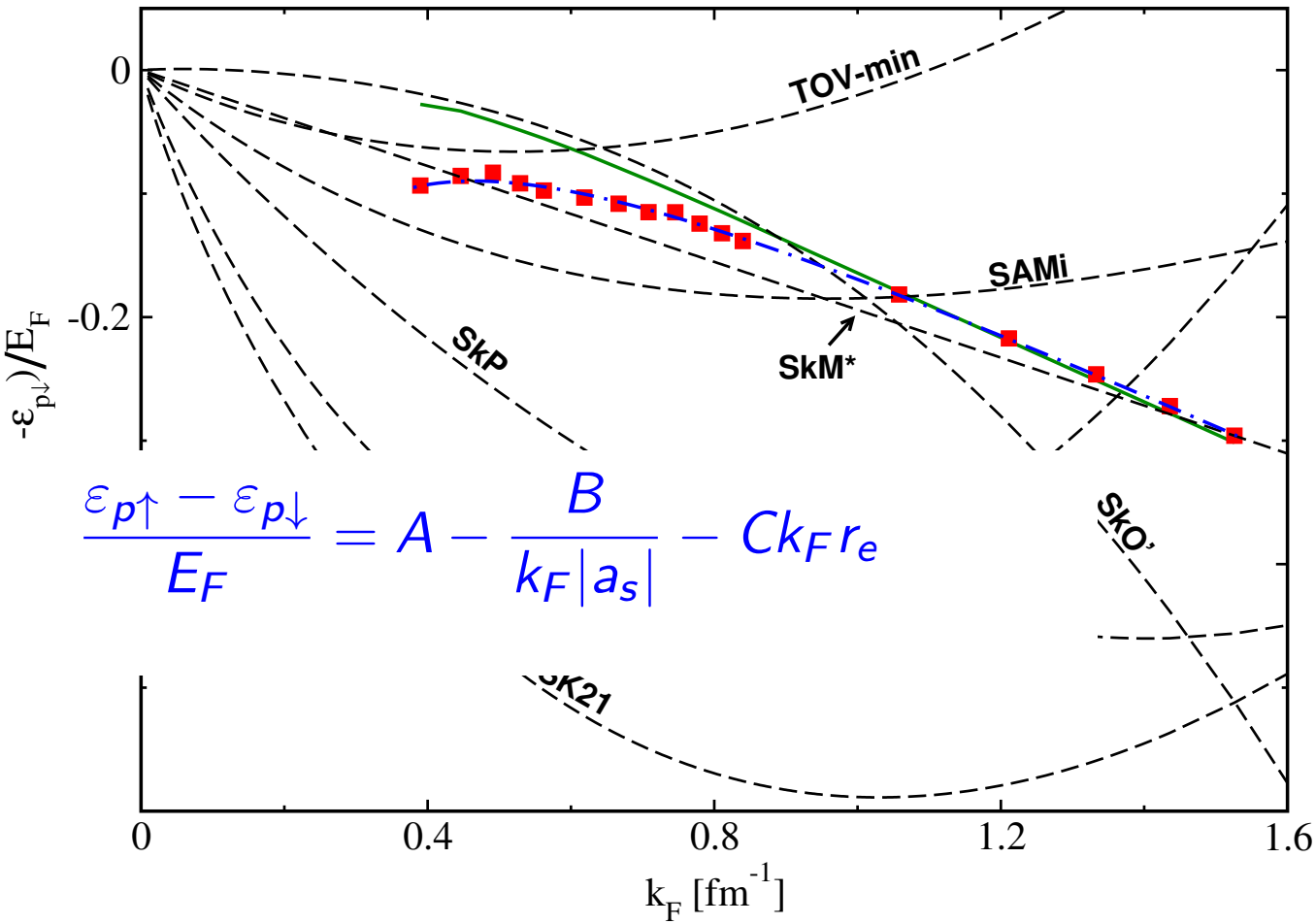

$$\frac{\varepsilon_{p\uparrow} - \varepsilon_{p\downarrow}}{E_F} = A - \frac{B}{k_F|a_s|} - Ck_F r_e$$

Conclusions

Summary:

- we have developed a MC method that works for general interactions providing rigourus upper–bounds on energy
- the use of CC type Wave–functions serves a dual pourpose:
  - extremely good guiding wave–function
  - provides expectation values for CC solutions (variational energies)
- robustness of algorithm allow to use approximations to the solution of CC equations (easy to get to triples etc.)
- 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 and finite nuclei
- estimate uncertaintes coming from interaction (public matrix elements can help here too)
- SRG with Quantum Monte Carlo?
- Finite-temperature? (maybe with CC–ansatz)