Quantum Monte Carlo with chiral Effective Field Theory Interactions (and at lower density)

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Advances in quantum Monte Carlo techniques for non-relativistic many-body systems

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Nuclear many-body problem

Need to solve:

$$\mathcal{H}\Psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_A; s_1, s_2, \cdots, s_A; t_1, t_2, \cdots, t_A) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_A; s_1, s_2, \cdots, s_A; t_1, t_2, \cdots, t_A)$$

where

$$H = -\frac{\hbar^2}{2m} \sum_{j=1,N} \nabla_j^2 + \sum_{j<k} v_{jk} + \sum_{j<k<l} V_{jkl}$$

s_i spin of *i*-th nucleon ($\pm\frac{1}{2}$)

t_i isospin of *i*-th nucleon ($\pm\frac{1}{2}$)

Quantum Monte Carlo:

$$\Psi(\tau \rightarrow \infty) = \lim_{\tau \rightarrow \infty} e^{-(\mathcal{H}-E_T)\tau} \Psi_V$$

$$\rightarrow \alpha_0 e^{-(E_0 - E_T)\tau} \Psi_0$$

Continuum Quantum Monte Carlo

Rudiments of Diffusion Monte Carlo:

Start somewhere and evolve

$$\psi(\mathbf{R},\tau) = \int G(\mathbf{R},\mathbf{R}',\tau)\psi(\mathbf{R}',0)d\mathbf{R}'$$

With a standard propagator

$$G(\mathbf{R},\mathbf{R}',\tau) = \langle \mathbf{R}|e^{-(H-E_0)\tau}|\mathbf{R}'\rangle$$

Cut up into many time slices

$$G(\mathbf{R},\mathbf{R}',\Delta\tau) \approx e^{-\frac{V(\mathbf{R})+V(\mathbf{R}')}{2}\Delta\tau} \left(\frac{m}{2\pi\hbar^2\tau}\right)^{\frac{3A}{2}} e^{-\frac{m|\mathbf{R}-\mathbf{R}'|^2}{2\hbar^2\tau}}$$

You probably also want to do importance sampling

$$\tilde{G}(\mathbf{R},\mathbf{R}',\Delta\tau) = \frac{\psi_I(\mathbf{R}')}{\psi_I(\mathbf{R})} G(\mathbf{R},\mathbf{R}',\Delta\tau)$$

Nuclear Hamiltonian

Easier said than done. Complicated Hamiltonian:

$$H = -\frac{\hbar^2}{2m}\sum_{j=1,N}\nabla_j^2 + \sum_{j<k} v_{jk} + \sum_{j<k<l} V_{jkl}$$

Phenomenological approach:

High-precision fits to NN scattering (Argonne)

$$V_2 = \sum_{j<k} v_{jk} = \sum_{j<k}\sum_{p=1}^{8} v_p(r_{jk}) O^{(p)}(j,k)$$

$$O^{p=1,8}(j,k) = (1, \sigma_j \cdot \sigma_k, S_{jk}, \mathbf{L}_{jk} \cdot \mathbf{S}_{jk}) \otimes (1, \tau_j \cdot \tau_k)$$

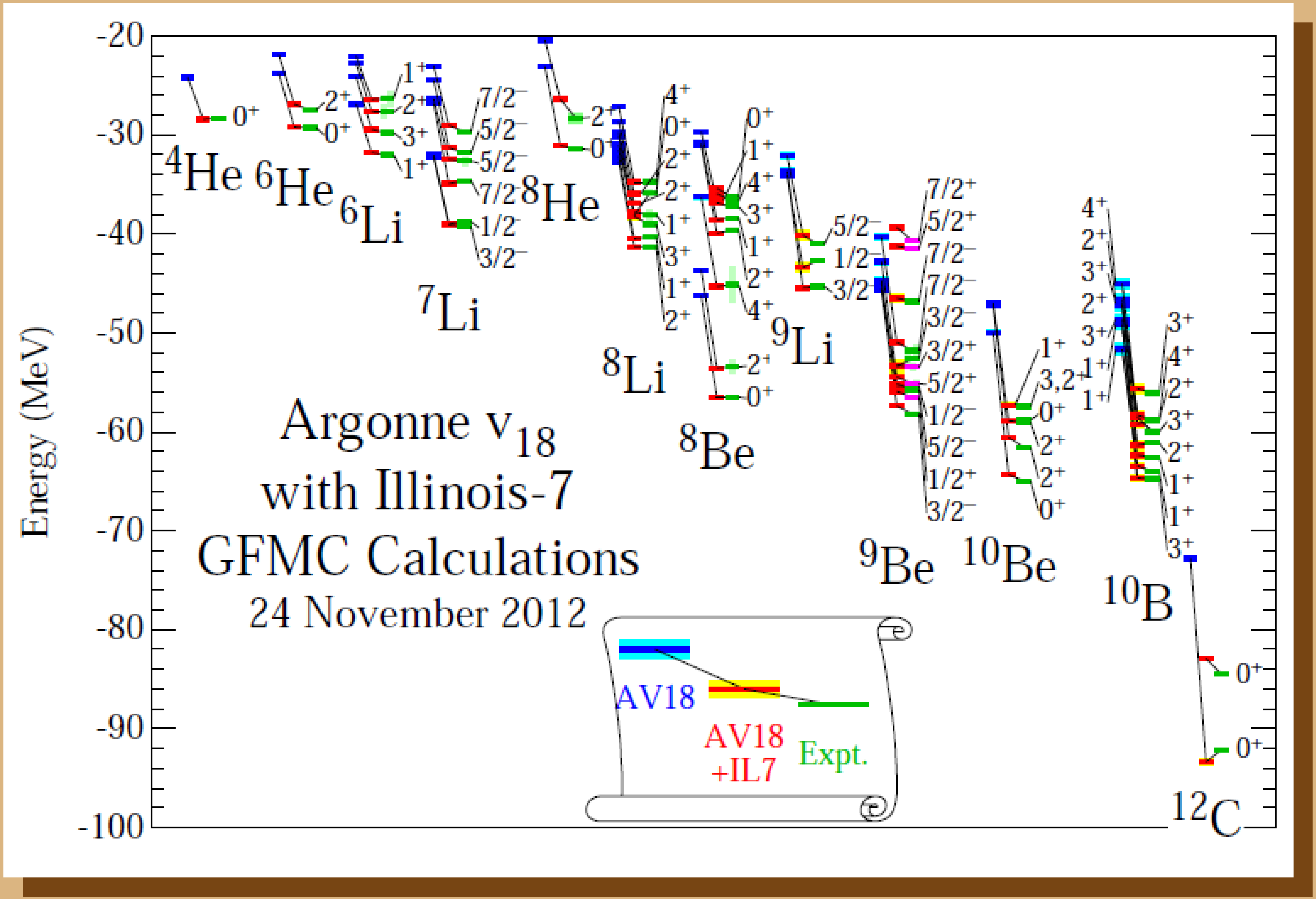
With tensor: $S_{jk} = 3(\hat{r}_{jk} \cdot \sigma_j)(\hat{r}_{jk} \cdot \sigma_k) - \sigma_j \cdot \sigma_k$

And spin, orbit: $\mathbf{S}_{jk} = \frac{\hbar}{2}(\sigma_j + \sigma_k)$

$$\mathbf{L}_{jk} = \frac{\hbar}{2\imath}(\mathbf{r}_j - \mathbf{r}_k) \times (\nabla_j - \nabla_k)$$

Phenomenological Hamiltonian

Very successful program (Carlson, Pieper, Wiringa, ...)



Credit: Steve Pieper

Quantum Monte Carlo

Enter Schmidt-Fantoni 1999: Auxiliary Field Diffusion Monte Carlo

GFMC needs $2^A \frac{A!}{Z!(A-Z)!}$ numbers, AFDMC would like only $4A$

(also see: Sarsa, Fantoni, Schmidt, Pederiva, PRC 2003)

Quantum Monte Carlo

Enter Schmidt-Fantoni 1999: Auxiliary Field Diffusion Monte Carlo

Take $V_2 = \sum_{j<k} v_{jk} = V_{\rm SI} + V_{\rm SD}$ and split

Spin-independent: $V_{\rm SI} = \sum_{j<k} \left[v_1(r_{jk}) + v_2(r_{jk}) \right]$

Spin-dependent: $V_{\rm SD} = \frac{1}{2} \sum_{j,\alpha,k,\beta} \sigma_{j,\alpha} \, A_{j,\alpha;k,\beta} \, \sigma_{k,\beta}$

For neutrons: 3N by 3N *A* matrix knows about spin-spin and tensor

Now diagonalize. Use eigendecomposition to create squares:

$$V_2 = V_{\rm SI} + \frac{1}{2} \sum_{n=1}^{3N} (O_n)^2 \lambda_n$$

Quantum Monte Carlo

Auxiliary Field Diffusion Monte Carlo (continued)

Handle squares through a Hubbard-Stratonovich transformation:

$$e^{-\frac{1}{2}\lambda O^2 \Delta\tau} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{x^2}{2}} e^{x\sqrt{-\lambda\Delta\tau}O}$$

This leads to the following short-time Green's function:

$$G(\mathbf{R}, \mathbf{R}', \Delta\tau) = \left(\frac{m}{2\pi\hbar^2\Delta\tau}\right)^{3A/2} \exp\left(-\frac{m|R - R'|^2}{2\hbar^2\Delta\tau}\right) e^{-V_{\mathrm{SI}}(R)\Delta\tau}$$
$$\prod_{n=1}^{3N} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx_n e^{-\frac{x_n^2}{2}} e^{x_n\sqrt{-\lambda_n\Delta\tau}O_n}$$

Use importance function (phase of walkers):

$$\psi_I(\mathbf{R}, S) = \prod_{i<j} f(r_{ij})\ \mathcal{A}\left[\prod_{i=1}^{N} \phi_\alpha(\mathbf{r}_i, s_i)\right] \qquad |s_i\rangle = a_i|\uparrow\rangle + b_i|\downarrow\rangle$$

Nuclear Hamiltonian: chiral EFT

How to go beyond in a systematic manner?

Exploit separation of scales: $a_{^1S_0} = (11\ \mathrm{MeV})^{-1}$

$m_\pi = 140\ \mathrm{MeV}$

$\Lambda_\chi \approx m_\rho \approx\ 800\ \mathrm{MeV}$

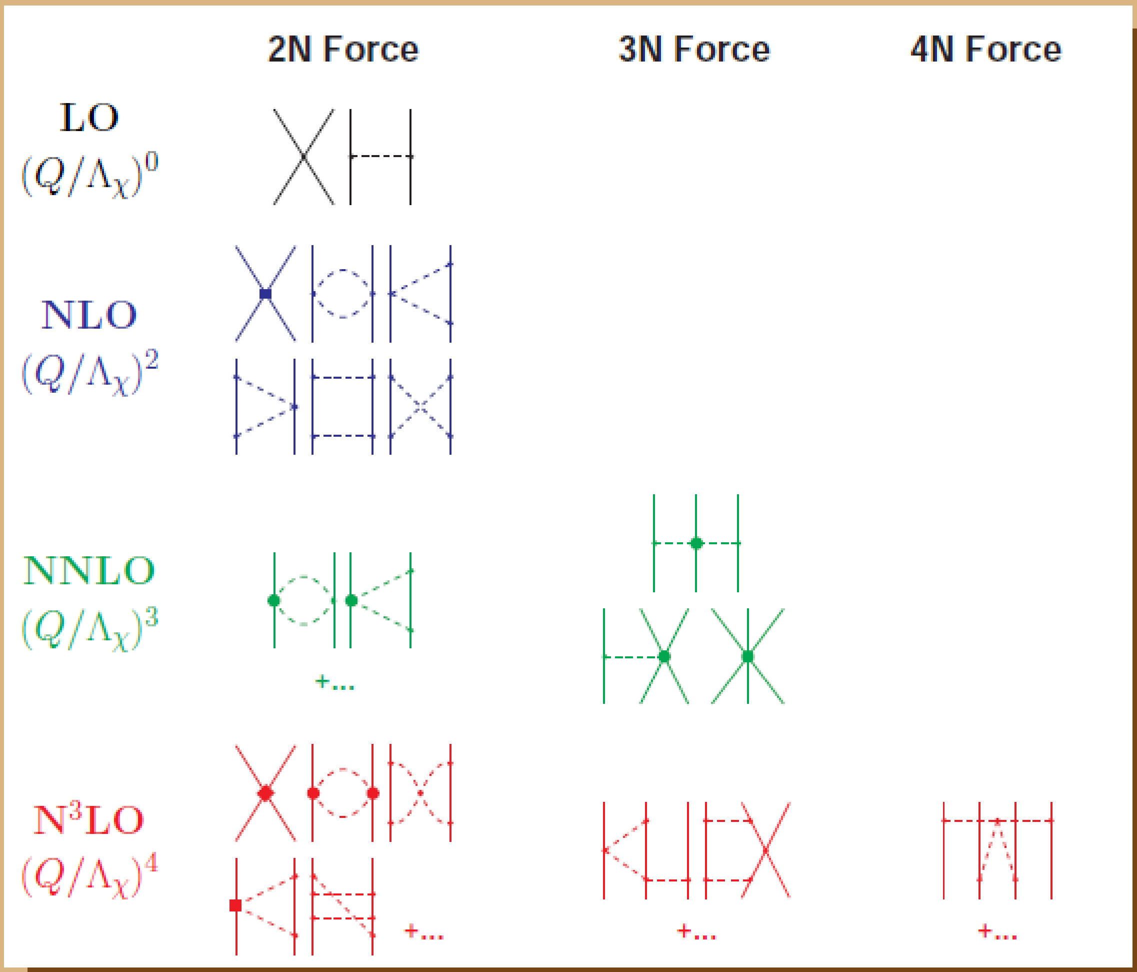
Chiral Effective Field Theory approach:

Use nucleons and pions as degrees of freedom

Systematically expand in $\dfrac{Q}{\Lambda_\chi}$

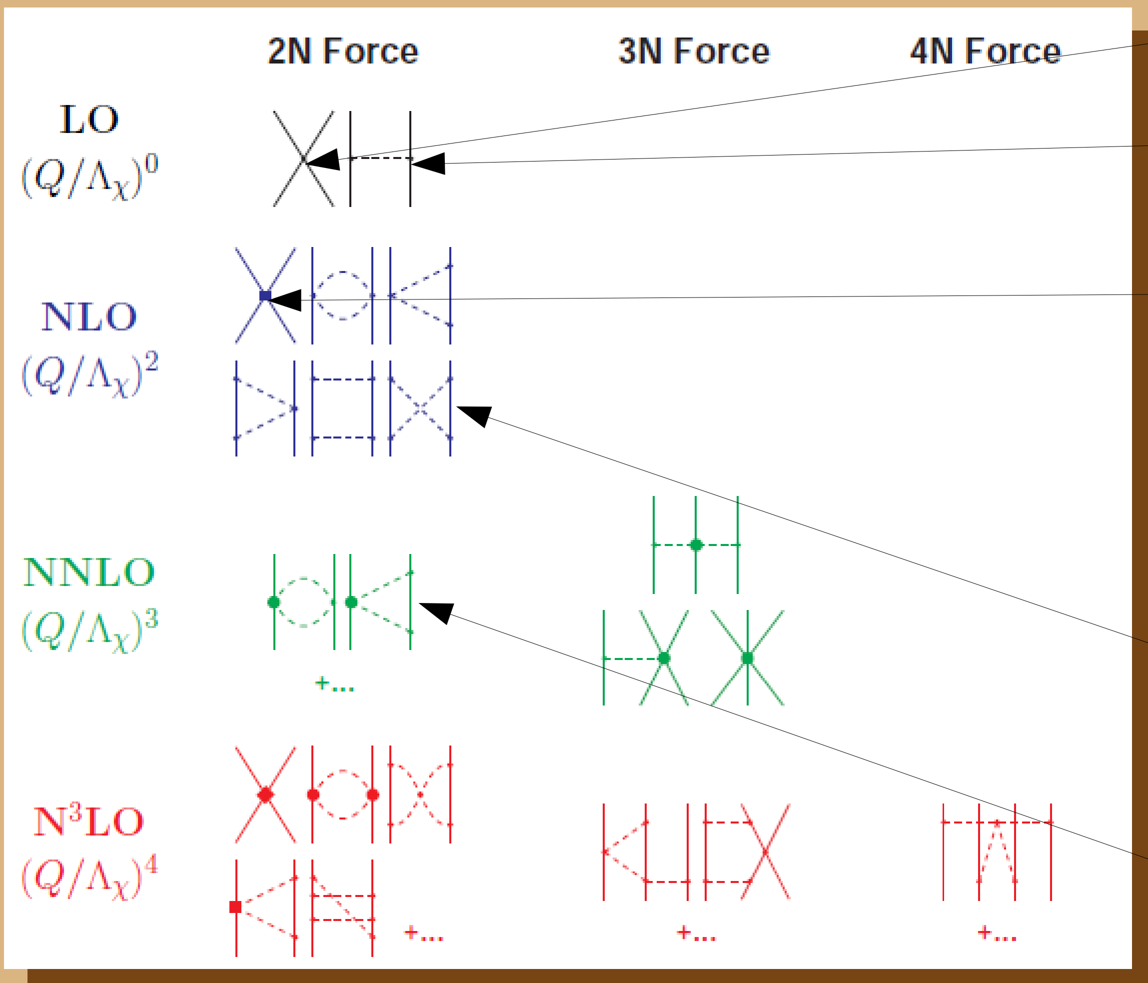
Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Meissner

Nuclear Hamiltonian: chiral EFT



- Attempts to connect with underlying theory (QCD)
- Systematic low-momentum expansion
- Consistent many-body forces
- Low-energy constants from experiment or lattice QCD
- Until now non-local in coordinate space (due to regulator and contacts), so unused in continuum QMC (see also: Lynn, Schmidt, PRC 2012)
- Power counting's relation to renormalization still an open question

Nuclear Hamiltonian: chiral EFT



$$V_{\rm ct}^{(0)} = C_S + C_T \, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

$$V_{1\pi}^{(0)} = -\left(\frac{g_A}{2f_\pi}\right)^2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \frac{(\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q})}{q^2 + m_\pi^2}$$

$$\begin{aligned} V_{\rm ct}^{(2)} &= C_1 \, q^2 + C_2 \, k^2 \\ &+ \left(C_3 \, q^2 + C_4 \, k^2\right) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \\ &+ i\frac{C_5}{2}(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\mathbf{q} \times \mathbf{k}) \\ &+ C_6 (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\ &+ C_7 (\boldsymbol{\sigma}_1 \cdot \mathbf{k})(\boldsymbol{\sigma}_2 \cdot \mathbf{k}) \end{aligned}$$

Long-studied
two-pion exchange

Contains couplings
from πN scattering

Regulator and dictionary:

$$f(p, p') = e^{-(p/\Lambda)^{2n}} e^{-(p'/\Lambda)^{2n}}$$

$$\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2 \qquad \mathbf{k} = (\mathbf{p}' + \mathbf{p})/2$$

$$\mathbf{p}' = (\mathbf{p}_1' - \mathbf{p}_2')/2 \qquad \mathbf{q} = \mathbf{p}' - \mathbf{p}$$

How to go beyond?

Combine power of Quantum Monte Carlo with consistency of chiral Effective Field Theory

Write down a local energy-independent NN potential

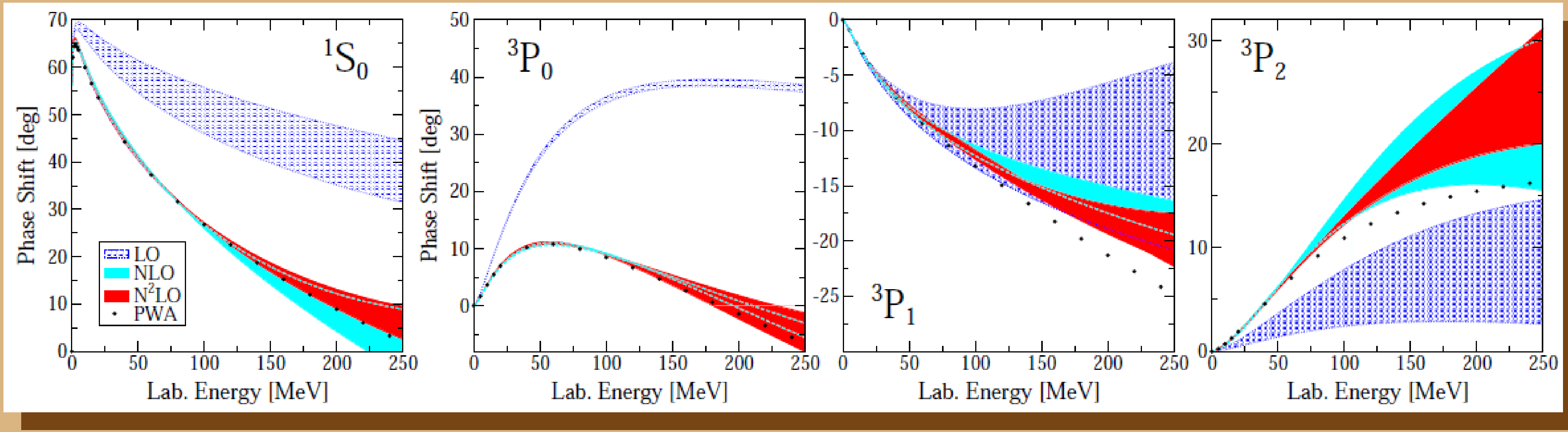
- Use local pion-exchange regulator: $f_{\text{long}}(r) = 1 - e^{-(r/R_0)^4}$
- Pick 7 different contacts at NLO, just make sure that when antisymmetrized they lead to a set obeying the required symmetry principles:

$$
\begin{aligned}
V_{\rm ct}^{(2)} &= C_1\, q^2 + C_2\, q^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
&+ \left(C_3\, q^2 + C_4\, q^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2\right) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \\
&+ i\, \frac{C_5}{2}\, (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \mathbf{q} \times \mathbf{k} \\
&+ C_6\, (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\
&+ C_7\, (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q})\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2
\end{aligned}
$$

How to go beyond?

Combine power of Quantum Monte Carlo with consistency of chiral Effective Field Theory

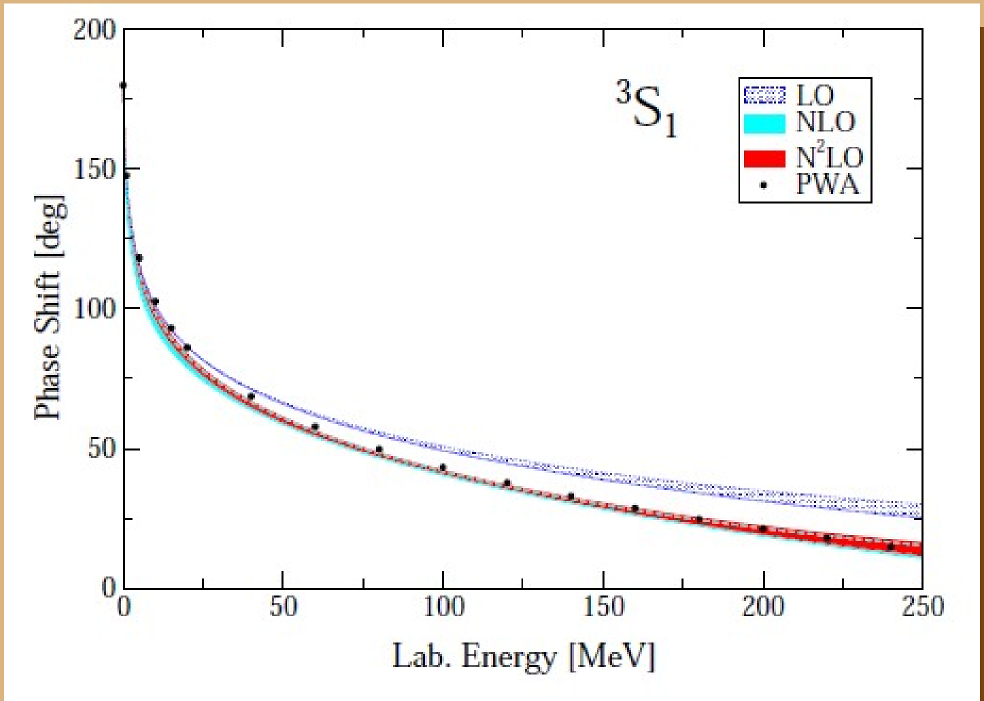
- Write down a local energy-independent NN potential
- Before doing many-body calculations, fit to NN phase shifts (*primum non nocere*)

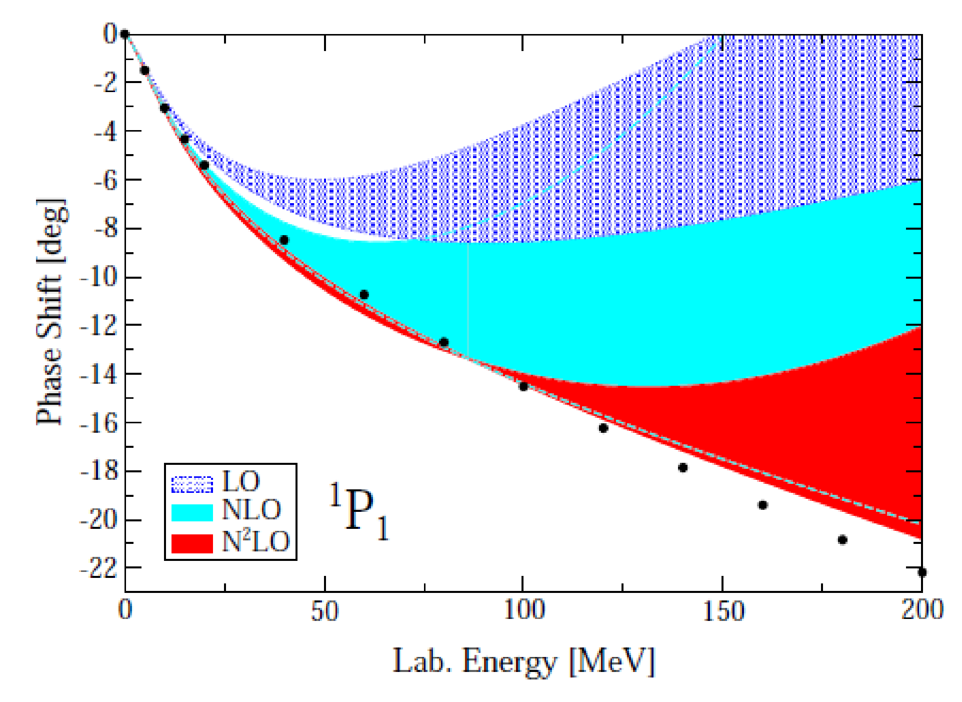


A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, arXiv:1303.6243

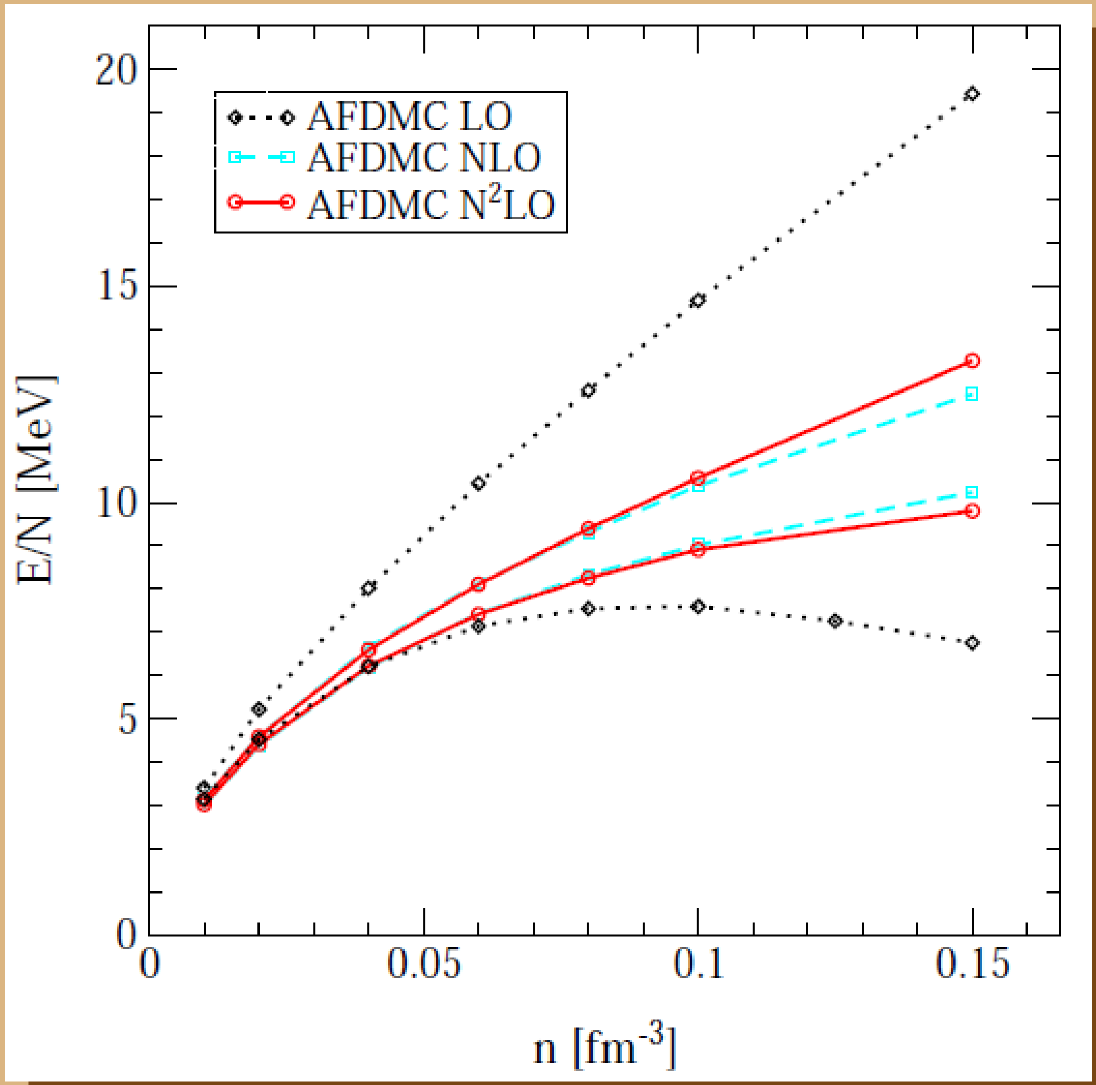
How to go beyond?

Fits currently being redone





Chiral EFT in QMC

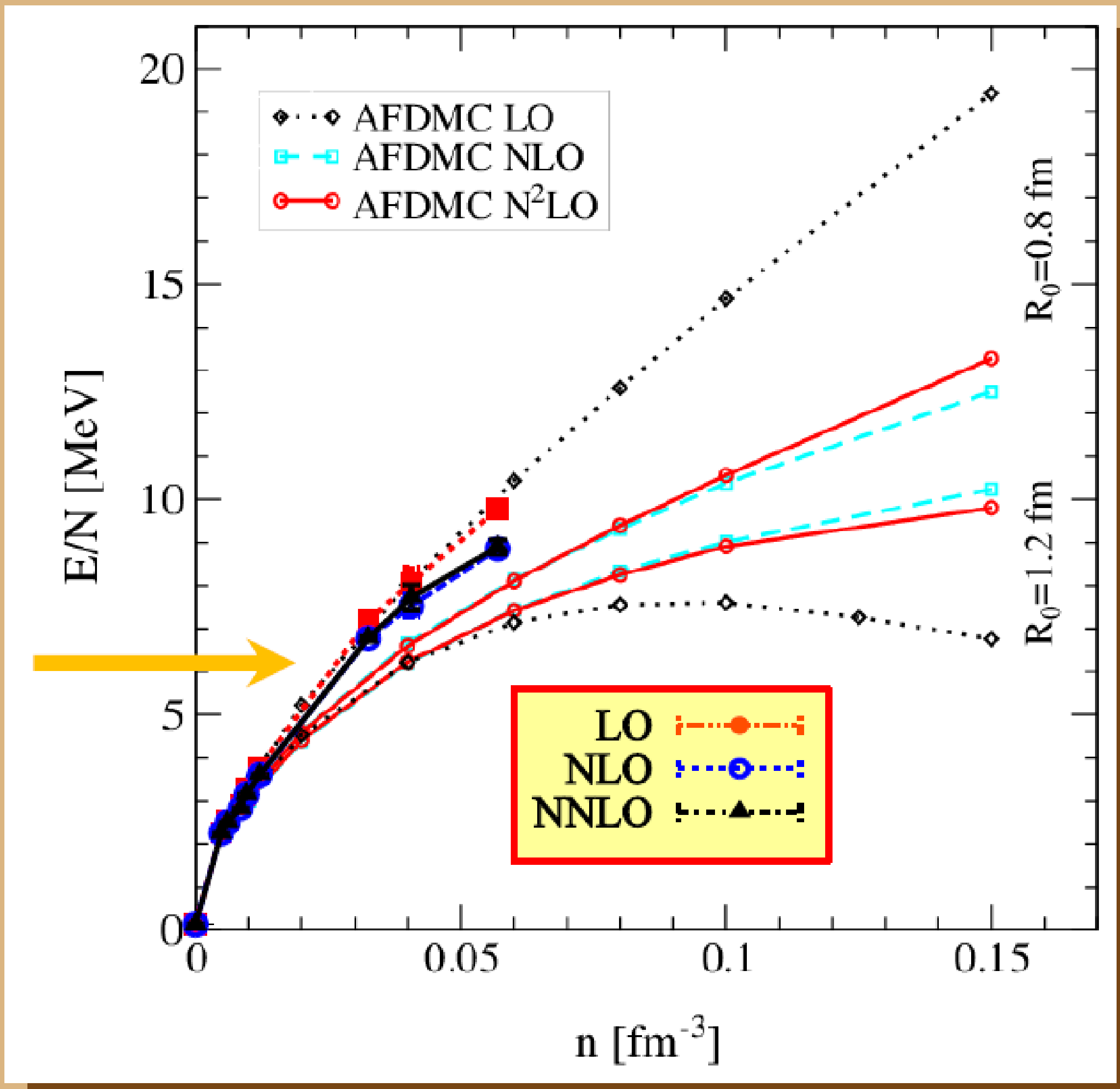


- Use Auxiliary-Field Diffusion Monte Carlo to handle the full interaction
- First ever non-perturbative systematic error bands
- Band sizes to be expected
- Many-body forces will emerge systematically

NEUTRONS

A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, arXiv:1303.6243

Chiral EFT in lattice QMC



- Complementary Quantum Monte Carlo approach that has already been using chiral EFT forces
- Preliminary results

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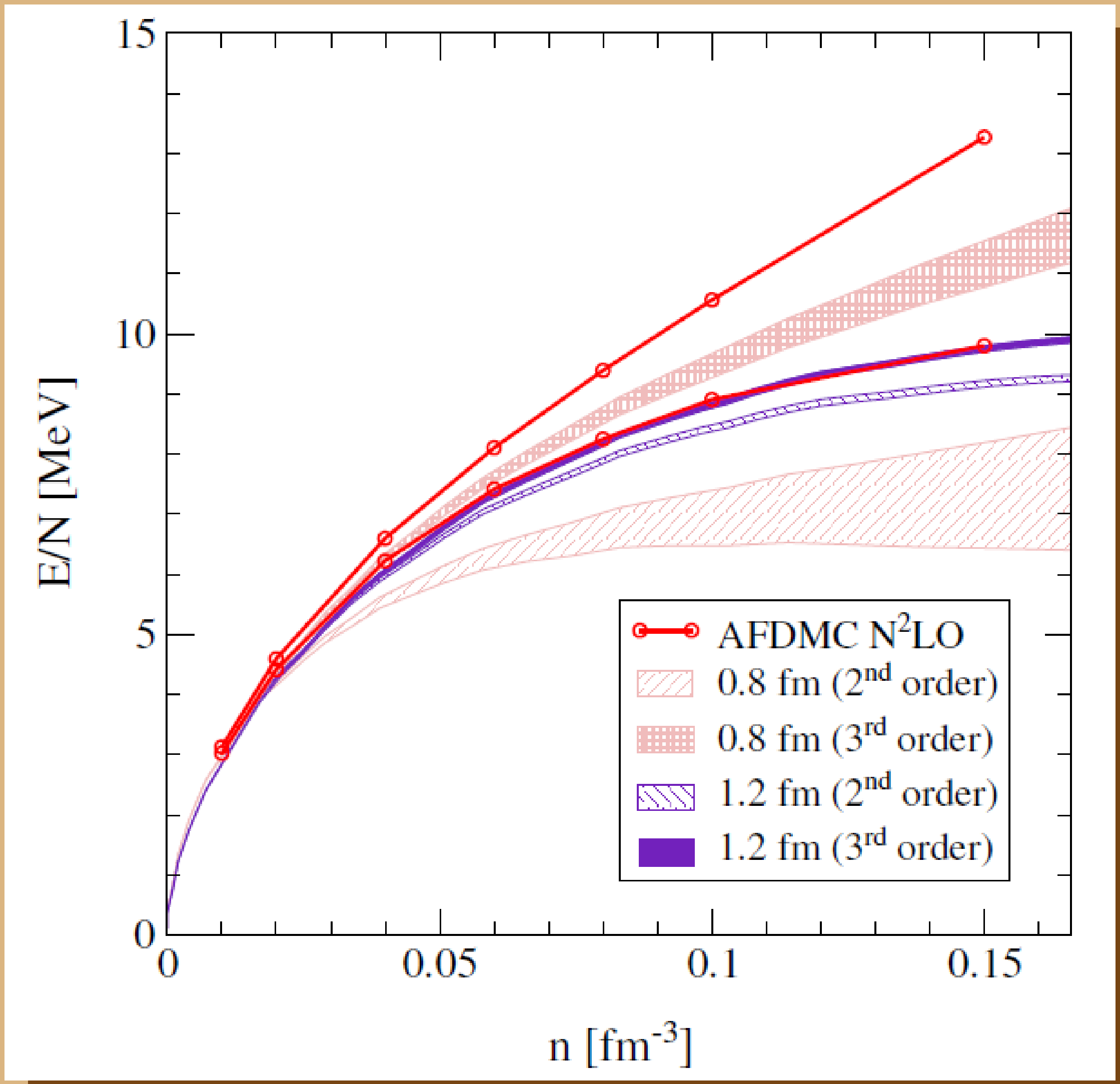
Dean Lee/nuclear lattice EFT collaboration

QMC vs MBPT



- Comparison with many-body perturbation approach
- MBPT bands come from diff. single-particle spectra
- Soft potential in excellent agreement with AFDMC
- Hard potential slower to converge

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A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, arXiv:1303.6243

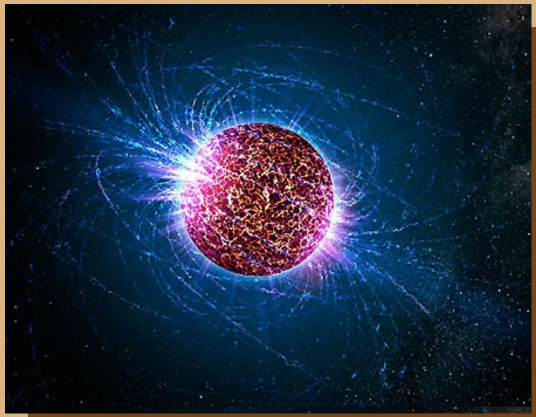
Now turn to lower densities

Simple interaction, rich physics

Lower densities

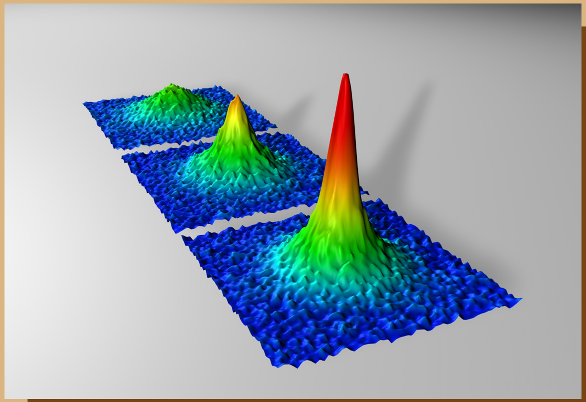
Neutron stars

- MeV scale
- $O(10^{57})$ neutrons



Cold atoms

- peV scale
- $O(10)$ or $O(10^5)$ atoms

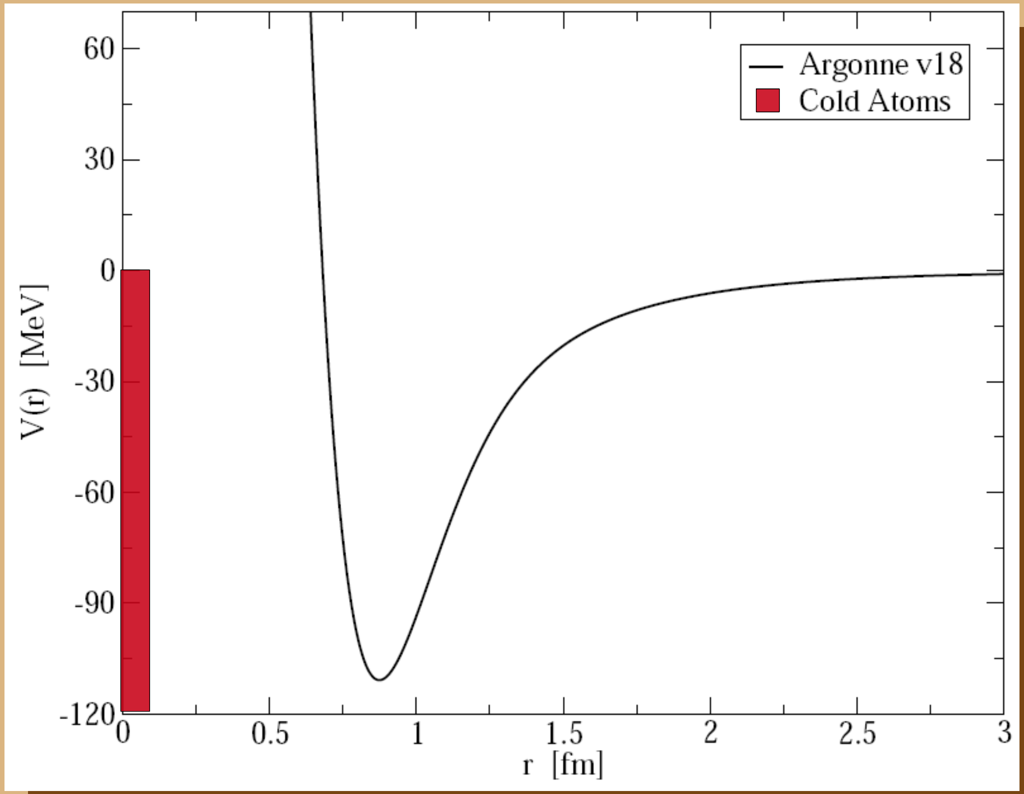


- Very similar E/E_{FG}
- Intermediate to strong coupling

Reminder: $E_{FG} = 3/5 N E_F$, $E_F = \hbar^2 k_F^2 / 2m$, $\rho = g k_F^3 / 6\pi^2$

Hamiltonian: unity in diversity

Things are much simpler at low density



Neutron matter

$^1S_0$ scattering phase shift

a = -18.5 fm, r_e = 2.7 fm

Cold atoms

Near a broad Feshbach resonance

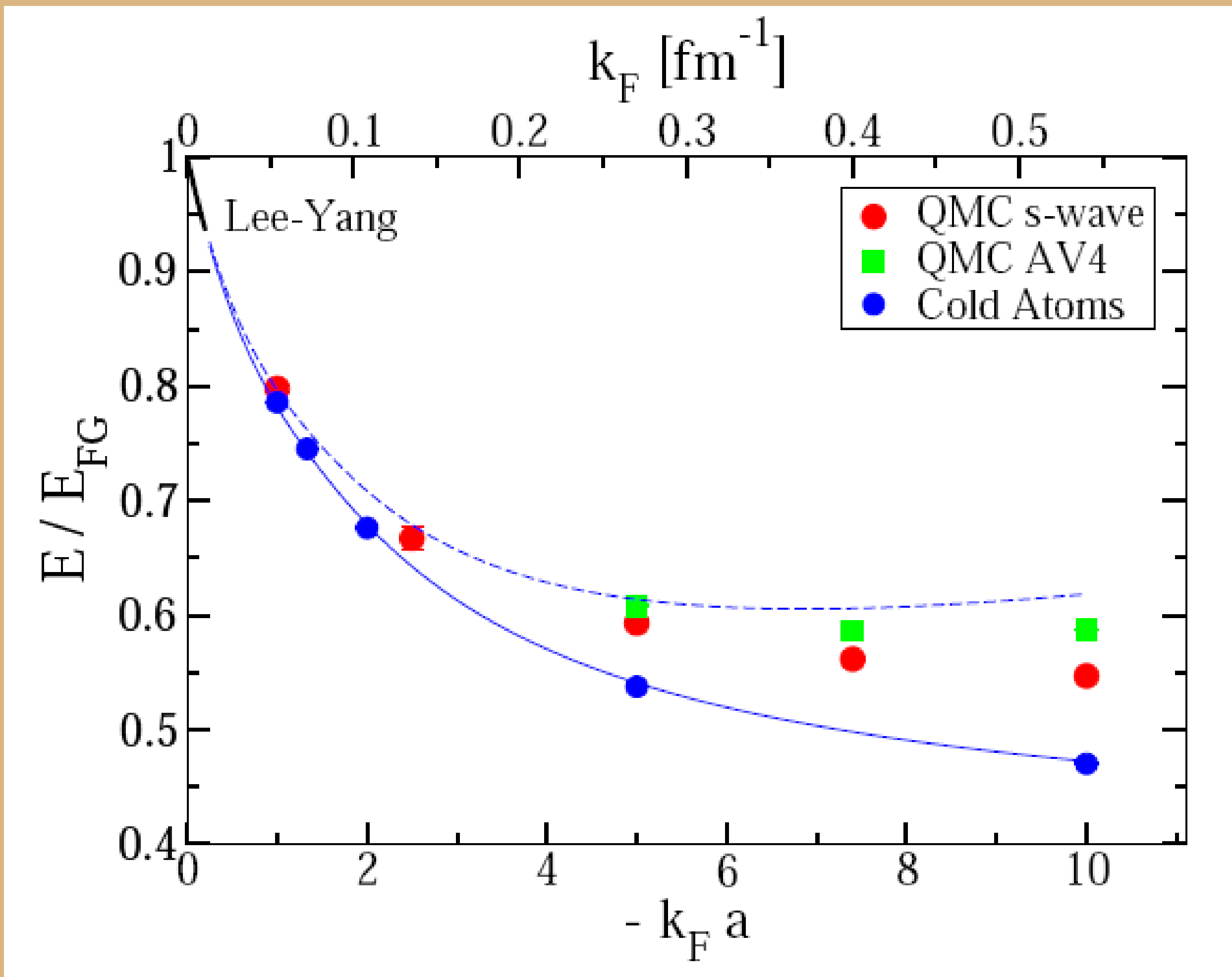
a = tunable, r_e =infinitesimal

Equal Populations

Equation of state

$$\uparrow\uparrow \quad + \quad \downarrow\downarrow$$

Equations of state



- Results identical at low density
- Range important at intermediate density (dashed line: linear dependence on range)
- Other channels start to matter at larger density

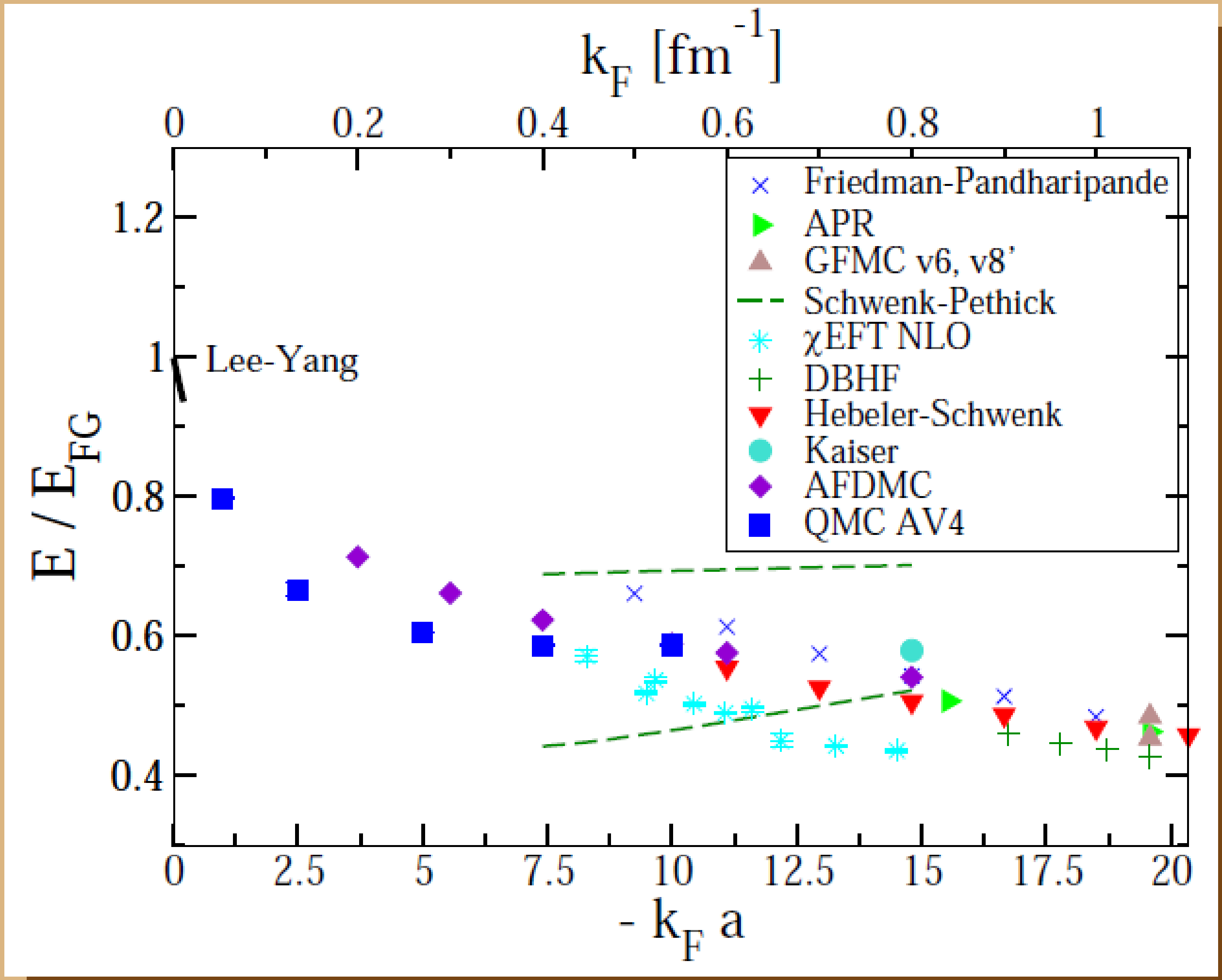
NEUTRONS

ATOMS

A. Gezerlis and J. Carlson, Phys. Rev. C **77**, 032801 (2008)

J. Carlson, S. Gandolfi, AG, Prog. Theor. Exp. Phys. **2012**, 01A209

Equations of state: comparison



- Lowest densities on the market; agreement with Lee-Yang trend
- At higher densities all calculations are in qualitative agreement

NEUTRONS

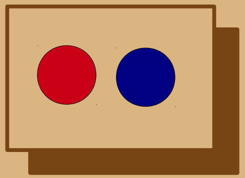
A. Gezerlis and J. Carlson, Phys. Rev. C **81**, 025803 (2010)

The DFT connection

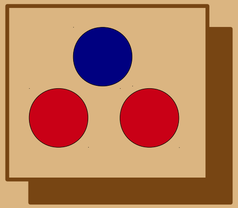
Microscopic constraints for Skyrme functionals
(“Skyrme” basically means “contact”)

Take zero-range forces:

$$v_{12} = t_0(1 + x_0 P_\sigma)\delta(\mathbf{r}_1 - \mathbf{r}_2) + \ldots$$



$$v_{123} = t_3\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_2 - \mathbf{r}_3)$$



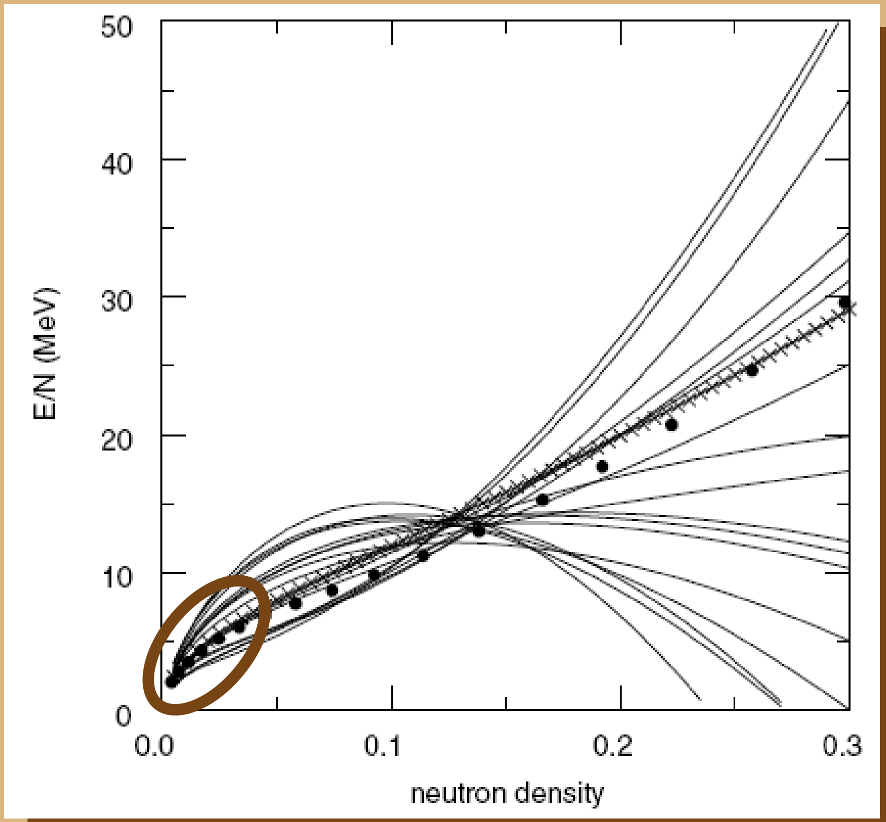
Simplest functional follows:

$$\mathcal{E} = \frac{\hbar^2}{2m}\tau + \frac{3}{8}t_0\rho^2 + \ldots + \frac{1}{16}t_3\rho^3$$

The DFT connection

Microscopic constraints for Skyrme functionals

- Large spread in predictions
- Dependable calculations are useful



NEUTRONS

B. A. Brown, Phys. Rev. Lett. **85**, 5296 (2000).

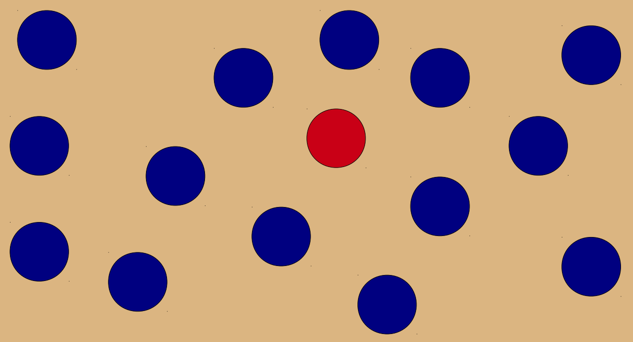
Very Unequal Populations

The Neutron Polaron

$$\uparrow\uparrow\uparrow \quad + \quad \downarrow$$

The neutron polaron

One impurity in a sea of fermions



Neat way to address: Chevy Ansatz

$$|\Psi\rangle = \phi_0 |\mathrm{FG}\rangle |\boldsymbol{p}\rangle + \sum_{\substack{k>k_F \\ q\leq k_F}} \phi_{k,q} \widehat{a}^\dagger_k \widehat{a}_q |\mathrm{FG}\rangle |\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{k}\rangle$$

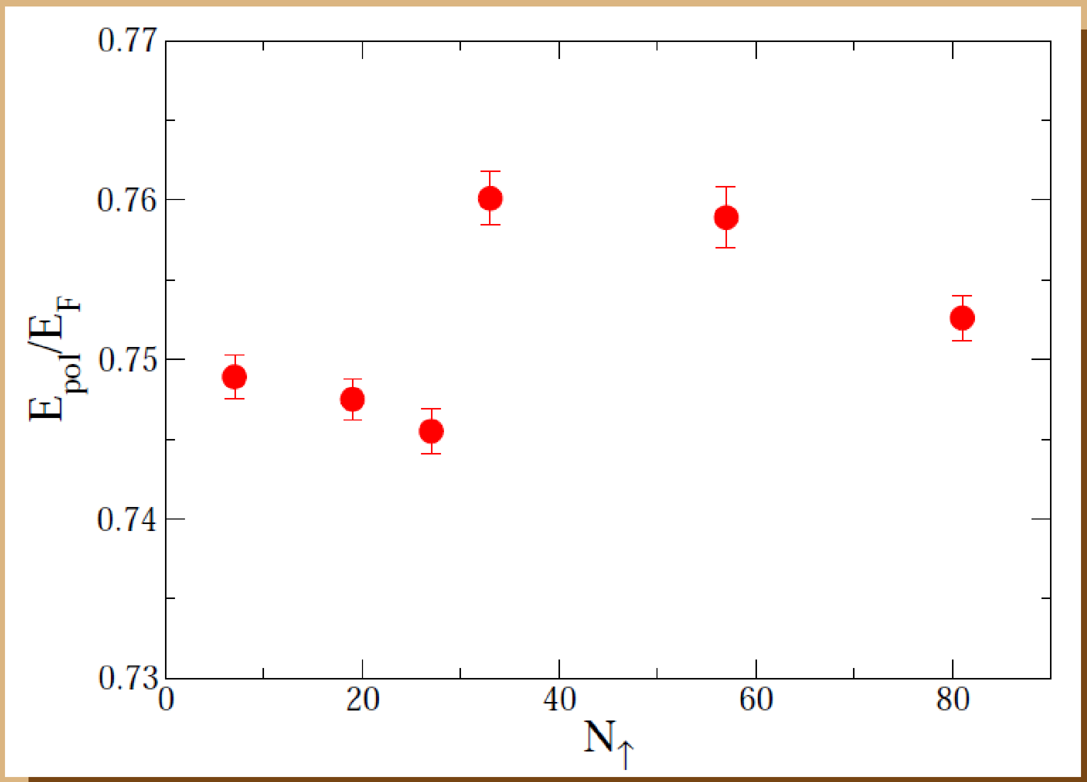
Take a Hamiltonian of your liking and minimize with respect to the ϕ_0 and $\phi_{k,q}$ parameters

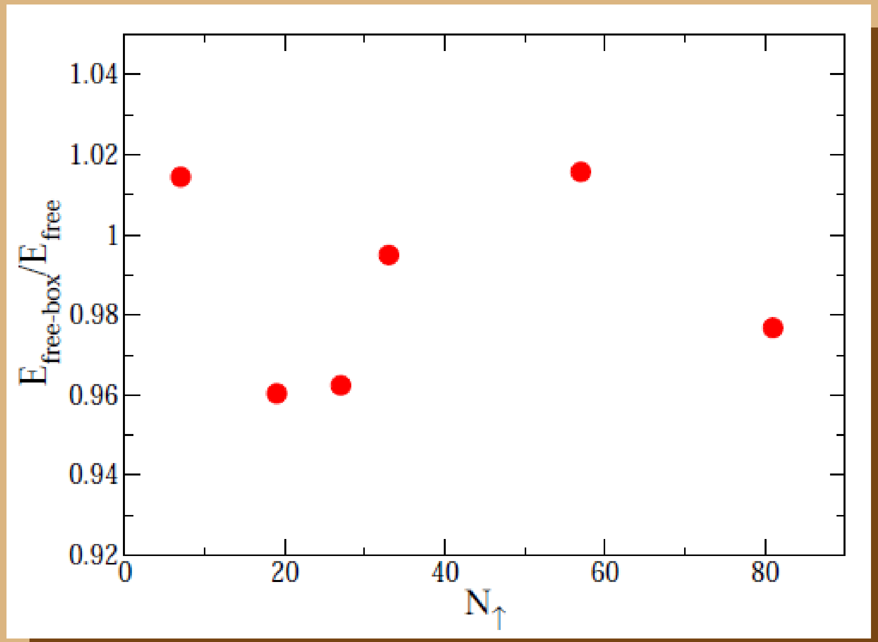
Calculate the binding energy of a single impurity

The neutron polaron

Check Ansatz with Quantum Monte Carlo

Behavior identical to free gas
(exception: $N = 7 : L \approx 4r_e$)





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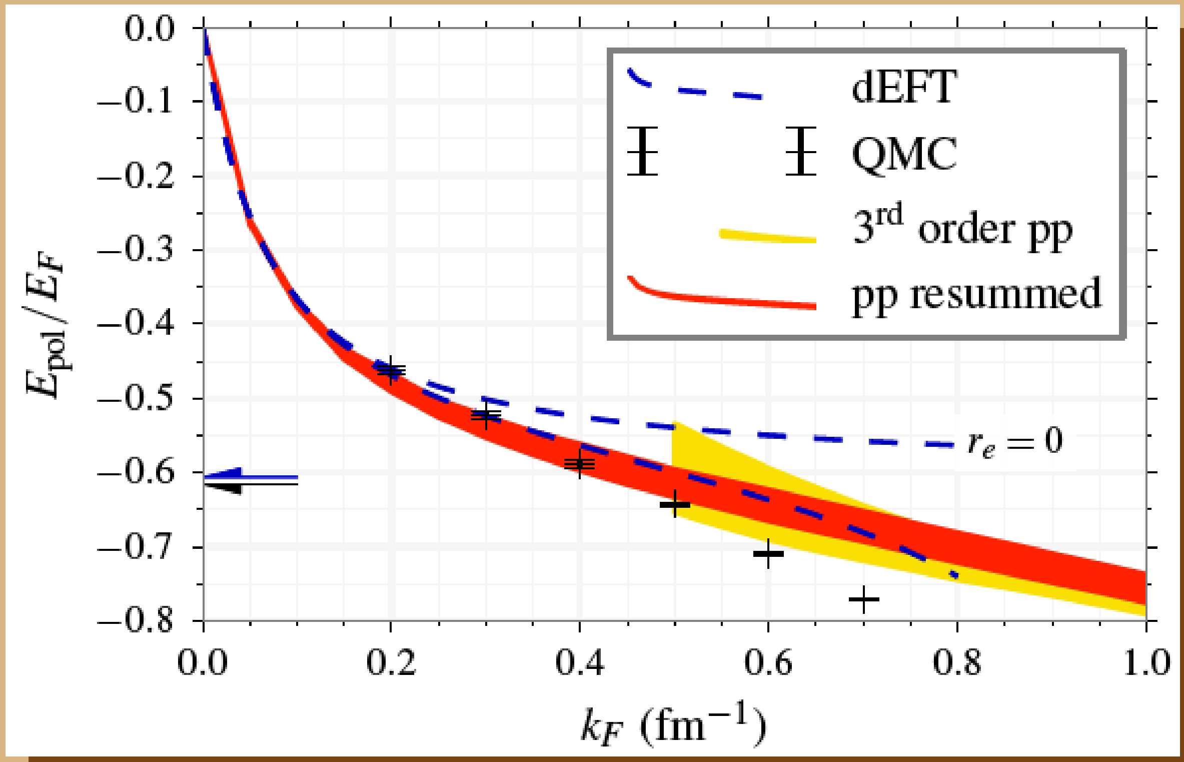
M. M. Forbes, A. Gezerlis, K. Hebeler,
T. Lesinski, A. Schwenk, *to be submitted to PRL* (2013)

The neutron polaron

Different many-body method benchmarking



- Low density universal
- Chevy Ansatz captures large part of the physics
- Diagrammatics quantify beyond s-wave contribs (ditto for AFDMC)

NEUTRONS

M. M. Forbes, A. Gezerlis, K. Hebeler,
T. Lesinski, A. Schwenk, *to be submitted to PRL* (2013)

The neutron polaron

New constraint from neutrons

Only four densities:

$$\rho = \rho_\uparrow + \rho_\downarrow$$

$$\mathbf{s} = \rho_\uparrow - \rho_\downarrow$$

$$\tau = \tau_\uparrow + \tau_\downarrow$$

$$\mathbf{T} = \tau_\uparrow - \tau_\downarrow$$

Quasi-standard density dependence:

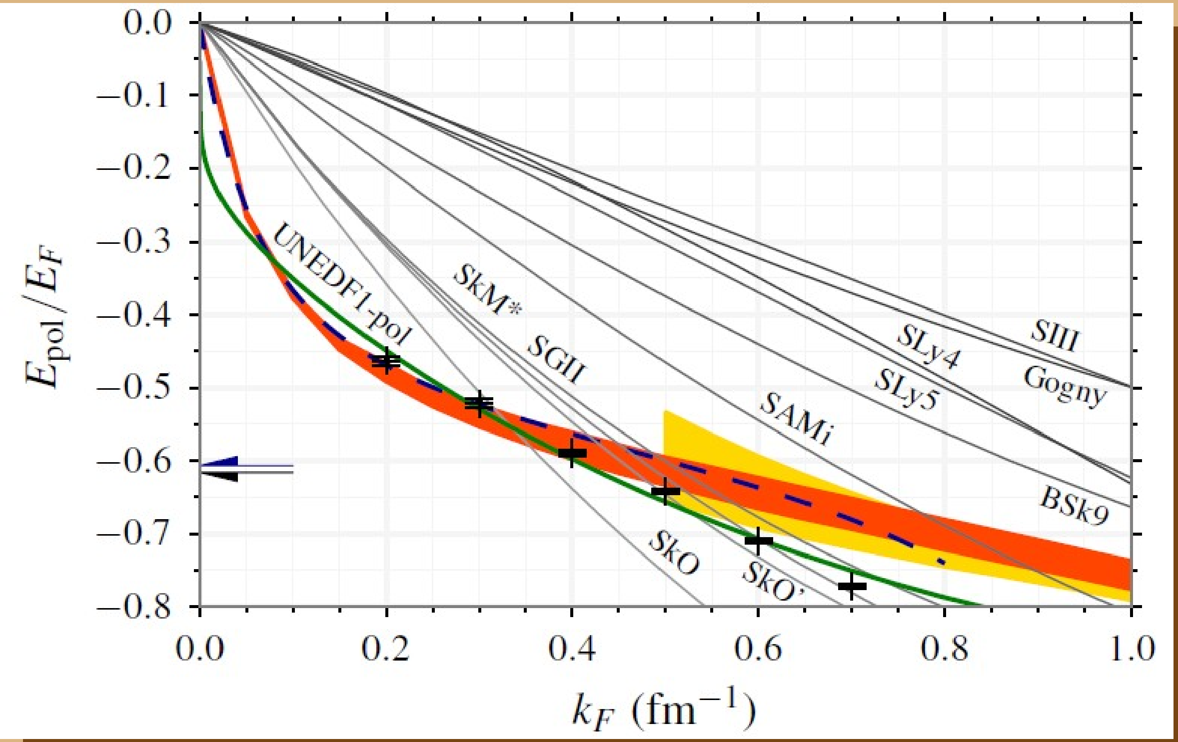
$$\begin{aligned} C^\rho &= C^{\rho,0} + C^{\rho,D} \rho^\gamma \\ C^s &= C^{s,0} + C^{s,D} \rho^\delta \end{aligned}$$

Resulting functional:

$$\begin{aligned} \mathcal{E}_{\mathrm{PNM}} = \frac{\hbar^2}{2m}\tau &+ C_1\,\rho^2 + C_2\,\rho^{2+\gamma} \\ &+ C_3\,\rho\tau \\ &+ C_4\,\mathbf{s}^2 + C_5\,\mathbf{s}^2\rho^\delta \\ &+ C_6\,\mathbf{s}\cdot\mathbf{T} \end{aligned}$$

The neutron polaron

New constraint on density functionals



- Microscopic input
- Most functionals are way off the Schroedinger equation output
- Green curve: playing around with time-even and time-odd exponents

NEUTRONS

M. M. Forbes, A. Gezerlis, K. Hebeler, T. Lesinski, A. Schwenk, *to be submitted to PRL* (2013)

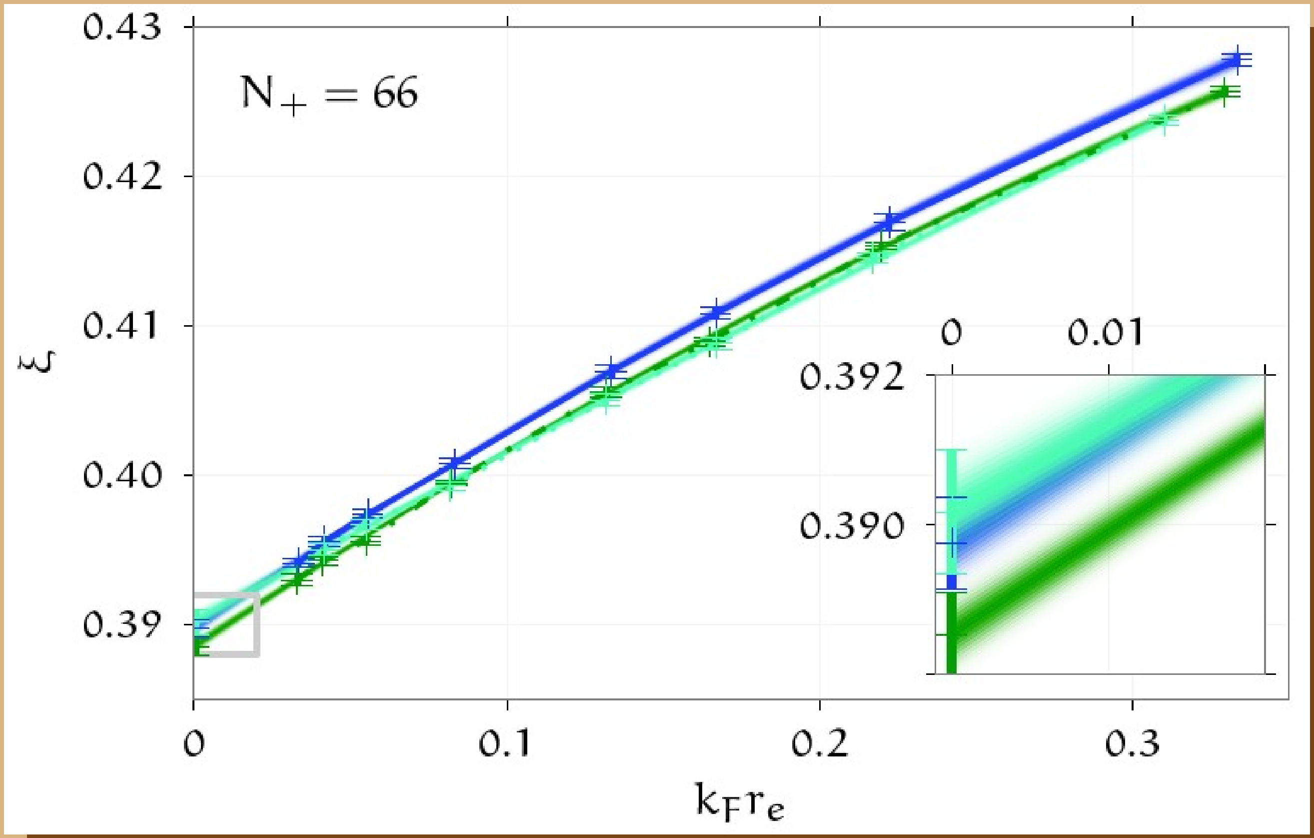
Fermions at unitarity

Explore effective-range dependence and finite-size effects

$$\uparrow\uparrow \quad + \quad \downarrow\downarrow$$

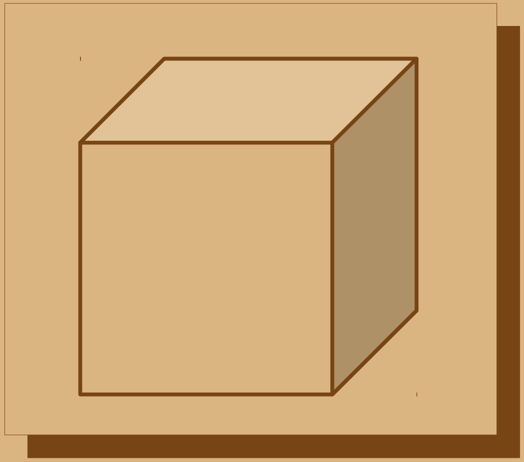
New QMC results

Carefully extapolated to zero effective range



We have:

- analyzed dependence on particle number for the first time
- re-optimized the variational wavefn
- carefully extrapolated to zero range



M. M. Forbes, S. Gandolfi, and A. Gezerlis, Phys. Rev. A. **86**, 053603 (2012).

DFT for superfluids: SLDA

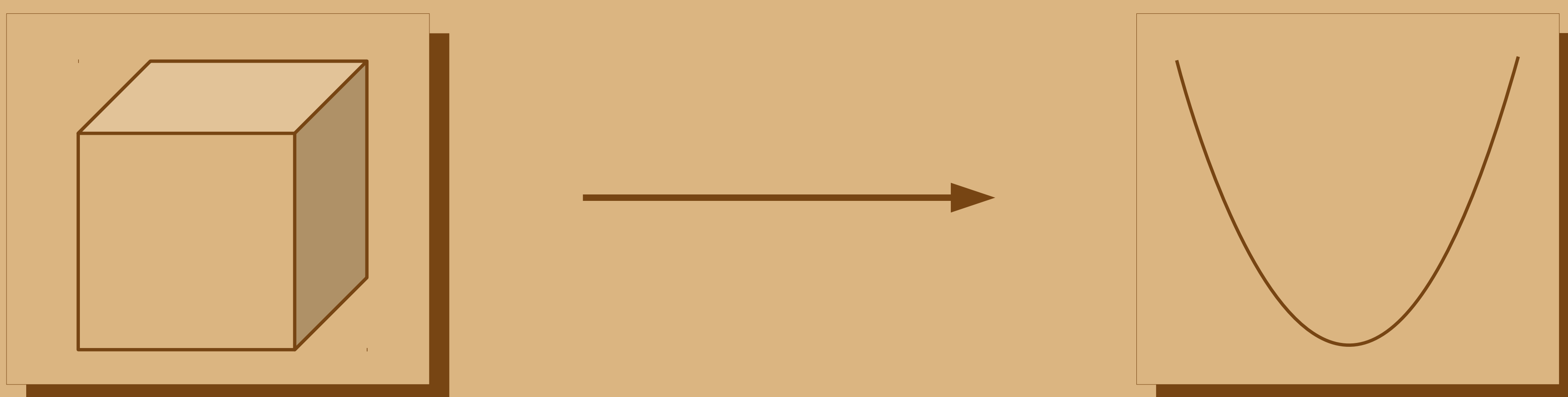
Bogoliubov-de Gennes + normal state interactions

Superfluid Local Density Approximation: $\mathcal{E} = \alpha\frac{\tau}{m} + \beta\frac{3(3\pi^2)^{2/3}}{10}n^{5/3} + g\nu^\dagger\nu$

Three densities: n (number), τ (kinetic), ν (anomalous)

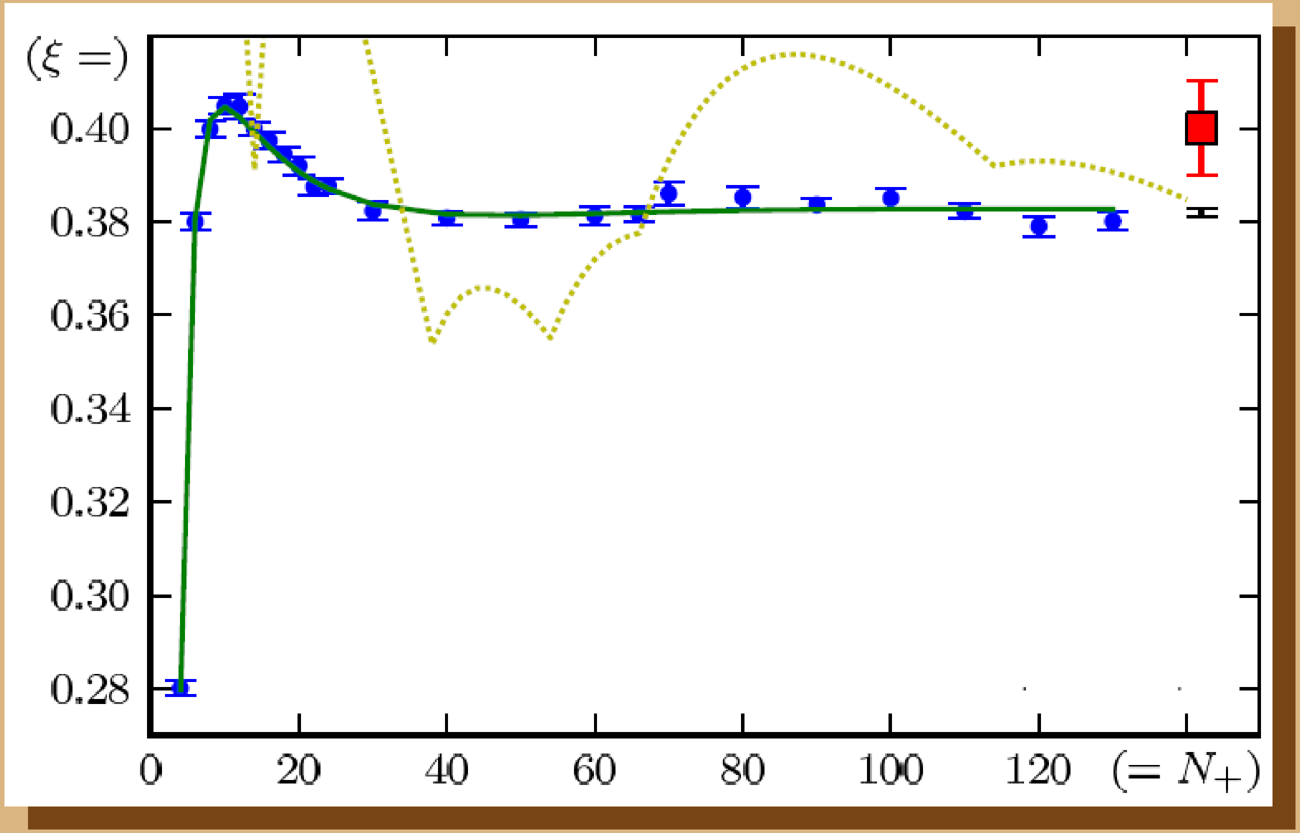
Three parameters: α (effective mass), β (self-energy), g (pairing)

Fit parameters in the continuum, make predictions on trapped systems

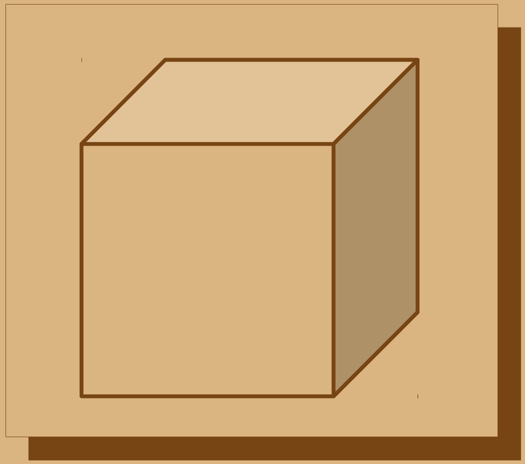


New DFT results

QMC + SLDA in a box



- No gradient corrections to be accounted for
- Allows us to reach the thermodynamic limit
- No pairing term in the functional leads to large shell corrections



M. M. Forbes, S. Gandolfi, and A. Gezerlis, Phys. Rev. Lett. **106**, 235303 (2011).

Conclusions

- Chiral EFT can now be used in continuum Quantum Monte Carlo methods
- We can directly test the perturbativeness of different orders
- Cold-atom experiments can constrain nuclear theory
- Neutron matter calculations impact both neutron-star phenomenology and heavy nuclei fits