Quantum Monte Carlo calculations with nonlocal chiral interactions

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Neutron rich matter and neutron stars

Collaborators
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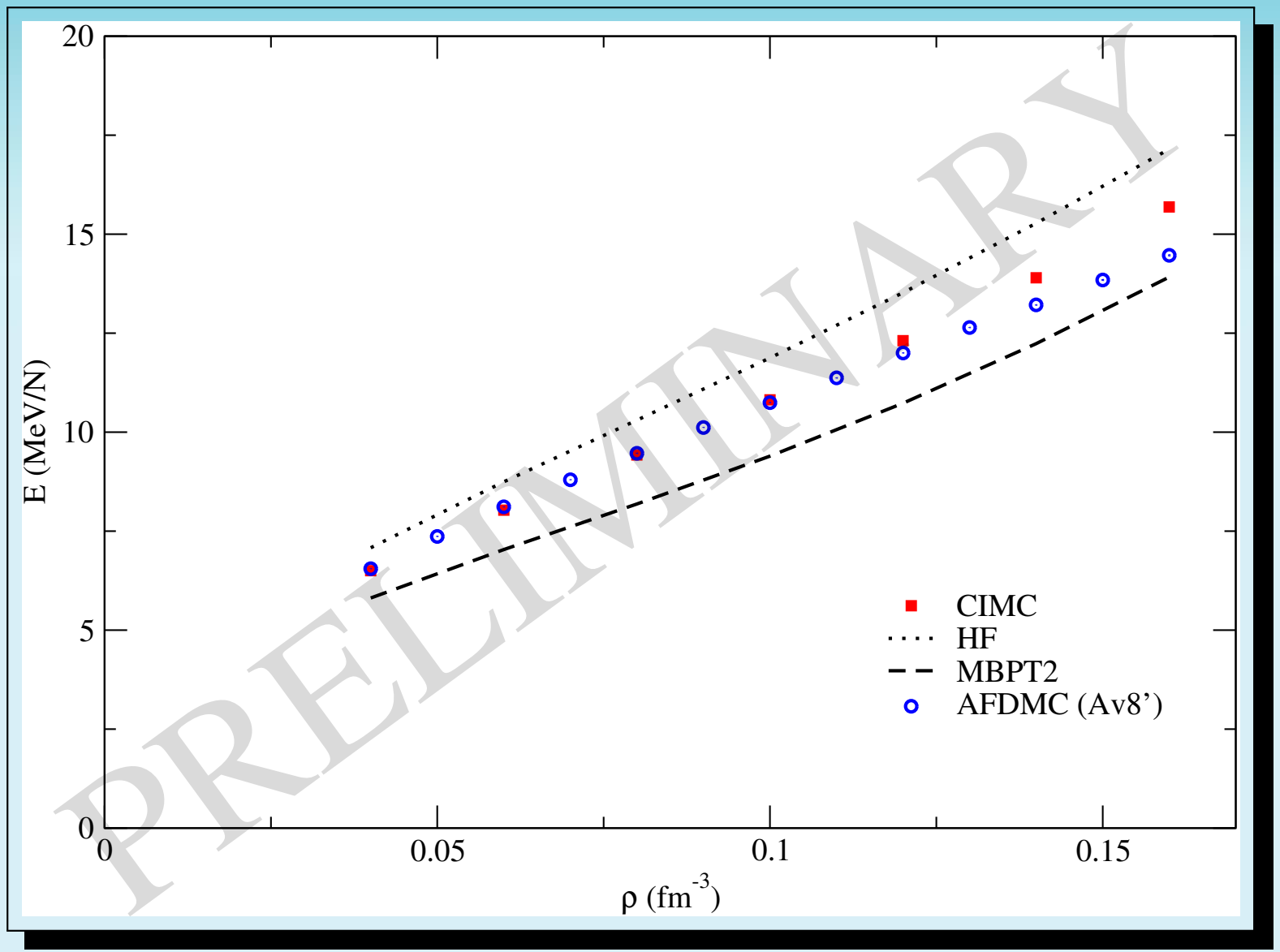
New Fock space QMC for non-local χEFT



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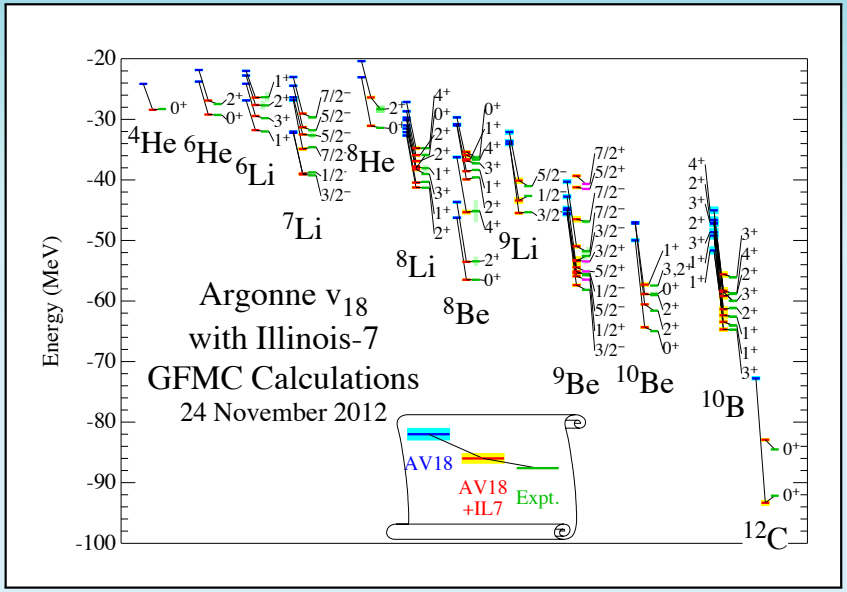
Monte Carlo with a modern interaction

- Diffusion based Monte Carlo (GFMC) is one of the most accurate methods for light nuclei
- Also widely used in condensed matter, quantum chemistry ...



Pieper et al (ANL)

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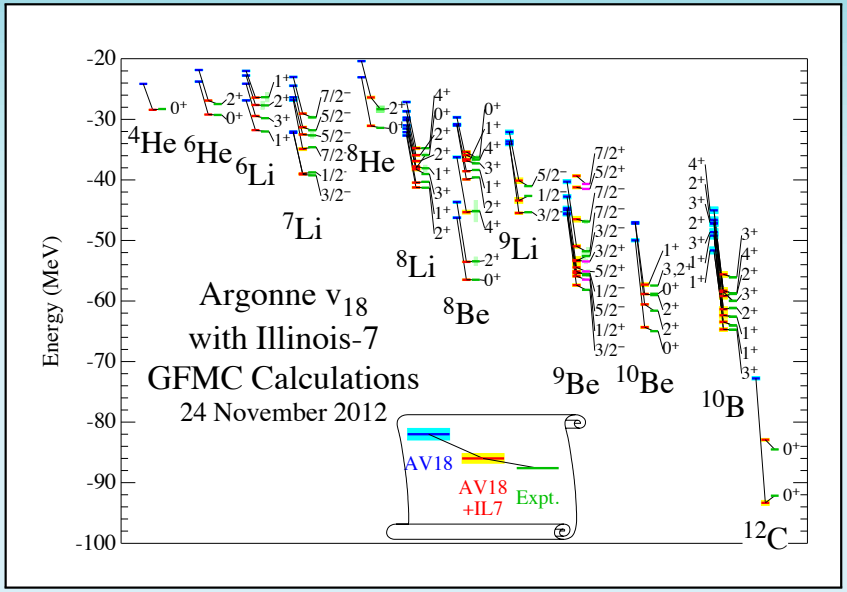
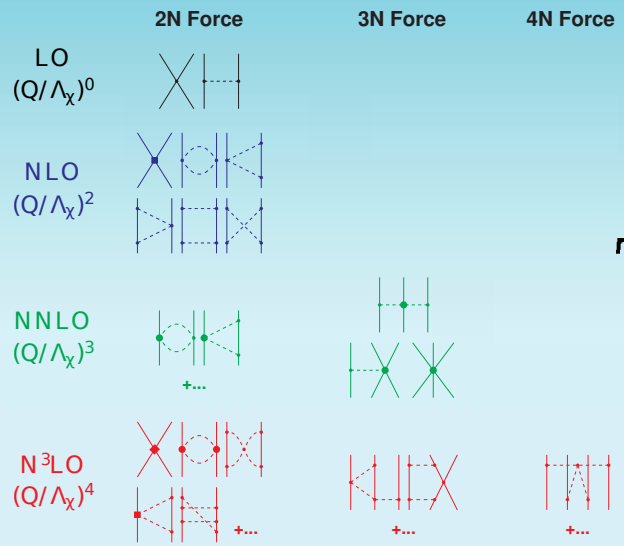


Pieper et al (ANL)

Standard GFMC/AFDMC only works for local interactions

Urbana-Argonne-Illinois models

Postmodern χ-EFT interactions



The χ-EFT interactions are non-local

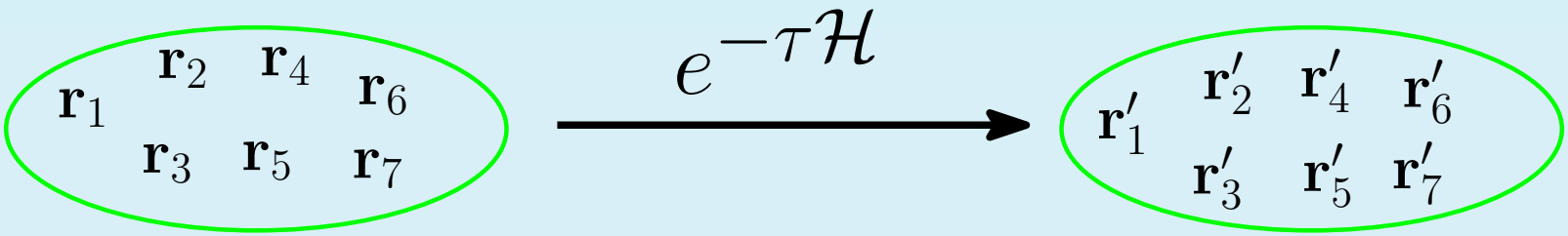
How to do χ-EFT + QMC?

- Develop DMC for non-local interactions
  (need to go to Fock space)
- Try to 'localize' χ-EFT, then use standard (AF)DMC
  `A. Gezerlis' talk.`

Standard Diffusion Monte Carlo

Use the power method to solve the Schrödinger equation

$$|\Psi_{\text{Ground State}}\rangle = \lim_{N\to\infty} \left(e^{-\tau H}\right)^N |\Psi_{\text{Initial State}}\rangle$$



- Interpret the matrix elements of $e^{-\tau H}$ as probabilities
- Propagation = Diffusion + Branching
- Only local Hamiltonians

Diffusion Monte Carlo in Fock space

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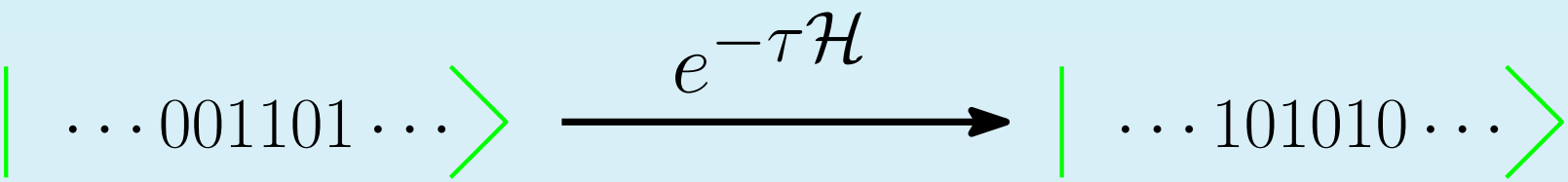
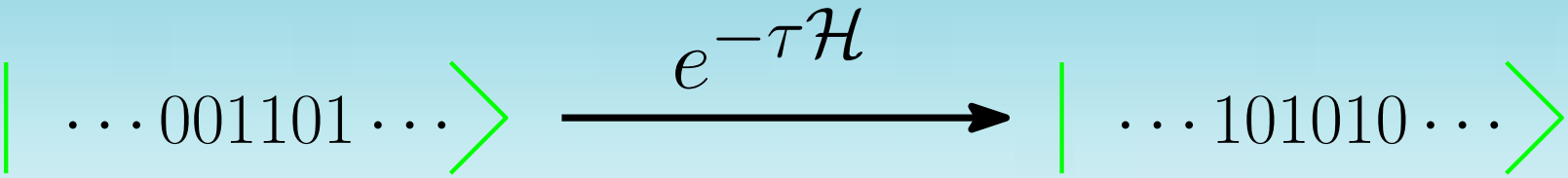


- Interpret the matrix elements of $e^{-\tau H}$ as probabilities
- Propagation = Diffusion + Branching
- **Non-local Hamiltonians possible**

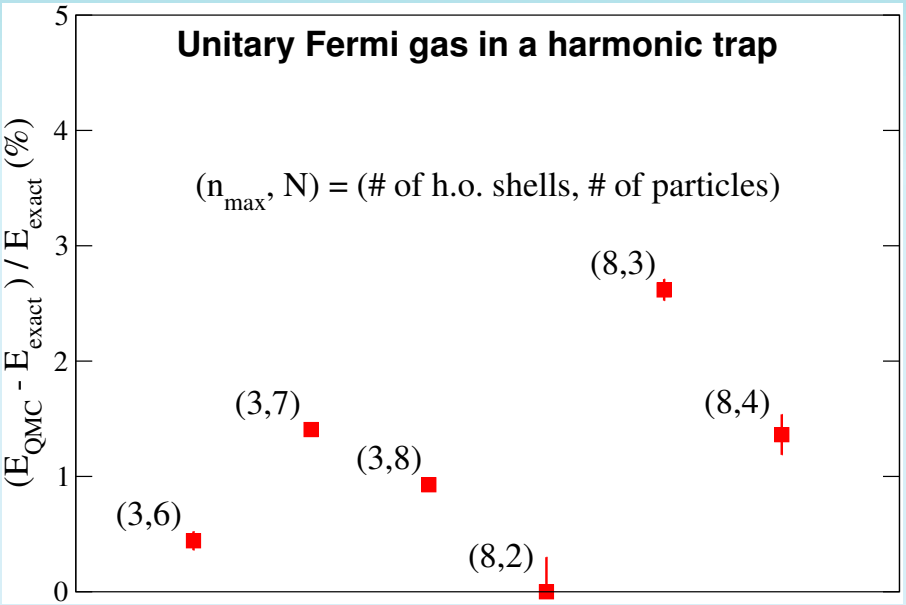
Diffusion Monte Carlo in Fock space

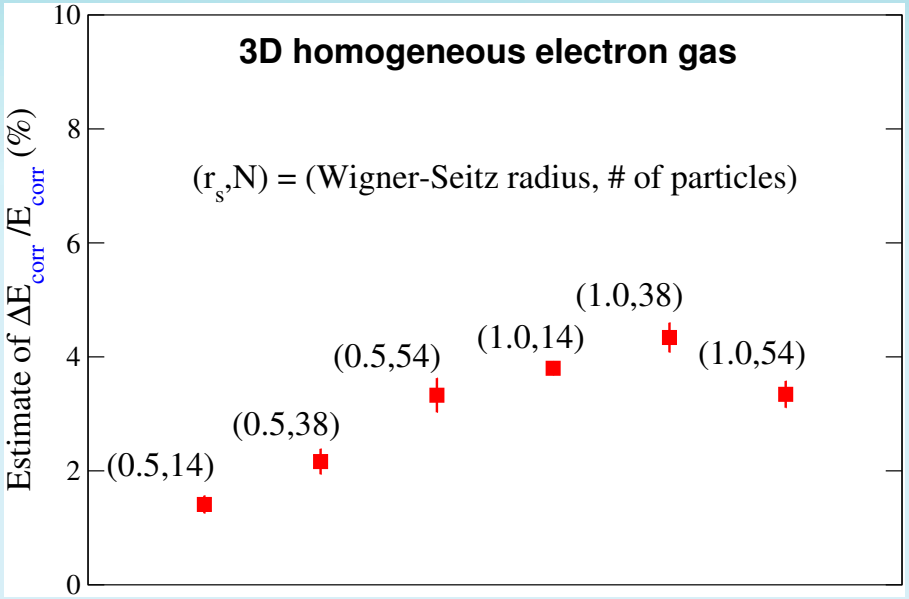


Challenges

- Efficient sampling of $e^{-\tau H}$ ✓
- Avoid the sign problem with the fixed node/phase condition ✓
- But, maintain the variational upper bound for the energy ✓
- **Good wave functions** to impose the fixed node/phase condition

Systematics

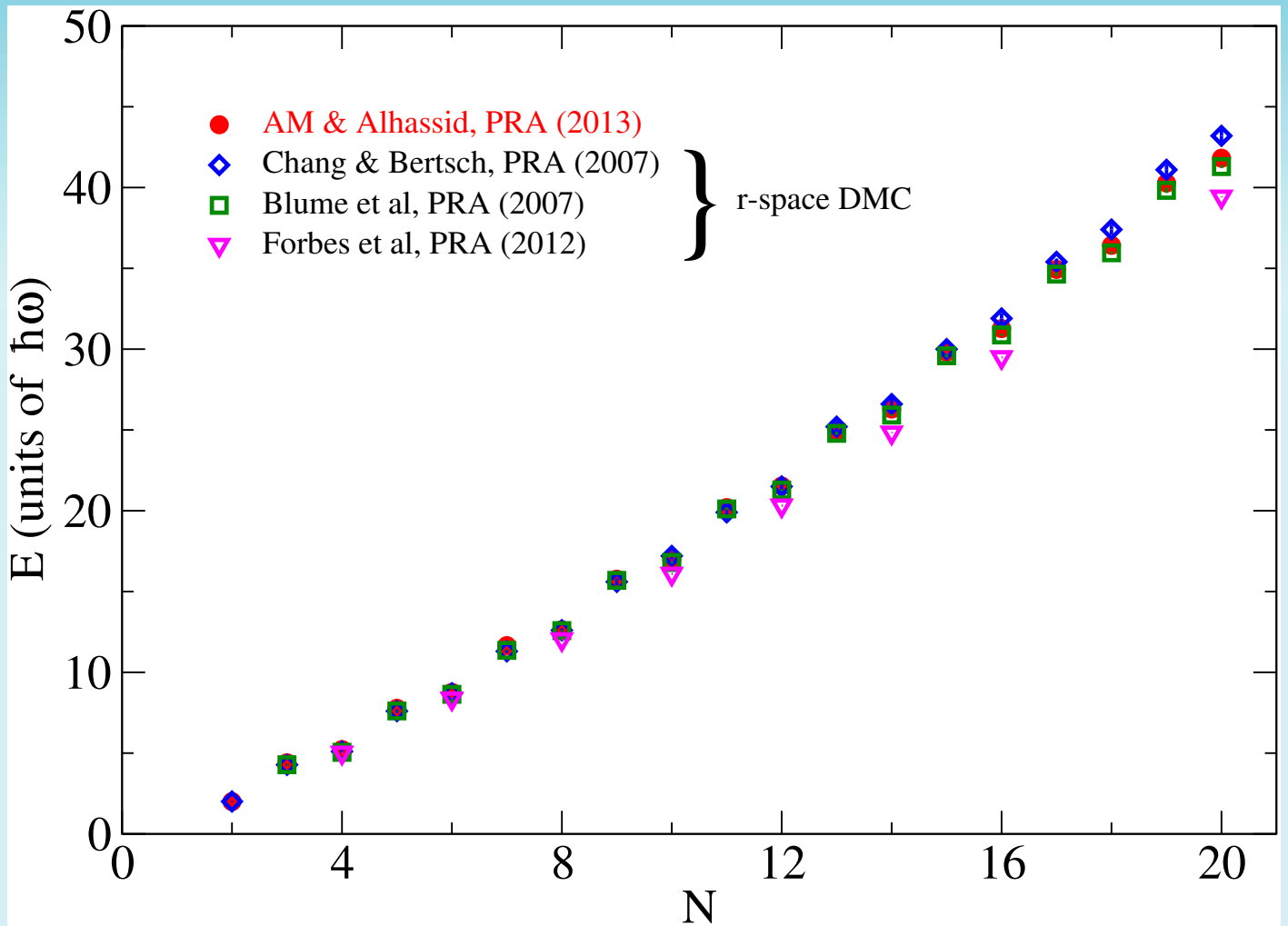




AM & Alhassid, PRA, in press (2013) [arxiv:1304.1645]

Roggero, AM & Pederiva, PRB **88**, *115138 (2013)*

Benchmarking for trapped unitary fermi gas



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Fixing the sign problem with Coupled Cluster w.f.

$$|\Phi_{CC}\rangle = e^{T}|\Phi_0\rangle$$

$$T = \sum t_i^a a_a^\dagger a_i + \sum t_{ij}^{ab} a_a^\dagger a_b^\dagger a_i a_j + \ldots$$

Benefits

- Possible to systematically improve the guiding wf
  CCD (CCSD) $\rightarrow$ CCDT (CCSDT) $\rightarrow \ldots$
- Well tested in many systems

Challenge

- Calculating overlaps $\langle \cdots 0100110 \cdots | \Phi_{CC} \rangle$

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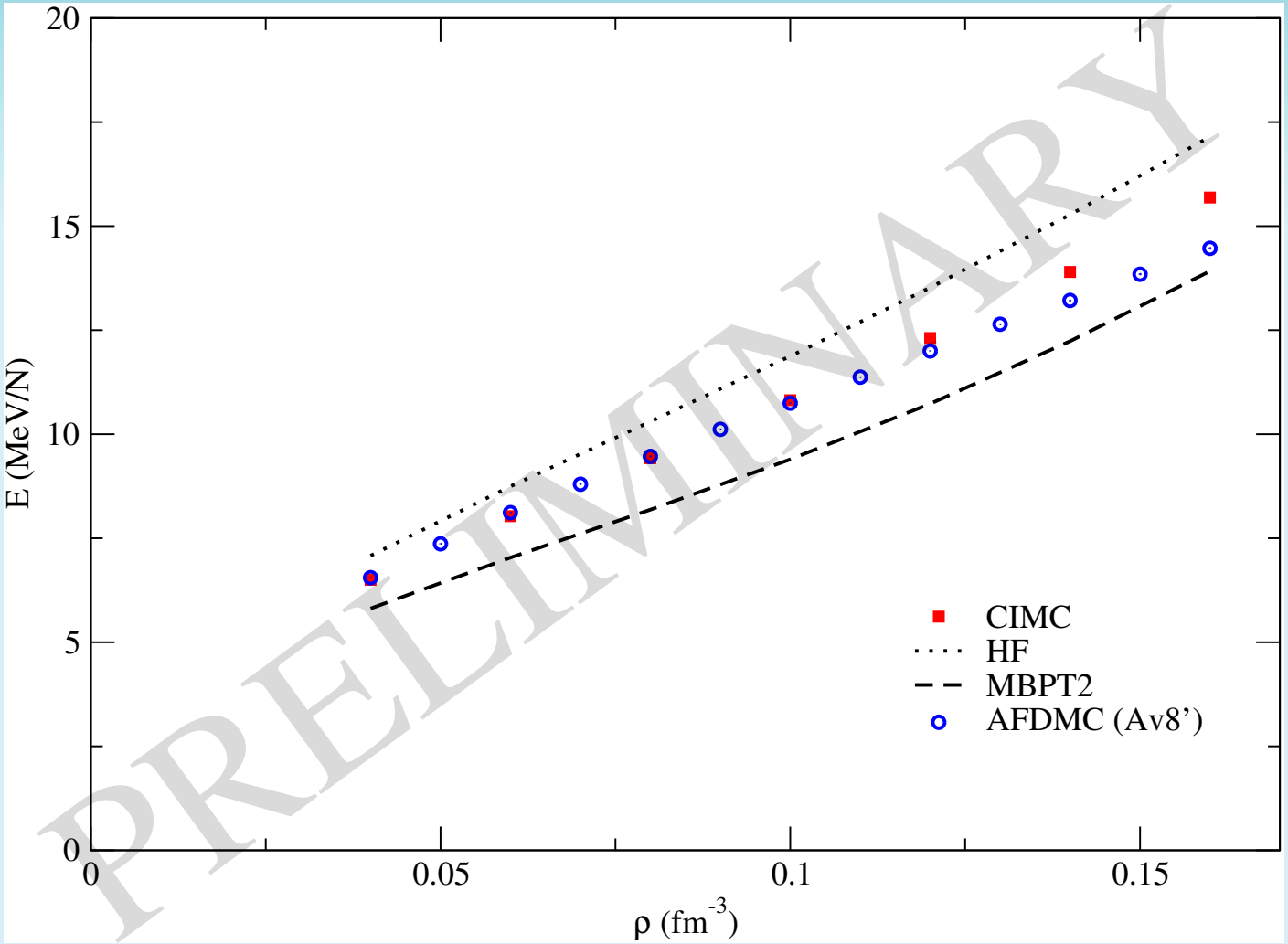
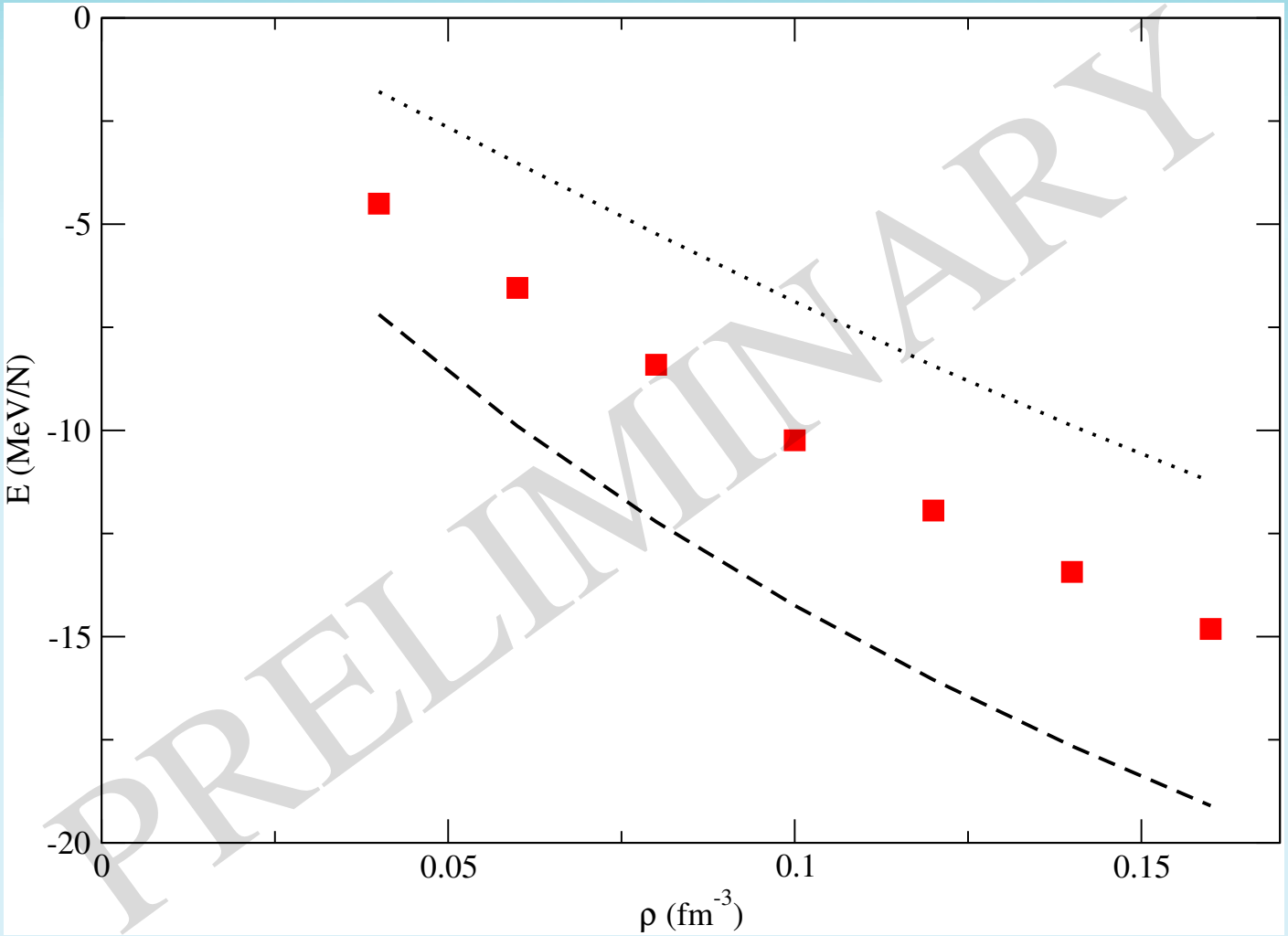
  New recursive algorithm

Neutron matter with NNLO$_{opt}$



Nuclear matter with $NNLO_{opt}$



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Take home messages

- We have a new Fock space QMC method
- QMC calculations with non-local chiral interactions are now possible
- Fixed-phase bias can be systematically improved with CC type wave functions
- 3b forces present no technical challenges (but, more expensive)