Quantum Monte Carlo for the Configuration Interaction framework

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Main issues

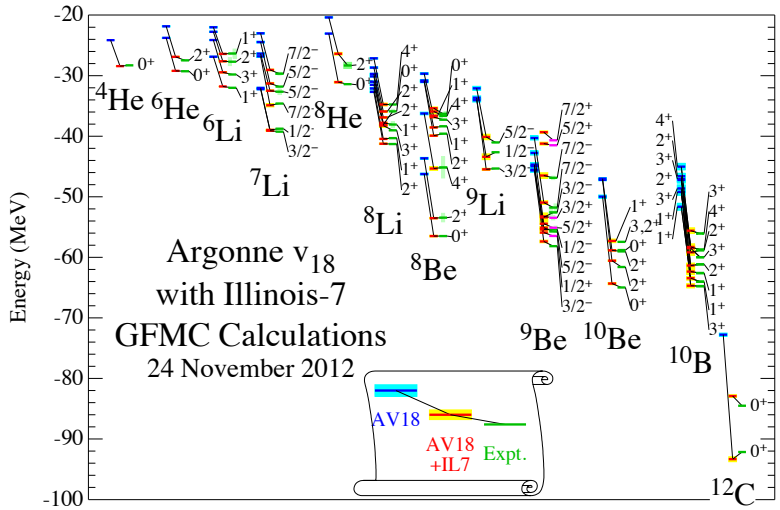
- QMC *a la* fixed-node GFMC in CI/k-space
  QMC with non-local (χ EFT) forces

- Variational energies from CC wave functions
  Standard CC theory is non-variational

- Momentum distribution in QMC
  Very difficult in standard r-space MC

Monte Carlo with a modern interaction

- GFMC is one of the most accurate methods for light nuclei
- AFDMC can potentially be pushed to larger systems/matter
- Great combination of accuracy and scaling



Pieper et al (ANL)

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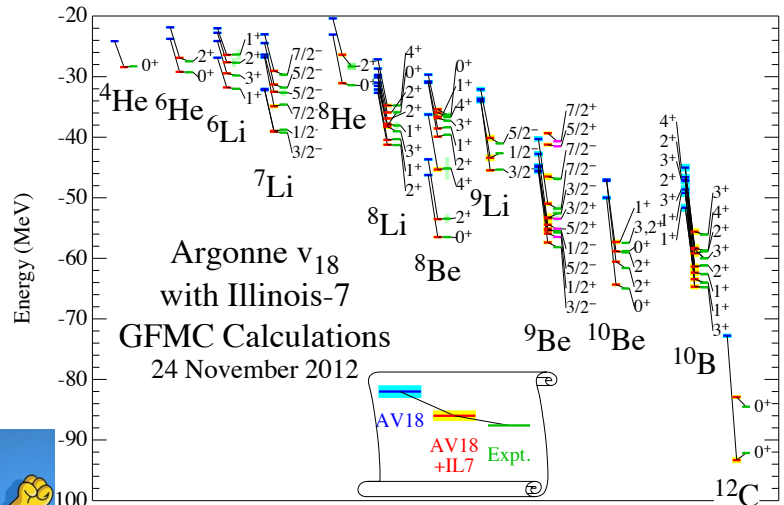

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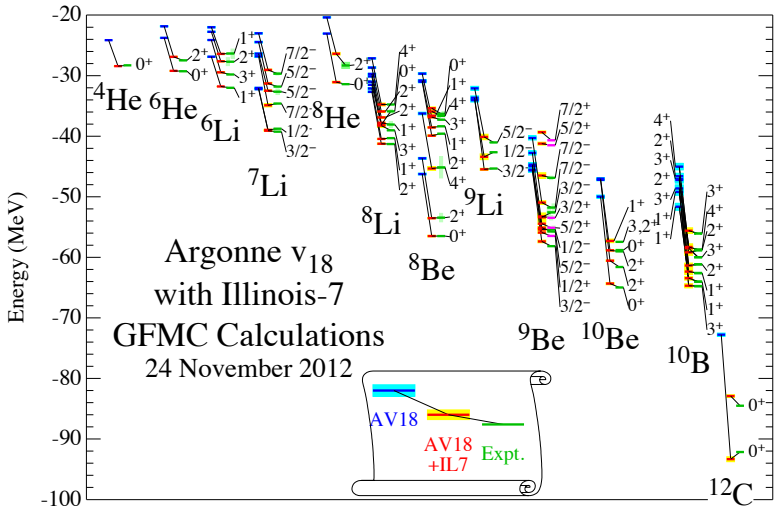
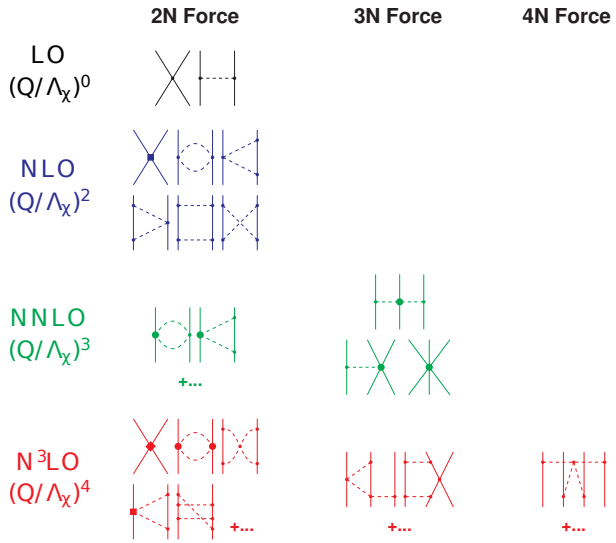


Pieper et al (ANL)

Only works for interactions local in r-space

Urbana-Argonne-Illinois models

Postmodern interactions



Machleidt & Entem, Phys. Rept. (2011)

- Effective
- Cutoff-dependent
- Non-local

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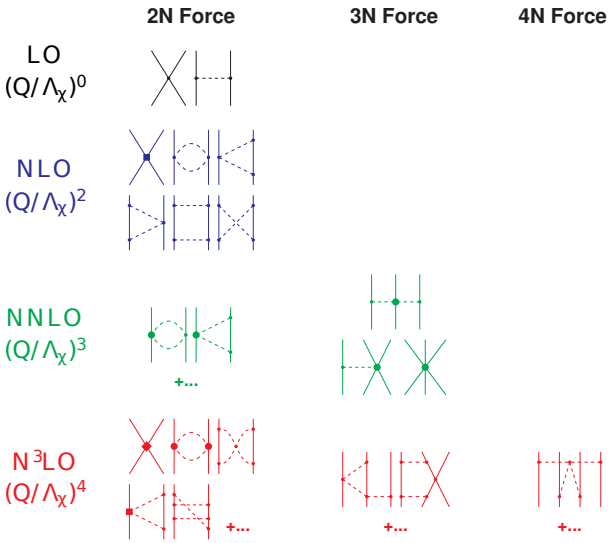

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Cannot apply r-space GFMC/AFDMC

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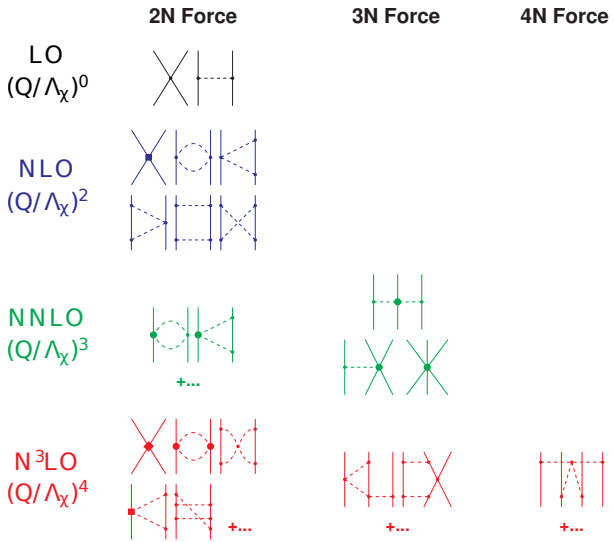

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Cannot apply r-space GFMC/AFDMC

The natural framework is CI/k-space

$$H = \sum_{i}^{\Omega} \varepsilon_{ij} a_i^\dagger a_j + \sum_{ijkl}^{\Omega} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k + \ldots$$

What else is out there?

- Direct diagonalization
  - When feasible most accurate
  - Bad scaling (current limit, dim. $\sim 10^{10}$)
  - Monte Carlo SM can push it further
- Monte Carlo with auxiliary fields (SMMC, Lattice EFT)
  Sign problem
  - Shifted contour
  - Complex Langevin
  - Lefschetz thimble?
    Cristoforetti, di Renzo & Scorzato, PRD (2012)
    Cristoforetti, di Renzo, AM & Scorzato, arxiv:1303:7204 (2013)
    AM, Cristoforetti & Scorzato, in preparation (2013)
- Localize the EFT + AFDMC

  Gezerlis et al (2013)

Configuration interaction Monte Carlo

- Use the power method

$$|\Psi_{\text{Ground State}}\rangle = \lim_{N\to\infty} \mathcal{P}^N |\Psi_{\text{Initial State}}\rangle$$

  - Occupation number basis : $|\mathbf{n}\rangle = |\ldots 0101\ldots\rangle$
  - Interpret $\mathcal{P}_{\mathbf{mn}}$ as transition probabilities

- Propagator
  - Simplest choice: $\mathcal{P} = (1 - \Delta\tau H)$
  - In reality we use more efficient propagators : $e^{-\Delta\tau(H-E_T)}$

Configuration interaction Monte Carlo

$$\mathcal{P} = 1 - \Delta\tau H \rightarrow |\Psi_{\tau+\Delta\tau}\rangle = \mathcal{P}|\Psi_\tau\rangle$$

$$\Psi_{\tau+\Delta\tau}(\mathbf{m}) = \sum_{\mathbf{n}} \langle \mathbf{m}|\mathcal{P}|\mathbf{n}\rangle \Psi_\tau(\mathbf{n})$$

$$= \sum_{\mathbf{n}} \left(\frac{\langle \mathbf{m}|\mathcal{P}|\mathbf{n}\rangle}{\sum_{\mathbf{m}} \langle \mathbf{m}|\mathcal{P}|\mathbf{n}\rangle} \right) \left(\sum_{\mathbf{m}} \langle \mathbf{m}|\mathcal{P}|\mathbf{n}\rangle \right) \Psi_\tau(\mathbf{n})$$

$$= \sum_{\mathbf{n}} \underbrace{p(\mathbf{m},\mathbf{n})}\, \underbrace{w(\mathbf{n})}\, \Psi_\tau(\mathbf{n})$$

Transition probability — Branching

MC sampling not possible if $p(\mathbf{m},\mathbf{n}) < 0$

$\Longrightarrow \langle \mathbf{m}|H|\mathbf{n}\rangle > 0 \longrightarrow$ sign problem

Exception: pure pairing H *AM, Alhassid & Bertsch, PRC (2011)*

Configuration interaction Monte Carlo

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- There is a sign problem for the generic case
- We need to somehow construct non-negative propagators

Transition probability Branching

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Hard problem: Propagator

How to choose a non-negative propagator?

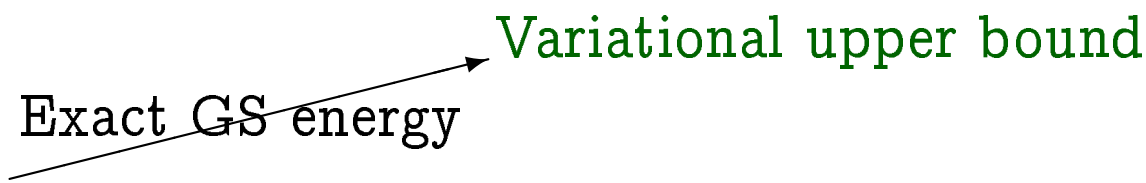
Borrow from lattice-GFMC (discrete, finite Hilbert space)

ten Haaf et al PRB (1995)

- Use importance sampling to circumvent the sign problem

$$\mathcal{P} \longrightarrow \mathcal{P}_{\text{new}}(\Phi_G) \geq 0$$

- But there is a price



- Better $\Phi_G \implies$ tighter bound
- $E_{CIMC} \leq \langle \Phi_G | H | \Phi_G \rangle$

AM & Alhassid, arxiv:1304.1645 (2013)

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How to choose the importance function Φ_G?

bund

~~Exact GS energy~~

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Harder problem: wave function

The importance function should be:

- Accurate/Flexible: Should be able to include the major correlations in the system
- Calculable : Need a fast algorithm to calculate it on a computer (fast = at most polynomial in N and/or Ω)

- Plenty of experience in r-space (~ 50 years)
- Almost none is CI/k-space
- 'Fourier' transform of r-space wave functions (e.g. Jastrow-Slater) does not work

Harder problem: wave function

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Can we get known CI w.f.s to work with MC?

- Plenty of experience in r-space (~ 50 years)
- Almost none is CI/k-space
- 'Fourier' transform of r-space wave functions (e.g. Jastrow-Slater) does not work

Antisymmetric geminal power

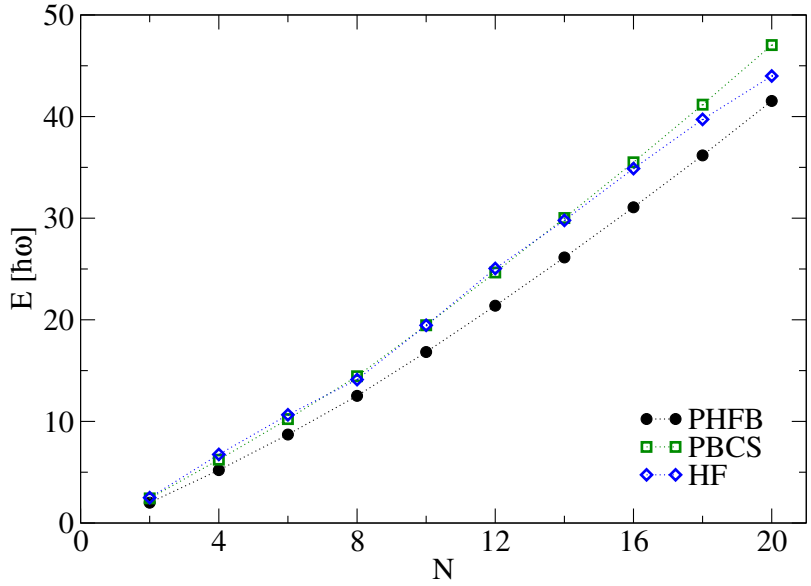
- For even N

$$|\Phi_{\mathrm{AGP}}\rangle = \left(\phi_{ij} a_i^\dagger a_j^\dagger\right)^{N/2} |0\rangle$$

- For odd N, we put the additional particle in a general sp orbital
- Fast algorithms : $\langle \mathbf{n}|\Phi_G\rangle$ is a Pfaffian ($\sim N^3$).
- Very flexible : can include different kinds of 2b correlations
- HFB, BCS, HF are special cases

Trapped unitary fermi gas

- Atoms in a harmonic trap
- Contact interaction among $\uparrow$ and $\downarrow$ spins only
- In this case $\langle \mathbf{n} | \Phi_G \rangle$ is a determinant!



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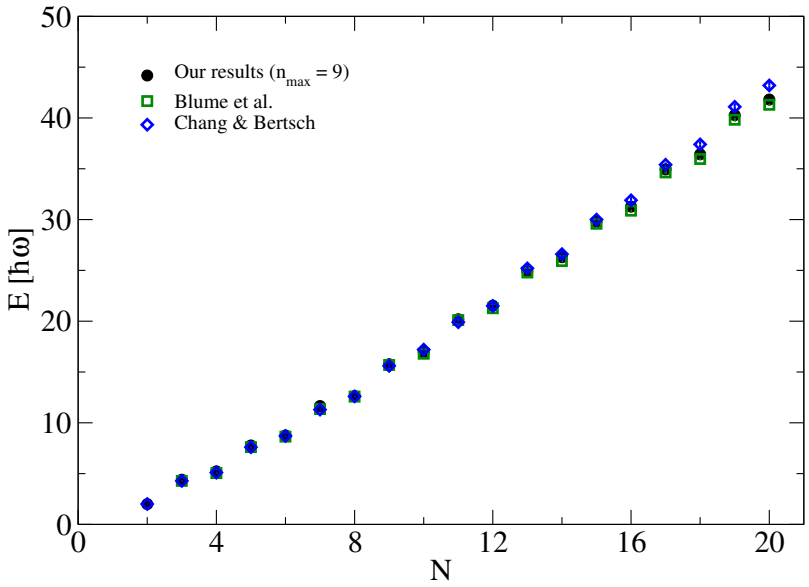

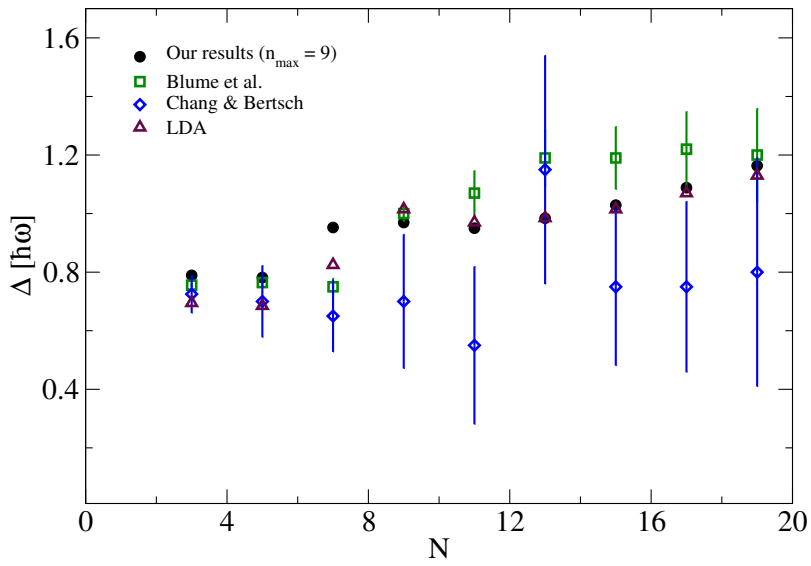

Coupled Cluster wave functions

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

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

- Different truncations for T lead to different approximations CCD, CCSD, CCSDT ...
- Accurate: CCSD(T) is 'gold standard' in chemistry ✓
- Energies not variational in the standard approach ✗

Can we calculate $\langle n|\Phi_{CC}\rangle$ quickly?

The magic formula

Start with Coupled Cluster Doubles (good for uniform systems):

$$\Phi^{m}_{CCD}\left(\begin{smallmatrix} p_1 p_2 \cdots p_m \\ h_1 h_2 \cdots h_m \end{smallmatrix}\right) = \Phi_{CCD}(\mathbf{n})$$

for

$$|\mathbf{n}\rangle = a^{\dagger}_{p_1} \ldots a^{\dagger}_{p_m} a_{h_1} \ldots a_{h_m} |\Phi_{HF}\rangle$$

Recursive formula:

$$\Phi^{m}_{CCD}\left(\begin{smallmatrix} \cdots \\ \cdots \end{smallmatrix}\right) = \sum_{\gamma=2}^{m} \sum_{\mu<\nu}^{m} (-)^{\gamma+\mu+\nu} t^{p_\mu p_\nu}_{h_1 h_\gamma} \Phi^{m-2}_{CCD}\left(\begin{smallmatrix} \cdots \\ \cdots \end{smallmatrix}\right)$$

Roggero, AM & Pederiva, arxiv:1304.1549 (2013)

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- Can be easily generalized to CCSD, CCSDT ...
- Scaling only with # ph
- No scaling with particle number or basis size!

Roggero, AM & Pederiva, arxiv:1304.1549 (2013)

Results for 3DEG

- The 3d electron gas is the 'longest range' Hamiltonian.
- Opposite limit of the contact interaction
- Good benchmark, many calculations available

How to do CIMC?

- Lattice in momentum space
- Single particle basis = plane waves
- Include all sp states up to some k_{max}

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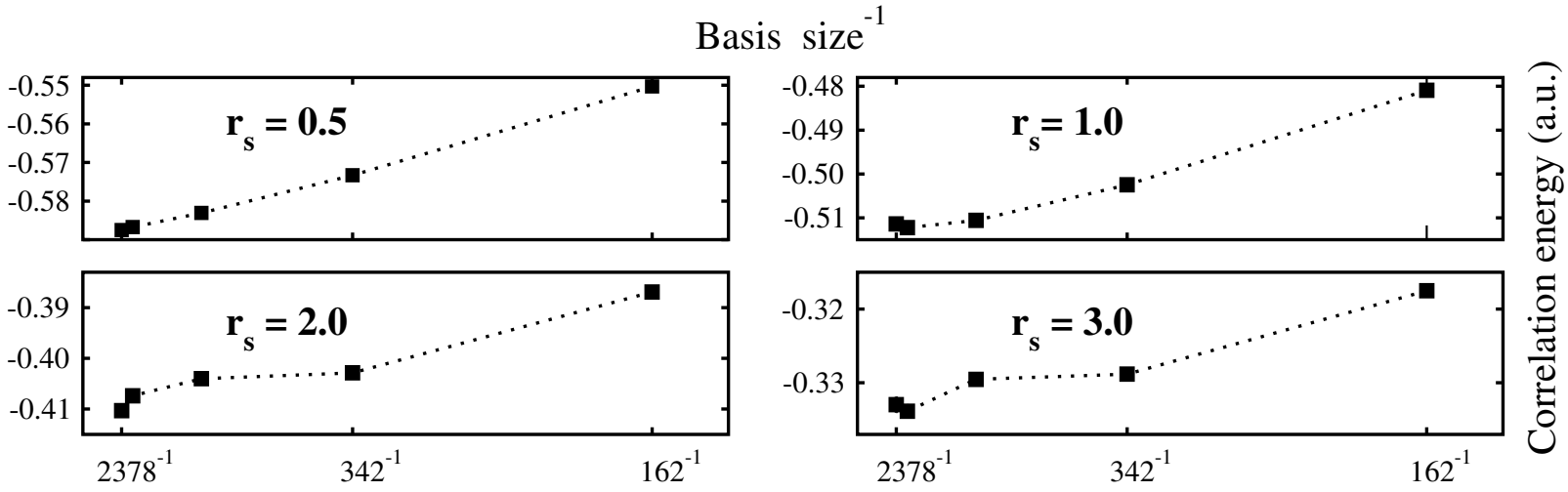

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- CCD + CIMC captures $\sim 95\%$ of the correlation energy
- No adjustable parameters in the wf
- Accuracy comparable to r-space MC
- Can improve systematically: CCDT, ...

Roggero, AM & Pederiva, arxiv:1304.1549 (2013)

What have we acheived, so far?

- Formulated 'Fixed-node' GFMC in CI/k-space ✓
- Shown how to use two well known classes of accurate wave functions as importance functions ✓
- Supervariational energies from CC wave functions
  Remember

$$E_{GS} \leq E_{CIMC} \leq \langle \Phi_G | H | \Phi_G \rangle$$

  when $\Phi_G \equiv \Phi_{CC}$

$$E_{GS} \leq E_{CIMC} \leq \langle \Phi_{CC} | H | \Phi_{CC} \rangle \quad \checkmark\checkmark\checkmark!!!$$

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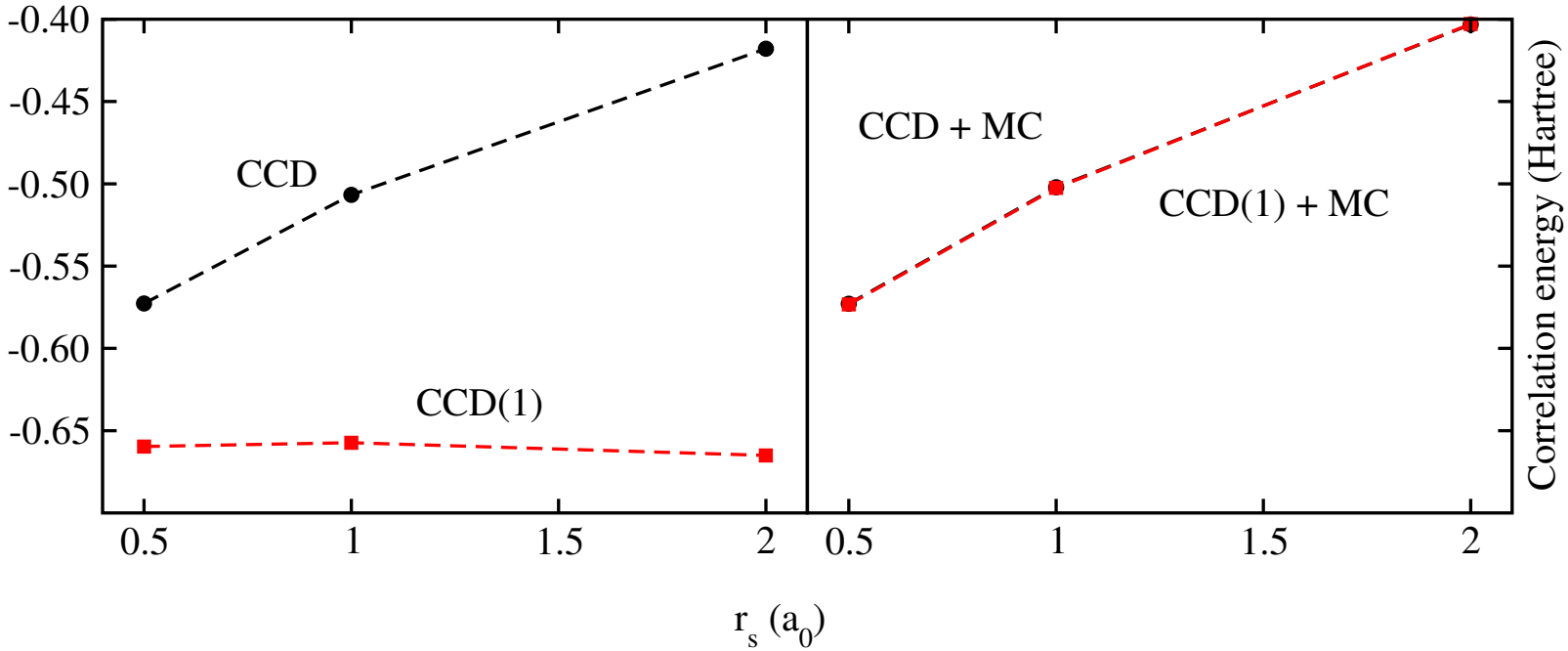
But, we can do better ...

Sign-structure important, not exact amplitudes



- CCD(1) = CCD wf with amplitudes taken from 2nd order perturbation theory
- Huge saving in computational time
- Can be very important for CCSD(T)

Fringe benefits: momentum distribution

- Very hard to calculate in r-space MC
- Howver, its diagonal in k-space ✓
- We can even calculate pure estimators ✓
  - Typically in DMC/GFMC one calculates $\langle \Phi_G | \mathcal{O} | \Psi \rangle$
  - Not the same as $\langle \Psi | \mathcal{O} | \Psi \rangle$, if $[\mathcal{O}, H] \neq 0$
  - But in CIMC we can calculate $\langle \Psi | \mathcal{O} | \Psi \rangle$ using the Feynman-Hellmann theorem

$$\langle \Psi | n_k | \Psi \rangle = \left. \frac{\partial \langle H + \alpha n_k \rangle}{\partial \alpha} \right|_0 = \langle \Phi_G | n_k | \Psi \rangle - \text{const.} \times \text{cov}(E, n_k)$$

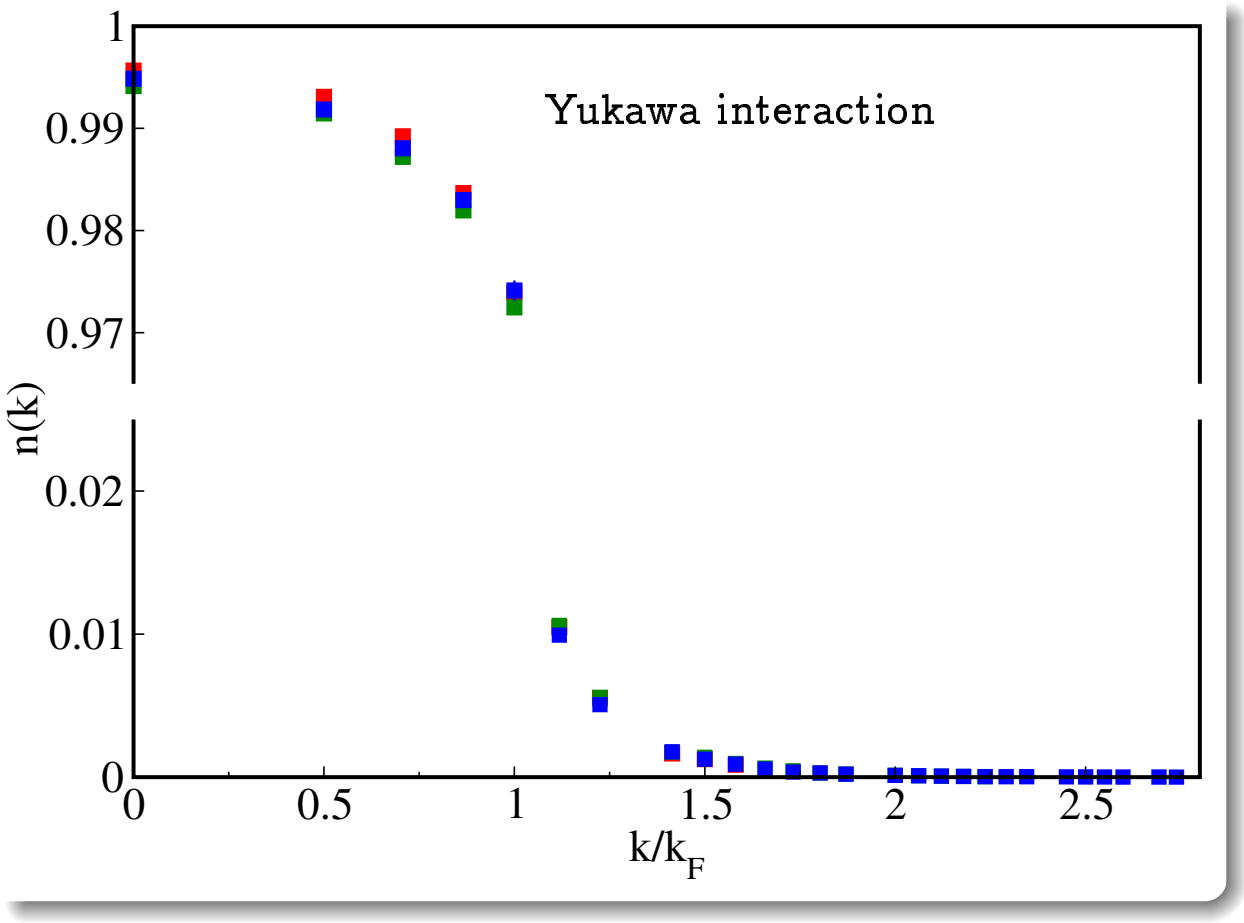
No need to calculate numerical derivatives! ✓

Gaudin & Pitarke, PRL (2007)

Roggero, AM & Pederiva, in preparation

Fringe benefits: momentum distribution

- Very hard to calculate in r-space MC
- Hc
- W



$\rangle$

$\mathrm{ov}(E, n_k)$

Roggero, AM & Pederiva, in preparation

Take home messages

- Can we do fixed-node GFMC in CI/k-space with non-local interactions?
  Yes, we can!
- Can we get variational energies from CC wave functions?
  We can get supervariational energies
- We have pure estimators for the momentum distribution
- The time for benckmarking is over. Now, onward to nuclei!

Fixing the sign problem in Fock space

- Comes from the Hamiltonian (if $H_{mn} > 0$ for $m \neq n$)
- Carrying walker sign leads to a null state
- No concept of 'continuity' in discrete Fock space
- Node fixing not possible 

Fixed 'sign' Hamiltonian

$$[\mathcal{H}_\gamma]_{mn} = \delta_{mn}\{H_{nn} + (1+\gamma)\sum_{s_{nn'}>0} \Phi_G(n')H_{n'n}\Phi_G(n)^{-1}\}$$
$$+ (1-\delta_{mn})\{\gamma\Theta(s_{mn}) + \Theta(-s_{mn})\}H_{mn}$$

where $s_{mn} = \text{sign}\{\Phi_G(m)H_{mn}\Phi_G(n)^{-1}\}$

Fixing the sign problem in Fock space

$$[\mathcal{P}_\gamma]_{\mathbf{mn}} = \Phi_G(\mathbf{m}) \left\{ \delta_{\mathbf{mn}} - \Delta\tau \left([\mathcal{H}_\gamma]_{\mathbf{mn}} - E_T \delta_{\mathbf{mn}} \right) \right\} \Phi_G^{-1}(\mathbf{n})$$

- $\mathcal{H}_{\gamma=-1} = H$
- $\mathcal{H}_{0 \le \gamma \le 1}$ has no sign problem by construction
- GS energies of $\mathcal{H}_{0 \le \gamma \le 1}$ provide upper bounds for the GS energy of H
- So does any linear extrapolation to $\gamma = -1$

ten Haaf et al., PRB (1995); Sorella & Capriotti, PRB (2000); Beccaria, PRB (2001)
AM & Alhassid, arxiv:1304.1645 (2013)

Our tightest upper bound for GS energy of H is :

$$E_{CIMC} = \mathbf{2E}_{GS}[\mathcal{H}_{\gamma=0}] - \mathbf{E}_{GS}[\mathcal{H}_{\gamma=1}]$$