Quantum Monte Carlo for Chiral Efective Field Theory potentials

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G. Hagen (ORNL), T. Papenbrock (UT)

Cortona - 29 Oct, 2013

Outline of the talk

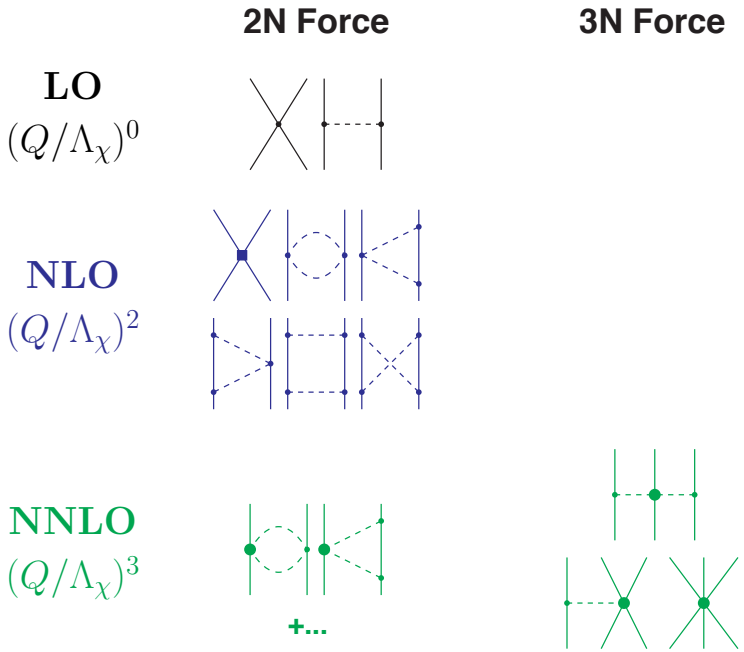
- Motivations
  - χ-EFT interactions
  - Monte Carlo and non–local potentials
- Configuration Interaction Monte Carlo
  - Quantum Monte Carlo in 2nd quantization
  - Sign-Problem and Coupled Cluster wave–functions
- Applications
  - (Benchmark) Coulomb gas in momentum–space
  - Neutron matter

Chiral Effective Field Theory (χ-EFT) interactions

- pions interact weakly at small energies (Goldstone bosons)

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

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



- short range contact–interaction + pions
- many–body forces predicted in model–independent way

R. Machleidt, D. R. Entem,
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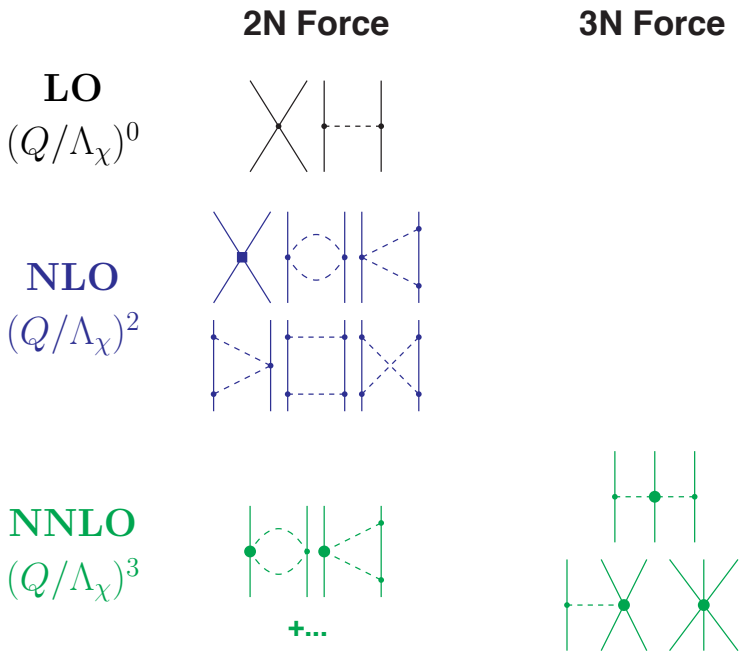

- short range contact–interaction + pions
- many–body forces predicted in model–independent way
- non–local in coordinate–space ($\geq$NLO)

$$H\Psi(x) = T\Psi(x) + V(x)\Psi(x)$$
$$\rightarrow T\Psi(x) + \int dy\ V(x,y)\ \Psi(y)$$

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Locality is needed for conventional QMC

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

Monte Carlo methods

Use a projection operator to filter the ground–state

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

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

the projection is then performed stochastically.

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The Standard Way

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

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

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

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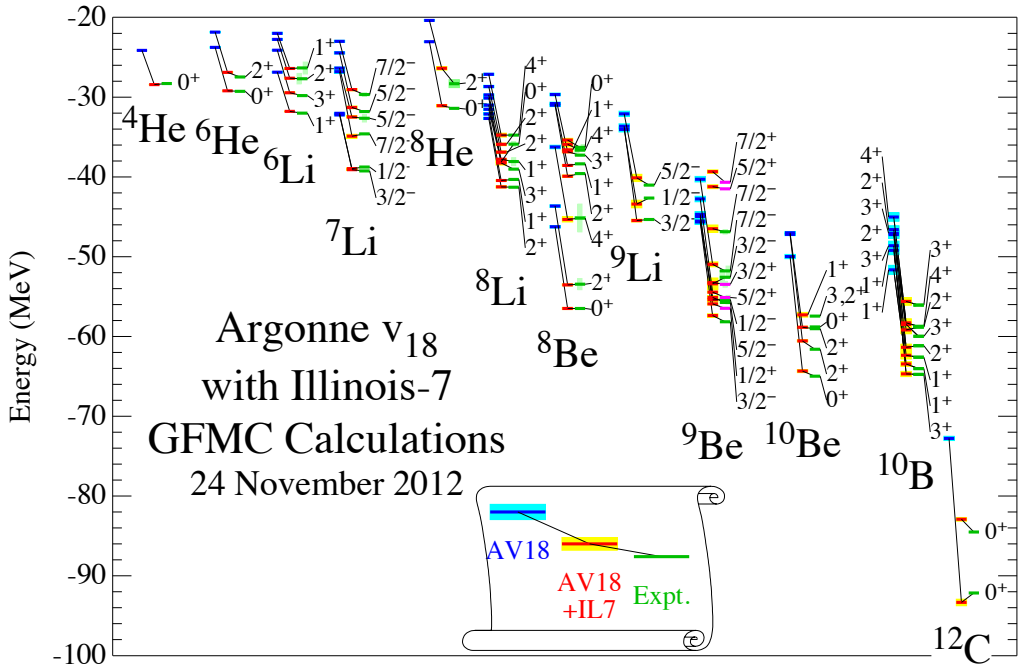

S. Pieper, R. Wiringa et. al (ANL)

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The Standard Way

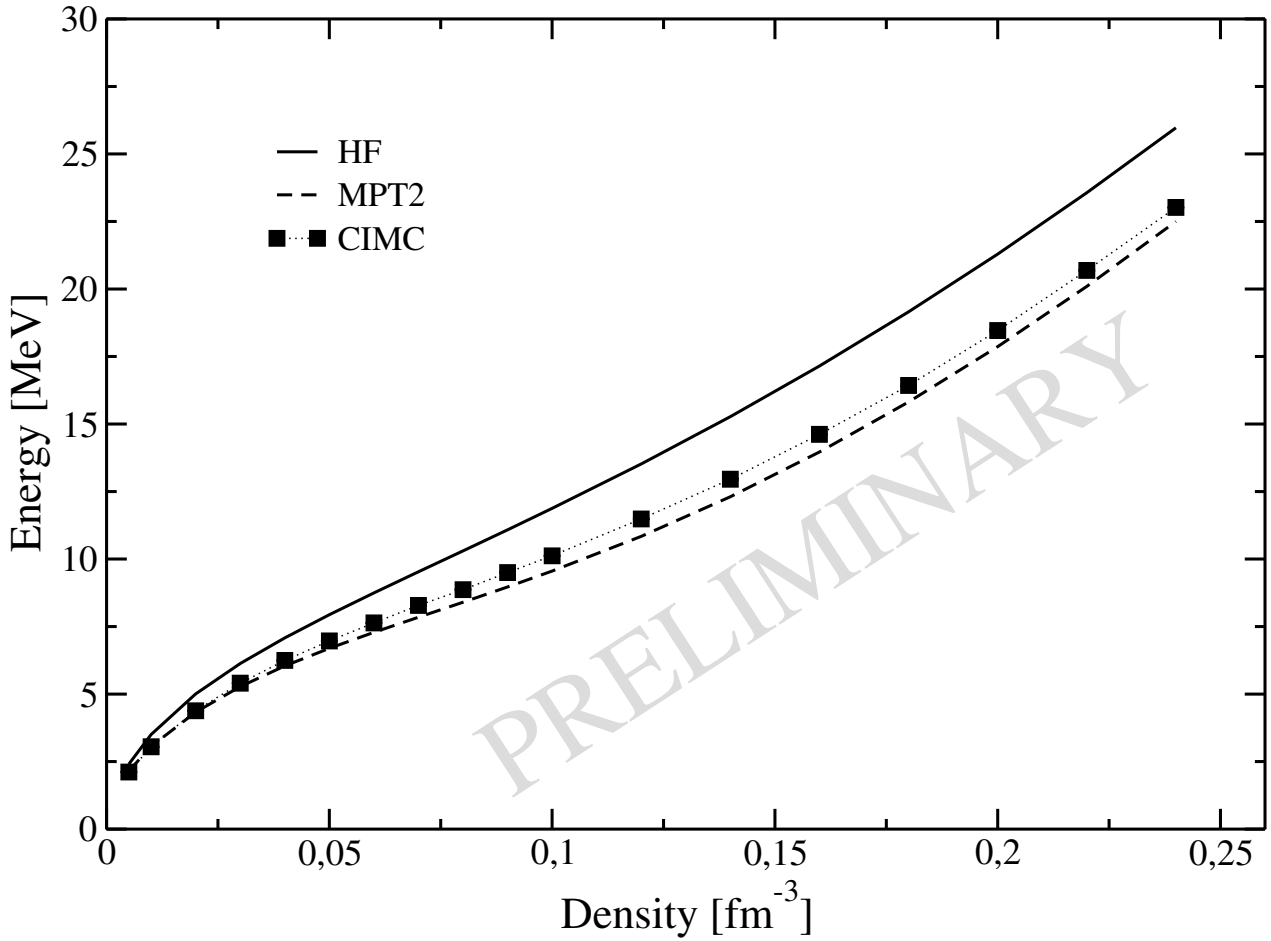
- work in coordinate–space
- for non–local interactions the projector doesn't factor

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

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

Neutron Matter with χ-EFT interactions at N2LO

We considered χ-EFT interaction at N2LO using the LEC coming from the optimized *POUNDerS* analysis [Ekstrom et al., PRL 110, 192502 (2013)]



Help from Second Quantization

$$\hat{H} = \sum_{a}^{\Omega} \epsilon_a \hat{a}_a^\dagger \hat{a}_a + \frac{1}{2} \sum_{ijkl}^{\Omega} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l + \ldots$$

- A general V_{ijkl} leads to non–local interactions
  - $\longrightarrow$ locality is a very stringent condition!!

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The Second Quantized Way (Configuration Interaction MC)

- work in occupation number basis: $|\mathbf{n}\rangle = |\dots 01100010 \dots\rangle$
- for any interaction the projector can be written as

$$\begin{aligned} \langle \mathbf{m}|\hat{P}|\mathbf{n}\rangle &= \left(\frac{\langle \mathbf{m}|\hat{P}|\mathbf{n}\rangle}{\sum_{\mathbf{m}} \langle \mathbf{m}|\hat{P}|\mathbf{n}\rangle} \right) \left(\sum_{\mathbf{m}} \langle \mathbf{m}|\hat{P}|\mathbf{n}\rangle \right) \\ &= p(\mathbf{m},\mathbf{n}) w(\mathbf{n}) \end{aligned}$$

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$$= p(\mathbf{m},\mathbf{n}) \quad w(\mathbf{n}) \longleftarrow p(\mathbf{m},\mathbf{n}) > 0$$

Circumventing the sign–problem

In coordinate–space we deal with the the sign problem using the so–called "fixed–node approximation" which employs an approximate ansatz Ψ_T:

$$P(\mathbf{m},\mathbf{n}) \;\rightarrow\; P_{FN}(\mathbf{m},\mathbf{n}) = \Psi_T(\mathbf{m}) P(\mathbf{m},\mathbf{n}) \Psi_T^{-1}(\mathbf{n})$$

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A good Ψ_T should be

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–> we found an efficient way to use Coupled Cluster wave–functions!!

Towards χ-EFT interactions

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

[A. R., A. Mukherjee and F. Pederiva **Phys. Rev. B 88,115138**]

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Coulomb

$$\langle p|\hat{V}|p'\rangle \propto \frac{1}{(p-p')^2}$$

- depends only on mom. transfer $q = p - p'$
- diagonal in spin space
- real matrix elements

NNLO χ-EFT

$$\langle p|\hat{V}|p'\rangle \propto V_{1\pi}(p-p') + V_{2\pi}(p,p') + V_{cont}(p,p')$$

- depends separately on p and p'
- non–trivial spin–isospin structure
- complex matrix elements

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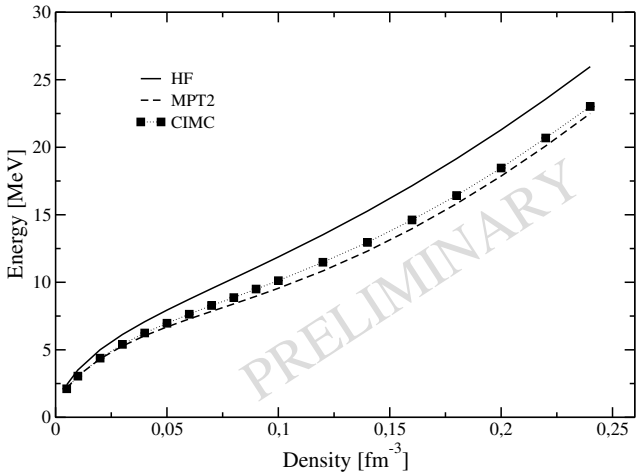
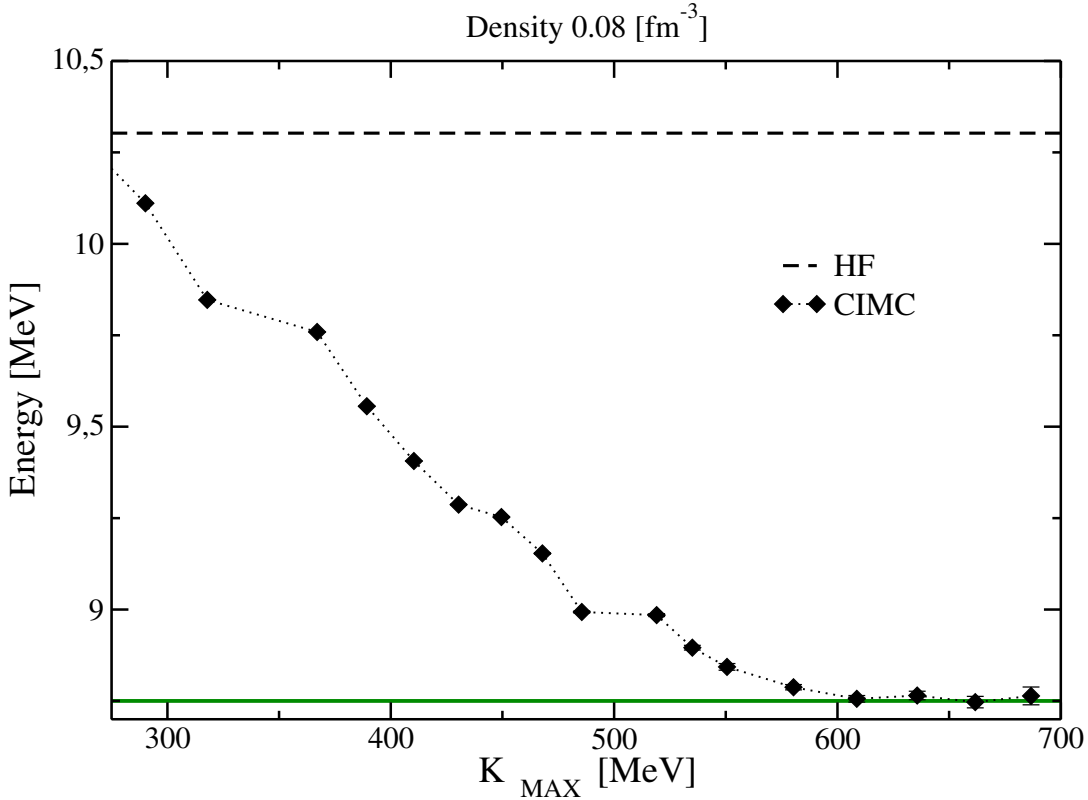
CIMC can be extended to the complex case, preserving

$$\langle \Psi_0|\hat{H}|\Psi_0\rangle \leq \langle \Psi_{CIMC}|\hat{H}|\Psi_{CIMC}\rangle \leq \langle \Psi_T|\hat{H}|\Psi_T\rangle$$

Neutron Matter with χ-EFT interactions at N2LO

- single–particle space $\mathcal{S} = \{$ plane waves $| \; k^2 <= K^2_{MAX} \}$





Conclusions

Summary:

- we have developed a MC method that works for general interactions providing rigourus upper–bounds on energy
- the use of Coupled Cluster Wave–functions serves a dual pourpose:
  - extremely good guiding wave–function
  - provides variational energies for CC solutions

Future work:

- three–body forces
- finite nuclei
- response functions [Pederiva's talk]

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Thanks for your attention

Wave–functions for Importance Sampling

A very accurate way to account for correlations in a generic Fock–space is the Coupled Cluster ansatz:

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

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

Is the CCD wave–function even quick to evaluate in SD space?

We need to calculate

$$\Phi^m_{\mathrm{CCD}}\left(\begin{smallmatrix} p_1 p_2 \cdots p_m \\ h_1 h_2 \cdots h_m \end{smallmatrix}\right) = \Phi_{\mathrm{CCD}}(\mathbf{n}) \quad \text{for} \quad |\mathbf{n}\rangle = a^\dagger_{p_1}\dots a^\dagger_{p_m} a_{h_1}\dots a_{h_m}|\Phi_{\mathrm{HF}}\rangle$$

It turns out that one can write a **recursive formula** ([arXiv:1304.1549])

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

Benchmark: Coulomb gas in momentum–space

[A. R., A. Mukherjee and F. Pederiva **Phys. Rev. B 88,115138**]

- weakly and strongly correlated regimes accessible tuning a single density–parameter: r_s (Wigner–Seitz radius)
- single–particle space $\mathcal{S} = \{ \text{ plane waves } | \; k^2 <= K^2_{MAX} \}$

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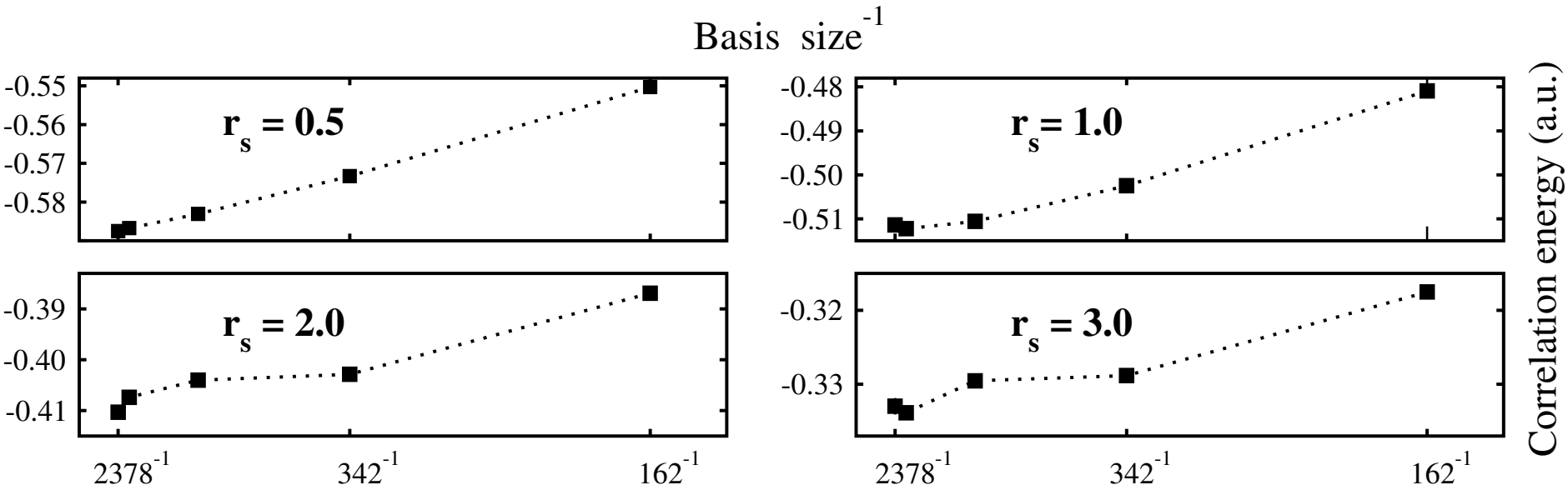

Results compare well with R–space MC with *state of the art* WF.