Diffusion Monte Carlo in momentum space based on Coupled Cluster wave functions

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Otranto - 31 May, 2013

Outline of the talk

- Ab–initio methods for nuclear structure
  - Direct Diagonalization
  - Monte Carlo
- Configuration Interaction Monte Carlo
  - Quantum Monte Carlo in Fock space
  - Importance Sampling and Sign-Problem
  - Coupled Cluster solutions as trial wave–functions
- Benchmark case: 3D Electron Gas
- Conclusions

Ab-initio methods for nuclear structure

A = 3,4 Several *exact* methods:

- Faddev-Yakubovsky,EIHH,NCSM,..
  (see eg. Kamada [PRC.64.044001])

A >4 Very few *ab–initio* methods

- Hamiltonian matrix diagonalization in basis–function space: NCSM (Navrátil [J.Phys.G.36.083101])
- Stochastic approach in R–space: GFMC

Direct Diagonalization

- choose model single–particle space $\mathcal{S}$
- write the Hamiltonian in the Hilbert space spanned by the N–particle Slater Determinants $|\mathbf{n}\rangle$, where $\mathbf{n} = \{n_a\}$, $n_a = 0, 1$ and $a \in \mathcal{S}$.

$$\hat{H} = \sum_{a \in \mathcal{S}} \epsilon_a \hat{a}_a^\dagger \hat{a}_a + \frac{1}{2} \sum_{abcd \in \mathcal{S}} V_{abcd} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c \hat{a}_d + \dots$$

- write interaction in the model–space
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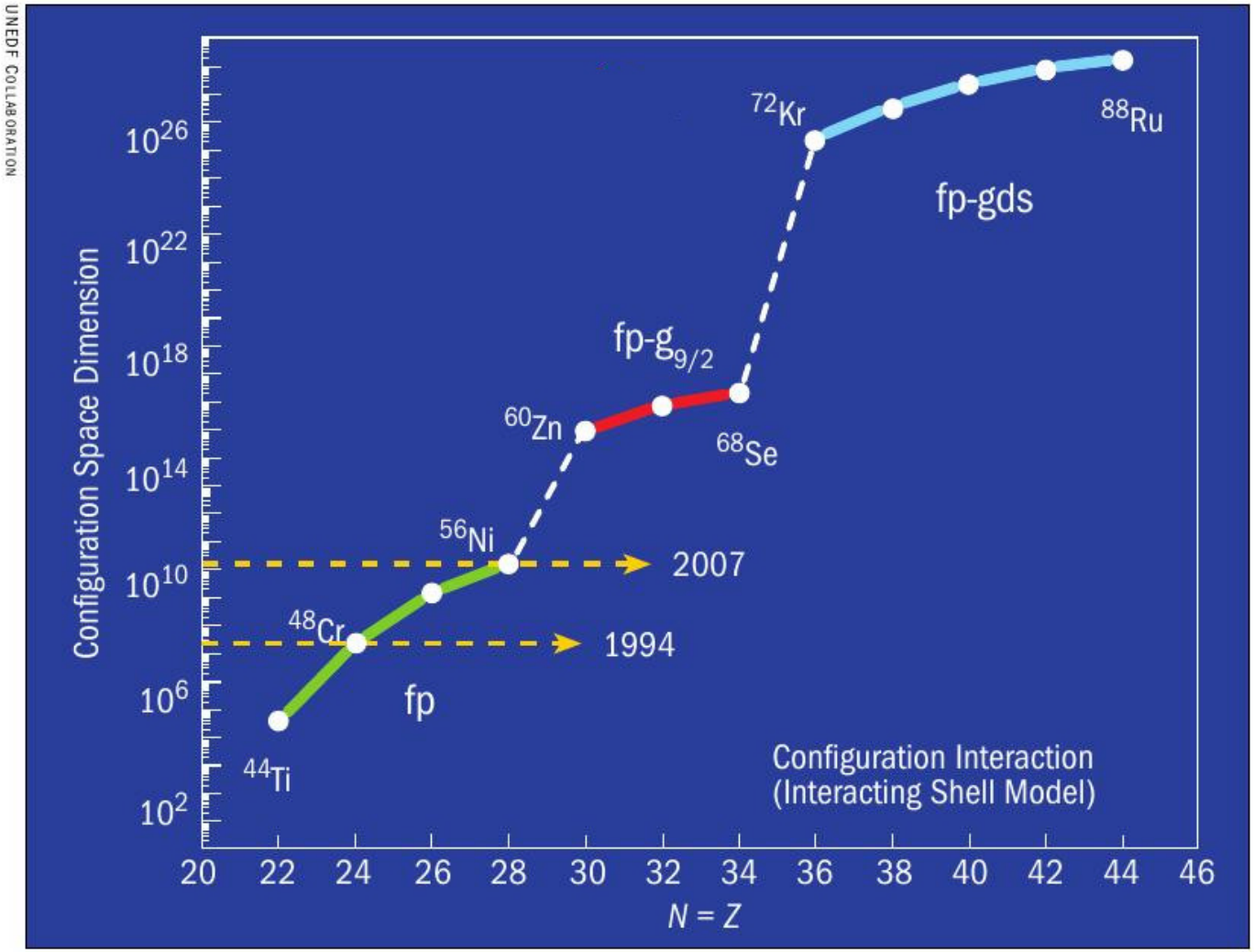
Problem

computational cost $\propto$ to dimension of the A-particle Hilbert space!

Direct Diagonalization



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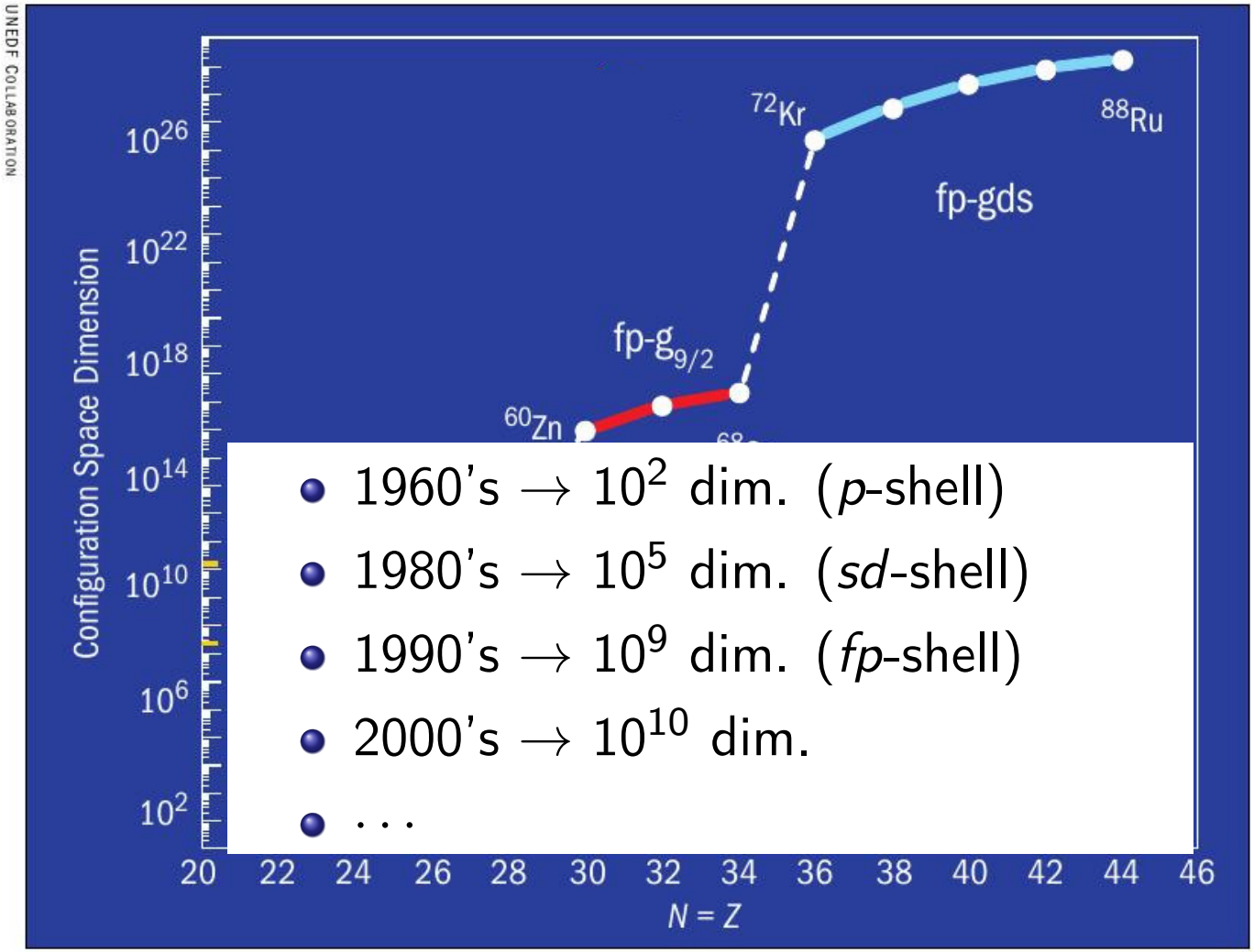

- 1960's $\rightarrow 10^2$ dim. (p-shell)
- 1980's $\rightarrow 10^5$ dim. (sd-shell)
- 1990's $\rightarrow 10^9$ dim. (fp-shell)
- 2000's $\rightarrow 10^{10}$ dim.
- ...

Monte Carlo methods

Use a projection operator to filter the ground–state

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

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

the projection is then performed stochastically.

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- can handle much larger systems
- virtually exact results
- formulation in R–space limits the choice of interactions to a limited class (ie. Argonne-Urbana family)

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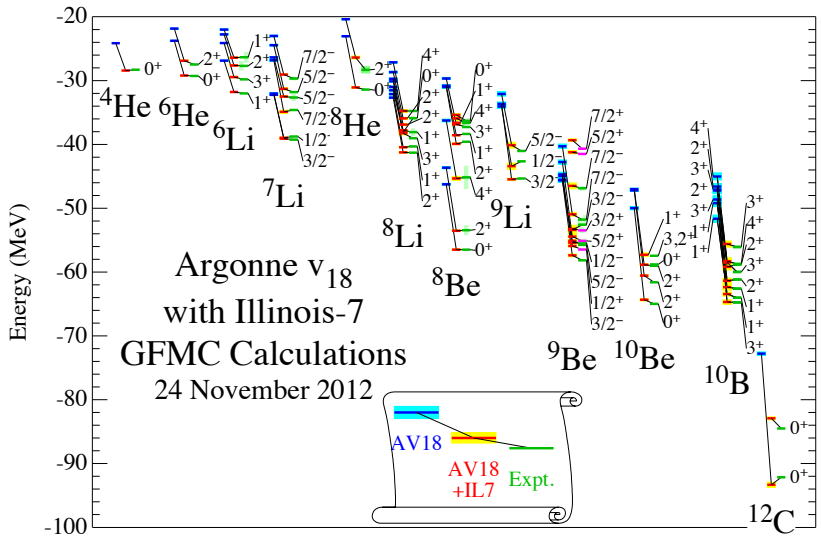

S. Pieper, R. Wiringa et. al (ANL)

What is missing?

We need an ab–initio method that has both:

- a level of accuracy comparable to few-body techniques (DD methods)
- favorable scaling with system–size (MC methods)
- ability to treat general interactions

In general R–space MC are not efficient when used with non–local (ie. momentum dependent) interactions, which unfortunately are very important in many fields:

- χ–EFT potentials in Nuclear Physics
- pseudopotentials in Solid–state Physics

What has been done so far?

- keep R–space as the stage and express EFT potentials in local form (eg. Gezerlis [arXiv:1303.6243])
  - can account only for a limited number of terms
- perform MC in Fock–space
  - use HS–transform to linearize interaction (eg. SMMC: Alhassid [Int.J.Mod.Phys.B15.1447])
    - limited only to certain types of interactions (sign problem)
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    - Configuration Interaction Monte Carlo (**[arXiv:1304.1645]**)

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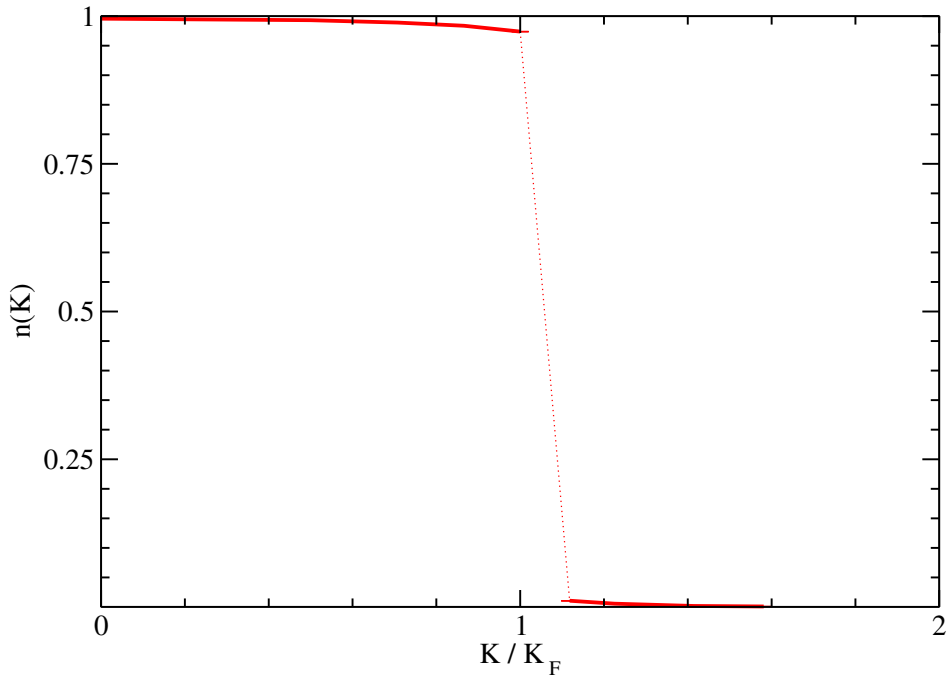
yet another advantage in working on a Fock–space

access to quantities that are extremely difficult to estimate in R–space

- in k–space $\rightarrow$ Momentum Distributions

Easy-access to Momentum Distribution

Preliminary results for $A = 66$ particles with Yukawa interaction



major improvement on current R–space MC methods
(eg. see Holzmann et al [PRL.107.110402])

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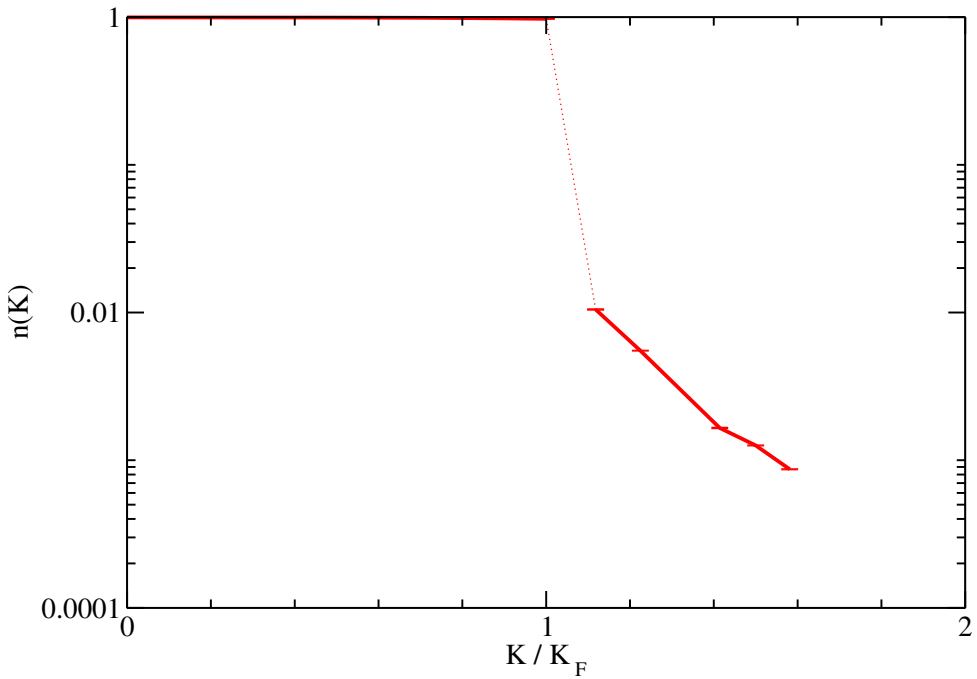

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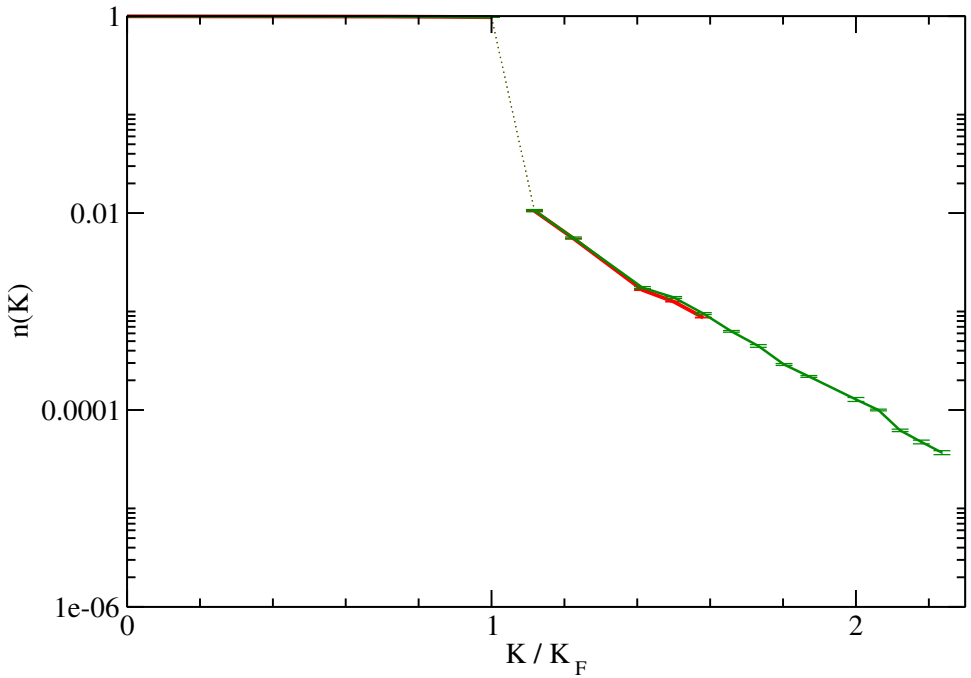

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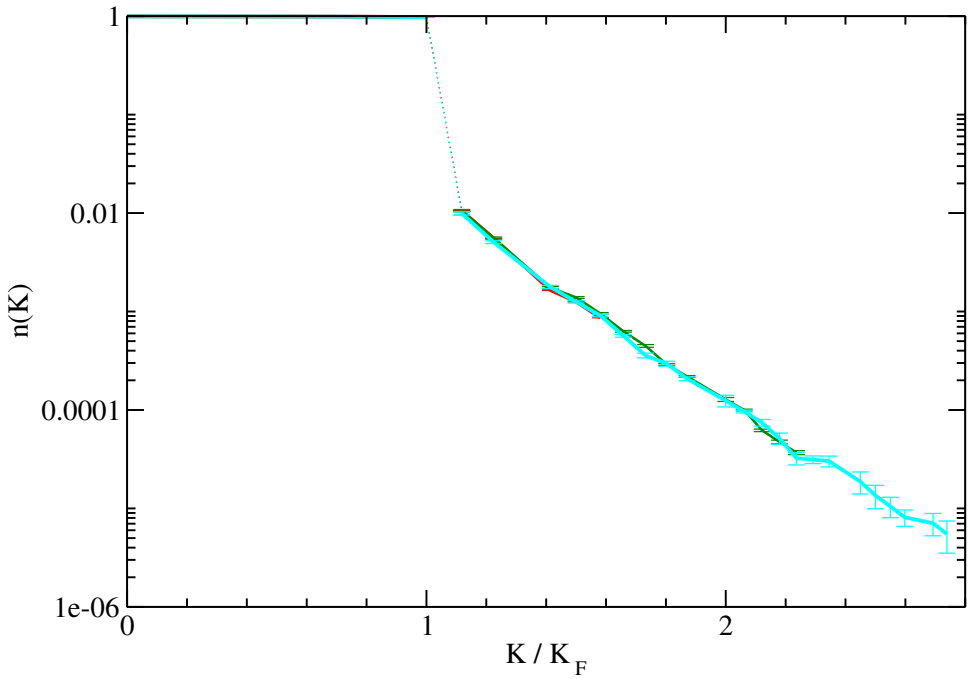

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$$\hat{P} = \hat{1} - \Delta\tau \left(\hat{H} - E_T \right) \rightarrow |\Psi_{\tau+\Delta\tau}\rangle = \hat{P}|\Psi_\tau\rangle$$

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

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

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MC sampling possible if $p(\mathbf{m}, \mathbf{n}) > 0 \rightarrow \langle \mathbf{m}|\hat{H}|\mathbf{n}\rangle > 0$ are problematic !

Configuration Interaction Monte Carlo

In R–space the sign problem is circumvented using the so–called "fixed–node approximation" which employs importance sampling

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

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In SD space we can do something similar (Ceperley et al.[PRB.51.13039])

$$\langle \mathbf{m}|\tilde{P}|\mathbf{n}\rangle = 1 - \Delta\tau\Psi_T(\mathbf{m})\left(\tilde{H}(\mathbf{m},\mathbf{n}) - E_T\right)\Psi_T^{-1}(\mathbf{n})$$

$$\tilde{H}(\mathbf{m},\mathbf{n}) = \begin{cases} H(\mathbf{m},\mathbf{n}) & \text{if } s(\mathbf{n},\mathbf{n}) < 0 \\ 0 & \text{if } s(\mathbf{n},\mathbf{n}) > 0 \end{cases}$$

$$\tilde{H}(\mathbf{n},\mathbf{n}) = H(\mathbf{n},\mathbf{n}) + \sum_{s(\mathbf{m},\mathbf{n})>0} s(\mathbf{m},\mathbf{n})$$

where $s(\mathbf{n},\mathbf{n}) = \Psi_T(\mathbf{m})H(\mathbf{m},\mathbf{n})\Psi_T^{-1}(\mathbf{n})$.

Wave–functions for Importance Sampling

A good Ψ_T should be

- flexible enough to incorporate relevant correlations in the system
- quick to evaluate

In R–space

- almost 50 years of experience in optimizing WF
- extremely good forms are available (Slater/BCS-Jastrow,..)

In K–space

- almost no experience
- FT of R–space WF doesn't work (high–k tails)

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: $\hat{T} = \hat{T}_2 = \frac{1}{2}\sum_{ij,ab} t_{ij}^{ab}\hat{a}_a^\dagger\hat{a}_b^\dagger\hat{a}_j\hat{a}_i$.

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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])

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

Benchmark: 3DEG in momentum–space [arXiv:1304.1549]

- 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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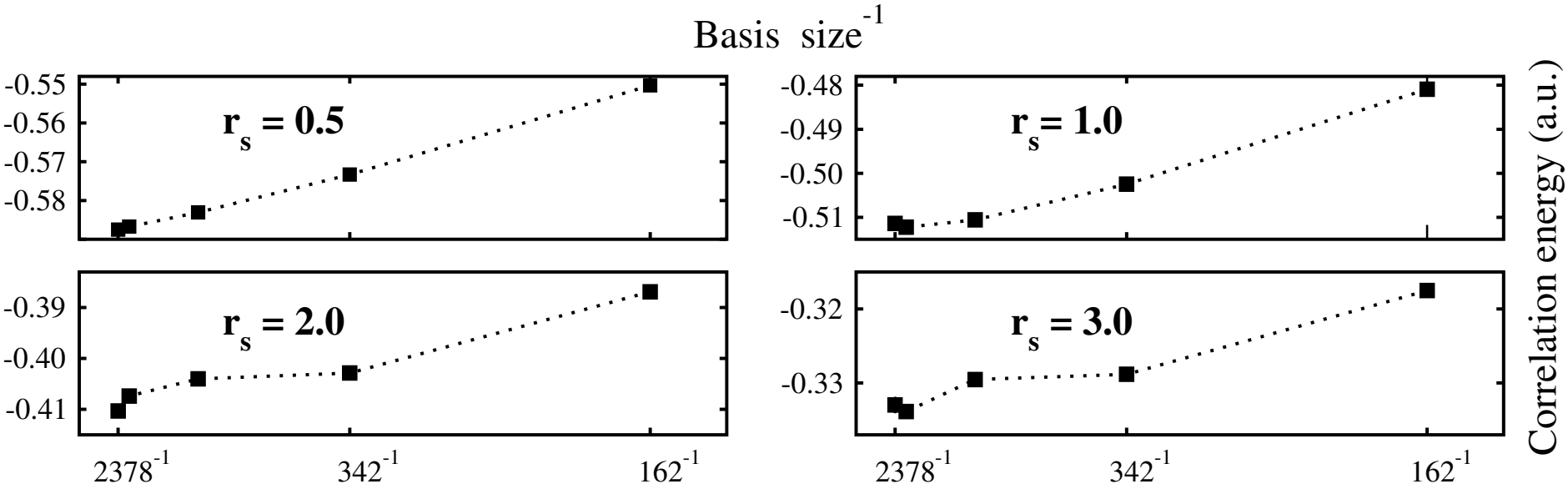

Results compare well with R–space MC with *state of the art* WF.

Conclusions

Summary:

- we have extended MC methods to work in general CI–space 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
- access to accurate momentum distributions

Perspectives:

- including higher–order correlations in CC wf
- consider spin–isospin dependent interaction ($\rightarrow \chi$-EFT)
- response functions

Thanks for your attention