

PROGRESS IN UNDERSTANDING THE PROPERTIES OF MANY-BODY SYSTEMS BY QUANTUM MONTE CARLO SIMULATIONS

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Collaborators

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 - Alessandro Roggero (U-Trento/INFN)
 - Lorenzo Contessi (U-Trento/INFN)
- } strange systems

Punchline

- **Ab-initio calculations are feasible not only for few-body systems but also for many-body systems ($A=13$ -few hundreds).**

Outline

- Methods for solving the non relativistic many-body Schroedinger's equation
- Nuclear (state dependent) interactions
- k-space methods
- Excited states
- Conclusions

Physics in the next talk by Diego Lonardoni

The non relativistic many-body problem

Many problems of interest in physics can be addressed by solving a *non-relativistic quantum problem* for N interacting particles:

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

where $|\Psi\rangle$ is the N particle state, and

$$\hat{H} = \sum_{i=0}^N -\frac{\hat{p}_i^2}{2m_i} + \hat{V}(1, 2, 3, \dots, N)$$

The potential can be as simple as the Coulomb potential, or as complicated as, for instance, the Argonne AV18 + UIX or some EFT nucleon-nucleon force (local or non local).

A general solution

There is an interesting, general way of solving the many-body Schrodinger problem, at least for the ground state. Let us consider the following operator, that we call “propagator” ($\hbar=1$):

$$e^{-(\hat{H}-E_0)\tau}$$

where E_0 is the ground state eigenvalue. If we apply it to an arbitrary state $|\Psi\rangle$ we obtain:

$$e^{-(\hat{H}-E_0)\tau}|\Psi\rangle = \sum_{n=0}^{\infty} c_n e^{-(E_n-E_0)\tau} |\Psi_n\rangle$$

where:

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$$

A general solution

In the limit of large τ it is easily seen that:

$$\lim_{\tau \rightarrow \infty} e^{-(\hat{H} - E_0)\tau} |\Psi\rangle = c_0 |\Psi_0\rangle$$

provided that the initial state is not orthogonal to the ground state.

NB: This is an example within the more general class of “*power methods*”.

All this is very general: no mention is made either of the details of H or of the representation of the states.

Projection Monte Carlo algorithms are based on a *stochastic implementation* of this “imaginary time propagation”. Different flavours correspond to the choice of a **specific representation** of the propagator and/or of the **specific Hilbert space** used.

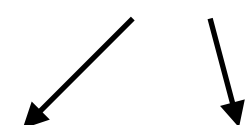
Projection Monte Carlo

The stochastic implementation of the imaginary time propagator is made by *sampling a sequence of states* in some Hilbert space. Each state is sampled starting from the previous one with a probability given by the propagator.

For instance, if the potential depends on the **coordinates of the particles only**, the formulation is relatively simple. First, we approximate our state with an expansion on a finite set of points in space:

$$|\Psi\rangle \sim \sum_{i=1}^{M_w} \langle R_i | \Psi \rangle |R_i\rangle$$

Particle coordinates




$$|R_i\rangle = \delta(R - R_i)$$

$$R \equiv \{\vec{r}_1 \dots \vec{r}_N\}$$

$$\langle R | \Psi \rangle \equiv \Psi(R)$$

Wavefunction in coordinate space



Projection Monte Carlo

We should also write the propagator in coordinates space, so that:

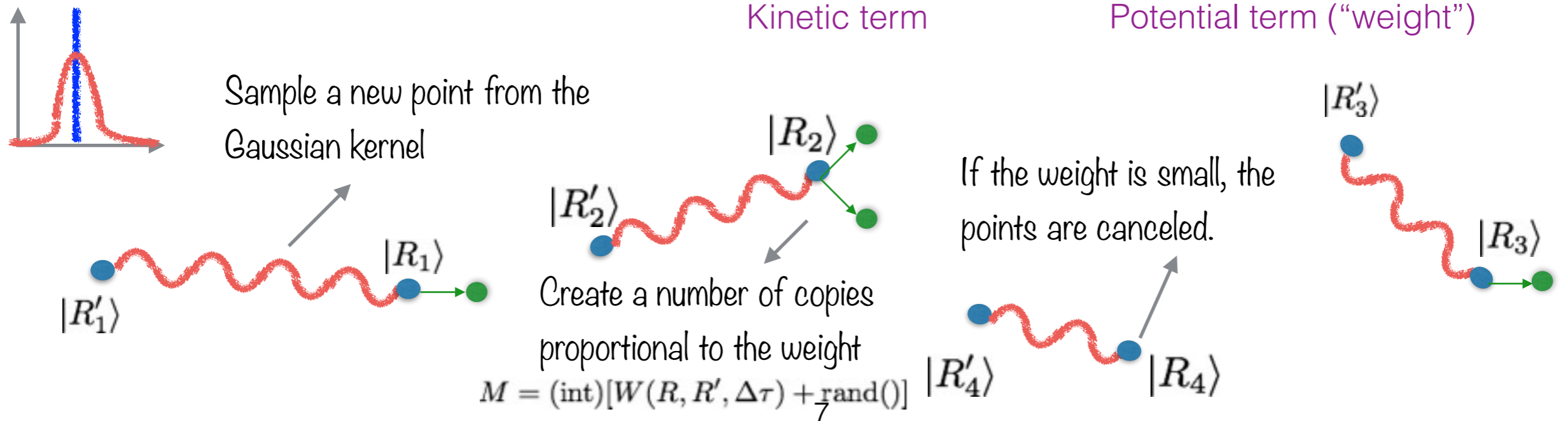
$$\langle R | \Psi(\tau) \rangle = \langle R | e^{-(\hat{H} - E_0)\tau} | R' \rangle \langle R' | \Psi(0) \rangle$$

In the limit of “short” τ (let us call it “ $\Delta\tau$ ”), the propagator can be broken up as follows (Trotter-Suzuki formula):

$$\langle R | e^{-(\hat{H} - E_0)\Delta\tau} | R' \rangle \sim e^{-\frac{(R - R')^2}{2 \frac{\hbar}{m} \Delta\tau}} e^{-\left(\frac{V(R) + V(R')}{2} - E_0\right)\Delta\tau}$$

Kinetic term

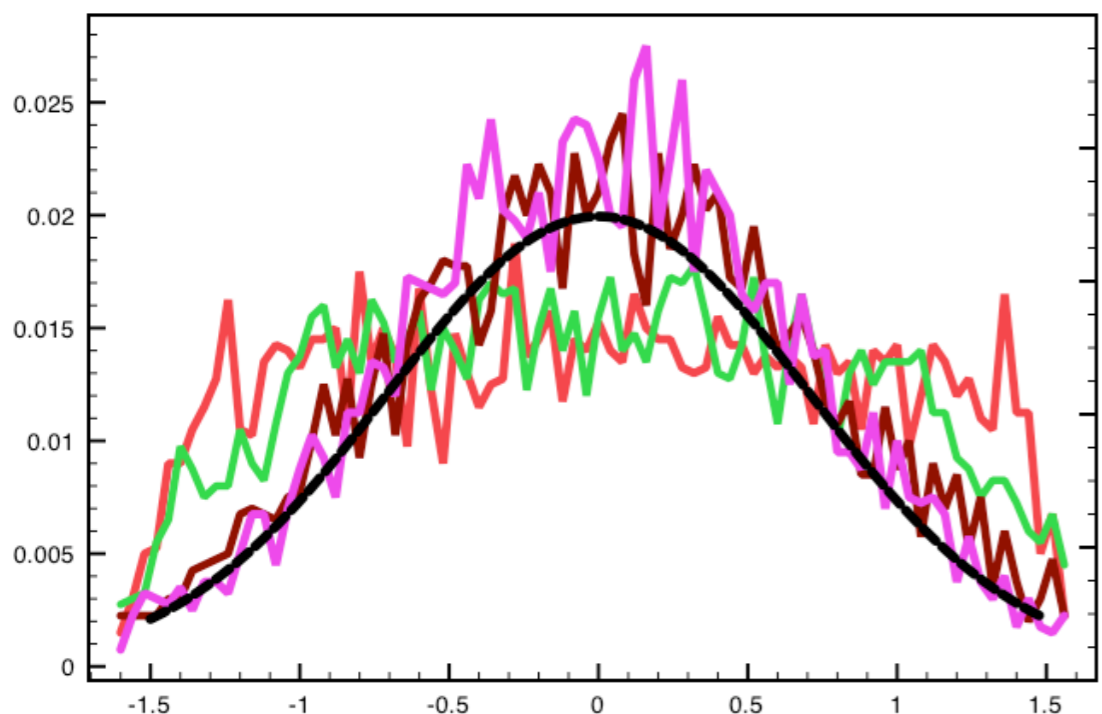
Potential term (“weight”)



Projection Monte Carlo

The “infinite time step limit”, and therefore the projection of the ground state can be reached by iterating the propagation for a large number of cycles.

EXAMPLE: harmonic oscillator in one dimension:



$$H = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2$$

Evolution of the histogram of a population of points from a uniform distribution in $[-1.5, 1.5]$ after 10 (red line), 100 (green), 1000 (purple), and 5000 (brown) cycles with time step $\Delta\tau = 0.01$. The black line is the exact solution (the ground state wave function)

Projection Monte Carlo

Once the convergence to the ground state is reached it is possible to use the sampled configurations to evaluate expectations of observables of interest in a Monte Carlo way. For example, if we want to compute the **energy**, we can use some test function and evaluate the following ratio:

$$\frac{\sum_k \hat{H} \Psi_T(R_k)}{\sum_k \Psi_T(R_k)}$$

This is the Monte Carlo estimate of:

$$\frac{\int dR \Psi_0(R) \hat{H} \Psi_T(R)}{\int dR \Psi_0(R) \Psi_T(R)} = \frac{\langle \Psi_0 | \hat{H} | \Psi_T \rangle}{\langle \Psi_0 | \Psi_T \rangle} = \frac{\langle \Psi_T | \hat{H} | \Psi_0 \rangle}{\langle \Psi_T | \Psi_0 \rangle} = E_0$$

Known issues

- The naive algorithm does not work for any realistic potential. In general the random walk needs to be guided by an **“importance function”**. In a correct formulation there is no bias on the results.
- The algorithm works (strictly speaking) only for the **“mathematical” ground state** of the Hamiltonian, which is always a symmetric (bosonic) wavefunction. Fermions live on an **“mathematical excited state”** of $H!$ **⇒ SIGN PROBLEM**. Workarounds exist, but the results are biased. However, **in many cases it is possible to estimate the bias**.

Sign Problem

One of the major issues in Quantum Monte Carlo calculations comes from the fact that Fermions live in an excited state (in mathematical sense) of the Hamiltonian. This means that if we want to preserve the normalisation of the Fermionic ground state (using for instance E_0^A instead of E_0 the propagation:

$$e^{-(\hat{H} - E_0^A)\tau} |\Psi\rangle = \sum_{n=0}^{\infty} c_n e^{-(E_n - E_0^A)\tau} |\Psi_n\rangle$$

Antisymmetric
(fermionic) ground state

Symmetric (bosonic)
ground state

leads to

$$\lim_{\tau \rightarrow \infty} e^{-(\hat{H} - E_0^A)\tau} = c_0 e^{-(E_0 - E_0^A)\tau} |\Psi_0\rangle + c_0^A |\Psi_0^A\rangle$$

Always > 0 (it's a theorem!)

therefore quantities that are symmetric (like the variance of any operator...) will grow exponentially in imaginary time compared to the expectation of any antisymmetric function. This is the essence of the so called the "sign problem".

Sign Problem

In order to cope with the sign problem it is useful to introduce some approximations. In particular, the general idea is to solve a modified Schroedinger equation with additional boundary conditions.

- For **real-valued wave functions**, the nodes (zeros) of the solutions must correspond to the nodes of some trial wavefunctions
- **(FIXED NODE APPROXIMATION)**
- For **complex valued wave functions**, we have two options:
 - A. Constrain the phase of the solution to be equal to the phase of some trial wave function **(FIXED PHASE APPROXIMATION)**
 - B. Constrain the sign of the real part of the wave function (or some suitable combination) to preserve the sign **(CONSTRAINED PATH APPROXIMATION)**

Many-nucleon systems

Nuclear physics experiments teach us that the nucleon-nucleon interaction depends on the relative **spin** and **isospin** state of nucleons. This fact can be formally related to the **fundamental symmetry properties of QCD**, and it is necessary in any realistic interactions that can be used in a many-body calculation

EXAMPLE: One of the most celebrated model nucleon-nucleon (NN) interaction is the so-called **Argonne AVX potential**, defined by:

$$\langle R, S, T | V_X \rangle = \sum_{i=1}^X v_i(r_{ij}) \hat{O}^i$$

R B Wiringa, V G J Stoks, and R Schiavilla
PRC 51, 38 (1995)

EX: AV8

$$\{\mathbb{I}, \vec{\sigma}_i \cdot \vec{\sigma}_j, S_{ij}, \hat{L}_{ij} \cdot \frac{1}{2}(\vec{\sigma}_i + \vec{\sigma}_j)\} \otimes \{\mathbb{I}, \vec{\tau}_i \cdot \vec{\tau}_j\}$$

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Spin representation
in term of Pauli matrices

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Spin-orbit

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Spin-orbit

Isospin

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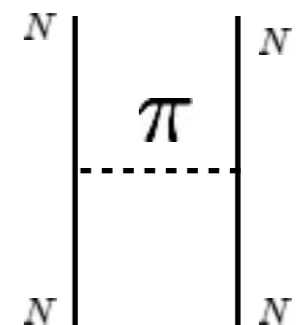
Spin-orbit

Isospin

Here S_{ij} is the tensor operator

$$S_{ij} \equiv 3(\hat{r}_{ij} \cdot \vec{\sigma}_i)(\hat{r}_{ij} \cdot \vec{\sigma}_j) - \vec{\sigma}_i \cdot \vec{\sigma}_j$$

that characterises the “one-pion exchange” part of the interaction.



Projection MC many-nucleon systems

We can apply our (very general) propagator to a state that is now given by the particle positions (the “R”), and the spin/isospin state of each nucleon (the “S”).

Problem

In the stochastic evolution, spins are subject to factors like:

$$\langle R, S | e^{-\sum_{ij} v_{\sigma\sigma}(r_{ij}) \vec{\sigma}_i \cdot \vec{\sigma}_j \Delta\tau} | R, S' \rangle$$

But:

$$\vec{\sigma}_i \cdot \vec{\sigma}_j |S\rangle = \begin{cases} -3/4 |S\rangle & \text{if } i, j \text{ in } S = 0 \text{ state} \\ 1/4 |S\rangle & \text{if } i, j \text{ in } S = 1 \text{ state} \end{cases}$$

The action of the propagators depends on the relative spin state of each pair of nucleons

Projection MC many-nucleon systems

Multicomponent wave functions are needed!

How large is the system space? For a system of A nucleons, Z protons, the number of states is $2^A \binom{A}{Z}$

	A	Pairs	Spin \times Isospin
${}^4\text{He}$	4	6	8×2
${}^6\text{Li}$	6	15	32×5
${}^7\text{Li}$	7	21	128×14
${}^8\text{Be}$	8	28	128×14
${}^9\text{Be}$	9	36	512×42
${}^{10}\text{Be}$	10	45	512×90
${}^{11}\text{B}$	11	55	2048×132
${}^{12}\text{C}$	12	66	2048×132
${}^{16}\text{O}$	16	120	32768×1430
${}^{40}\text{Ca}$	40	780	$3.6 \times 10^{21} \times 6.6 \times 10^9$
8_n	8	28	128×1
${}^{14}_n$	14	91	8192×1

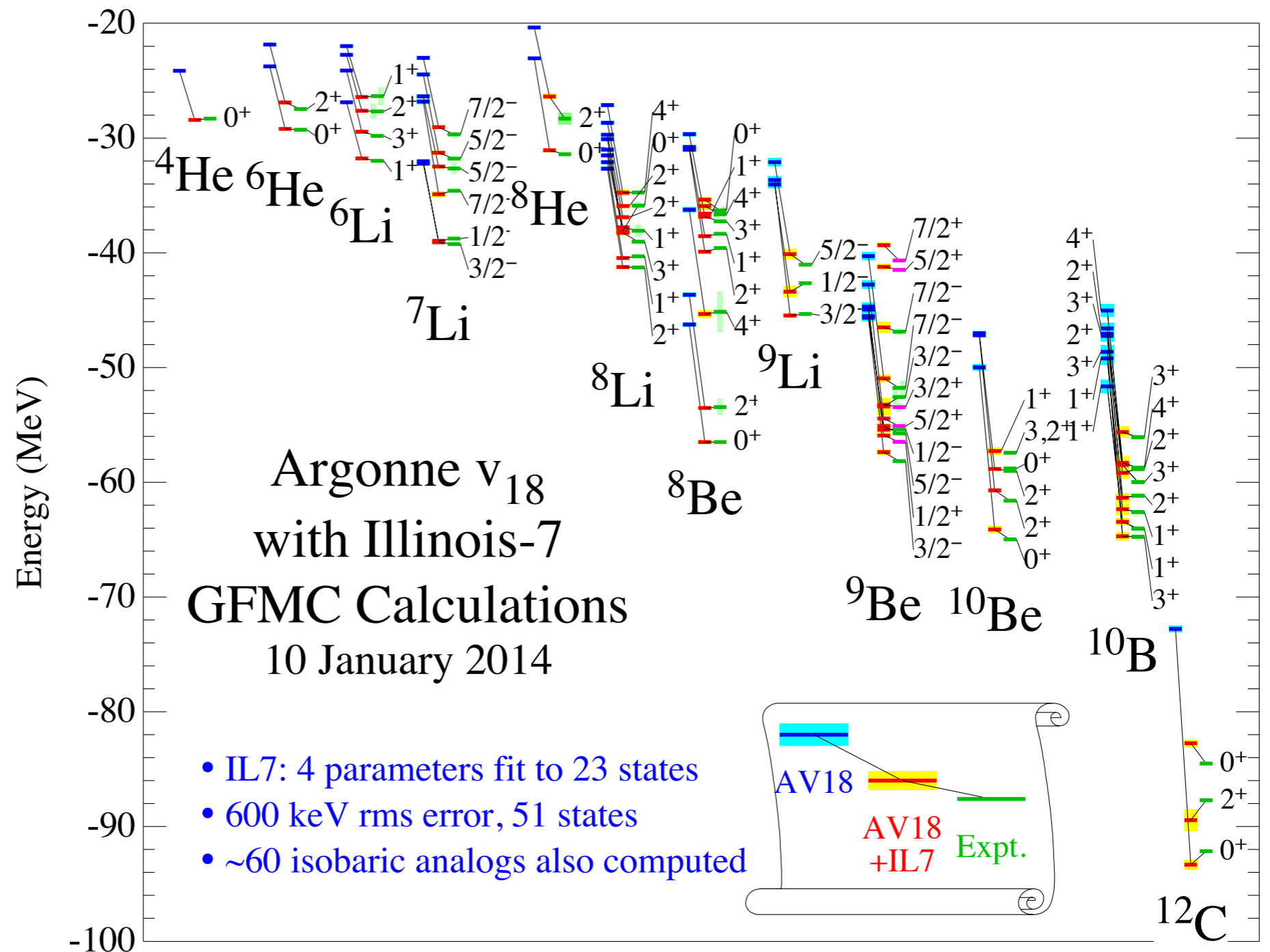
Number of states in many nucleon wave functions for a few selected nuclei

- Very accurate results, possibility of using accurate wave functions for the evaluation of general estimators (e.g. response functions)
- Due to the high computational cost, application limited so far to $A \leq 12$: **COMPUTATIONAL CHALLENGE!**

Projection MC many-nucleon systems

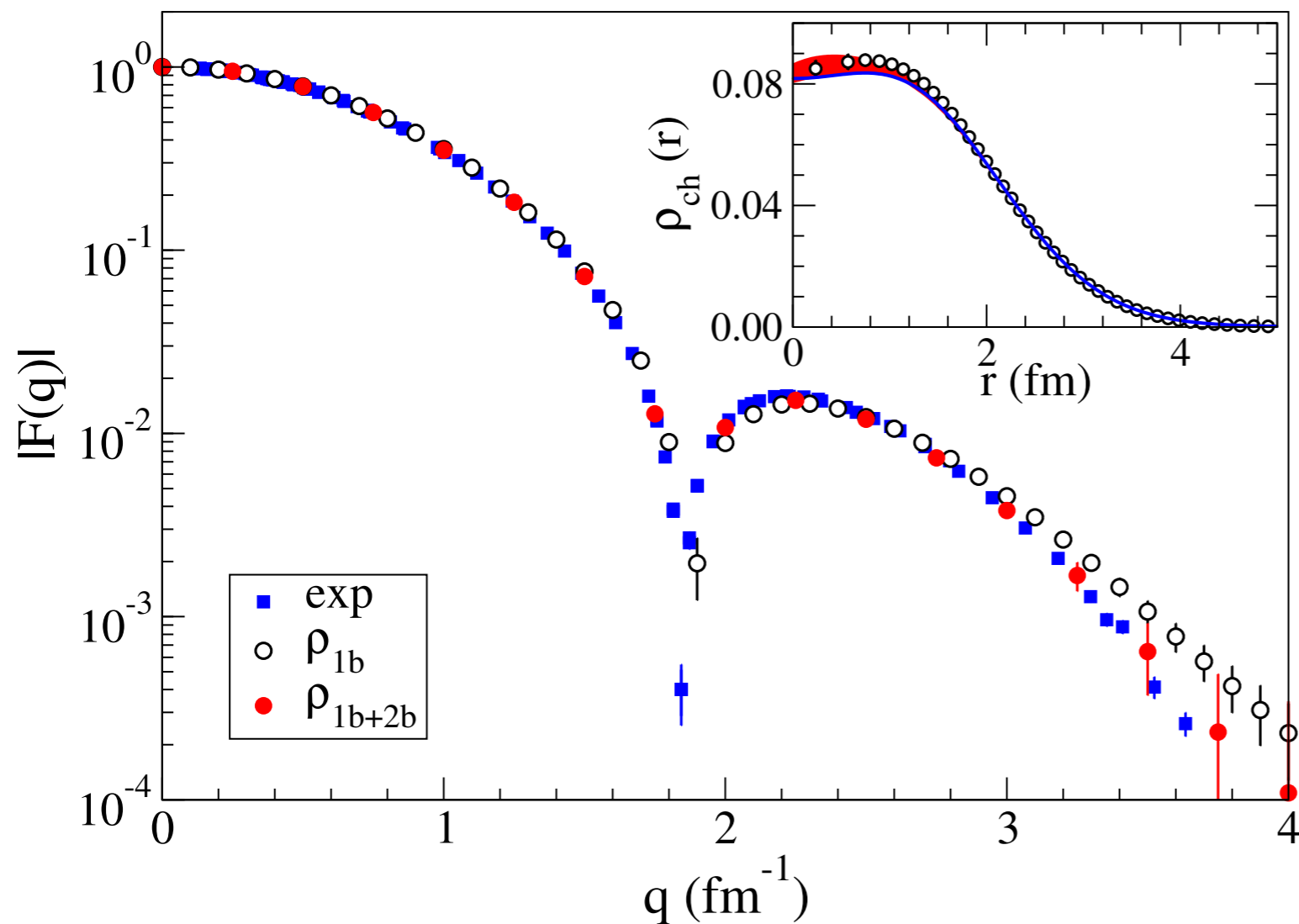
Very accurate results have been obtained in the years for the ground state and some excitation properties of nuclei with $A \leq 12$ by the Argonne based group (GFMC calculations by Pieper, Wiringa, Carlson, Schiavilla...).

These calculations include two- and three-nucleon interactions.



Courtesy of R. Wiringa, ANL

Projection MC many-nucleon systems



GFMC calculations also provide very good ab-initio estimates of quantities other than the energy. Here, for example, is reported the computation of the charge form factor of ^{12}C compared to experimental data (I. Sick)

An alternative: AFDMC

Stefano Fantoni & Kevin Schmidt, 1999

The computational cost can be reduced in a Monte Carlo framework by introducing a way of **sampling over the space of states**, rather than summing explicitly over the full set.

For simplicity let us consider only one of the terms in the interaction.

We start by observing that:

Linear combination
of spin operators for
different particles

$$\sum_{i < j} v(r_{ij}) \vec{\sigma}_i \cdot \vec{\sigma}_j = \frac{1}{2} \sum_{i; \alpha, j; \beta} \sigma_{i; \alpha} A_{i; \alpha, j; \beta} \sigma_{j; \beta} = \sum_{n=1}^{3A} \lambda_n \hat{O}_n^2$$

Then, we can linearize the operatorial dependence in the propagator by means of an integral transform:

auxiliary fields → Auxiliary Field Diffusion Monte Carlo

$$e^{-\frac{1}{2} \lambda \hat{O}_n^2 \Delta \tau} = \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2}} e^{-x \sqrt{\lambda \Delta \tau} \hat{O}_n}$$

Hubbard-Stratonovich transformation

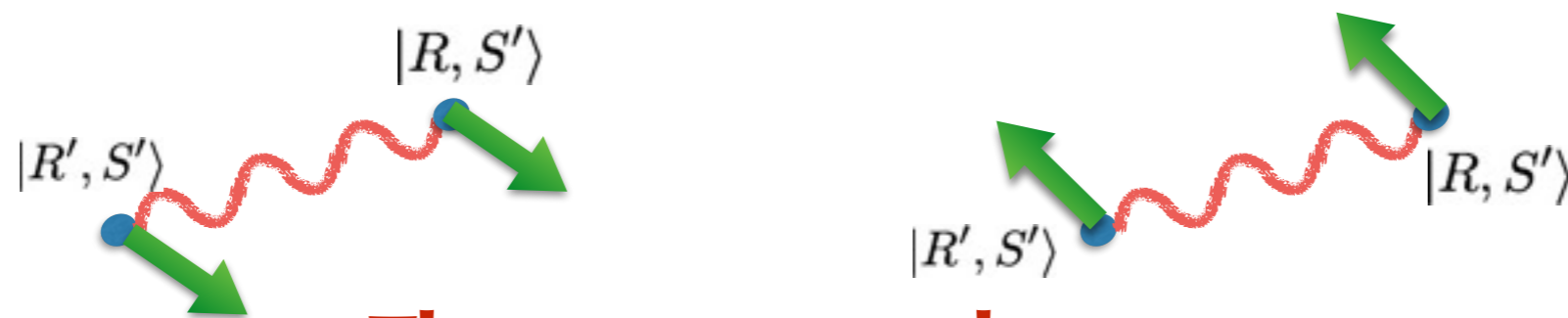
An alternative: AFDMC

The operator dependence in the exponent has become **linear**.

In the Monte Carlo spirit, the integral can be performed by sampling values of x from the Gaussian $e^{-\frac{x^2}{2}}$. For a given x the action of the propagator will become:

$$e^{-x\sqrt{\lambda\Delta\tau}\hat{O}_n}|S\rangle = \prod_{k=1}^{3A} e^{-x\sqrt{\lambda\Delta\tau}\phi_n^k\sigma_k}|S\rangle$$

In a space of spinors, each factor corresponds to a rotation induced by the action of the Pauli matrices



**The sum over the states
has been replaced by sampling rotations!**

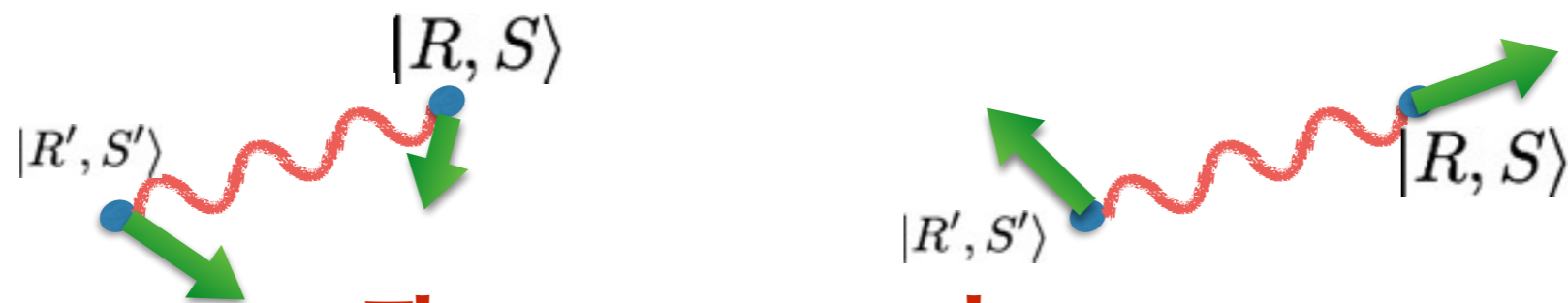
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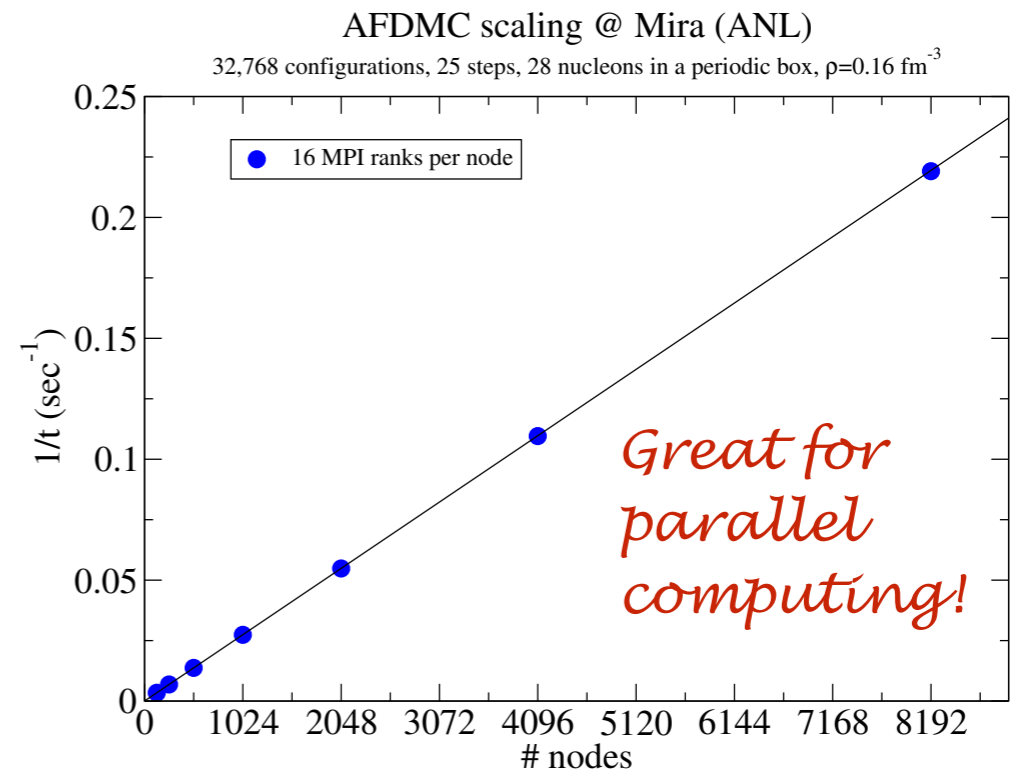
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The crucial advantage of AFDMC is that the scaling of the required computer resources is no longer exponential: **the cost scales as A^3** (the scaling required by the computation of the determinants in the antisymmetric wave functions) **→ LARGER SYSTEMS ACCESSIBLE!**

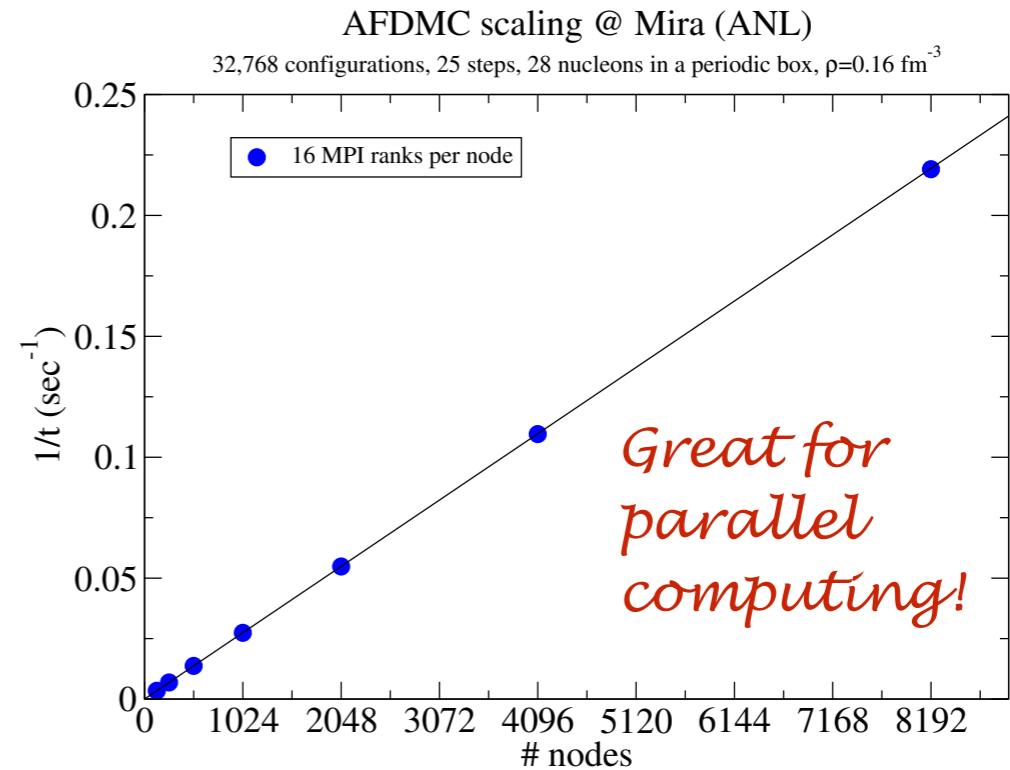
Problems

- The HS transformation can be used **ONLY FOR THE PROPAGATOR** **Accurate wave functions** require an operatorial dependence! **Cluster expansion introduced and working!**
- Extra variables **→** larger fluctuations and autocorrelations.
- Some problems in treating **nuclear spin-orbit (however now works for AV7')**.
- **Three-body forces** (extremely important in nuclear physics) can be reduced by a HS transformation **only for pure neutron systems**. (However, there is progress on **density dependent 3-body forces that can be used in the propagator!!**)



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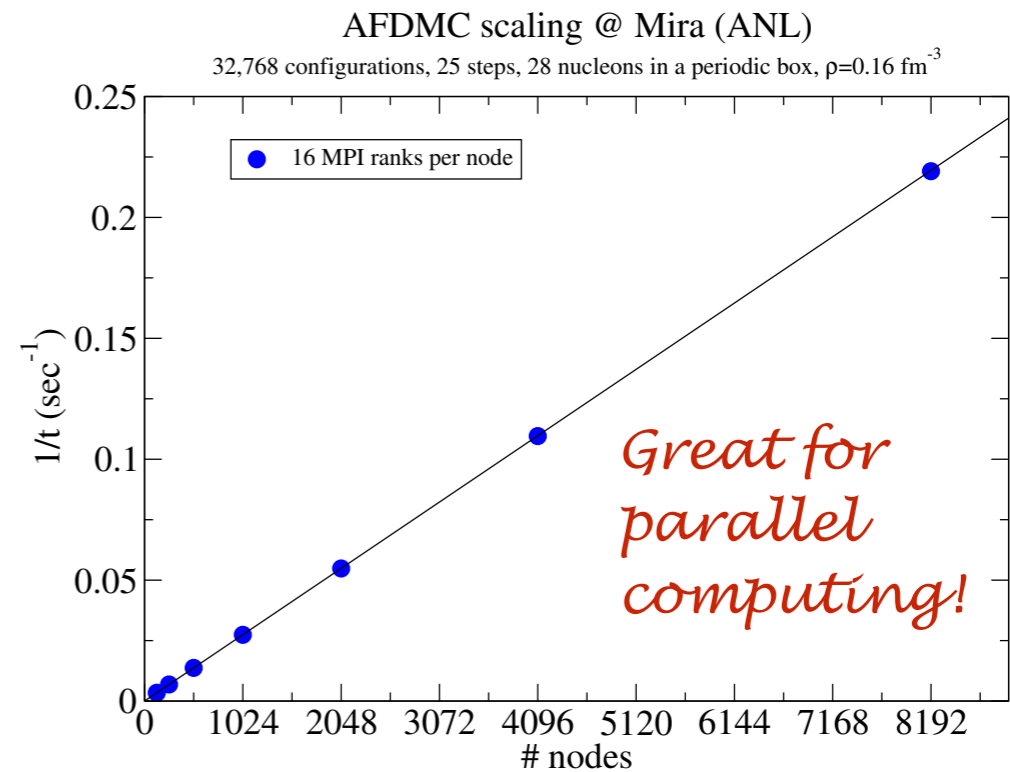
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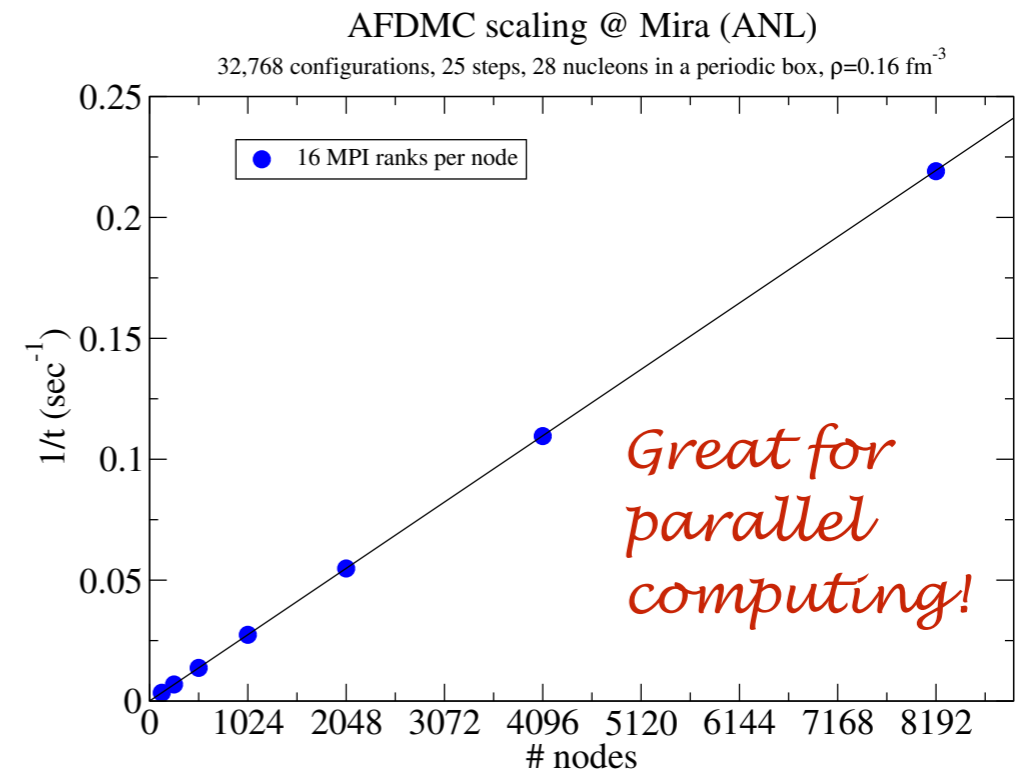
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Fock space calculations

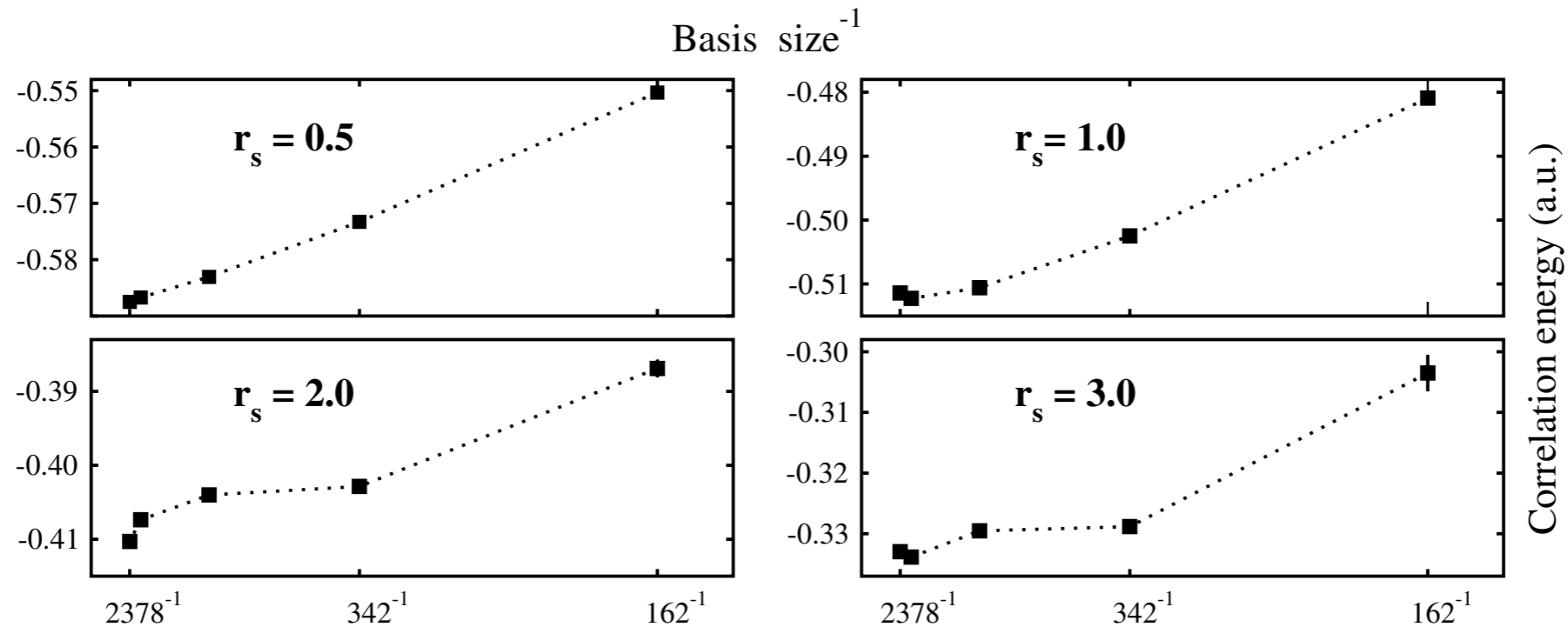
The stochastic power method can also be used in Fock space. In this case the propagator acts on the occupation number of a basis set used to span the Hilbert space of the solution of a given Hamiltonian. In particular, given two basis states $|\mathbf{m}\rangle$ and $|\mathbf{n}\rangle$ the quantity:

$$\langle \mathbf{m} | \mathcal{P}_{\Delta\tau} | \mathbf{n} \rangle = \langle \mathbf{m} | 1 - (\hat{H} - E_0) \Delta\tau | \mathbf{n} \rangle$$

is interpreted as the probability of the system of switching the occupation of the state $|\mathbf{n}\rangle$ into the occupation of the state $|\mathbf{m}\rangle$. This propagation has in principle the same properties of the coordinates space version.

**IMPLEMENTED IN TRENTO: CONFIGURATION INTERACTION
MONTE CARLO (CIMC)** (A.Roggero, A.Mukehrjee, FP)

Configuration Interaction Monte Carlo

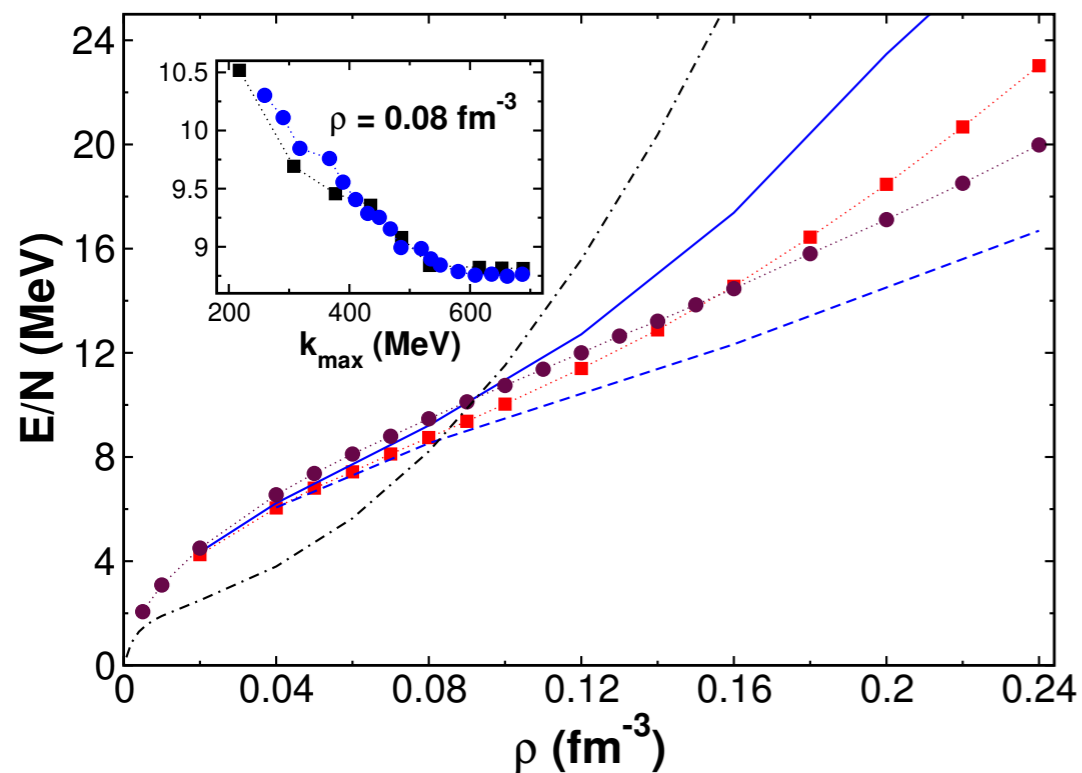


Alessandro Roggero, Abhishek Mukherjee, and Francesco Pederiva Phys. Rev. B **88**, 115138 (2013)

A first test of this algorithm was the evaluation of the equation of state of the three-dimensional homogeneous electron gas, for which very accurate results are already available. In this case the Hamiltonian is very simple, and includes the contribution of a uniform cancelling background of positive charge.

As importance function we used the overlaps computed by COUPLED CLUSTERS at the doubles level (CCD) method.

Configuration Interaction Monte Carlo



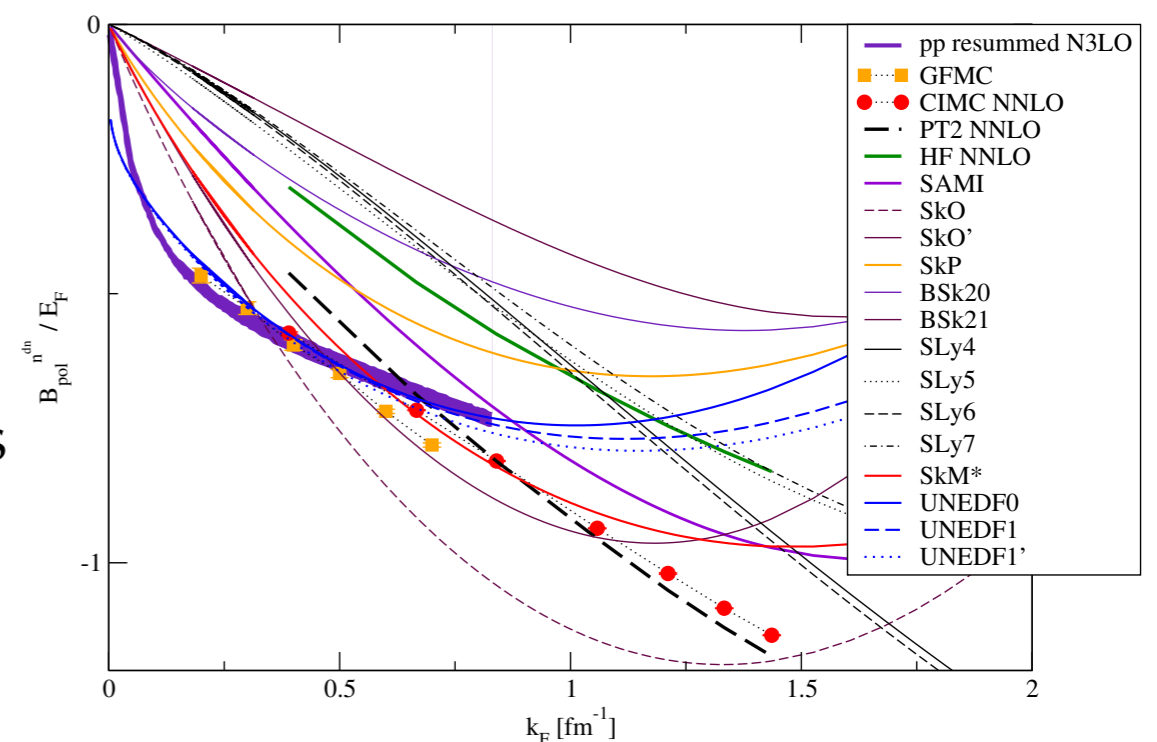
Alessandro Roggero, Abhishek Mukherjee, Francesco Pederiva
PRL, in press (2014)

On the right the energy of a neutron polaron, always computed with the same Hamiltonian and CIMC.

Alessandro Roggero, Abhishek Mukherjee, Francesco Pederiva
in preparation

One of the main advantages of using an algorithm in Fock space is the possibility of using non-local Hamiltonians, such as the recent chiral EFT based Hamiltonians.

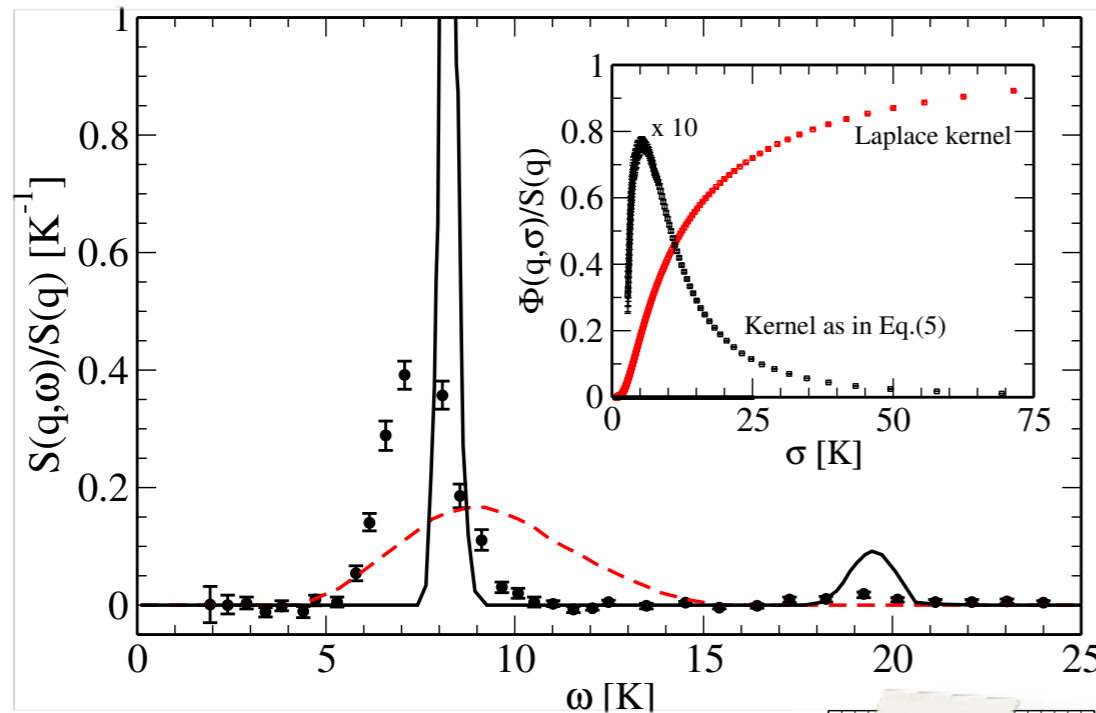
Here on the left, the computation of the equation of state of pure neutron matter with the N2LO interaction of Machleidt et al.



Response Functions

From QMC
calculations

Alessandro Roggero, Francesco Pederiva, and Giuseppina Orlandini, Phys. Rev. B **88**, 094302 (2013)

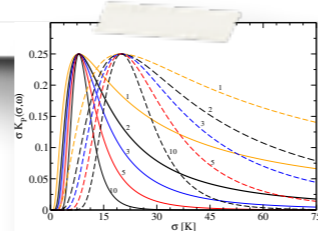


$$S_{\hat{O}}(\mathbf{q}, \omega) = \sum_{\nu} |\langle \Psi_{\nu} | \hat{O}(\mathbf{q}) | \Psi_0 \rangle|^2 \delta(E_{\nu} - \omega)$$

$$= \langle \Psi_0 | \hat{O}^{\dagger}(\mathbf{q}) \delta(\hat{H} - \omega) \hat{O}(\mathbf{q}) | \Psi_0 \rangle$$

$$\Phi(\mathbf{q}, \sigma) = \int K(\sigma, \omega) S_{\hat{O}}(\mathbf{q}, \omega) d\omega.$$

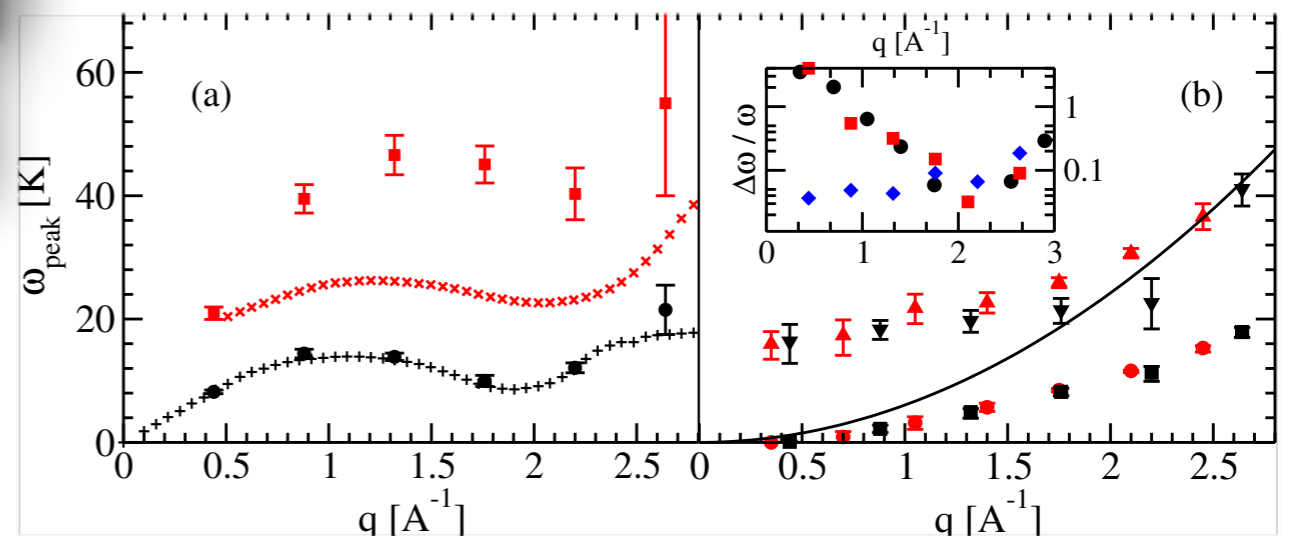
The natural choice within QMC is a Laplace kernel, very inefficient and amplifying the ill-posedness of the inversion problem.



Better kernel: **SUMUDU**

$$K_P(\sigma, \omega) = N \left[\frac{e^{-\mu \frac{\omega}{\sigma}}}{\sigma} - \frac{e^{-\nu \frac{\omega}{\sigma}}}{\sigma} \right]^P$$

- Still “natural” in the language of QMC
- “Bell shaped”, and therefore more efficient and less prone to inversion ambiguities.



Conclusions

- Quantum Monte Carlo methods for projecting the ground state of an arbitrary Hamiltonian can be formulated for general Hamiltonians and Hilbert spaces, and are (and will be) applied to a very wide range of physical systems of interest.
- The “sign problem” is still unsolved: approximations generally needed for many-fermion systems.
- Propagators can be elaborated in order to increase the numerical efficiency of the algorithm (there is recent progress along this direction).
- Large A systems interacting via spin/isospin dependent Hamiltonians can be treated by “standard” formulations or by introducing auxiliary degrees of freedom (AFDMC).
- Methods have been devised to project the ground state in an arbitrary Fock space (in particular momentum space)
- An efficient way of computing general response functions has been indicated. Development is in progress.