
Istituto Nazionale di Fisica Nucleare

IS MONSTRE (Modeling Nuclear Structure and Reactions)

# QUANTUM MONTE CARLO METHODS

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Collaborations

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# QUANTUM MONTE CARLO IN MONSTRE

Two main lines of action in the development of Quantum Monte Carlo algorithms:

- Projection methods defined in the space of Slater determinants (Configuration Interaction Monte Carlo, CIMC). This is particularly useful for nuclear structure problems, since it is not limited to Hamiltonians expressed in the coordinate basis (Roggero, Barbieri)

- Variational methods using neural networks to approximate the many-body wavefunction of the system ("Neural wavefunctions"). This method provides very accurate predictions for the observables in a variational context (➔ no sign problem) (Lovato)

*A couple remarks…*

- Quantum Monte Carlo methods have now reached a certain level of maturity. However, there is still room for improvements and extensions of the method.

- QMC provides a very useful mind frame for those who want to get into quantum computing.

# CONFIGURATION INTERACTION MONTE CARLO

Originally the idea was to develop ana algorithm working in “momentum space” for non-local Hamiltonians.

The wavefunction of an interacting many-fermion system can be expanded on a basis of Slater determinants $|\Phi_i\rangle$ built for instance from the orbitals coming from an Hartree-Fock calculation:

$$|\Psi^{\mathrm{FCI}}\rangle \equiv \sum_i C_i |\Phi_i\rangle$$

Usually, the wavefunction is optimized by computing the matrix elements $H_{ij} = \langle \Psi_i | \hat{H} | \Phi_i \rangle$ and diagonalizing. Eigenvalues and eigenvectors provide the spectrum and the expansion coefficients of the corresponding wavefunctions. Diagonalization (see e.g. the NCSM method) is expensive and currently limited to $A \simeq 20$

ain idea

Replace diagonalization with a *stochastic projection method* capable to give the overlaps of the ground state wavefunction with the chosen basis $|\Phi_i\rangle$ encoded, for instance, in terms of occupation numbers or momentum. In general this works very well in second quantization.

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

# CONFIGURATION INTERACTION MONTE CARLO

Projection methods are based on imaginary time propagation. Defining the (non unitary) propagator $\mathcal{P}$ as:

$$\mathcal{P} = \exp\Big[-(\hat{H} - E_0)\delta t\Big]$$

where $E_0$ is an estimate of the ground state energy, we have:

$$\lim_{N\to\infty} \mathcal{P}^N |\Psi\rangle = |\Psi_0\rangle$$

Where $|\Psi_0\rangle$ is the ground state of the Hamiltonian. If $\delta t$ is small one can expand the propagator obtaining:

$$\mathcal{P}|\Psi\rangle \simeq [(1 - (\hat{H} - E_0)\delta t]|\Psi\rangle$$

If we expand on the basis $|\Phi_i\rangle$ truncated to $M$ states, the expression can be recast as:

$$\langle\Phi_j|\Psi(t+\delta t)\rangle \equiv \langle\Phi_j|\mathcal{P}|\Psi(t)\rangle = \sum_{i=1}^{M}\langle\Phi_j|\mathcal{P}|\Phi_i\rangle\langle\Phi_i|\Psi(t)\rangle \simeq \sum_{i=1}^{M}\langle\Phi_j|[(1 - (\hat{H} - E_0)\delta t]\Phi_i\rangle\langle\Phi_i|\Psi(t)\rangle$$

As in standard QMC method the sum over the $M$ states can approximated by a sum over a number $M_w$ of "walkers" in the space of the Slater determinants. The probability of jumping from one state to the next is given by the matrix element of the propagator in the r.h.s. of the equation above.

# CONFIGURATION INTERACTION MONTE CARLO

As in standard QMC method the sum over the $M$ states can approximated by a sum over a number $M_w$ of "walkers" in the space of the Slater determinants. The probability of jumping from one state to the next is given by:

$$p(i,j) = \frac{\langle \Phi_j | \mathcal{P} | \Phi_i \rangle}{\sum_{i=1}^{M} \langle \Phi_j | \mathcal{P} | \Phi_i \rangle} \equiv \frac{\langle \Phi_j | \mathcal{P} | \Phi_i \rangle}{g(j)}$$

Beware that this definition is valid iff the matrix elements of the propagator are positive! This sets a strong constraint on the maximum propagation time, which must be less than $2/(E_{max}\text{-}E_0)$, where $E_{max}$ is the highest eigenvalue of $H$ in the model space considered. The denominator $g(j)$ becomes a "weight" that reflects the change in normalization during the propagation.

To this elementary scheme we have added two ingredients:

- Importance sampling to guide the walkers
- Exponential propagator

# RECENT PROGRESS

A set of calculations was originally performed on the electron gas (and a few other Coulombic systems) and neutron matter with an N2LO chiral interaction, but without 3NF.

A few years ago, Carlo Barbieri and Pierre Arthuis proposed to work on the extension of the formalism to interactions containing 3NF. These are necessary to address the problem of nuclear matter, but also to discuss correctly nuclides far away from the stability valley and close to the drip line.

$$H_3 = \frac{1}{36} \sum_{pqrstu} \bar{v}_{pqrstu} a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$

**PROPOSAL:** Use the Normal Ordered 2 Body Approximation (NO2BA):

$$H_3 = \frac{1}{6} \sum_{ijk} \bar{v}_{ijkijk} + \frac{1}{2} \sum_{ijpq} \bar{v}_{ijpijq} : a_p^\dagger a_q :$$
$$+ \frac{1}{4} \sum_{ipqrs} \bar{v}_{ipqirs} : a_p^\dagger a_q^\dagger a_s a_r :$$
$$+ \cancel{\frac{1}{36} \sum_{pqrstu} \bar{v}_{pqrstu} : a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s :}$$

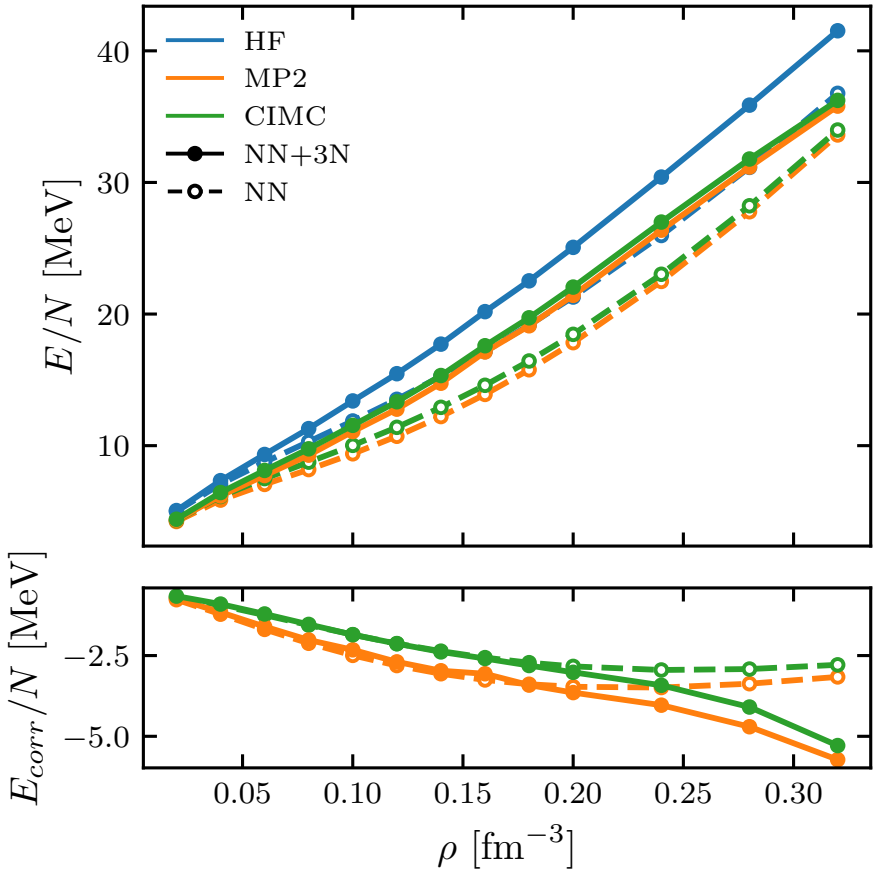
Dropping the last term introduces a small truncation error.

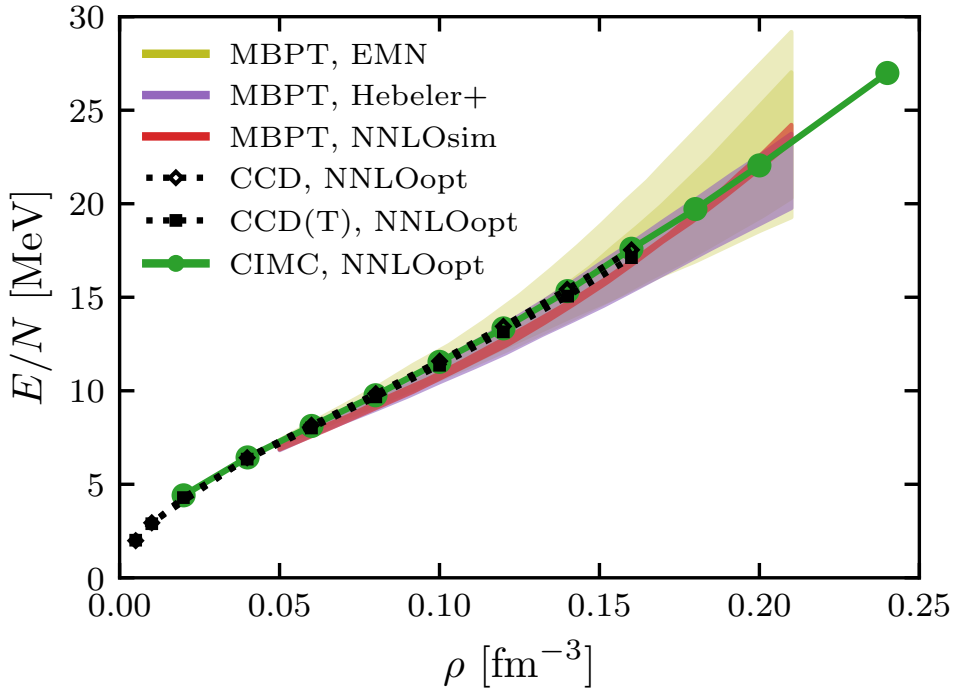
# RECENT PROGRESS

The algorithm was tested on Pure Neutron Matter with a N2LO chiral interaction in the NO2BA

Pierre Arthuis, Carlo Barbieri, FP, and Alessandro Roggero, Phys. Rev. C **107**, 044303 (2023)

Equation of state of PNM (66 neutrons)

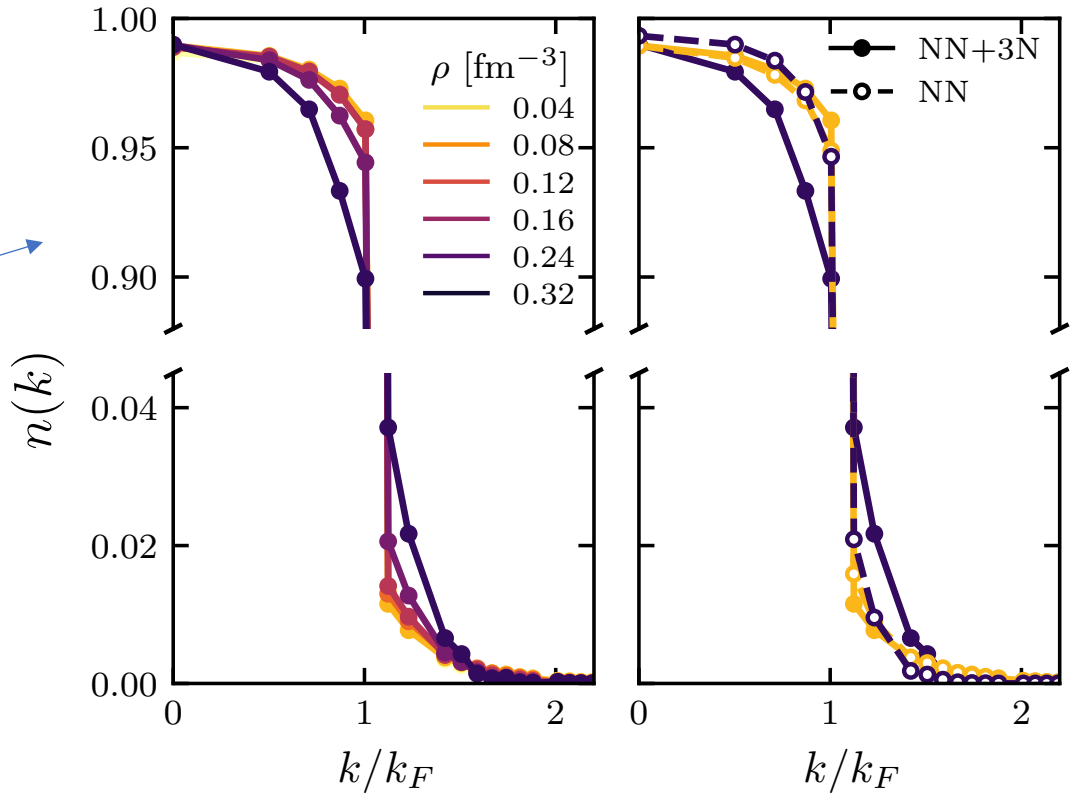


# RECENT PROGRESS

CIMC gives access to a number of other observables that are quite difficult to compute when using the standard approach in coordinate systems. One of them is for example the momentum distribution. Since we are working essentially expanding the wavefunction in terms of determinants of plane waves, it is sufficient in order to evaluate the momentum distribution to create a histogram of the frequency of the occupation of states with given momentum. Results are obviously very clean.

$n(k)$ for 66 neutrons at different densities, including 3NF




$n(k)$ for 66 neutrons at densities $0.5n_0$ and $2n_0$, with and without 3NF

# RECENT PROGRESS

A bit less straightforward is the computation of the static structure factor $S(q)$, which is defined as:

$$S(q) = \int_0^\infty d\omega S(q,\omega) = \langle \Psi_0 | \rho(q)^\dagger \rho(q) | \Psi_0 \rangle$$

where:

$$S(q,\omega) = \sum_n |\langle \Psi_n | \rho(q) | \Psi_0 \rangle|^2 \, \delta(E_n - E_0 - \omega)$$

In a CIMC calculation $S(q)$ needs to be computed as a mixed estimator

$S_l(q)$

$$S_{mixed}(\mathbf{q},\tau) = \frac{\sum_{l=1}^{N_\tau} w_G(l,\tau) \frac{\langle \Phi_G | \hat{S}(\mathbf{q}) | D_l \rangle}{\langle \Phi_G | D_l \rangle}}{\sum_{l=1}^{N_\tau} w_G(l,\tau)}$$

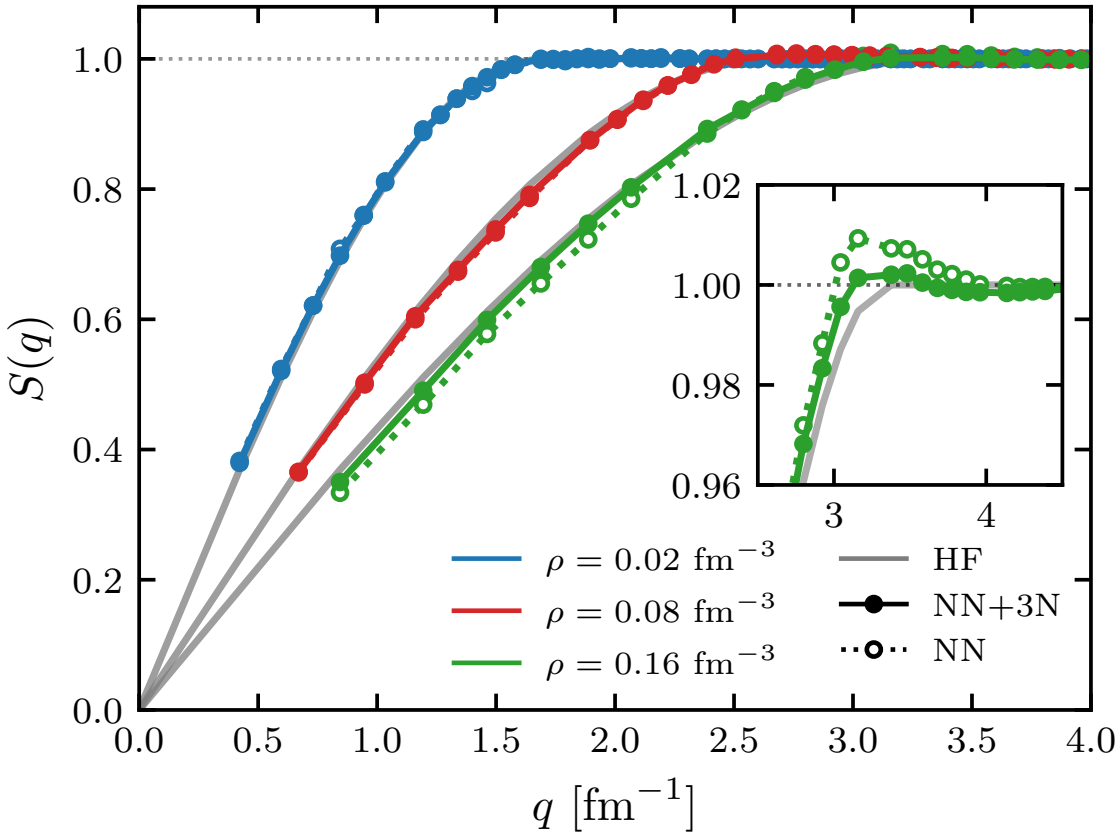
The operator to be averaged needs in turn to be computed as a sum of a diagonal and off-diagonal parts:

$$S_l(\mathbf{q}) = \langle D_l | \hat{S}(\mathbf{q}) | D_l \rangle + \sum_{m \neq l} \frac{\langle \Phi_G | D_m \rangle \langle D_m | \hat{S}(\mathbf{q}) | D_l \rangle}{\langle \Phi_G | D_l \rangle}$$

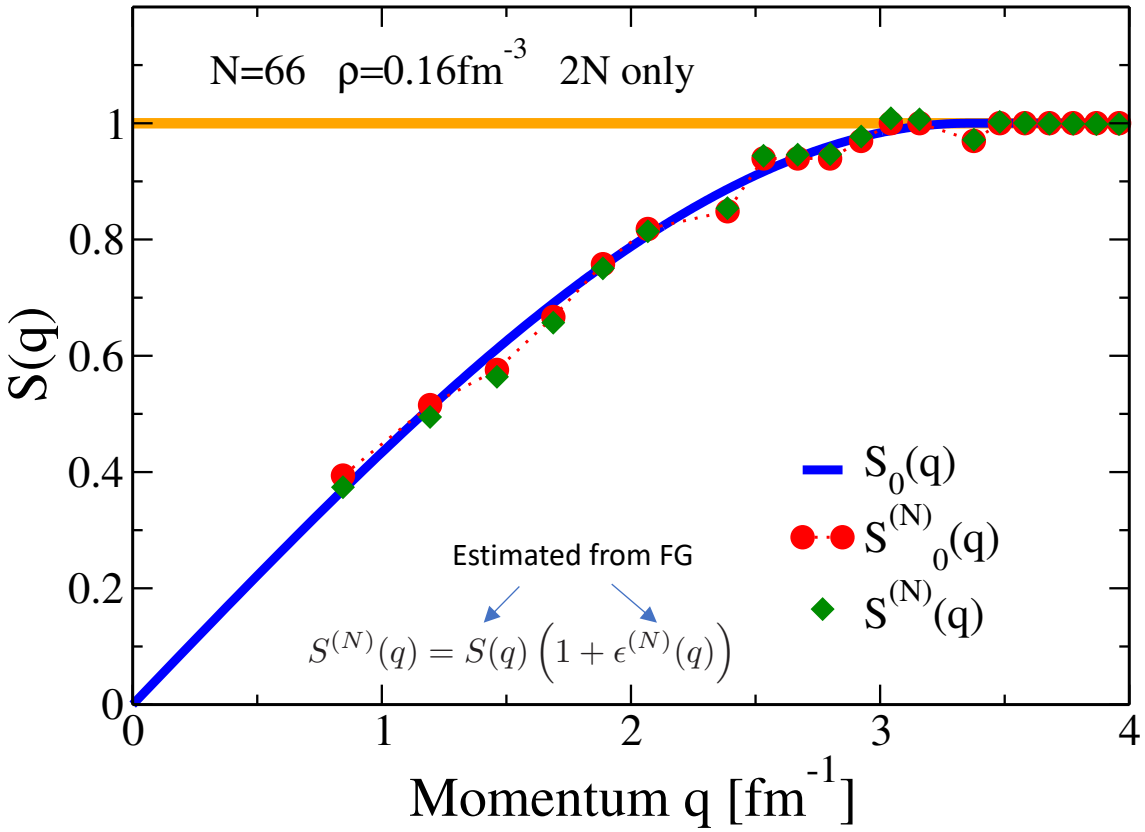
$$= S_l^D(\mathbf{q}) + S_l^O(\mathbf{q}) \, .$$

# RECENT PROGRESS

Static structure factor




S(q) for 66 neutrons at different densities with and without the inclusion of 3NF




Corrections for finite size effects (mostly shell effects) need to be included. This is done with an analysis based on the comparison with the Fermi gas results.

# NEURAL WAVEFUNCTIONS

Neural networks (NN), as universal approximants, can be used to implement highly correlated many-body wavefunctions that are then optimized by optimizing the NN parameters.

Recently this method was combined with CIMC in simple models in order to explore the potential benefits. A first application was made to the study of a simple pairing model with an Hamiltonian:

$$H = \sum_{p=1}^{P} d_p N_p - \sum_{p,q=1}^{P} g_{pq} A_p^\dagger A_q$$

$$N_p = \sum_\sigma a_{p\sigma}^\dagger a_{p\sigma} \qquad [A_p, A_q^\dagger] = \delta_{pq}(1 - N_p)$$

$$A_p^\dagger = a_{p+}^\dagger a_{p-}^\dagger \qquad [N_p, A_q^\dagger] = 2\delta_{pq} A_p^\dagger$$

$$A_p = a_{p-} a_{p+} \qquad [N_p, A_q] = -2\delta_{pq} A_p$$

We also considered a Richardson-Gaudin model:

$$H = \sum_{p=1}^{P} d_p N_p - 2g \sum_{p,q=1}^{P} \sqrt{(\alpha - d_p)(\alpha - d_q)} A_p^\dagger A_q$$

Both models can be exactly solved! (Important for comparison)

# NEURAL WAVEFUNCTIONS

In this case we perform a simple variational calculation to estimate:

$$E_V \equiv \frac{\langle \psi_V | H | \psi_V \rangle}{\langle \psi_V | \psi_V \rangle}$$

as a function of the parameters in the wavefunction. The latter is represented in terms of occupation number states:

Probability to be sampled

$$E_V = \sum_N \frac{|\langle N|\psi_V\rangle|^2}{\langle \psi_V|\psi_V\rangle} E_L(N) \quad \text{where} \quad E_L(N) = \frac{\langle N|H|\psi_V\rangle}{\langle N|\psi_V\rangle} \quad \text{is the local energy.}$$

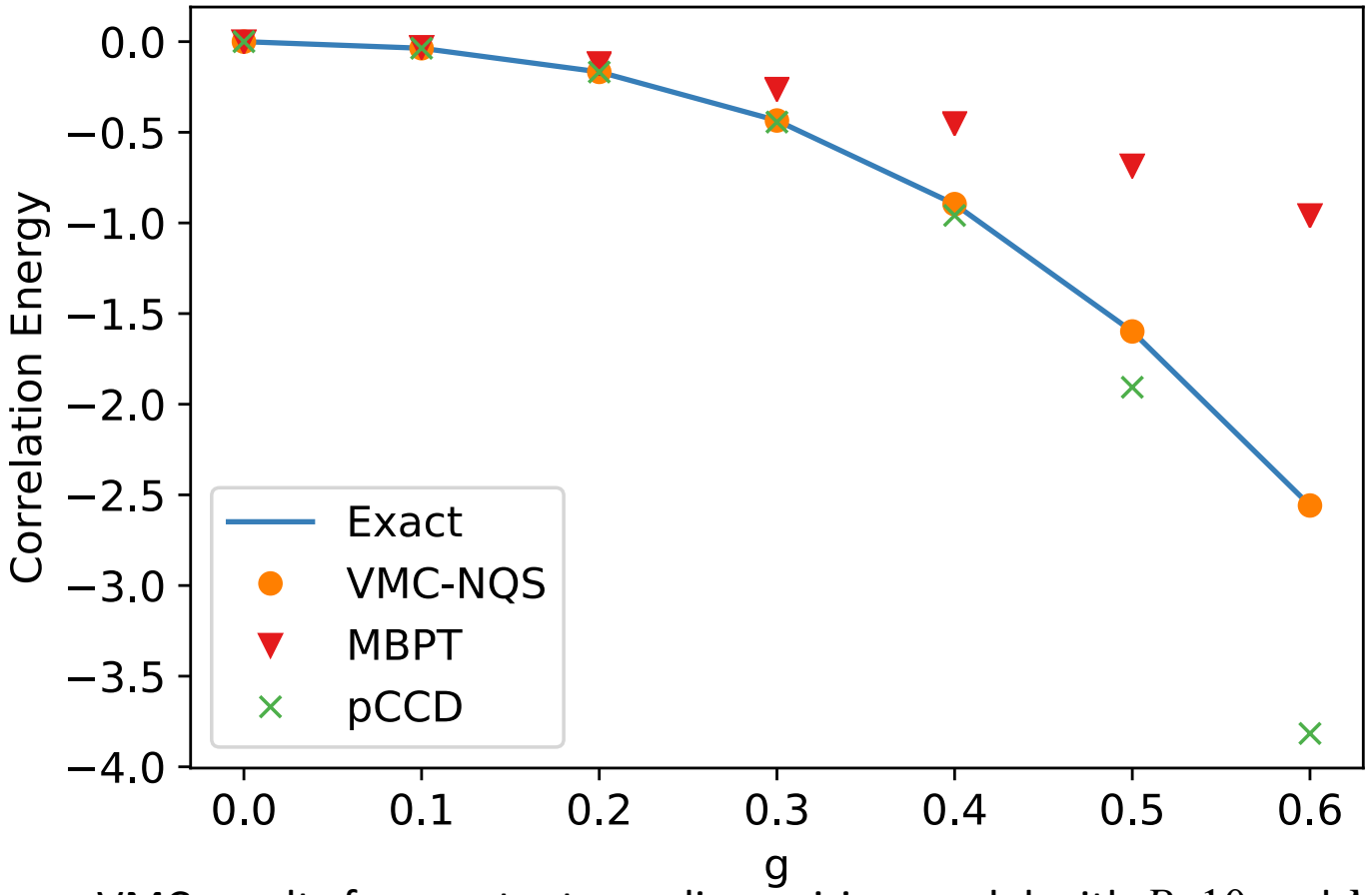
The variatioinal ansatz is a so-called neural wave function:

$$\psi_V(N) \equiv \langle N|\,\psi_V\rangle = e^{\mathcal{U}(N)} \tanh(\mathcal{V}(N))$$

where $\mathcal{U}(N)$ and $\mathcal{V}(N)$ are fully connected neural networks (FCNNs).
The model space is given in terms of the number $P$ of levels that can be occupied by the $M$ pairs of Fermions.
The states $|N\rangle$ are then given by $P$ bits, $M$ of which have value $1$ and P-M have value $0$.

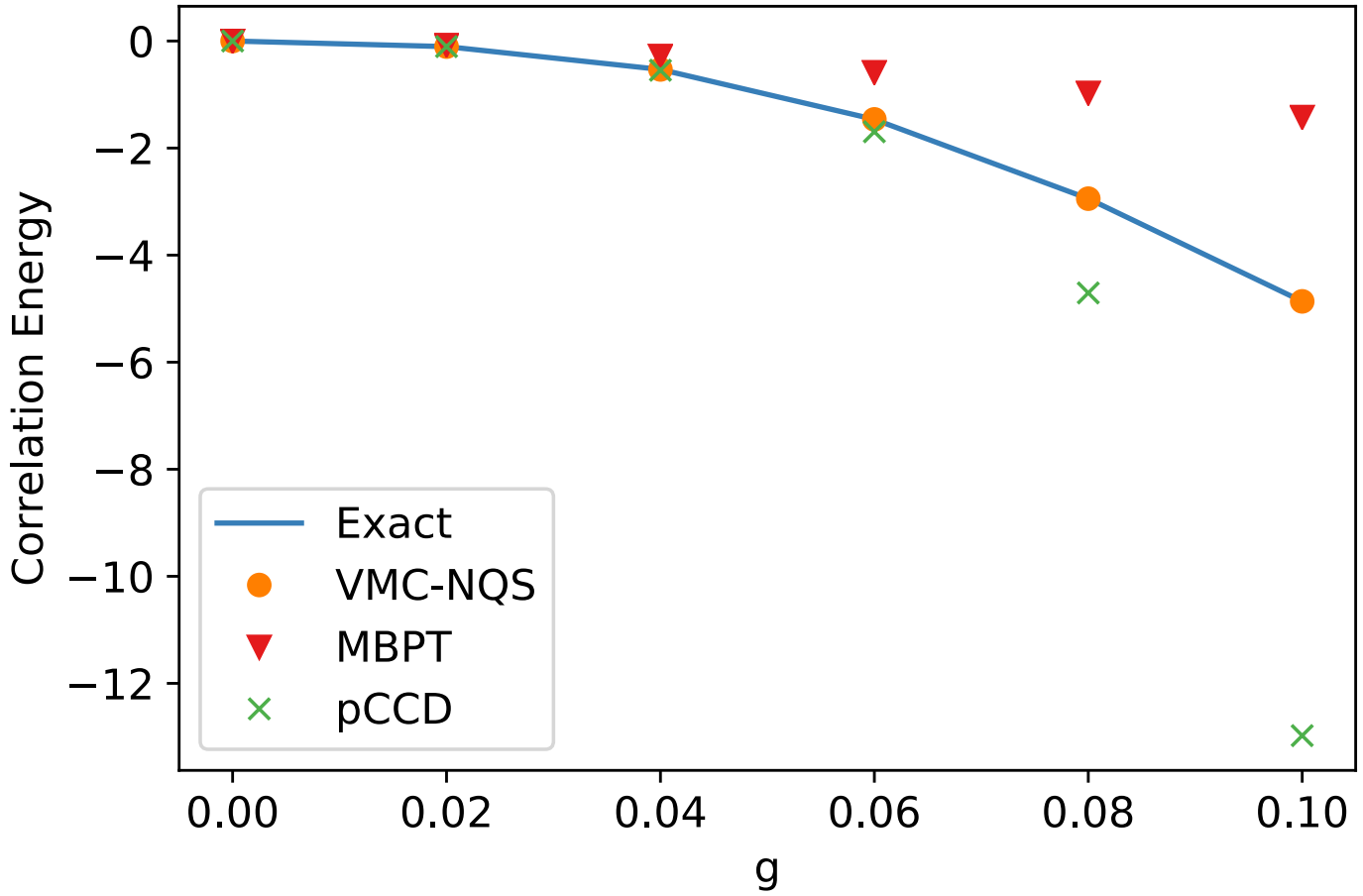
# NEURAL WAVEFUNCTIONS

Mauro Rigo, Benjamin Hall, Morten Hjorth-Jensen, Alessandro Lovato, and FP, Phys. Rev. E **107**, 025310 (2023)




VMC results for constant coupling pairing model with $P$=10 and $M$=5 as a function of the interaction strength $g$, compared to CC, MBPT and exact results. Notice that pCCD calculations do not respect the variational principle.

# NEURAL WAVEFUNCTIONS




VMC results for a separable coupling pairing model with $P$=10 and $M$=5 as a function of the interaction strength $g$, compared to CC, MBPT and exact results. Notice that pCCD calculations do not respect the variational principle.

# PIANI PER IL PROSSIMO FUTURO

- Extension of the CIMC to the case of symmetric nuclear matter. Recent calculations show that the situation is a bit more under control than it was just a few years ago. However, it is still worth checking the results coming from chiral forces in the non-local formulation.

- Computation of other observables, also in nuclei. In particular there is a proposal by Carlo Barbieri to use this formalism to compute optical potentials (a PRIN was also submitted on the subject)

- Use of neural wave functions in configuration space for more realistic interactions (effective chiral or phenomenological). This somewhat simplifies the computation of generic observables

- Extension of the use of NWF in coordinates for strange systems. We recently started a collaboration with A. Drago and A. Di Donna (a master student in Ferrara) for the study of light hypernuclei. This opens the way to the pursuing a few ideas concerning the properties of supersaturated matter (for astrophysical applications)