

# MONTE CARLO METHODS

## — PART 3

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# Fermions

Many-Fermion systems require a wavefunction that is antisymmetric under exchange of particles.

From a strictly mathematical point of view, the search of an antisymmetric ground state corresponds to the search of an excited state of the Hamiltonian. In fact, the absolute ground state of the Hamiltonian is always a nodeless function. A heuristic argument justifying this statement, is based on the form of the Green's function:

$$\begin{aligned}\langle R | e^{-(H-E_0)\tau} | R' \rangle &\approx \langle R | e^{-[V(R)-E_0]\frac{\Delta\tau}{2}} e^{-T\tau} e^{-[V(R')-E_0]\frac{\Delta\tau}{2}} | R' \rangle + o(\Delta\tau^3) \\ &= \left[ \frac{1}{2\pi\hbar^2/m\Delta\tau} \right]^{\frac{3A}{2}} e^{-\frac{(R-R')^2}{2\hbar^2/m\Delta\tau}} e^{-\left[ \frac{V(R)+V(R')}{2} - E_T \right] \Delta\tau}\end{aligned}$$

This expression is strictly positive definite at all imaginary times. Therefore any point in configuration space can be propagated to any point of the domain of the Hamiltonian. Therefore the ground state can be zero only on the boundaries of this domain (where eventually one can have infinite absorption)

# Fermions

The difficulty in projecting out the component of a generic wavefunction along the ground state is known as **SIGN PROBLEM**. The name comes from the fact that a naïve way of looking at it is simply to observe that a wavefunction changing sign in space cannot be sampled, because it is not a probability density.

This way of looking at the sign problem is too simple-minded. Let us assume that we have an approximation of the ground state of the many-Fermion system. The minimum condition required is that it has a component in the same subspace as the exact solution (i.e. it has the correct symmetry requirements).

Formally, we can stabilize the right component in the imaginary time propagation simply by changing the reference eigenvalue.

$$\Psi(R, \tau) = e^{-(H-E_0^A)\tau} \Psi(R) = e^{-(E_0-E_0^A)\tau} c_0 \Psi_0(R) + c_0^A \Psi_0^A(R) + \sum_{n \neq 0} e^{-(E_n-E_0^A)\tau} c_n \Psi_n(R)$$

Exponentially diverging

Stable

Exponentially decaying

# Fermions

The exponentially growing component along the symmetric ground state does not change the expectation of the Hamiltonian, if we use as a function to project from an antisymmetric function  $\Psi_T^A$ :

$$E_0^A = \frac{\langle \Psi(R, \tau) | \hat{H} \Psi_T^A \rangle}{\langle \Psi(R, \tau) | \Psi_T^A \rangle} = \frac{\int dR [e^{-(E_0 - E_0^A)\tau} c_0 \Psi_0(R) + c_0^A \Psi_0^A(R)] \hat{H} \Psi_T^A(R)}{\int dR [e^{-(E_0 - E_0^A)\tau} c_0 \Psi_0(R) + c_0^A \Psi_0^A(R)] \Psi_T^A(R)} \quad \text{for large } \tau$$

The denominator yields a finite value, because of the symmetry of the functions:

$$\begin{aligned} & \int dR [e^{-(E_0 - E_0^A)\tau} c_0 \Psi_0(R, 0) + c_0^A \Psi_0^A(R, 0)] \Psi_T^A(R) = \\ & = \int dR e^{-(E_0 - E_0^A)\tau} c_0 \Psi_0(R) \Psi_T^A(R) + \int dR c_0^A \Psi_0^A(R) \Psi_T^A(R) \end{aligned}$$

The same holds for the numerator, considering that

$$\hat{H} \Psi_T^A \approx E_0^A \Psi_0^A + \text{components along excited states}$$



# Fermions

The previous expression might give the idea that imaginary time projection works as well also for excited states (*the change in sign is not a problem by itself!*)

However, in a Diffusion Monte Carlo calculation the estimate of the eigenvalue is always approximate when we take a finite number of samples. The standard deviation of the answer depends on the variance of the  $\hat{H}\Psi_T^A$  (in MC sense):

$$\sigma^2(\hat{H}\Psi_T^A) = \left\langle \left( \hat{H}\Psi_T^A \right)^2 \right\rangle - \left\langle \hat{H}\Psi_T^A \right\rangle^2$$

Let us consider the expectation of the square of  $\hat{H}\Psi_T^A$

$$\frac{\langle \Psi(R, \tau) \hat{H} | \hat{H}\Psi_T^A \rangle}{\langle \Psi(R, \tau) | \Psi_T^A \rangle} = \frac{\int dR \left[ e^{-(E_0 - E_0^A)\tau} c_0 \Psi_0(R) + c_0^A \Psi_0^A(R) \right] \left( \hat{H}\Psi_T^A(R) \right)^2}{\langle \Psi(R, \tau) | \Psi_T^A \rangle} =$$

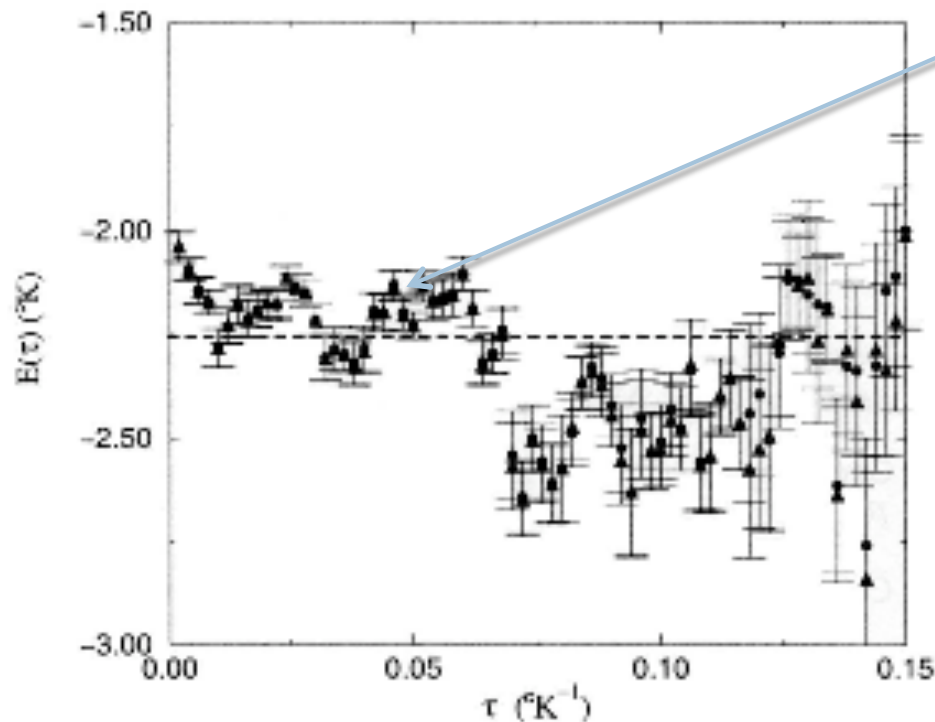
Exponentially diverging (bad)

Decaying (OK)

$$= \frac{\int dR e^{-(E_0 - E_0^A)\tau} c_0 \Psi_0(R) \left( \hat{H}\Psi_T^A(R) \right)^2}{\langle \Psi(R, \tau) | \Psi_T^A \rangle} + \frac{\int dR c_0^A \Psi_0^A(R) \left( \hat{H}\Psi_T^A(R) \right)^2}{\langle \Psi(R, \tau) | \Psi_T^A \rangle}$$

# Fermions

We are left with a contradictory statement: the energy converges to the exact eigenvalue with an exponentially growing statistical error. In other words, the signal to noise ratio decays exponentially.



$$\frac{1}{E_0^F - E_0^B} \approx 0.05 \text{K}^{-1}$$

*Evolution of the mean value of energy in a DM C calculation with free nodes for 14  $^3\text{He}$  particles. Note that the error bars rapidly increase with imaginary time.*

# Fermions

Another way of looking at the sign problem is that of considering the evolution of *signed* walkers

Let us consider the ground state of a many-Fermion system. We can always separate the positive and the negative parts of the wavefunction as follows:

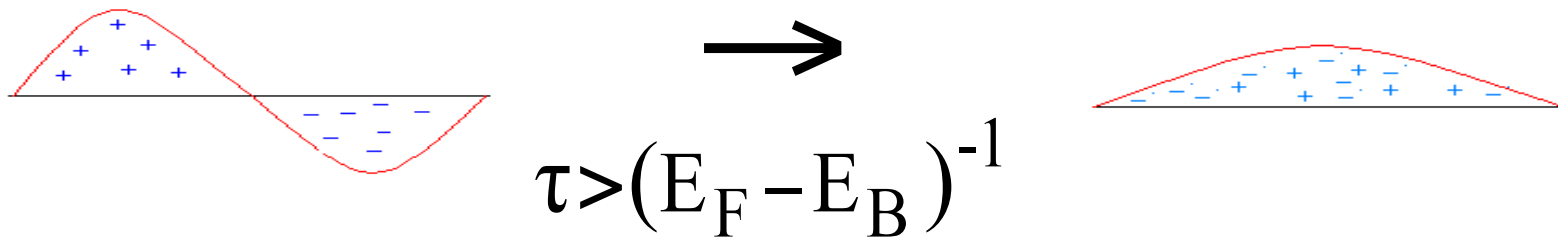
$$\Psi_0^A(R) = \Psi^+(R) - \Psi^-(R)$$

where both  $\Psi^+$  and  $\Psi^-$  are positive definite, and therefore good candidates for being densities of walkers. We can imagine to sample separately the two parts of the wavefunction using two different sets of walkers  $R^+$  and  $R^-$ . These walkers will contribute to estimates with different signs:

$$E_0^A \approx \frac{\sum_i \hat{H} \Psi_T^A(R^+) - \sum_i \hat{H} \Psi_T^A(R^-)}{\sum_i \Psi_T^A(R^+) - \sum_i \Psi_T^A(R^-)}$$

# Fermions

However, the imaginary time evolution will drive both populations to the same distribution, proportional to the absolute ground state of the Hamiltonian.



The consequence is that all estimates have an exponentially increasing noise (the denominator in the quotient previously defined annihilates exponentially, and the signal to noise ratio decays as well)

*Antisymmetry is not a local property of the solution. Therefore the stability of the antisymmetric solution cannot be achieved by modifying the local behavior of the propagator (e.g. by importance sampling). One needs to break an overall “plus-minus” symmetry of the Hamiltonian.*

# Fixed node approximation

The success of the Diffusion Monte Carlo method is due to the fact that an approximate version exist, proposed originally by J. Anderson, that allows for computing with decent accuracy properties of many-Fermion systems of physical interest. This approximation is called *FIXED-NODE*.

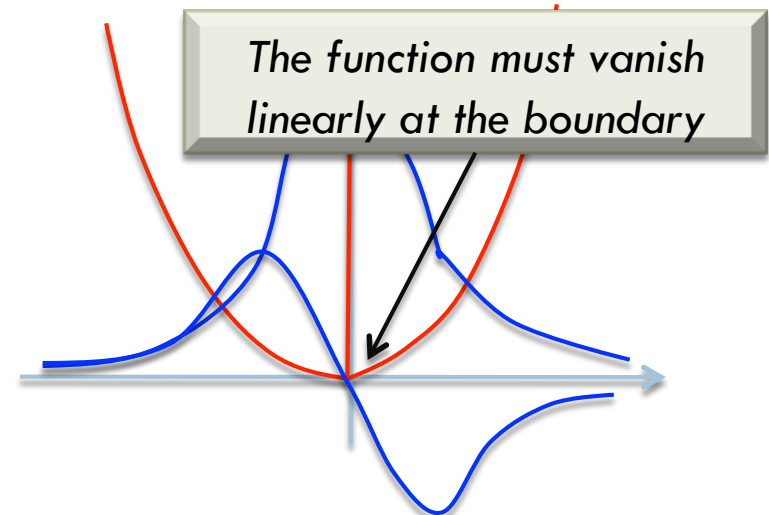
From a formal point of view, the FN approximation starts from a trial solution of the Hamiltonian to be studied. The Hamiltonian is then redefined as follows:

$$\hat{H} = \hat{H}_0 + V_{FN}$$

where

$$V_{FN}(R) = \begin{cases} 0 & \text{if } \Psi_T^A(R) > 0 \\ \infty & \text{if } \Psi_T^A(R) < 0 \end{cases}$$

The fixed-node potential changes the boundary conditions of the problem, imposing an infinite absorption rate in correspondence of the nodes of  $\Psi_T^A$ .



# Fixed node approximation

Obviously, at this point we are not solving any more the original problem, but a *different* problem. How are the solutions related to each other?

The equation that is solved by the DMC becomes:

$$\begin{cases} (\hat{H}_0 + \delta_{FN})\chi(R) = E_{FN}\chi(R) \\ \chi(R)\Psi_T^A(R) \geq 0 \end{cases}$$

Under certain conditions  $E_{FN}$  is an upper bound for the eigenvalue  $E_0^A$ . The following argument might be made general for any set of symmetries  $\mathcal{A}$  defining the subspace of the Hilbert space we are interested in. However, we will limit ourselves to the case of the group of permutations of particles, considering therefore only the case of an antisymmetric state.

# Fixed node approximation

The conditions for having an upper bound are the following:

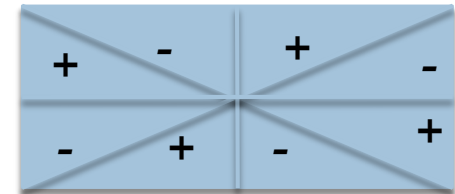
- ✓ The trial wavefunction must be real;
- ✓ An operator  $A$  exists such that it transforms the wavefunction maintaining  $H$  invariant (this is obviously true for permutations of particles in presence of local interactions);
- ✓  $[H,A]=0$ , and  $A$  is an hermitean projector (true for permutations);
- ✓ The trial wavefunction must belong to a one-dimensional representation of the symmetry group considered. This is true for the ground state of the Hamiltonian, both symmetric and antisymmetric;
- ✓  $H$  must not have other delta terms;

# Fixed node approximation

If the Hamiltonian is invariant under the group of permutations, and the wavefunction transforms like a real one-dimensional representation of the group of permutations, the nodal surface does not change. Therefore:

$$\delta_{FN}(R) \neq 0 \text{ iff } \chi(R) = 0 \text{ or } P\chi(R) = 0$$

Under these conditions, the variational theorem holds:



$$E_0^A \leq \frac{\langle P\Psi_T^A | \hat{H} P\chi(R) \rangle}{\langle P\Psi_T^A | P\chi(R) \rangle} = \frac{\langle P\Psi_T^A | \hat{H} \chi(R) \rangle}{\langle P\Psi_T^A | \chi(R) \rangle} = \frac{\langle \Psi_T^A | (\hat{H} + \delta_{FN}(R)) \chi(R) \rangle}{\langle \Psi_T^A | \chi(R) \rangle} = E_{FN}$$

*"Tiling" property*

Equality holds only if the **nodal surface of the trial function is exact**.

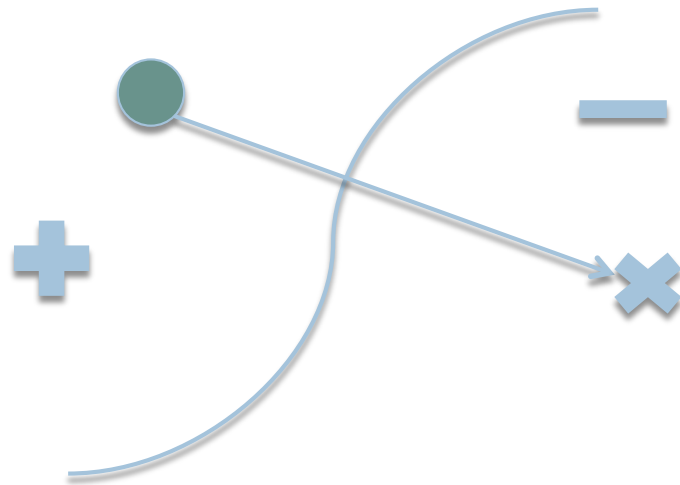
On the other hand, the fixed-node eigenvalue has to be lower than the variational estimate of the energy on the antisymmetric trial function. We have therefore:

$$E_0^A \leq E_{FN} \leq E_T^A$$



# Fixed node approximation

The implementation of the fixed node in a DMC code is extremely easy.  
It is sufficient to kill walkers trespassing the nodal surface.



*If an acceptance-rejection scheme is implemented, then the move can simply be rejected*

# Complex wavefunctions

The situation is much less satisfactory when we have to do with complex wavefunctions. Hamiltonians not invariant under time reversal do not admit real eigenfunctions. Sometimes (e.g. in the case of minimal electromagnetic coupling) it is possible to solve the problem for the sum or difference of the wavefunction and the complex conjugate. However, in general this is not possible.

In this case we cannot use the fixed node approximation! An easy workaround is represented by the fixed-phase approximation. A simple way of introducing it is the following. Let us consider the expectation of the Hamiltonian:

$$E_0^A = \frac{\langle \Psi(R, \tau) | \hat{H} \Psi_T^A \rangle}{\langle \Psi(R, \tau) | \Psi_T^A \rangle} = \frac{\int dR \Psi^*(R, \tau) \hat{H} \Psi_T^A(R)}{\int dR \Psi^*(R, \tau) \Psi_T^A(R)} = \frac{\int dR \Psi^*(R, \tau) \Psi_T^A(R) \frac{\hat{H} \Psi_T^A(R)}{\Psi_T^A(R)}}{\int dR \Psi^*(R, \tau) \Psi_T^A(R)}$$

# Complex wavefunctions

We can always write the wavefunctions as modulus times the phase:

$$\Psi(R, \tau) = |\Psi(R, \tau)| e^{i\phi(R, \tau)} \quad \Psi_T^A(R) = |\Psi_T^A(R)| e^{i\phi_T^A(R)}$$

Substituting we obtain:

$$E_0^A = \frac{\int dR |\Psi(R, \tau)| |\Psi_T^A(R)| e^{i\phi(R, \tau) - i\phi_T^A(R)} \frac{\hat{H}\Psi_T^A(R)}{\Psi_T^A(R)}}{\int dR |\Psi(R, \tau)| |\Psi_T^A(R)| e^{i\phi(R, \tau) - i\phi_T^A(R)}}$$

The fixed-phase approximation consists of assuming:

$$\phi(R, \tau) \equiv \phi_T^A(R)$$

This means that the density of walkers to be sampled is the product of the moduli of the importance function and of the projected wavefunction.

# Complex wavefunctions

The fixed phase approximation corresponds to taking in the Green's function the real part of the local kinetic energy, rather than the complex expression.

$$G(R, R', \Delta\tau) =$$

$$= \exp \left[ \frac{\left( -\frac{\hbar^2}{2m} \operatorname{Re} \left( \frac{\nabla^2 \Psi_T^A(R)}{\Psi_T^A(R)} \right) + \frac{\hat{V} \Psi_T^A(R)}{\Psi_T^A(R)} - \frac{\hbar^2}{2m} \operatorname{Re} \left( \frac{\nabla^2 \Psi_T^A(R')}{\Psi_T^A(R')} \right) + \frac{\hat{V} \Psi_T^A(R')}{\Psi_T^A(R')} \right) - E_0^A}{2} \right]$$

Observables are computed as:

$$\langle \hat{O} \rangle = \frac{1}{\# \text{ samples}} \sum_{i=1}^{\# \text{ samples}} \operatorname{Re} \left\{ \frac{\hat{O} \Psi_T^A(R_i)}{\Psi_T^A(R_i)} \right\}$$

# Complex wavefunctions

The fixed phase is not the only approximation that can be used in the case of complex wavefunctions.

An alternative that is often used is the so-called “constrained path” approximation. In this case the walkers are constrained to the region in which the trial wavefunction has positive real part.

At the same time the drift term must be redefined as

$$R_{drifted} = R' + \frac{\nabla \text{Re}\{\Psi_T^A(R_i)\}}{\text{Re}\{\Psi_T^A(R_i)\}} \Delta\tau$$

Observables are computed as:

$$\langle \hat{O} \rangle = \frac{1}{\# \text{ samples}} \sum_{i=1}^{\# \text{ samples}} \frac{\hat{O} \text{Re}\{\Psi_T^A(R_i)\}}{\text{Re}\{\Psi_T^A(R_i)\}}$$

# Complex wavefunctions

- For the fixed phase approximation it is possible to prove an upper bound property only in the case of local spin-isospin independent interactions. When the interaction is operatorial, as in the case of many nucleon systems, the upper bound property is not guaranteed.
- The constrained path approximation cannot be proved to be an upper bound in any case.
- There is in principle no way to understand a priori which approximation is more accurate. In nuclear physics, often the constrained path is used, but in recent calculations we found that the fixed-phase gives lower energies.
- For Hamiltonians in which the wavefunction can be taken real (e.g. two dimensional quantum dots immersed in a perpendicular magnetic field), the comparison between fixed-phase, constrained path and fixed node shows that using complex wavefunctions usually leads to higher estimates of the energy.

# Nuclear Hamiltonians

The nucleon nucleon interaction poses a particular challenge for the implementation of DMC techniques. The main reason is the fact that the interaction depends on the relative spin/isospin of the nucleons, and in general it is non local.

A class of realistic two-body local potential is the so-called Argonne VX (AVX). Such potentials have the form:

$$V(ij) = \sum_{i < j} \sum_{p=1}^{X\tau_i} v_p(r_{ij}) O^{(p)}(i,j)$$

As an example consider the potential AV8. The operators are:

$$O^{p=1\dots 8} = (\mathbf{1}, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}, \mathbf{L} \cdot \mathbf{S}) \otimes (\mathbf{1}, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_i)$$

where:

$$S_{ij} = 3(\mathbf{r}_{ij} \cdot \boldsymbol{\sigma}_i)(\mathbf{r}_{ij} \cdot \boldsymbol{\sigma}_j) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \quad \mathbf{L} = \frac{1}{2i}(\mathbf{r}_i - \mathbf{r}_j) \times (\nabla_i - \nabla_j)$$

$$\mathbf{S} = \frac{1}{2}(\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_j)$$

# Variational Monte Carlo

Wave function with operatorial Jastrow 2 body and 3 body correlations should be used to impose correct cusp conditions in each channel, i.e. to ensure that:

$$\frac{H\psi_T(R)}{\psi_T(R)} < \infty$$

If this condition is satisfied, fluctuations in the local energy will be small and the calculation very rapidly converging. However, for a realistic nuclear Hamiltonian this implies that the wavefunction itself has an operatorial form:

$$|\psi_T(R)\rangle = \left[ 1 + \sum_p \sum_{i<j} u_p(r_{ij}) \hat{O}_p \right] |\psi_0(R)\rangle$$

*Mean field  
function made  
up of single  
particle spinors*

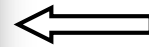


# VMC and Nuclear Hamiltonians

The **standard VMC technique** is easy to apply only if the interaction is purely central, or whenever the wavefunction can be written as a product of eigenfunctions of  $S_z$ .

For realistic potentials the presence of quadratic spin and isospin operators imposes that a **MULTICOMPONENT WAVEFUNCTION** is used

$$\frac{A!}{Z!(A-Z)!} 4^A$$



*The huge number of states limits present calculations to  $A \leq 14$*

# Auxiliary Fields

*The use of auxiliary fields and constrained paths is originally due to S. Zhang for condensed matter problems (S.Zhang, J. Carlson, and J.Gubernatis, PRL74, 3653 (1995), Phys. Rev. B55. 7464 (1997))*

*Application to the Nuclear Hamiltonian is due to S.Fantoni and K.E. Schmidt (K.E. Schmidt and S. Fantoni, Phys. Lett. 445, 99 (1999))*

The method consists of using the **Hubbard-Stratonovich** transformation in order to reduce the spin operators appearing in the Green's function from **quadratic** to **linear**

# Auxiliary Fields

For simplicity, let us consider a system made of neutrons only (no isospin).  
the n-n interaction can be re-written in a matrix form

$$V = V_{si} + V_{sd} = V_{si} + \sum_{i\alpha j\beta} \sigma_{i\alpha} A_{i\alpha;j\beta} \sigma_{j\beta}$$

where the  $3N \times 3N$  matrix  $A$  is a combination of the various  $v(p)$  appearing in the interaction.  $A$  is **real** and **symmetric**, and it can be diagonalized:

$$\sum_{j\beta} A_{i\alpha;j\beta} \Psi_{j\beta}^n = \lambda_n \Psi_{i\alpha}^n$$

Because the matrix is symmetric, eigenvalues and eigenvectors are real.

# Auxiliary Fields

Let us now define a new set of operators from the linear combinations of the original operators that diagonalize the interaction:

$$O_n = \sum_{i\alpha} \sigma_{i\alpha} \psi_{i\alpha}^n$$

The spin dependent part of the interaction can now be expressed as

$$V_{sd} = \frac{1}{2} \sum_{n=1}^{3N} \lambda_n O_n^2$$

# Auxiliary Fields

We can apply the Hubbard-Stratonovich transformation to the Green's function for the spin-dependent part of the potential:

$$e^{-V_{sd} \Delta\tau} \cong \prod_{n=1}^{3N} e^{-\frac{1}{2} \lambda_n O_n^2 \Delta\tau} \quad \leftarrow \text{Commutators neglected! (Trotter-Suzuki again...)}$$

$$e^{-\frac{1}{2} \lambda_n O_n^2 \Delta\tau} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx_n \exp \left\{ -\frac{x_n^2}{2} - \sqrt{-\lambda_n \Delta\tau} x_n O_n \right\}$$

The  $x_n$  are auxiliary variables to be sampled. The effect of the  $O_n$  is a rotation matrix to be applied to the spinorial components of each particle.

# Auxiliary fields



## *Additional remarks*

- **Spin-orbit terms** can be treated in a similar way (with some extra care)
- **Fermion sign problem still in place**, with the previously discussed difficulty of dealing with wave functions which are complex.

# AN EXAMPLE: COMPUTATION OF PAIRING GAP IN NEUTRON AND NUCLEAR MATTER

- **“Superfluidity” of nuclei** as been long known. Attractive components of the NN force induce a pairing among nucleons. A few outcomes of it are the even-odd staggering of binding energies or anomalies on the momentum of inertia.
- More recently superfluidity of bulk nuclear matter has been recognized to play a role in the **cooling process of neutron stars.**

# Nuclear Hamiltonian

The interaction between  $N$  nucleons can be written in terms of an Hamiltonian of the form:

$$H = \sum_{i=1}^N \frac{p_i^2}{2m_i} + \sum_{i < j} \sum_{p=1}^M v_p(r_{ij}) O^{(p)}(i, j) + V_3$$

where  $i$  and  $j$  label the nucleons,  $r_{ij}$  is the distance between the nucleons and the  $O^{(p)}$  are operators including spin, isospin, and spin-orbit operators.  $M$  is the maximum number of operators ( $M=18$  for the Argonne  $v_{18}$  potential).



# Nuclear Hamiltonian

The interaction used in this study is  $AV_8'$  cut to the first six operators.

$$O^{p=1\dots6} = (\mathbf{1}, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}) \otimes (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)$$

where

$$S_{ij} = 3(\mathbf{r}_{ij} \cdot \boldsymbol{\sigma}_i)(\mathbf{r}_{ij} \cdot \boldsymbol{\sigma}_j) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$$

**EVEN AT LOW DENSITIES THE DETAIL OF THE INTERACTION STILL HAS IMPORTANT EFFECTS (see Gezerlis, Carlson 2008)**

# Nuclear matter

## Wave Function

The *many-nucleon wave function* is written as the product of a **Jastrow factor** and an **antisymmetric mean field wave function**:

$$\psi(\mathbf{r}_1 \dots \mathbf{r}_N; \boldsymbol{\sigma}_1 \dots \boldsymbol{\sigma}_N; \boldsymbol{\tau}_1 \dots \boldsymbol{\tau}_N) = \prod_{i < j} \phi_J(r_{ij}) A(\mathbf{r}_1 \dots \mathbf{r}_N; \boldsymbol{\sigma}_1 \dots \boldsymbol{\sigma}_N; \boldsymbol{\tau}_1 \dots \boldsymbol{\tau}_N)$$

The functions  $\phi_J$  in the Jastrow factor are taken as the scalar components of the FHNC/SOC correlation operator which minimizes the energy per particle of SNM at saturation density  $r_0 = 0.16 \text{ fm}^{-3}$ . The antisymmetric product  $A$  is a Slater determinant of *plane waves*.

# Nuclear matter

## *Simulations*

*Most simulations are performed in a **periodic box**. The number of nucleons must be chosen in order to fill a shell of momenta in 3d. The smallest usable number is **28 nucleons** (14 p and 14 n). The density was changed varying the size of the simulation box.*

*Particular attention must be paid to **finite size effects**.*

- At the higher densities we performed a summation over the first shell of periodic replicas of the simulation cell.*
- Some checks against simulations with a **larger number of nucleons (N=76,108)** were performed at the extrema of the density interval considered.*

# $^1S_0$ gap in neutron matter

AFDMC should allow for an accurate estimate of the gap in **superfluid neutron matter**.

INGREDIENT NEEDED: A “SUPERFLUID” WAVEFUNCTION.

*Nodes and phase* in the superfluid are better described by a *Jastrow-BCS wavefunction*

$$\Psi_T(R) = \left[ \prod_{i < j} f_J(r_{ij}) \right] \phi_{BCS}(R, S)$$

where the BCS part is a Pfaffian of orbitals of the form

$$\phi(\mathbf{r}_{ij}, s_i, s_j) = \sum_a \frac{v_{k_a}}{u_{k_a}} e^{-i\mathbf{k} \cdot \mathbf{r}_{ij}} \chi(s_i, s_j)$$

***Coefficients from CBF calculations***

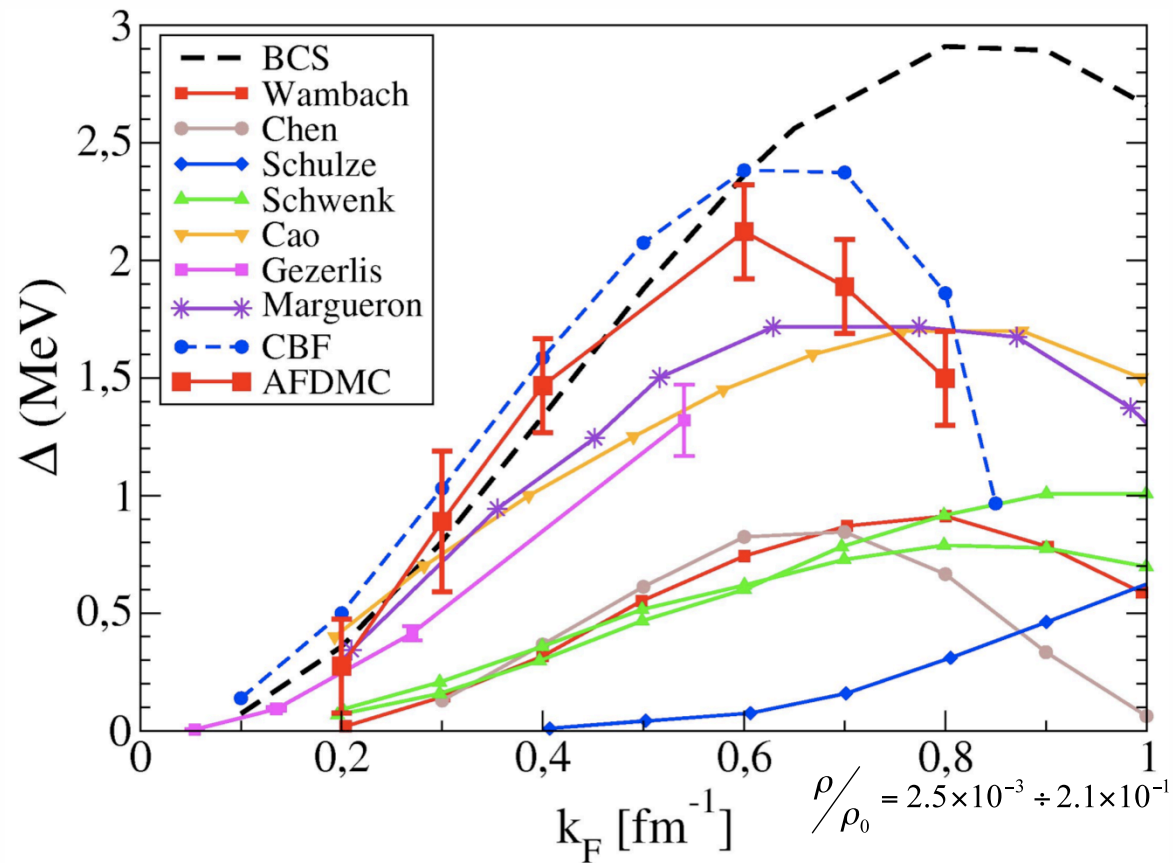
# Gap in neutron matter

The gap is estimated by the even-odd energy difference at fixed density:

$$\Delta(N) = E(N) - \frac{1}{2} [E(N+1) - E(N-1)]$$

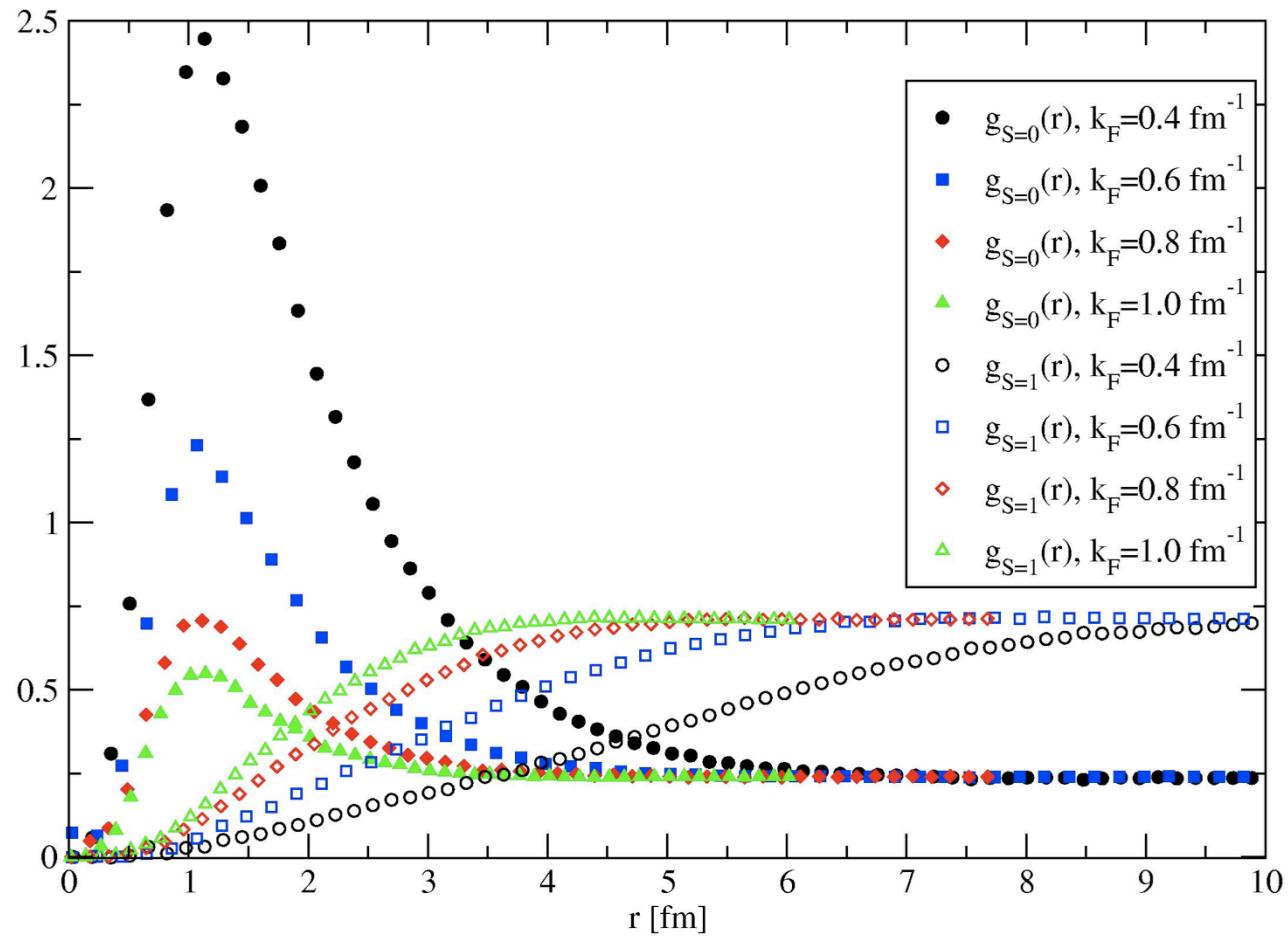
- For our calculations we used  $N=12-18$  and  $N=62-68$ . The gap slightly decreases by increasing the number of particles.
- The parameters in the pair wavefunctions have been taken by CBF calculations.

# Gap in Neutron Matter



Gandolfi S., Illarionov A., Fantoni S., P.F., Schmidt K., PRL 101, 132501 (2008)

# Pair correlation functions



# Gap in asymmetric matter

