Quantum stochastic methods for the N-body nuclear problem

P1:

Quantum Monte Carlo

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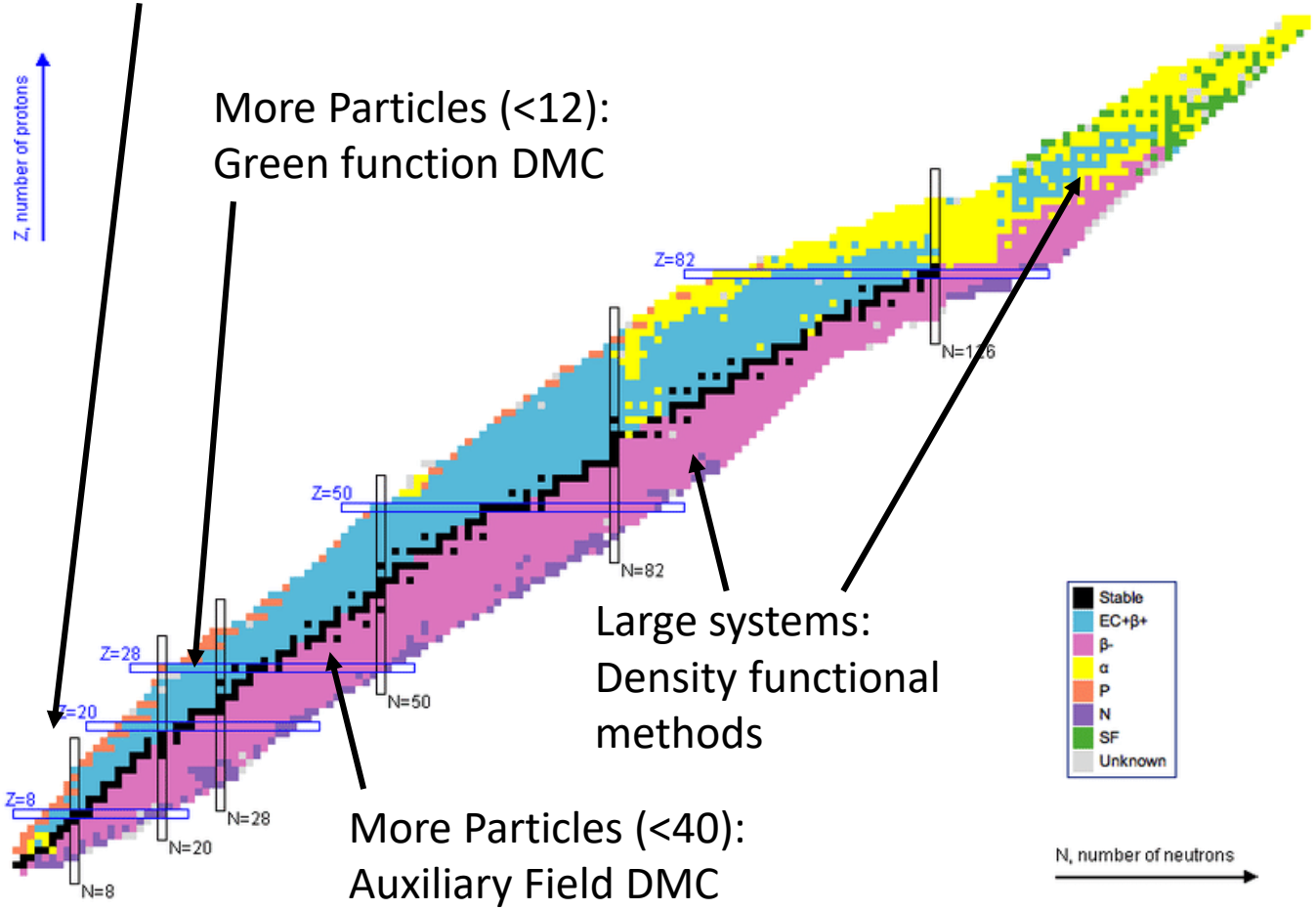
Introduction

Few Particles:
Exact diagonalization

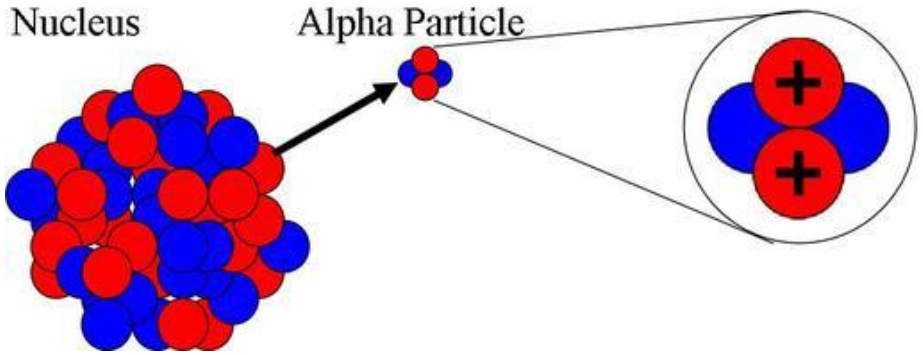
More Particles (<12):
Green function DMC



Large systems:
Density functional
methods

More Particles (<40):
Auxiliary Field DMC

- Variational Monte Carlo
- Diffusion Monte Carlo
  - Fermions, sign problem, and auxiliary fields
- Towards a density functional description
- Dynamical systems and in medium dynamics
- Phase-space approaches



http://physicsopenlab.org/2016/02/11/alpha-%CE%B1-radioactivity/

Henning, Greg. (2012). Stability of Transfermium Elements at High Spin: Measuring the Fission Barrier of 254

A key concept: the variational principle

Problem: find the ground state energy of a many-body quantum mechanical system.

Possible solution: find the wave function that minimizes the energy of a system.

$$H\,\Psi_{Gs} = E\,\Psi_{Gs}$$

- $E_{gs} = \min_{a} \langle \Psi_T^a | H | \Psi_T^a \rangle$

See e.g. Stochastic variational method
Y. Suzuki and K. Varga, (1998)

Expand the wave function in a base $\Psi_T^a = \sum_A c_A\,\phi_A$
i.e. the ground state energy is the lowest eigenvalue of H in a restricted H.S.

Vary the parameters of the wave function to find the minimum

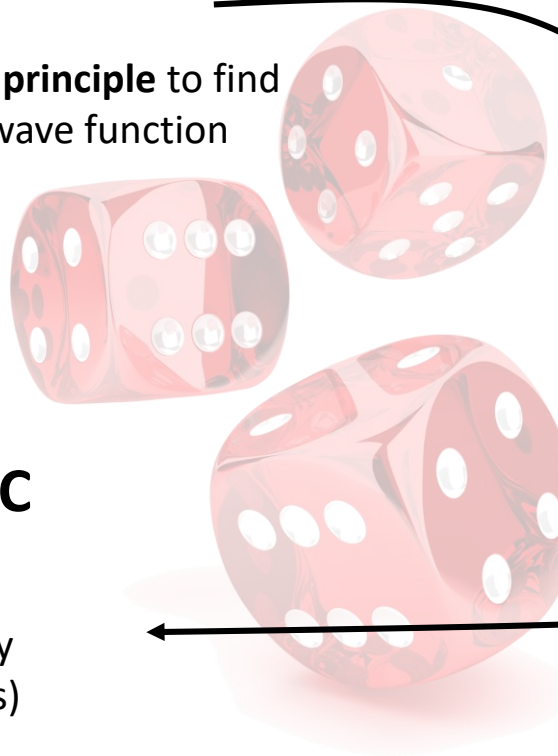
$$\partial_a \langle \Psi_T^a | H | \Psi_T^a \rangle = 0$$

In both cases the choice of the wavefunction is crucial

Quantum Monte Carlo is a class of ab initio, numerical, stochastic many-body methods able to solve a quantum problem (the non-relativistic Schrödinger equation in my case) with improvable uncertainties.

Variational Monte Carlo

- Exploits the **variational principle** to find the best parameterized wave function



Diffusion in imaginary time

- **Excited states** contributions exponentially suppressed
- **Need some approximation** to keep the sign problem under control
- **Many-fermions** accessible with the introduction of **Auxiliary fields**

Unconstrained MC

- Unbiased estimators
- (results only affected by stochastic uncertainties)

Towards more particle sector: Variational Monte Carlo

The idea: minimize the energy over a **set of parameters**

(instead of expanding the groundstate)

$$E_{gs} = \min_a \langle \psi_T^a | H | \psi_T^a \rangle$$

$$E_T = \langle \psi_T | H | \psi_T \rangle = \int \psi_T^*(\boldsymbol{X}) H \psi_T(\boldsymbol{X}) d\boldsymbol{X} = \int |\psi_T(\boldsymbol{X})|^2 \frac{H\psi_T(\boldsymbol{X})}{\psi_T(\boldsymbol{X})} d\boldsymbol{X}$$

M. Kalos and P. Whitlock, Monte Carlo methods (Wilei 2008)

W.K. Hastings, Biometrika **57** (1970) 97-109

Monte Carlo allows to calculate this integral efficiently!

Using the **Central Limit Theorem**!

Central limit theorem

M. Kalos and P. Whitlock, Monte Carlo methods (Wilei 2008)

$\boldsymbol{X}$ fitted with distribution $g(\boldsymbol{X})$

$$I = \int g(\boldsymbol{X})\, f(\boldsymbol{X}) d\boldsymbol{X} \quad \rightarrow \quad I_n = \lim_{n\to+\infty} \frac{1}{n} \sum_{\boldsymbol{X}\in g(\boldsymbol{X})} f(\boldsymbol{X})$$

$$P(I_n) = \frac{1}{\sqrt{2\pi\sigma_n^2}}\, e^{-\frac{(I_N - I)^2}{2\sigma_n^2}} \qquad \sigma_n \propto \frac{1}{\sqrt{n}}$$

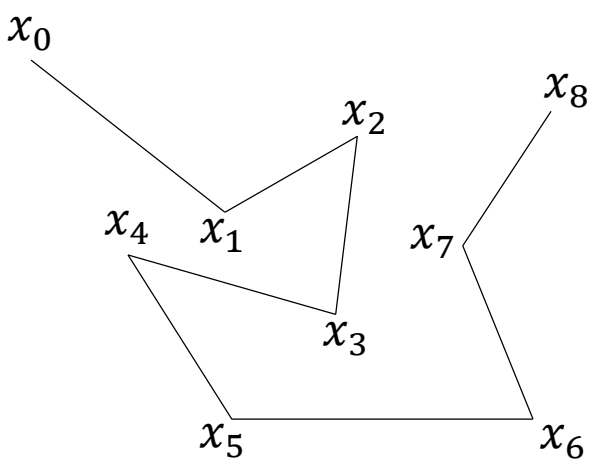
I know how to calculate this!

$$E_a = \int |\psi_T(\boldsymbol{X})|^2 \frac{H\psi_T(\boldsymbol{X})}{\psi_T(\boldsymbol{X})} d\boldsymbol{X} = \lim_{n\to+\infty} \frac{1}{n} \sum_{\boldsymbol{X}\in|\psi_T|^2} \frac{H\psi_T(\boldsymbol{X})}{\psi_T(\boldsymbol{X})}$$

How to sample $|\psi_T|^2$?

$$\sigma_n = \left\langle \left(\frac{H\psi_T(\boldsymbol{X})}{\psi_T(\boldsymbol{X})} \right)^2 \right\rangle - \left\langle \frac{H\psi_T(\boldsymbol{X})}{\psi_T(\boldsymbol{X})} \right\rangle^2 \propto \frac{1}{\sqrt{n}}$$

Sampling procedure: Markov Chains



Ensemble of points distributed as $\psi_T^2(\mathbf{x})$

Main idea:

Chain of points one derived from the other:

1) Move it with a **random walk**:

$$\boldsymbol{x}_{n+1}(x) = \boldsymbol{x}_n + \boldsymbol{\eta} \cdot Step$$

2) **Accept** the move only if the new position is "favorable":
extract a new $\xi = \text{Rand}[0,1]$ and accept only if

$$\frac{\psi_T^2(\boldsymbol{x}_{n+1})}{\psi_T^2(\boldsymbol{x}_n)} > \xi$$

When the number of steps is large, the coordinates are:

- distributed as $\psi_T^2(\mathbf{x})$
- Independent from the initial choice of $\boldsymbol{x}_0$

Look at the reference for the derivation:

M. Kalos and P. Whitlock, Monte Carlo methods (Wilei 2008)

Gagniuc, Paul A. (2017). Markov Chains: From Theory to Implementation and Experimentation. USA, NJ: John Wiley & Sons. pp. 1–235.

$$\eta = Rand[0,1]$$

Step is a parameter *

$\psi_T^2(\boldsymbol{x})$ is the probability we want to sample.

* (a part for the convergence speed, the simulation is independent from the Step)

Quantum VMC

Hastings, W.K. Biometrika 57 (1970) 97-109

M. Kalos and P. Whitlock, Monte Carlo methods (Wilei 2008)

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T. Skyrme
Nucl.Phys. 9 (1959) 615-634

J. Toulouse, C. J. Umrigar
Journal of Chemical Physics 126, 084102 (2007)

Trial wave function:

$$\psi_T = \left[\prod_{i=2}^{n} U_i(\boldsymbol{X}) \right] \phi^A(\boldsymbol{X})$$

Physical guess

- 2-body Schrödinger equation solution
- $U_3^{ijk} = U_2^{ij} + U_2^{ik} + U_2^{jj}$
- Skyrme wave functions Slater determinant

General assumption

- Expansion of the wavefunction in a basis. e.g. Hermite polinomial, Spline functions.

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Most of the energy in nuclear physics comes from **(iso-)spinorial correlation:**

Nuclear interaction include **spin-isospin operators** $(\sigma_1 \cdot \sigma_2, \tau_1 \cdot \tau_2, (\sigma_1 \cdot r_{ij})(\sigma_2 \cdot r_{ij}), \dots)$ and **many-body interactions.**

The nuclear Hamiltonian has **intrinsic errors:** we do not require chemical precision

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Trial wave function:

$$\psi_T = \left[\prod_{i=2}^{n} U_i(\boldsymbol{X})\right] \phi^A(\boldsymbol{X})$$

$$\phi^A = SD\left(\psi_1^A(\boldsymbol{x}_1), \psi_2^A(\boldsymbol{x}_2), .., \psi_N^A(\boldsymbol{x}_N)\right) = det\begin{pmatrix} \psi_1^A(\boldsymbol{x}_1) & \cdots & \psi_N^A(\boldsymbol{x}_1) \\ \vdots & \ddots & \vdots \\ \psi_1^A(\boldsymbol{x}_N) & \cdots & \psi_N^A(\boldsymbol{x}_N) \end{pmatrix}$$

Single particle wave functions

E.g. $\psi_i^A(\boldsymbol{x_j}) = e^{-\frac{r_j^2}{A_i^2}} \quad Y_{L,m} \left|\Sigma_j\right\rangle \quad \left|\mathrm{T}_j\right\rangle$

Spinorial part (see Auxiliary field QMC)

Spherical harmonics

Radial wave function (A_i is a variational parameter)

- Mean field
- Harmonic orbitals

Trial wave function:

V.R. Pandharipande (1971)

Trial wave function:

$$\psi_T = \left[\prod_{i=2}^{n} U_i(\boldsymbol{X})\right] \phi^A(\boldsymbol{X})$$

2b/3b correlations (Jastrow function):

$$U_{2b}(r_{ij}) = \mathcal{S}\left(\prod_{i,j}\left(\sum_p f^p(r_{ij})\ \ \hat{O}_{ij}^p\right)\right)$$

- **Symmetric** under particle exchange
- Accounts for the **two-body short-range behavior** of the wave function
- $\hat{O}^p$ are **spin- / isospin-projections** operators.

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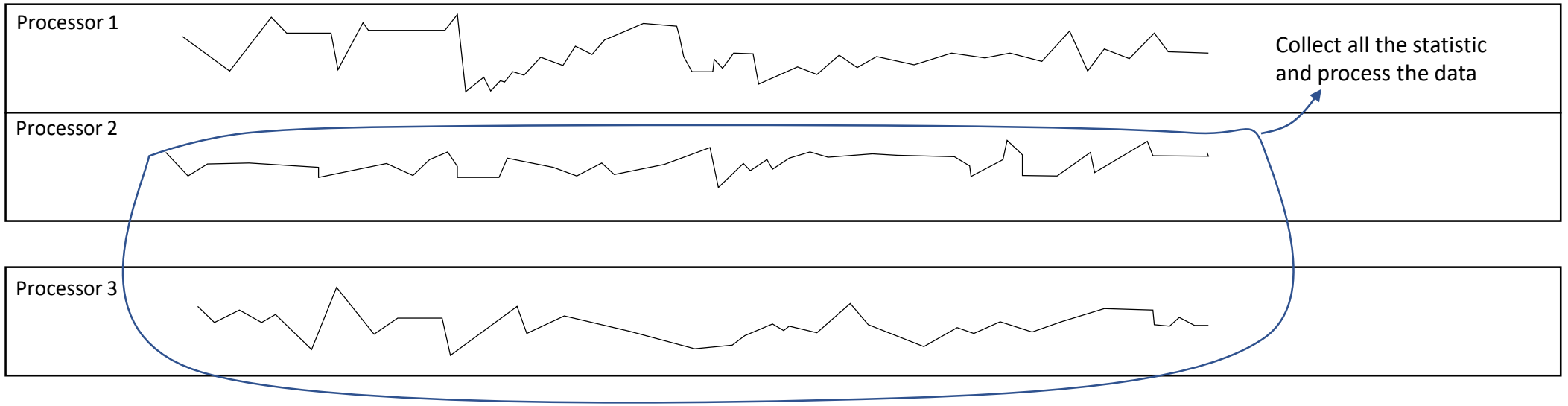
e.g. Hermite polinomial, Spline functions

Efficiency

Parallelization:

How to **parallelize** variational Monte Carlo?

Easy! Each processor takes care of a **different Marcov chain**.
No comunication is required untill you have to sum the expectation values!
It is **trivially** and almost perfectly **parallelizable**!



“Linear Method” Optimization

J. Toulouse and C. J. Umrigar, J. Chem. Phys. **126**, 084102 (2007)

Considering a ψ_T dependent from a **set of parameters** $\{p_1, \ldots, p_k\}$:

$$\left|\bar{\psi}_{\mathrm{T}}(\boldsymbol{p})\right\rangle = \frac{|\psi_T(\boldsymbol{p})\rangle}{\sqrt{\langle\psi(\boldsymbol{p})|\psi(\boldsymbol{p})\rangle}}$$

It can be **expanded**

$$\left|\bar{\psi}_{\mathrm{T}}^{lin}(\boldsymbol{p})\right\rangle = \left|\bar{\psi}_T(\boldsymbol{p}^0)\right\rangle = \sum_{i=1}^{N_p} \Delta p_i \left|\bar{\psi}_T^i(\boldsymbol{p}^0)\right\rangle$$

The first variation $\Delta\boldsymbol{p}$ that minimizes the energy

$$E_{lin}(\boldsymbol{p}) = \frac{\left\langle\bar{\psi}_{\mathrm{T}}^{lin}(\boldsymbol{p})|H|\bar{\psi}_{\mathrm{T}}^{lin}(\boldsymbol{p})\right\rangle}{\left\langle\bar{\psi}_{\mathrm{T}}^{lin}(\boldsymbol{p})\middle|\bar{\psi}_{\mathrm{T}}^{lin}(\boldsymbol{p})\right\rangle}$$

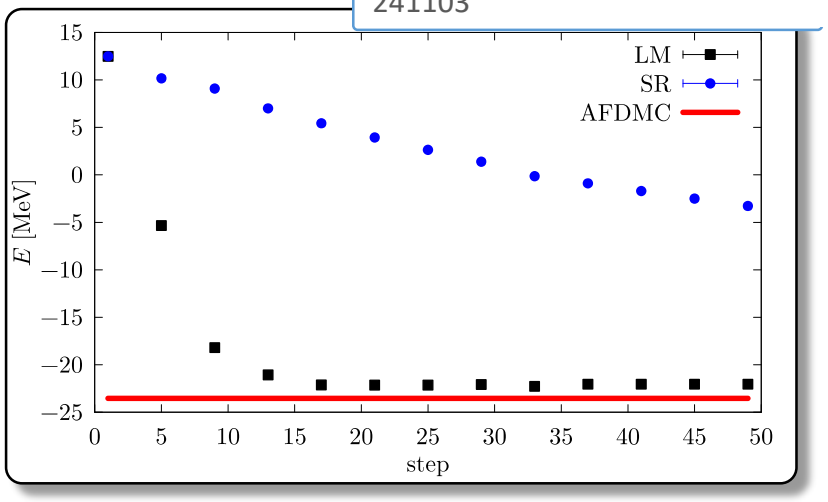
Can be found solving the linear equation

$$\bar{H}\,\Delta\boldsymbol{p} = \Delta E\,\bar{S}\,\Delta\boldsymbol{p}$$

$$\{\bar{H}\}_{ij} = \left\langle\bar{\psi}_{\mathrm{T}}^i(\boldsymbol{p})|H|\bar{\psi}_{\mathrm{T}}^j(\boldsymbol{p})\right\rangle$$

$$\{\bar{S}\}_{ij} = \left\langle\bar{\psi}_{\mathrm{T}}^i(\boldsymbol{p})\mid\bar{\psi}_{\mathrm{T}}^j(\boldsymbol{p})\right\rangle$$

S. Sorella, Phys. Rev. B 71 (2005) 241103



VMC : Pro and contra

Pro

- Access to the **groundstate** of large systems;
- **Optimization** can be used to find very **general states**;
- **Easily parallelizable**;
- **Improvable** numerical uncertainty.

Cons

- Sensible to the **parametrization** of the wavefunction
  (If the wavefunction is too correlated and complicated, it is difficult to find the correct parametrization);
- **Variational** (Best for groundstates);
- **Stochastic uncertainty**;
- **Not the cheapest method** for few-particles.

Diffusion and importance sampling

The integral to be calculated is:

$$E_{gs} = \frac{\langle \psi_{gs}|H|\psi_g\rangle}{\langle \psi_{gs}|\psi_g\rangle} = \frac{\int (\psi_{gs}^* \psi_g)\left(\frac{H\psi_g}{\psi_g}\right) d\boldsymbol{X}}{\int \psi_{gs}^* \psi_g} = \frac{1}{N}\lim_{n\to+\infty}\frac{1}{n}\sum_{\boldsymbol{X}\in\psi_{gs}^*\psi_g}\frac{H\psi_g(\boldsymbol{X})}{\psi_g(\boldsymbol{X})}$$

Function to be sampled

Estimator

Why not using $E_{gs} = \frac{\int \psi_{gs}^* H \psi_g}{\int \psi_{gs}^* \psi_g}$?

It will work but the algorithm would be very unstable.

http://users.jyu.fi/~veapaja/QMC/MC-lecture.pdf

M. Kalos and P. Whitlock, Monte Carlo methods (Wilei 2008)

$$H\,\psi_{gs} = (T+V)\psi_{gs} = E_0\,\psi_{gs}$$

To sample the groundstate we **diffuse in imaginary time** an arbitrary wave function:

$$|\psi_{gs}\rangle = e^{-(H-E_0)\tau}|\psi\rangle = c_0|\psi_{gs}\rangle + \sum_{n=1}^{\infty} c_n\, e^{-(E_n-E_0)\tau}|\psi_n\rangle \to^{\tau\to\infty} |\psi_0\rangle$$

$$\psi_{gs}^*\,\psi_g = lim_{\tau\to\infty}\, e^{-(H-E_0)\tau}\,\psi_g\psi \to \sum_n e^{-(H-E_0)\Delta\tau}\,\psi_g\psi \sim \sum_n e^{-T\,\Delta\tau} e^{-(V-E_0)\Delta\tau}\,\psi_g\psi$$

The idea is to do a chain of samples.

- Evolve a configuration of points for each $\Delta\tau$ until it samples the groundstate

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The idea is to do a **chain of samples:**

- Evolve a configuration of points for each $\Delta\tau$ until it samples the groundstate

Warning: this is the case of coordinate space diffusion!

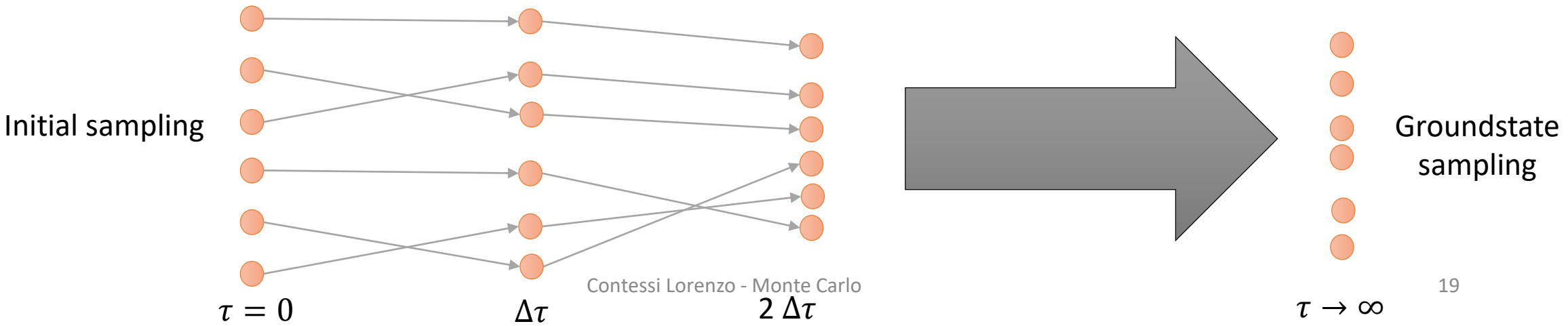
In **continuous coordinate space**:

$$\psi_{\{\tau+\Delta\tau\}}(\boldsymbol{r}) = \int \langle \boldsymbol{r}|e^{-(H-E_0)\Delta\tau}|\boldsymbol{r}'\rangle \, \langle \boldsymbol{r}'|\psi_{\{\tau\}}\rangle \, d\boldsymbol{r}' = \int G(\boldsymbol{r}' \to \boldsymbol{r}) \, \psi_{\{\tau\}}(\boldsymbol{r}') \, d\boldsymbol{r}'$$

$$G(\boldsymbol{r}' \to \boldsymbol{r}) = \langle \boldsymbol{r}|e^{-(H-E_0)\Delta\tau}|\boldsymbol{r}'\rangle = \langle \boldsymbol{r}|e^{-(T+V-E_0)\Delta\tau}|\boldsymbol{r}'\rangle =$$

-- **Trotter expansion** ($\Delta\tau$ is small) --

$$\langle \boldsymbol{r}|e^{-(T+V-E_0)\Delta\tau}|\boldsymbol{r}'\rangle = \langle \boldsymbol{r}|e^{-T\,\Delta\tau}|\boldsymbol{r}'\rangle\langle \boldsymbol{r}|e^{(E_0-V)\Delta\tau}|\boldsymbol{r}'\rangle \cdot O(\Delta\tau^2)$$



Sampling the groundstate: Imaginary time step diffusion

Warning: this is the case of coordinate space diffusion!

The green function is :

$$G(\boldsymbol{x}' \to \boldsymbol{x}, \Delta\tau) =$$

[few algebraic passages described in http://users.jyu.fi/~veapaja/QMC/MC-lecture.pdf M. Kalos and P. Whitlock, Monte Carlo methods (Wilei 2008)]

$$= \left(4\pi \frac{\hbar^2}{2m}\,\Delta\tau\right)^{\frac{3N}{2}} e^{-\frac{\left(\boldsymbol{x}-\boldsymbol{x}'-\Delta\tau\frac{\hbar^2}{2m}2\frac{\nabla\psi_g}{\psi_g}\right)^2}{4\,\Delta\tau}} e^{\Delta\tau\left(\frac{1}{2}\left(\frac{H\psi_g(\boldsymbol{x})}{\psi_g(\boldsymbol{x})}+\frac{H\psi_g(\boldsymbol{x}')}{\psi_g(\boldsymbol{x}')}\right)-E_T\right)} + O(\tau^3)$$

Random walk: $e^{-\frac{\left(\boldsymbol{x}-\boldsymbol{x}'-\Delta\tau\frac{\hbar^2}{2m}2\frac{\nabla\psi_g}{\psi_g}\right)^2}{4\,\Delta\tau}}$

Weight: $e^{\Delta\tau\left(\frac{1}{2}\left(\frac{H\psi_g(\boldsymbol{x})}{\psi_g(\boldsymbol{x})}+\frac{H\psi_g(\boldsymbol{x}')}{\psi_g(\boldsymbol{x}')}\right)-E_T\right)}$

Notice that hard interactions and many-body terms are not problematic

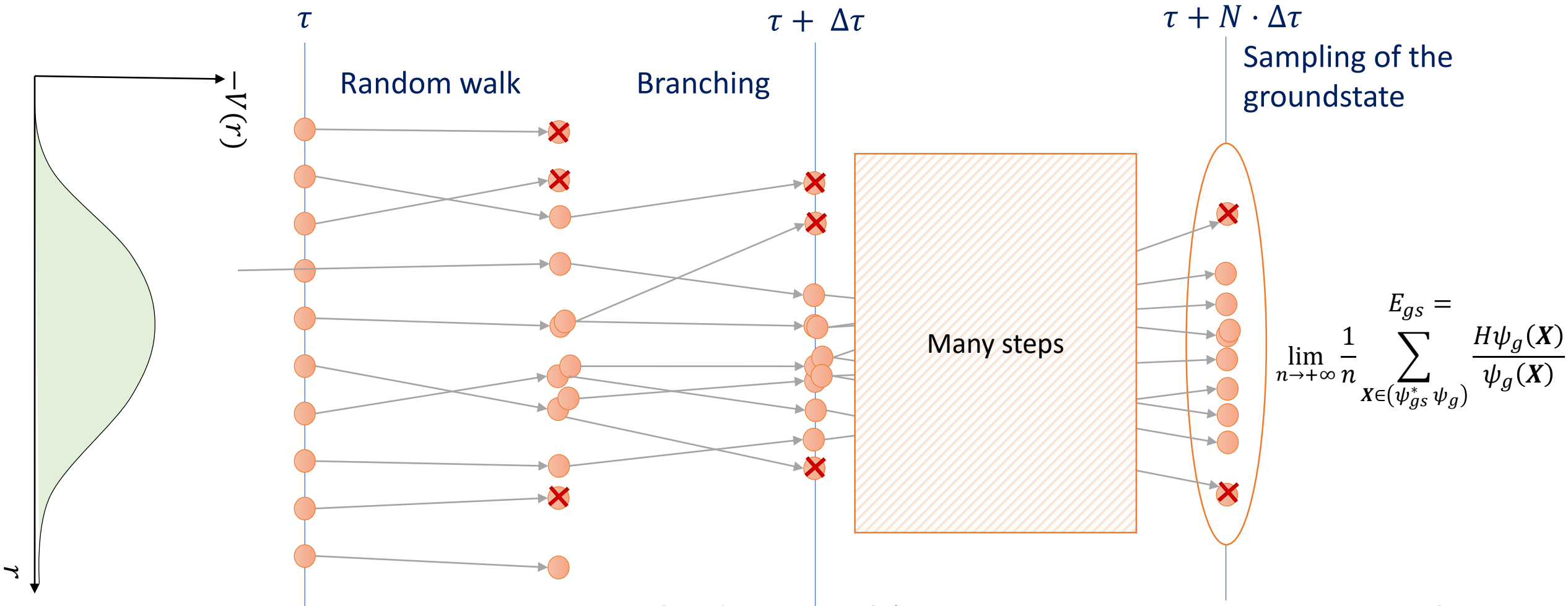
Move the walker with a gaussian walk

Weight of the configuration
- Multiply the estimator
- Branch the walkers

Weighting and branching

Weighting: attach to each sampling $e^{\Delta\tau\left(\frac{1}{2}\left(\frac{H\psi_g(x)}{\psi_g(x)}+\frac{H\psi_g(x')}{\psi_g(x')}\right)-E_T\right)}$

Branching: each configuration is cloned $\left[e^{\Delta\tau\left(\frac{1}{2}\left(\frac{H\psi_g(x)}{\psi_g(x)}+\frac{H\psi_g(x')}{\psi_g(x')}\right)-E_T\right)}+\mu\right]$ times from one step to the other.



For three particles the number of (spin / isospin) components **increases exponentially**!

$$(\overrightarrow{\sigma_2}\cdot\overrightarrow{\sigma_3})\begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ a_{\uparrow\uparrow\downarrow} \\ a_{\uparrow\downarrow\uparrow} \\ a_{\uparrow\downarrow\downarrow} \\ a_{\downarrow\uparrow\uparrow} \\ a_{\downarrow\uparrow\downarrow} \\ a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ 2a_{\uparrow\downarrow\uparrow} - a_{\uparrow\uparrow\downarrow} \\ 2a_{\uparrow\uparrow\downarrow} - a_{\uparrow\downarrow\uparrow} \\ a_{\uparrow\downarrow\downarrow} \\ a_{\downarrow\uparrow\uparrow} \\ 2a_{\downarrow\downarrow\uparrow} - a_{\downarrow\uparrow\downarrow} \\ 2a_{\downarrow\uparrow\downarrow} - a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix} \neq \begin{pmatrix} a'_{\uparrow\uparrow\uparrow} \\ a'_{\uparrow\uparrow\downarrow} \\ a'_{\uparrow\downarrow\uparrow} \\ a'_{\uparrow\downarrow\downarrow} \\ a'_{\downarrow\uparrow\uparrow} \\ a'_{\downarrow\uparrow\downarrow} \\ a'_{\downarrow\downarrow\uparrow} \\ a'_{\downarrow\downarrow\downarrow} \end{pmatrix}$$

n-body spinor → $\mathbf{2^N}$ components

Limited to $\sim$ 12 particles

Single particle spin base is not closed with respect to non-quadratic spin operators:

$\sigma_i \cdot \sigma_j$ operators mix the coefficients of the states.

D. Ceperley, G.V. Chester, M.H. Kalos (1977)

Using the **Hubbard-Stratonovich** transformation:

$$e^{-\frac{1}{2}\lambda O^2} = \frac{1}{\sqrt{2\pi}} \int dx \, e^{-\frac{x^2}{2} + \sqrt{-\lambda} x \, O}$$

AFDMC introduces a **new integral** for each operator transformation.

A quadratic operator can be transformed into a linear one,
at the price of an **integral** (per operator).

$$\overrightarrow{\sigma_i} \left(\begin{pmatrix} \alpha_1 a_\uparrow \\ \beta_1 \, a_\downarrow \end{pmatrix}_1 \otimes \dots \otimes \begin{pmatrix} \alpha_i a_\uparrow \\ \beta_i \, a_\downarrow \end{pmatrix}_i \otimes \dots \otimes \begin{pmatrix} \alpha_A a_\uparrow \\ \beta_A \, a_\downarrow \end{pmatrix}_A \right)$$

$$= \left(\begin{pmatrix} \alpha_1 a_\uparrow \\ \beta_1 \, a_\downarrow \end{pmatrix}_1 \otimes \dots \otimes \begin{pmatrix} \alpha_i' a_\uparrow \\ \beta_i' \, a_\downarrow \end{pmatrix}_i \otimes \dots \otimes \begin{pmatrix} \alpha_A a_\uparrow \\ \beta_A \, a_\downarrow \end{pmatrix}_A \right)$$

New scaling is $2\mathbf{N}$ instead of $2^{\mathbf{N}}$

Sign problem

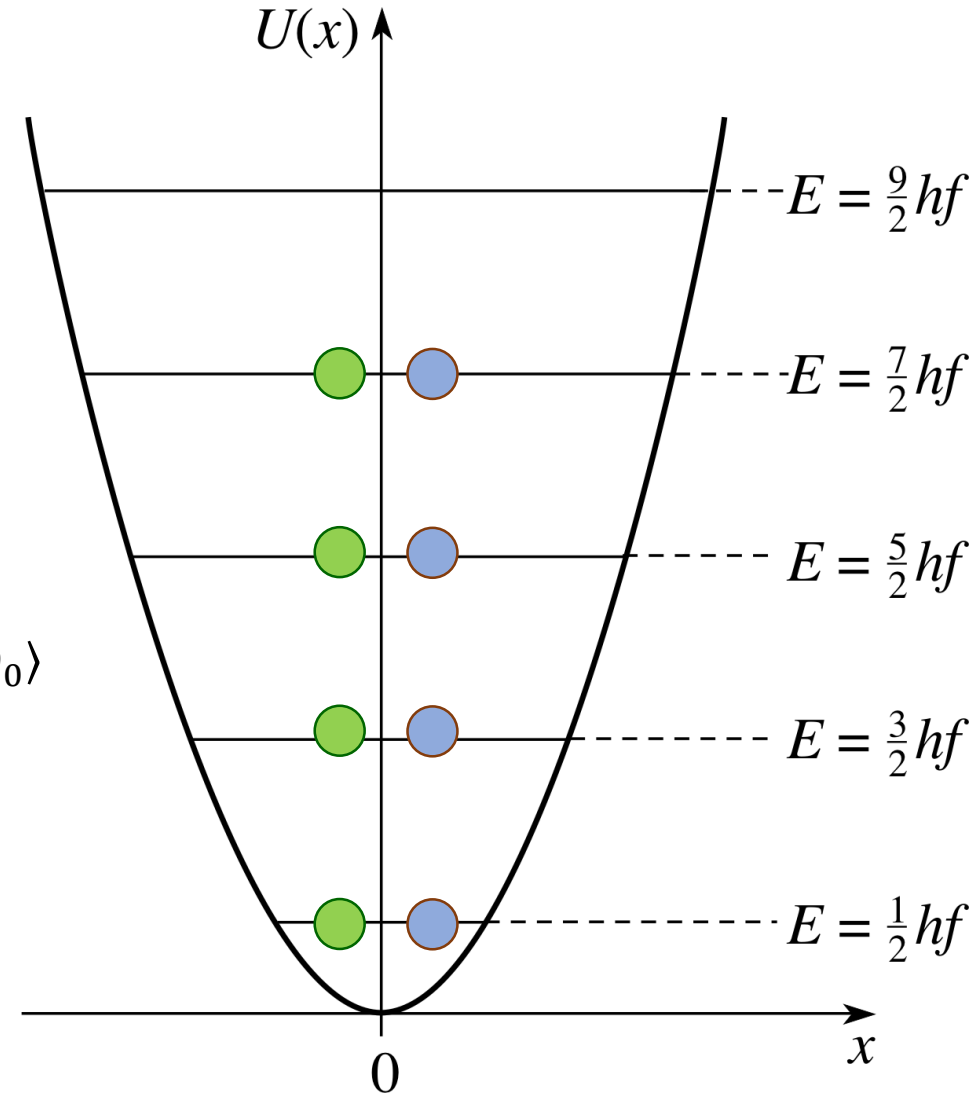
A classic quantum mechanical fermionic problem:

Harmonic oscillator without interparticle interaction.
The ground state is the **Hartree-Fock wavefunction**.

However, the **diffusion algorithm** is the same for **bosons and fermions**!

$$|\psi_0\rangle = e^{-(H-E_0)\tau}|\psi\rangle = c_0|\psi_0\rangle + \sum_{n=1}^{\infty} c_n\, e^{-(E_n-E_0)\tau}|\psi_n\rangle \rightarrow^{\tau\rightarrow\infty} |\psi_0\rangle$$

DMC will diffuse the walkers to the **bosonic groundstate**!



A classic quantum mechanical fermionic problem:

Harmonic oscillator without interparticle interaction.
The ground state is the **Hartree-Fock wavefunction.**

However, the **diffusion algorithm** is the same for **bosons and fermions**!

$$|\psi_0\rangle = e^{-(H-E_0)\tau}|\psi\rangle = c_0|\psi_0\rangle + \sum_{n=1}^{\infty} c_n\, e^{-(E_n-E_0)\tau}|\psi_n\rangle \rightarrow^{\tau\rightarrow\infty} |\psi_0\rangle$$

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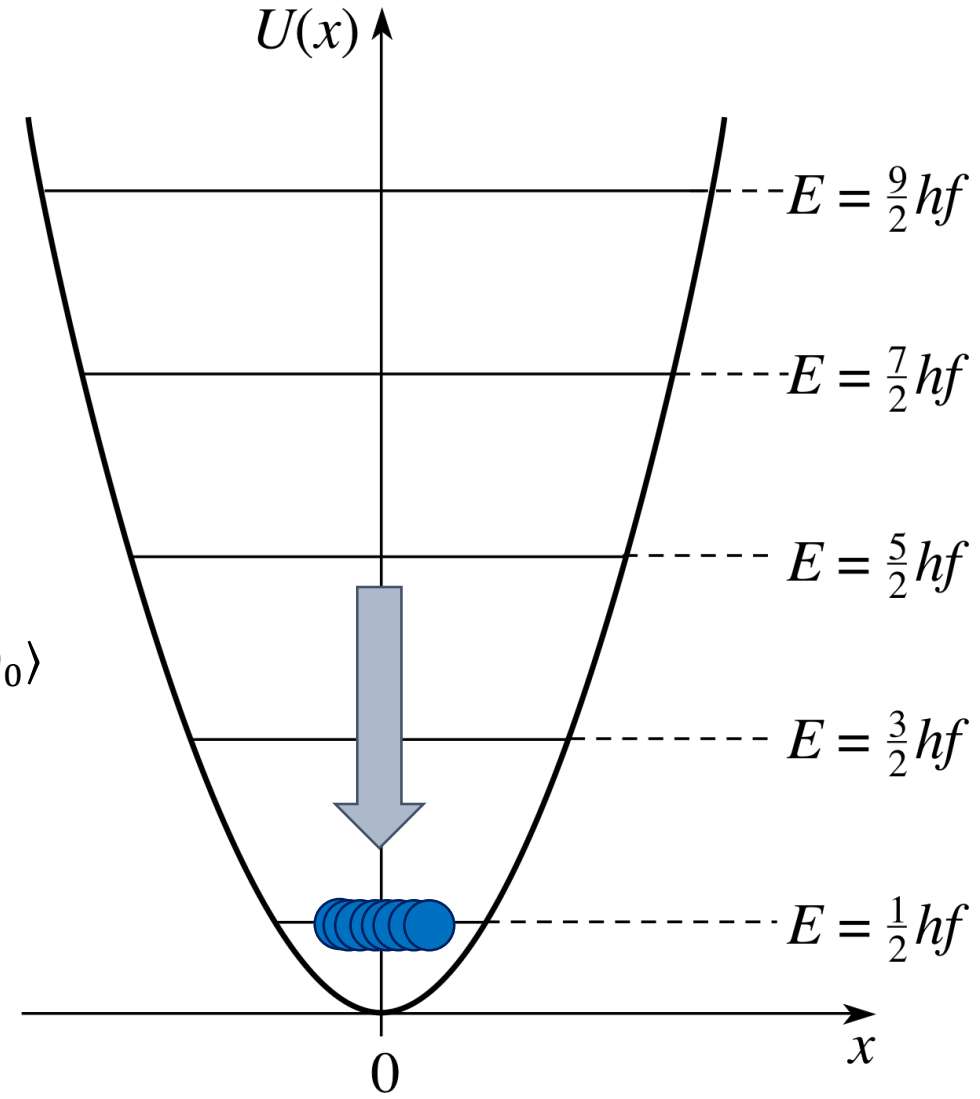


However the (energy) **estimator** is

$$E_{gs} = \frac{\langle \psi_{gs} | H | \psi_g \rangle}{\langle \psi_{gs} | \psi_g \rangle}$$

And

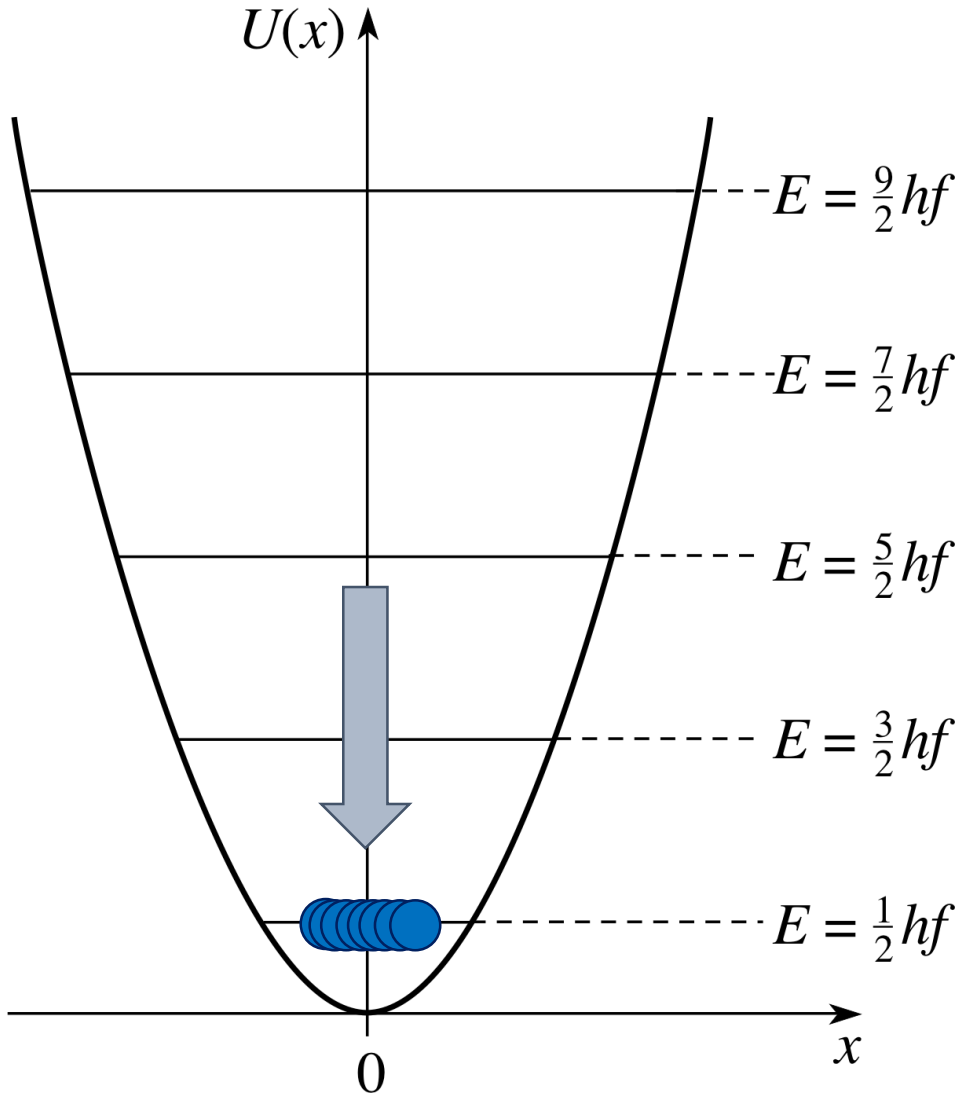
$$\langle \psi_{gs} | \psi_g \rangle \to 0$$

Since **bosonic and fermion wave functions are orthogonal**.

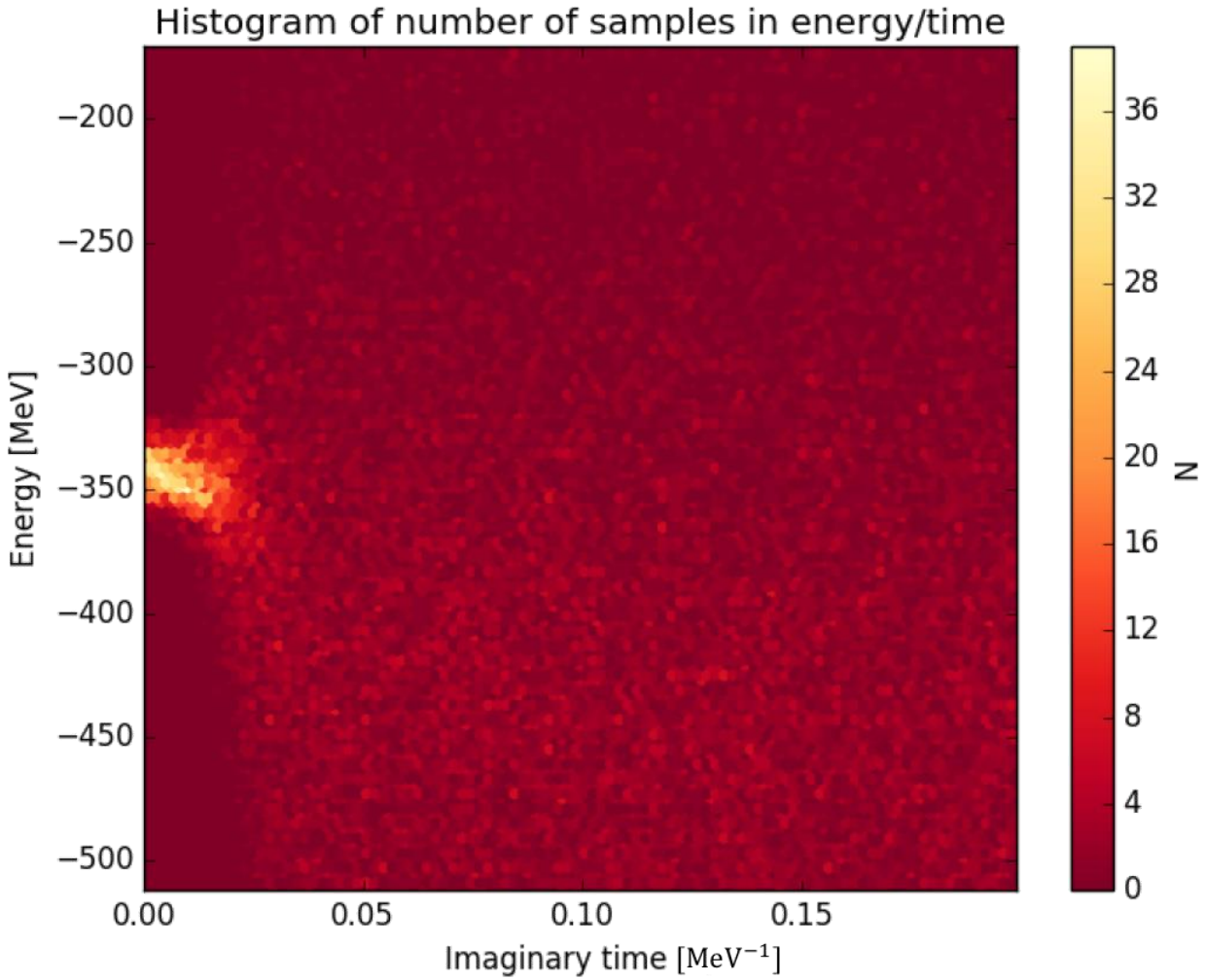
- The **mean estimator** is still correct
- The **error on the estimator blows up by the $\frac{\to 0}{\to 0}$ ratio**.

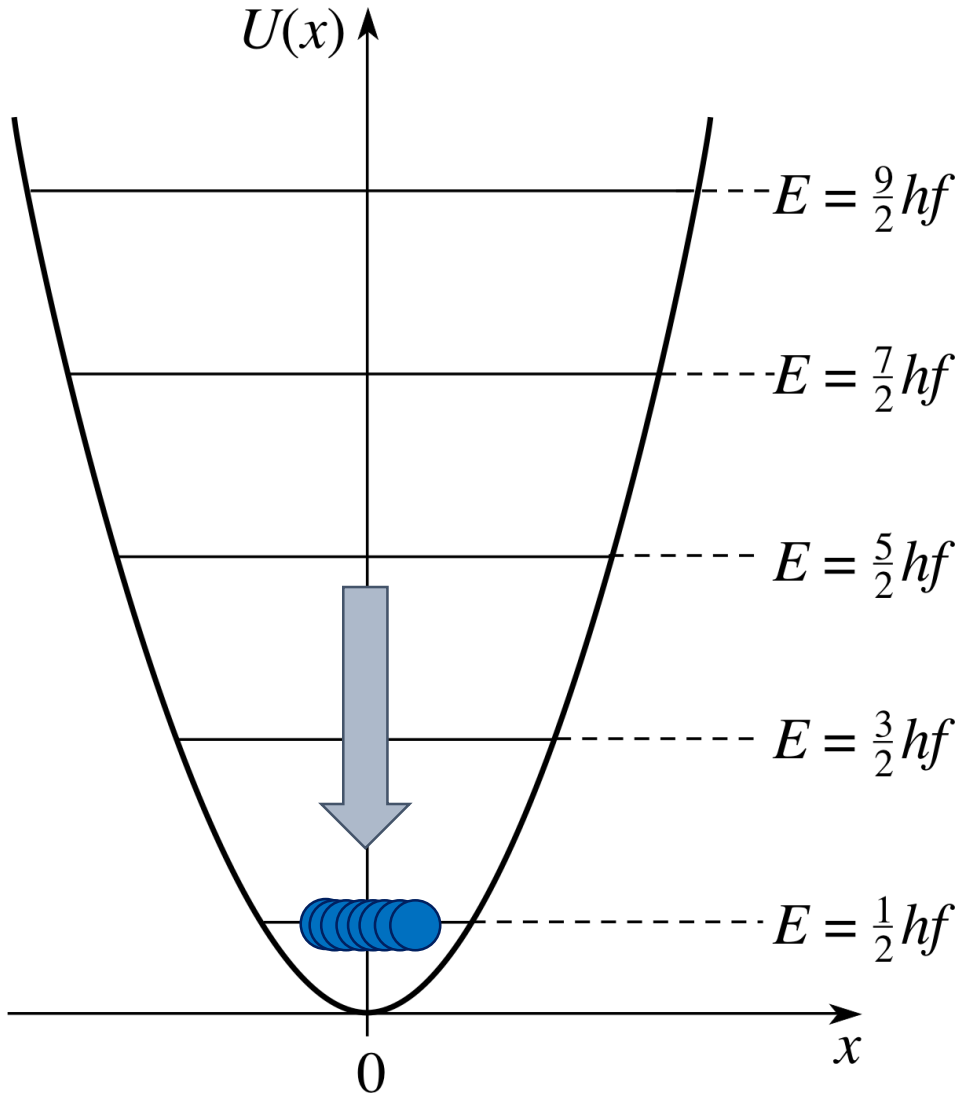
$$E_{gs} = \frac{\int \left(\psi_{gs}^* \psi_g\right) \left(\frac{H\psi_g}{\psi_g}\right)}{\int \psi_{gs}^* \psi_g}$$

On another point of view $\left(\psi_{gs}^* \psi_g\right)$ is **not a probability** since not strictly positive



Sign problem





Fixed node, fixed phase, and constrained path

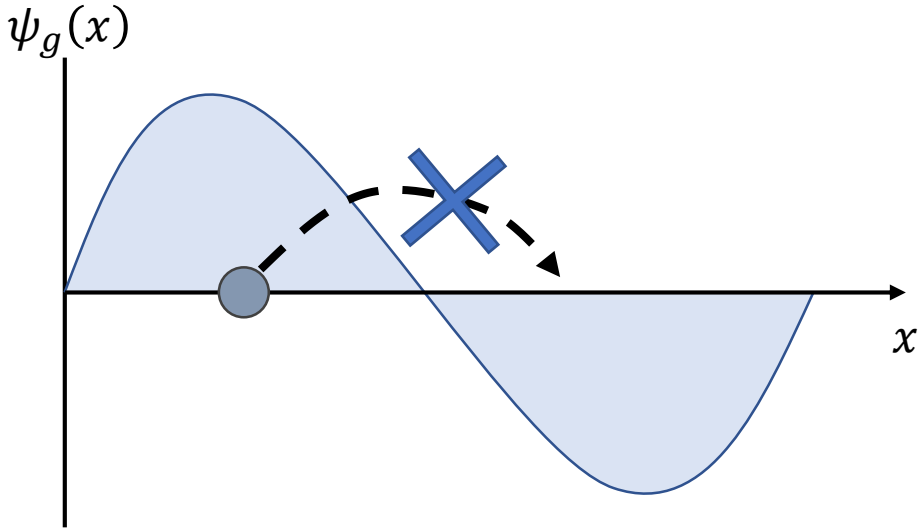
Fix the zeros of the diffused wave function to be the same as the guide wave function:

Any walker that try to pass from a positive to a negative area of the guide wave function **is removed**.

It introduces a bias, but it will make the sampled wave function **orthogonal to the bosonic one**.

$$E_{gs} = \frac{\int \left(\psi_{gs}^{*}\psi_{g}\right)\left(\frac{H\psi_{g}}{\psi_{g}}\right)}{\int \psi_{gs}^{*}\psi_{g}}$$

With fixed node: $\left(\psi_{gs}^{*}\psi_{g}\right) > 0$ is a well defined probability!



Fixed phase: for complex wave functions $\left(\psi_{gs}^{*}\psi_{g}\right) \in \Re^{+}$

Constrained path: an alternative is to sample only the real part $\mathrm{Re}\left(\psi_{gs}^{*}\psi_{g}\right)$

F. Bolton (1996)
S. Zhang (1997)

M. D. Jones, G. Ortiz, and D. M. Ceperley, Phys. Rev. E55, 6210 (1997)

Not constraining the phase will make the variance explode.

Signal to noise spoiling **can be delayed** tuning the guide wavefunction (ϵ parameter),
but we should start with an almost correct groundstate.

$$\tilde{\psi}_g = \sqrt{Re(\psi_g)^2 + \epsilon\, Im(\psi_g)^2}$$

with ϵ tuned to reduce the variance (e.g. $\epsilon \sim 0.20$)

$$E_{gs} = \frac{\int (\psi_{gs}^* \tilde{\psi}_g) \frac{\psi_g}{\tilde{\psi}_g} \left(\frac{H\psi_g}{\psi_g}\right)}{\int \psi_{gs}^* \psi_g}$$

gives enough time to see how far our
fixed-node energy is far from the true solution.

A physical exemple

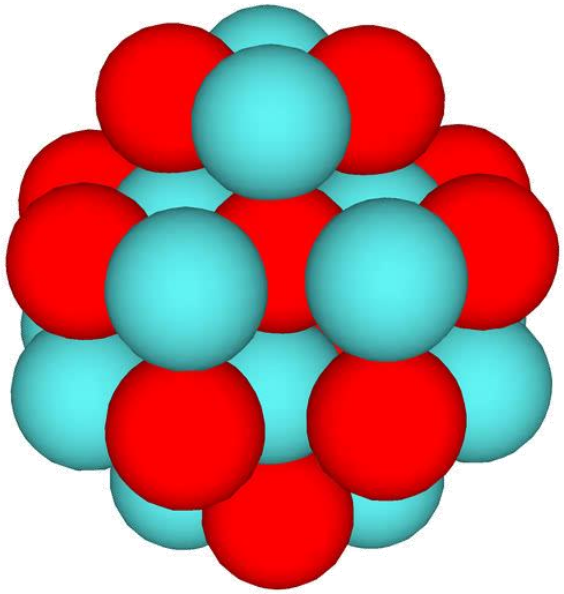
From
L. C., A. Lovato, F. Pederiva, A. Roggero, J. Kirscher and U. van Kolck, Phys.Lett.B 772 (2017), 839-848

^{16}O using Contact Effective Field theory at LO:

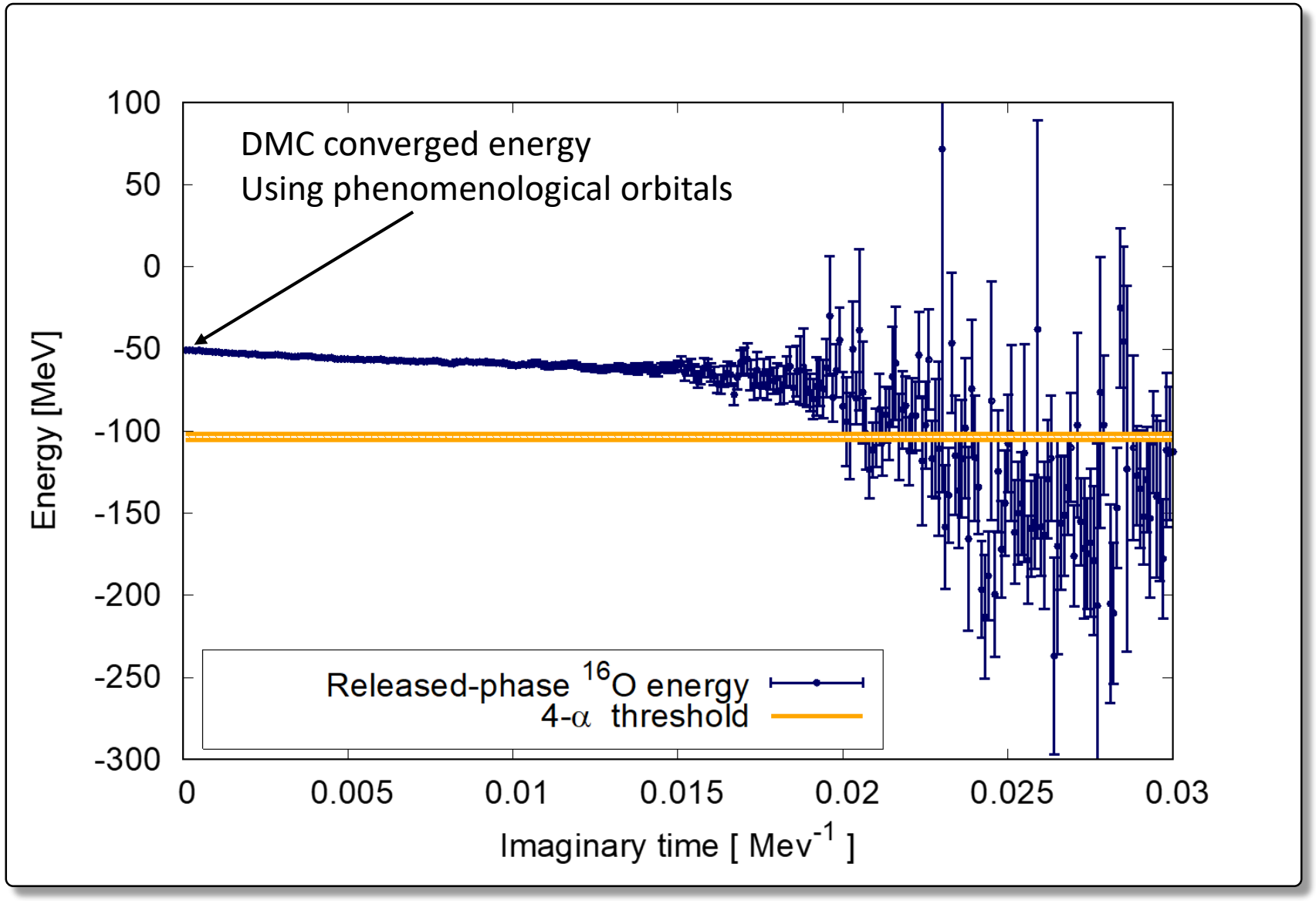
$$V^{LO} = \sum_{i<j} [C_0(\Lambda) + C_1(\Lambda)(\overrightarrow{\sigma_i} \cdot \overrightarrow{\sigma_j})\,] e^{-\frac{1}{2}|r_{ij}|^2\Lambda^2}$$
$$+D_0(\Lambda) \sum_{(i<j)\neq k} \left[e^{-\frac{\Lambda^2}{2}(|r_{ij}|^2+|r_{ik}|^2)} + e^{-\frac{\Lambda^2}{2}(|r_{ij}|^2+|r_{jk}|^2)} + e^{-\frac{\Lambda^2}{2}(|r_{jk}|^2+|r_{ik}|^2)}\right]$$

In particular for large cutoffs (e.g. $\Lambda = 8\ \mathrm{fm}^{-1}$)

- Performs well in few-body
- Do not stabilize larger nuclei at LO
  (corrections are needed)
  Es. ^{16}O



^{16}O Phenomenological orbitals

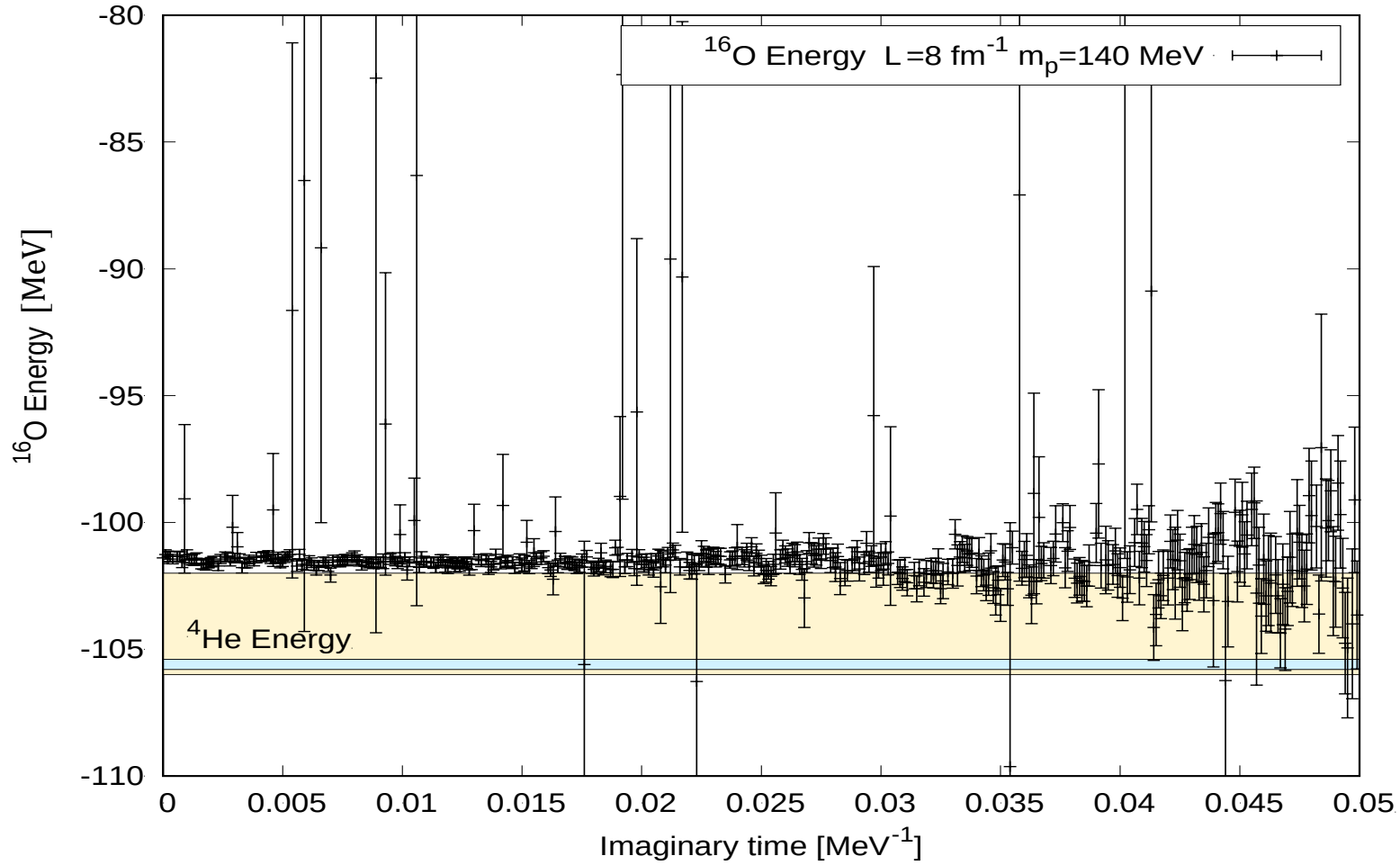


^{16}O Spline orbitals and correlations

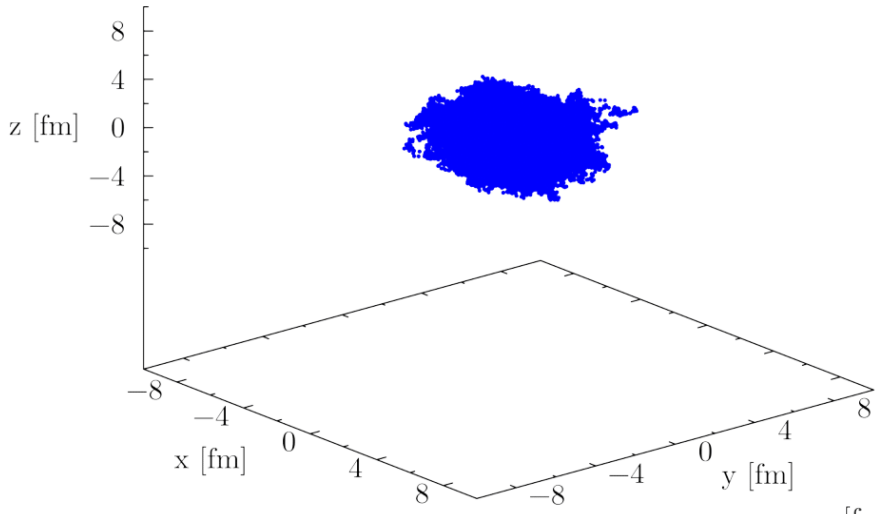
$m_\pi = 140$ MeV		
Λ [fm^{-1}]	^{16}O Energy [MeV]	4α treshold [MeV]
2	-97.19(6)	-92.68(8)
4	-92.23(14)	-94.52(9)
6	-97.51(14)	-100.24(8)
8	-100.97(20)	-104.2(2)
∞	$-115^{1(sys)}_{8(stat)}$	$-120^{1(sys)}_{8(stat)}$

- All the errors shown are statistical errors from Monte Carlo method.

^{16}O Spline orbitals and correlations

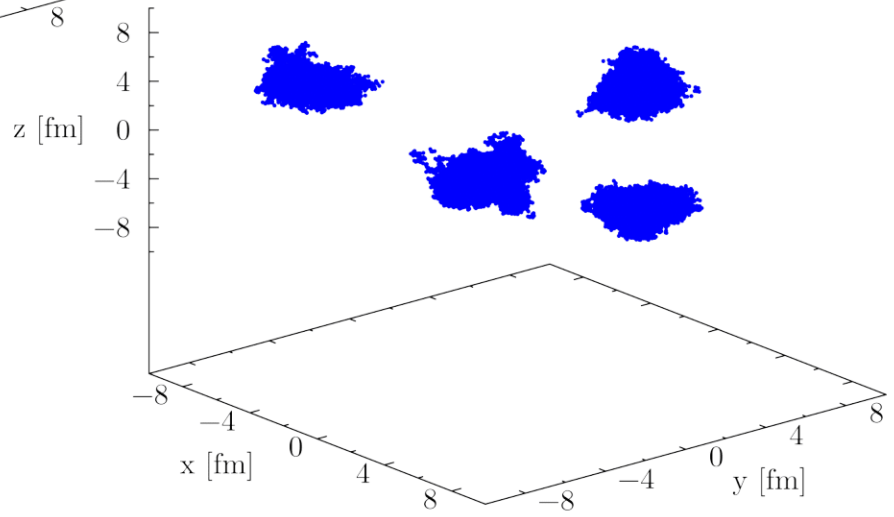


Oxygen density ($m_\pi = 140$ MeV)



$\Lambda = 2\ \mathrm{fm}^{-1}$

$\Lambda = 8\ \mathrm{fm}^{-1}$



Conclusions first part

Quantum Monte Carlo can solve high dimensional quantum problems.

Variational QMC is fast and precise, but relays on a good parametrization of the wavefunction

Green function QMC allows to extract the groundstate of the system using a diffusion in imaginary time

Auxiliary field QMC permits to find the groundstate energy of many-fermions

- Not positive wave functions (e.g. for many-fermions) will introduce the **Sign Problem**
- The Sign Problem **can be tamed but not removed** (fixed node, fixed phase, constraint path)