



# 993SM - Laboratory of Computational Physics lecture 12 - part 1 June 4, 2021

**Maria Peressi**

Università degli Studi di Trieste - Dipartimento di Fisica

Sede di Miramare (Strada Costiera 11, Trieste)

e-mail: [peressi@units.it](mailto:peressi@units.it)

tel.: +39 040 2240242

# Monte Carlo in quantum systems

VARIATIONAL MONTE CARLO (VMC)

M. Peressi - UniTS - Laurea Magistrale in Physics  
Laboratory of Computational Physics - Unit XII

# Variational Monte Carlo

A stochastic way of calculating **expectation values of observables** in many-body (in general) systems using a **trial wavefunction** which depends on PARAMETERS.

=> Which are the parameters that give

- ✓ the most reliable expectation value?
- ✓ the best trial wavefunction?

A method based on:

variational principle + Monte Carlo evaluation of integrals  
using importance sampling based on the Metropolis algorithm

# Variational Monte Carlo

- 1) Start from a **trial wavefunction** (wfc)
- 2) Calculate the **expectation value** of the many-body hamiltonian  $\mathcal{H}$  or in general of other observables  $\mathcal{O}$  on the wfc, transforming the integral into a form suitable for **MC integration**
- 3) **Change parameters and recalculate** the expectation value on the new wfc.
- 4) Iterate **to reach the best estimate of the expectation value**

With VMC one can obtain exact properties only if the trial wavefunction is an **exact** wavefunction of the system; it is a **variational** method to find the ground state.

# Variational Monte Carlo

- 1) Start from a **trial wavefunction** (wfc)
- 2) Calculate the **expectation value** of the many-body hamiltonian  $\mathcal{H}$  or in general of other observables  $\mathcal{O}$  on the wfc transforming the integral in a form suitable for **MC integration**
- 3) **Change parameters and recalculate** the expectation value on the new wfc.
- 4) Iterate **to reach the best estimate of the expectation value**

With VMC one can obtain exact properties only if the trial wavefunction is an **exact** wavefunction of the system; it is a **variational** method to find the ground state.

# Variational Monte Carlo

1) Start from a **trial wavefunction** (wfc)

*done in Lecture VII for a single-particle problem (harmonic oscillator)*

2) Calculate the **expectation value** of the many-body hamiltonian  $\mathcal{H}$  or in general of other observables  $\mathcal{O}$  on the wfc transforming the integral in a form suitable for **MC integration**

3) **Change parameters and recalculate** the expectation value on the new wfc.

4) Iterate **to reach the best estimate of the expectation value**

With VMC one can obtain exact properties only if the trial wavefunction is an **exact** wavefunction of the system; it is a **variational** method to find the ground state.

# Quantum averages - I

(Ground) state average:

$$\langle \mathcal{O} \rangle_{\psi} = \frac{\int \psi^*(R) \mathcal{O} \psi(R) dR}{\int |\psi(R)|^2 dR}$$

$R$ : compact notation for  
the whole set of variables  
of the many-body wfc

# Quantum averages - I

(Ground) state average:

$$\psi(R)\psi^{-1}(R)$$

$$\langle \mathcal{O} \rangle_{\psi} = \frac{\int \psi^*(R) \mathcal{O} \psi(R) dR}{\int |\psi(R)|^2 dR}$$



# Quantum averages - I

(Ground) state average:

$$\psi(R)\psi^{-1}(R)$$

$$\langle \mathcal{O} \rangle_{\psi} = \frac{\int \psi^*(R) \mathcal{O} \psi(R) dR}{\int |\psi(R)|^2 dR}$$

$$= \int \left[ \frac{|\psi(R)|^2}{\langle \psi | \psi \rangle} \right] \left[ \frac{\mathcal{O} \psi(R)}{\psi(R)} \right] dR \equiv \int \underline{w(R)} \underline{\mathcal{O}_L(R)} dR$$

probability  
(weighting  
factor)

“local” operator

# Quantum averages - II

integrals in many variables  $\{R\} \Rightarrow$   
suitable for importance sampling - Monte Carlo  
integration:

$$\langle \mathcal{O}_L \rangle = \int w(R) \mathcal{O}_L(R) dR \approx \frac{1}{M} \sum_{i=1}^M \mathcal{O}_L(R_i)$$

provided that the configurations  $i$   
are distributed with the probability

$$w(R_i) = \frac{|\psi(R_i)|^2}{\langle \psi | \psi \rangle}$$

$$\text{error} \sim 1/\sqrt{M}$$

# VMC on one trial wfc - I

Details for the calculation of quantum averages:

2) Calculate the **expectation value** of the many-body hamiltonian  $\mathcal{H}$  on the wfc transforming the integral into a form suitable for **MC integration**

---

2a) Equilibration phase:

a walker consisting of an initially random set of particle positions  $\{R\}$  is propagated according to the Metropolis algorithm, in order to equilibrate and start sampling  $|\psi(\{R\})|^2$ . If the problem is many-body, a new configuration can be obtained by moving just one particle and the others are unchanged.

2b) Accumulation phase:

New configurations are generated and energies and other observables are accumulated for statistical analysis.

# VMC on one trial wfc - II

## I. Equilibration phase:

1. Generate initial configuration using random positions for the particles.
2. For every particle\* in the configuration:
  1. Propose a move from  $\mathbf{r}$  to  $\mathbf{r}'$  ← **brute force sampling**
  2. Compute  $w = |\Psi(\mathbf{r}')/\Psi(\mathbf{r})|^2 = |\Psi(\mathbf{r}')|^2/|\Psi(\mathbf{r})|^2$
  3. Accept or reject move accordingly to Metropolis probability  $\min(1, w)$
3. Repeat configuration moves until equilibrated

## 2. Accumulation phase:

1. For every particle in the configuration:
  1. Propose a move from  $\mathbf{r}$  to  $\mathbf{r}'$
  2. Compute  $w = |\Psi(\mathbf{r}')/\Psi(\mathbf{r})|^2$
  3. Accept or reject move accordingly to Metropolis probability  $\min(1, w)$
  4. Accumulate the contribution to the local energy and other observables at  $\mathbf{r}$  (if move is rejected) or  $\mathbf{r}'$  (if move is accepted)
2. Repeat configuration moves until sufficient data are accumulated

In this algorithm, a new configuration is considered when one particle is moved, individually.

(\*) If the problem is many-body,  $\mathbf{r}$  and  $\mathbf{r}'$  are single-particle coordinates and therefore differ from  $\mathbf{R}$ .

# The variational principle - I

For the ground state:

if  $\psi(R)$  is a trial wavefunction and  $E_0$  is the exact ground state eigenvalue, we have:

$$\langle E \rangle_{\psi} \geq E_0$$

and the "=" holds if and only if the trial wavefunction is the exact ground state wavefunction ( $\psi \equiv \psi_0$ ).

# The variational principle - II

Basic idea for VMC:

calculate  $\langle \mathcal{O} \rangle$  over different trial wavefunctions  
and choose the best...

# VMC - standard procedure - I

1) Start from a **trial wavefunction with a set of parameters  $\alpha_0$**

2) Calculate the **expectation value** of the operator  $\mathcal{O}$  with a **MC integration**:

$$\langle \mathcal{O}_L \rangle_{\alpha_0} = \frac{\int |\psi_{\alpha_0}(R)|^2 \mathcal{O}_L(R) dR}{\int |\psi_{\alpha_0}(R)|^2 dR} = \int w_{\alpha_0}(R) \mathcal{O}_L(R) dR \approx \frac{1}{M} \sum_{i=1}^M \mathcal{O}_L(R_i^{\{\alpha_0\}})$$

3) **Change the set of parameters  $\alpha$  and recalculate** from scratch the expectation value on the new wfc:

$$\langle \mathcal{O}_L \rangle_{\alpha} = \frac{\int |\psi_{\alpha}(R)|^2 \mathcal{O}_L(R) dR}{\int |\psi_{\alpha}(R)|^2 dR} = \int w_{\alpha}(R) \mathcal{O}_L(R) dR \approx \frac{1}{M} \sum_{i=1}^M \mathcal{O}_L(R_i^{\{\alpha\}})$$

(  $\mathcal{O}_L(R)$  changes (contains the new parameters) but also the  $w(R)$  and hence the set of points  $\{R_i\}$  change)

4) Iterate **to reach the best estimate of the expectation value**

# VMC - standard procedure - II

Two problems:

1) time consuming

2) stochastic errors can be comparable to differences between expectation values for different sets of parameters

solution?



# “reweighting” technique

A better idea: use the same sampling for similar trial wfc,  $\psi_\alpha, \psi_{\alpha_0}$ .

Start from  $\alpha_0$ . Define:  $r_\alpha(R) \equiv \frac{|\psi_\alpha(R)|^2}{|\psi_{\alpha_0}(R)|^2}$

Remembering that:  $w_\alpha(R) = \frac{|\psi_\alpha(R)|^2}{\int |\psi_\alpha(R)|^2 dR}$ , and similar for  $w_{\alpha_0}$ , we have:

$$\begin{aligned} \langle \mathcal{O}_L \rangle_\alpha &= \frac{\int |\psi_\alpha(R)|^2 \mathcal{O}_L(R) dR}{\int |\psi_\alpha(R)|^2 dR} = \frac{\int r_\alpha(R) |\psi_{\alpha_0}(R)|^2 \mathcal{O}_L(R) dR}{\int r_\alpha(R) |\psi_{\alpha_0}(R)|^2 dR} = \\ &= \frac{\int r_\alpha(R) w_{\alpha_0}(R) \mathcal{O}_L(R) dR}{\int r_\alpha(R) w_{\alpha_0}(R) dR} \approx \frac{\sum_i r_\alpha(R_i) \mathcal{O}_L(R_i)}{\sum_i r_\alpha(R_i)} \end{aligned}$$

where the set  $\{R_i\}$  of  $M$  points is generated according to  $w_{\alpha_0}(R)$

(Check that:  $A(\alpha, \alpha_0) \equiv \frac{(\sum_i r_\alpha(R_i))^2}{\sum_i r_\alpha^2(R_i)} \approx M$  ; if not, generate other points)

# “zero-variance” property

(when applicable, very useful!)

**if a trial wavefunction is the exact one,**  
the variance of the numerical estimate of  $\langle \mathcal{O} \rangle$  ( $\langle \mathcal{H} \rangle$ )

is zero:

$$\sigma^2 \equiv \langle \psi | (\mathcal{H} - \langle \mathcal{H} \rangle)^2 | \psi \rangle = 0$$

**the criterion to find the best parameter set  
is precisely defined!**

(remark: applicable also to excited states if  
the exact excited state wfc is contained in the trial wfc set)

# possible problems/remarks

- nodes of the trial wfc: not a real problem, provided the trial moves are large enough to overcome nodes
- $\mathcal{H}(R)\psi(R)$  must be defined everywhere
- $\psi(R)$  must have the proper symmetry (bosons or fermions) and proper boundary conditions

# Trial wavefunction

The reliability of the VMC estimates  
are crucially dependent  
on the quality of the trial wfc

# Trial wavefunctions for many-body systems

The choice of trial wavefunction is critical in VMC calculations. All observables are evaluated with respect to the probability distribution  $|\Psi_T(\mathbf{R})|^2$ . The trial wavefunction,  $\Psi_T(\mathbf{R})$ , must well approximate an exact eigenstate for all  $\mathbf{R}$  in order that accurate results are obtained. Improved trial wavefunctions also improve the importance sampling, reducing the cost of obtaining a certain statistical accuracy.

Typical form chosen for the many-body trial wfc:

$$\psi = \exp \left[ \sum_{i < j}^N -u(r_{ij}) \right] \det[\theta_k(r_i, \sigma_i)]$$

Jastrow or two-body correlation function

Slater determinant on  
single-particle spin-orbitals

# Programs & scripts:

on moodle2

**metropolis\_gaussian.f90**

(see also: metropolis\_sampling.f90, Unit VII)

**metropolis\_parabola.f90**

**metropolis\_parabola\_vs\_a.f90**

**job\_gaussian**

**job\_parabola**

# Exercises

I) Harmonic oscillator solved with VMC : (a particularly simple example, where everything could be done also analytically, used to test the numerical algorithm)

$$\mathcal{H} = E_{kin} + E_{pot} = \frac{1}{2}p^2 + \frac{1}{2}x^2 \quad (\hbar = 1, m = 1)$$

I.a) Trial wfc.:

$$\psi(x) = Ae^{-\beta x^2} \quad \text{or} \quad Ae^{-x^2/(4\sigma^2)} \quad \text{with : } \beta = \frac{1}{4\sigma^2}$$

$$\left\{ \begin{array}{l} E_{pot,L}(x) \equiv \frac{E_{pot}\psi(x)}{\psi(x)} = \frac{1}{2}x^2 \\ E_{kin,L}(x) \equiv \frac{E_{kin}\psi(x)}{\psi(x)} = \frac{-\frac{1}{2}\frac{d^2}{dx^2}\psi(x)}{\psi(x)} = -2\beta^2 x^2 + \beta \end{array} \right.$$

$$\left\{ \begin{array}{l} \langle E_{pot} \rangle = \frac{\langle \psi | \frac{1}{2}x^2 | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\int \frac{1}{2}x^2 |\psi(x)|^2 dx}{\int |\psi(x)|^2 dx} = \frac{1}{2}\sigma^2 = \frac{1}{8\beta} \\ \langle E_{kin} \rangle = \frac{\langle \psi | -\frac{1}{2}\nabla^2 | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\int \left( \frac{1}{4\sigma^2} - \frac{x^2}{8\sigma^4} \right) |\psi(x)|^2 dx}{\int |\psi(x)|^2 dx} = \frac{1}{8\sigma^2} = \frac{1}{2}\beta \end{array} \right.$$

# Determining the ground state

$$\langle E_{pot,L} \rangle = \frac{1}{8\beta}, \quad \langle E_{kin,L} \rangle = \frac{1}{2}\beta \quad \frac{d\langle E_{tot,L}(\beta) \rangle}{d\beta} = 0 \implies \beta = \frac{1}{2}, E_{tot} = \frac{1}{2}$$

$(\alpha = \sqrt{2}/2)$

But also, looking at the variance:

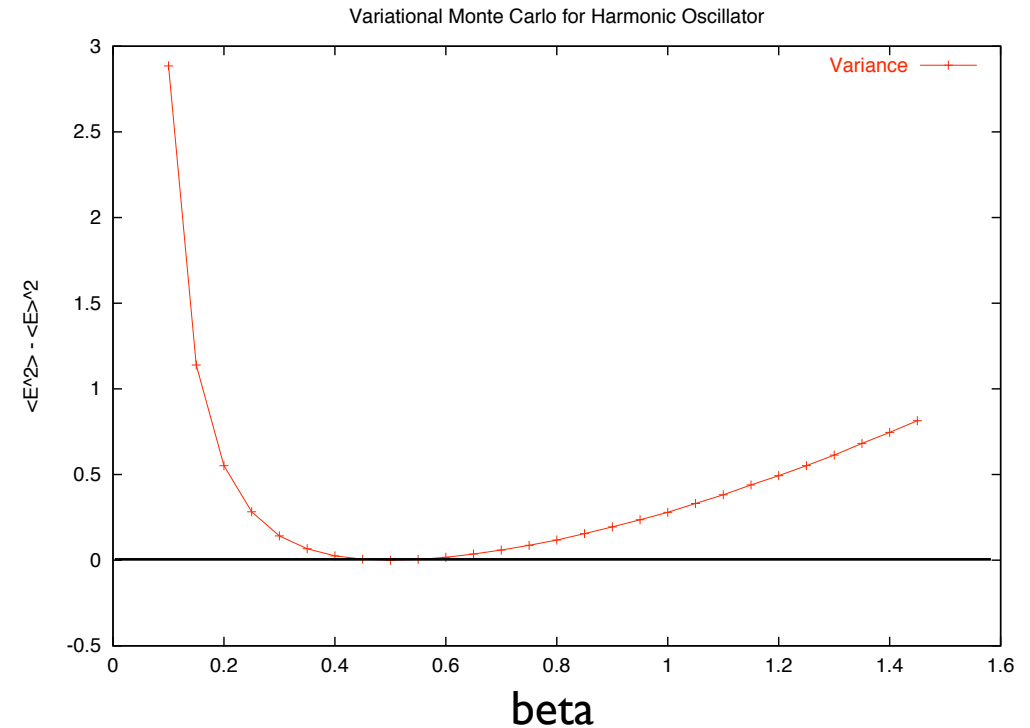
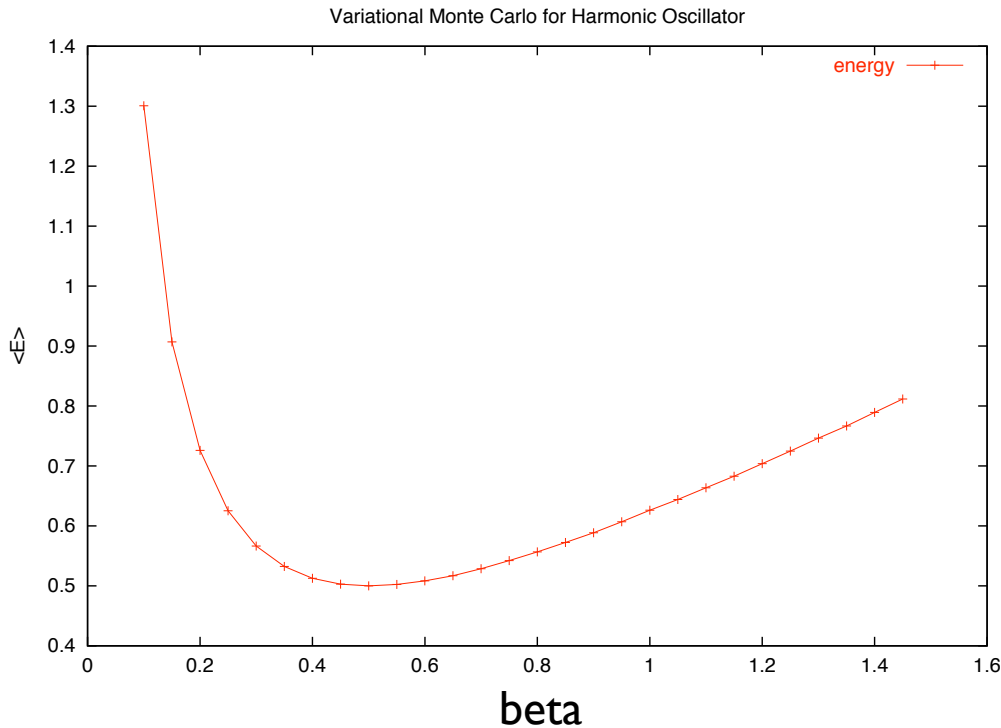
$$\begin{aligned} \sigma_E^2 &= \langle E_{tot,L}^2 \rangle - \langle E_{tot,L} \rangle^2 = \\ &= \left\langle \left( \frac{1}{2}x^2 - 2\beta^2 x^2 + \beta \right)^2 \right\rangle - \left( \frac{1}{8\beta} + \frac{1}{2}\beta \right)^2 = \\ &= \frac{1}{32\beta^2} + \frac{1}{2}\beta^2 - \frac{1}{4} \end{aligned}$$

For the exact ground state:

$$\beta = \frac{1}{2} \implies \sigma_E = 0$$



Notice the zero-variance property for this problem:



(\*)  
300 walkers and MCSteps = 10,000

(\*) In this simple case, even a single walker is enough.

**Many independent walkers** starting at different random points in the configuration space could be necessary for a better sampling **in more complicate systems** (a single walker might have trouble locating all of the peaks in the distribution; using a large number of randomly located walkers improves the probability that the distribution will be correctly generated)

# Exercises

## I) Harmonic oscillator solved with VMC:

$$\mathcal{H} = E_{kin} + E_{pot} = \frac{1}{2}p^2 + \frac{1}{2}x^2$$

### I.b) Trial wfc.:

(reasonable choice:

satisfies boundary conditions; correct symmetry; only one parameter)

$$\psi(x) = \begin{cases} B(a^2 - x^2), & \text{for } |x| < a; \\ 0, & \text{for } |x| > a. \end{cases} \quad \text{Normalization: } \int_{-a}^a B^2(a^2 - x^2)^2 dx = 1 \implies B^2 = \frac{15}{16a^5}$$

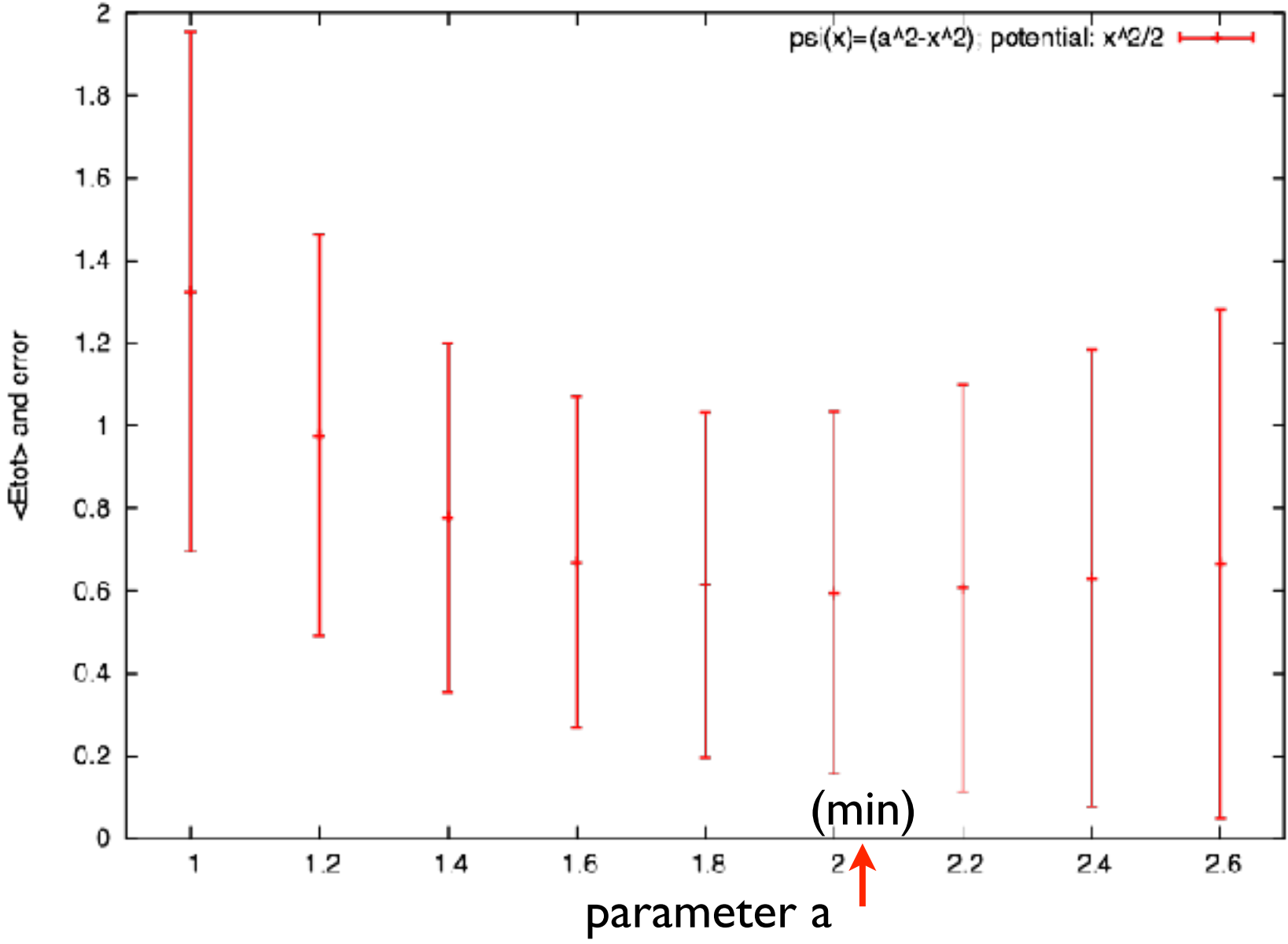
$$E_L(x) = \frac{\mathcal{H}\psi(x)}{\psi(x)} = \left( \frac{1}{a^2 - x^2} + \frac{1}{2}x^2 \right)$$

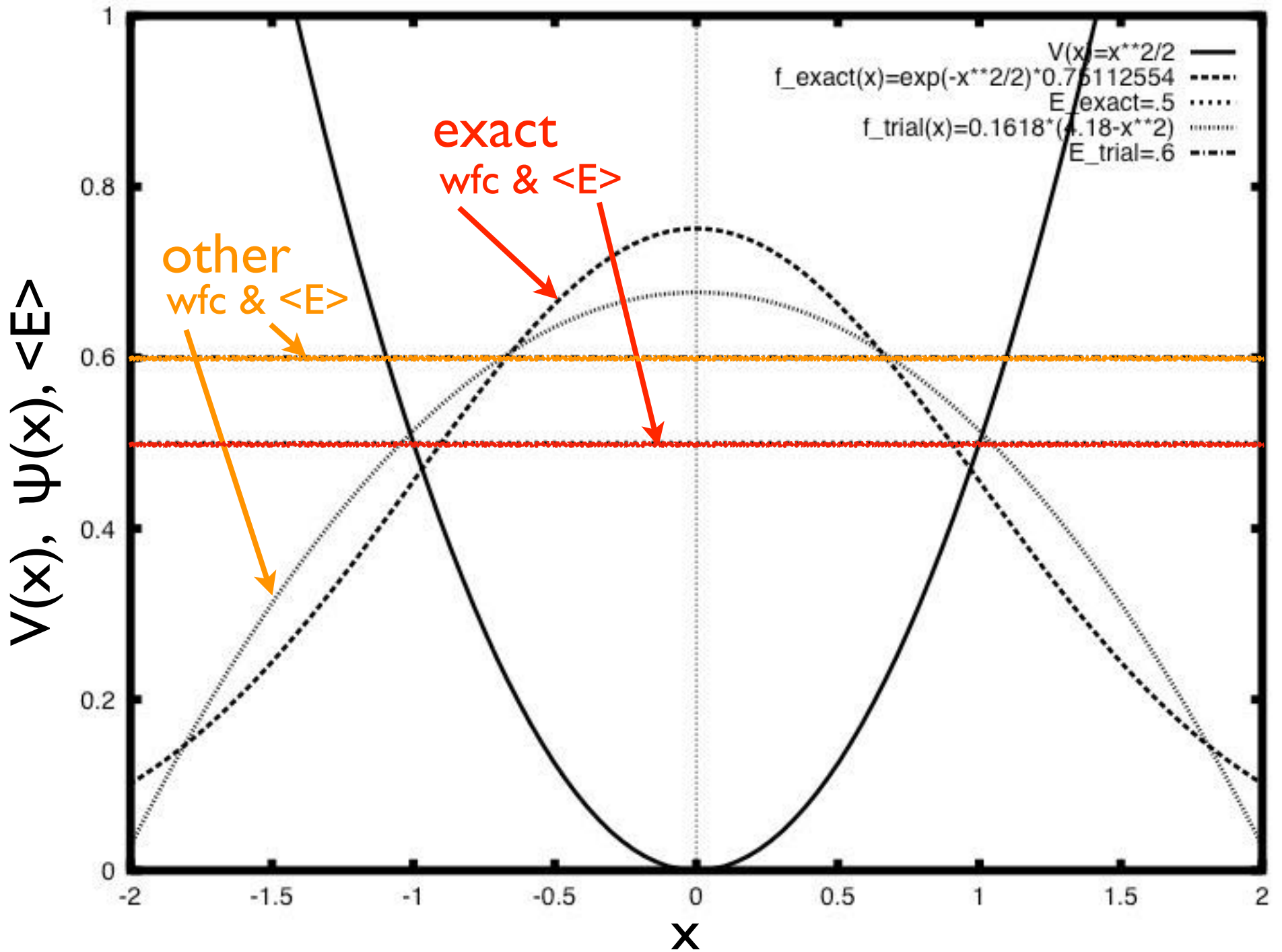
(in this case the problem can be analytically solved:)

$$\begin{aligned} \langle E_{tot,L} \rangle &= \int_{-a}^a \frac{|\psi(x)|^2}{\langle \psi | \psi \rangle} E_L(x) dx = \int_{-a}^a B^2(a^2 - x^2)^2 \left( \frac{1}{a^2 - x^2} + \frac{1}{2}x^2 \right) dx \\ &= \int_{-a}^a B^2(a^2 - x^2) dx + \frac{B^2}{2} \int_{-a}^a x^2(a^2 - x^2)^2 dx = \frac{5}{4a^2} + \frac{a^2}{14} \end{aligned}$$

$$\frac{d\langle E_{tot,L}(a) \rangle}{da} = 0 \implies a^2 = \sqrt{\frac{35}{2}}, \quad E_{tot} \approx 0.6$$

Notice: the zero-variance property does not hold for this class of trial wfc's!  
and the energy minimum does not correspond to the variance minimum





# Exercises

## 2) Anharmonic oscillator solved with VMC:

$$\mathcal{H} = E_{kin} + E_{pot} = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \frac{1}{8}x^4$$

Trial wfc.:

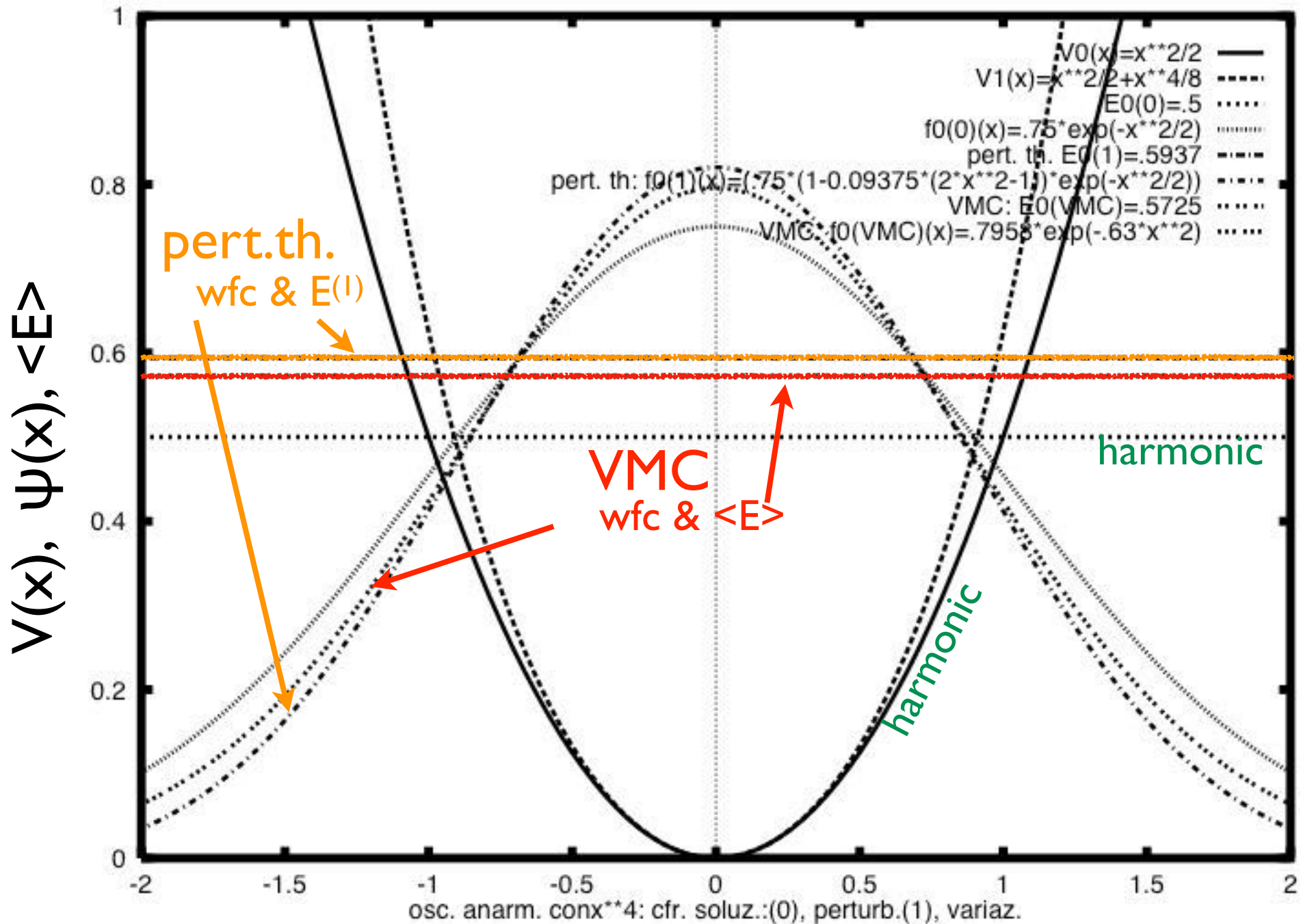
$$\psi(x) = Ae^{-\beta x^2}$$

(also in this case the problem can be analytically solved:)

$$\langle E_{tot,L} \rangle = \left( \frac{1}{2} - 2\beta^2 \right) \frac{1}{4\beta} + \beta + \frac{3}{128\beta^2}$$

$$\frac{d\langle E_{tot,L} \rangle}{d\beta} = 0 \implies \beta(4\beta^2 - 1) = \frac{3}{8} \implies \beta \approx 0.63, \quad E_{tot} \approx 0.5725$$

(better than 1st order perturbation theory)



# managing input/output

**job\_parabola** Note: it must be **executable!**

make it with: (\$prompt)> chmod u+x job\_parabola

run with: (\$prompt)> ./job\_parabola

```
for sigma in 0.5 0.6 0.7 0.8 0.9 1.; do
```

```
cat > input << EOF
```

```
1000
```

```
$sigma
```

```
0.
```

```
5.
```

```
EOF
```

```
./a.out < input >> dati
```

( >> means “append” )

### 3) Hydrogen atom solved with VMC:

$$H = -\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{r}$$

A 3D problem which can be reduced to 1D, using the radial part of the laplacian operator in polar coordinates:

$$H = -\frac{\hbar^2}{2m} \left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right] - \frac{e^2}{r}$$

Use atomic units  $(\hbar = 1, m = 1, e^2 = 1 \implies E \text{ in Hartree})$

Consider a s-type trial wfc with a radial part:  $\psi_\alpha(r) = e^{-\alpha r}$

$$E_L(r) = \frac{H\psi_\alpha(r)}{\psi_\alpha(r)} = -\frac{1}{2} \left[ \alpha^2 - \frac{2\alpha}{r} \right] - \frac{1}{r}$$



### 3) Hydrogen atom solved with VMC:

$$E_L(r) = \frac{H\psi_\alpha(r)}{\psi_\alpha(r)} = -\frac{1}{2} \left[ \alpha^2 - \frac{2\alpha}{r} \right] - \frac{1}{r}$$

$$\Rightarrow \langle E_L \rangle = \int_0^\infty \frac{\psi_\alpha^2(r)}{\langle \psi_\alpha | \psi_\alpha \rangle} E_L(r) d\mathbf{r} = \int_0^\infty \frac{4\pi r^2 \psi_\alpha^2(r)}{\langle \psi_\alpha | \psi_\alpha \rangle} E_L(r) dr$$

NOTES: using spherical coordinates and 1D integral, pay attention to:

- Generation of new position: must be  $r \geq 0$
- Probability of being btw  $r$  and  $r+dr$ : is  $\propto 4\pi r^2$

### 3) Hydrogen atom solved with VMC:

The harmonic oscillator program **metropolis\_gaussian.f90** or what you have done can be adapted to this problem by changing the form of the trial wave function and local energy:

Accumulate 
$$E_L(r) = \frac{H\psi_\alpha(r)}{\psi_\alpha(r)} = -\frac{1}{2} \left[ \alpha^2 - \frac{2\alpha}{r} \right] - \frac{1}{r}$$

generating points and accepting or rejecting them according to the ratio

$$w = \left( \frac{r'}{r} \right)^2 \left| \frac{\psi(r')}{\psi(r)} \right|^2$$

### 3) Hydrogen atom solved with VMC:

Hints:

- use nmcs = 100.000
  - Max variation of  $r = 4$  Bohr; adapt it to keep the acceptance ratio of the order of 50%
- => use also the zero variance property!

Alternative approach keeping the full 3D problem:

- consider cartesian (x,y,z) coordinates
- no need of limiting the walk; probability automatically set correctly

# He atom solved with VMC:

If we use atomic units with  $\hbar = m_e = e = 1$ , the Hamiltonian for the motion of the two electrons can be written

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}},$$

where  $r_{12} = |\mathbf{r}_{12}| = |\mathbf{r}_1 - \mathbf{r}_2|$ . The terms  $-2/r_i$  represent the negative (attractive) potential energy between each electron with charge  $-1$  and the Helium nucleus with charge  $+2$ , and the term  $+1/r_{12}$  represents the positive (repulsive) potential energy between the two electrons.

## A simple choice of variational trial wave function

(1) If the repulsive term  $1/r_{12}$  were not present, then the Hamiltonian would be that of two independent Hydrogen-like atoms. It can be shown that the energy and ground state wave function of a Hydrogen-like atom whose nucleus has charge  $Z$  are given by

$$E_0 = -\frac{Z^2}{2}, \quad \psi_0 \sim e^{-Zr}.$$

The wave function of the combined atom with two non-interacting electrons would be the product of two such wave functions:

$$\psi(\mathbf{r}_1, \mathbf{r}_2) \sim e^{-2r_1} e^{-2r_2}.$$

This suggests a trial wave function of the form

$$\Psi_{T,\alpha} = e^{-\alpha r_1} e^{-\alpha r_2},$$

similar to what was done for the Hydrogen atom. If the electron-electron interaction is neglected, then the average energy with this wave function can be calculated

$$\left\langle -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} \right\rangle = 2 \times \frac{\alpha^2}{2} - 2 \times \alpha,$$

# He atom solved with VMC:

(2)  
H with interaction,  
 $\psi$  without correlation

which has a minimum at  $\alpha = 1$ , which gives  $\langle E \rangle = -1$ . The experimentally measured ground state energy is  $E_0 = -2.904$ . In fact, the average energy can be evaluated exactly for this trial wave function even if the electron-electron interaction is included:

$$\left\langle -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}} \right\rangle = \alpha^2 - \frac{27}{8}\alpha,$$

which has a minimum at  $\alpha = 27/16$ , which gives  $\langle E \rangle = -2.8477$ . This shows that the repulsion between the electrons is important and lowers the energy.

(3)

## Padé-Jastrow wave function

The textbook suggest using a trial wave function

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = e^{-2r_1} e^{-2r_2} e^{\frac{r_{12}}{2(1+\alpha r_{12})}},$$

with  $\alpha$  as a variational parameter. The local energy with this wave function can be calculated

$$E_L(\mathbf{r}_1, \mathbf{r}_2) = -4 + \frac{\alpha}{(1+\alpha r_{12})} + \frac{\alpha}{(1+\alpha r_{12})^2} + \frac{\alpha}{(1+\alpha r_{12})^3} - \frac{1}{4(1+\alpha r_{12})^4} + \frac{\hat{\mathbf{r}}_{12} \cdot (\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2)}{(1+\alpha r_{12})^2}.$$

H with interaction,  
 $\psi$  with correlation, extremely simple form

```

double eLocal(double *rElectron1, double *rElectron2) {
    // value of trial wave function for walker n
    double r1 = 0, r2 = 0, r12 = 0;
    for (int d = 0; d < 3; d++) {
        r1 += rElectron1[d] * rElectron1[d];
        r2 += rElectron2[d] * rElectron2[d];
        r12 += (rElectron1[d] - rElectron2[d]) *
            (rElectron1[d] - rElectron2[d]);
    }
    r1 = sqrt(r1);
    r2 = sqrt(r2);
    r12 = sqrt(r12);
    double dotProd = 0;
    for (int d = 0; d < 3; d++) {
        dotProd += (rElectron1[d] - rElectron2[d]) / r12 *
            (rElectron1[d] / r1 - rElectron2[d] / r2);
    }
    double denom = 1 / (1 + alpha * r12);
    double denom2 = denom * denom;
    double denom3 = denom2 * denom;
    double denom4 = denom2 * denom2;
    double e = - 4 + alpha * (denom + denom2 + denom3)
        - denom4 / 4 + dotProd * denom2;
    return e;
}

```

```

double Psi(double *rElectron1, double *rElectron2) {

    // value of trial wave function for walker n
    double r1 = 0, r2 = 0, r12 = 0;
    for (int d = 0; d < 3; d++) {
        r1 += rElectron1[d] * rElectron1[d];
        r2 += rElectron2[d] * rElectron2[d];
        r12 += (rElectron1[d] - rElectron2[d])
            * (rElectron1[d] - rElectron2[d]);
    }
    r1 = sqrt(r1);
    r2 = sqrt(r2);
    r12 = sqrt(r12);
    double Psi = - 2*r1 - 2*r2 + r12 / (2 * (1 + alpha*r12));
    return exp(Psi);

}

```