## Exercise Lecture VIII

# Variational Monte Carlo (VMC)

### 1. Quantum oscillator in 1D: variational approach (see Fig. 1)

Consider the hamiltonian of the quantum harmonic oscillator  $\mathcal{H}=p^2/2+x^2/2$  (having choosen  $m=k=\hbar=1$ ). We want to solve it numerically with VMC. To this purpose consider two different choices for the trial wavefunction:

$$\psi(x) = \begin{cases} B(a^2 - x^2), & \text{for } |x| < a; \\ 0, & \text{for } |x| > a. \end{cases}$$
 (1.a)

or:

$$\psi(x) = Ae^{-\beta x^2} \tag{1.b}$$

with a and  $\beta$  variational parameters, A and B proper normalization constants.

(a) Calculate

$$\langle E \rangle = \langle E_L \rangle = \frac{1}{M} \sum_{i=1}^{M} E_L(x_i),$$

with

$$E_L(x) = \frac{\mathcal{H}\psi(x)}{\psi(x)}$$
 (local energy)

and with the  $x_i$  distributed according  $\psi(x)^2$ . Using the trial wavefunction (1.b), remind the exercise concerning the Metropolis sampling of a gaussian function, Lecture VII; see the code metropolis\_gaussian.f90. See metropolis\_parabola.f90 for (1.a).

(b) Verify numerically and analytically that the variational solution gives in the two cases:

$$(1.a)$$
:  $a = (35/2)^{1/4} \approx 2.0453$ ;  $\langle E \rangle = 0.6$ 

(1.b):  $\beta = \frac{1}{2}$ ;  $\langle E \rangle = 0.5$ 

(In this case the exact analytic solution is known,  $E_0 = 0.5$ ; however, in case (1.a) the minimum of  $\langle E \rangle$  as a function of a is rather flat: use steps of 0.01 for a and n = 100000 Metropolis accumulation steps to appreciate the minimum)

(c) Instead of solving the problem by minimizing  $\langle E_L \rangle$ , solve it minimizing the variance:

$$\sigma^2 = < E_L^2 > - < E_L >^2;$$

you should observe that in the case (1.a) the minimum of the variance is positive, whereas in the case (1.b) is zero.

(Important: note the usefulness of the "zero variance property"; the EXACT minimum of  $\sigma^2$  is 0 is the class of the trial wavefunctions contains the exact result, whereas in general the minimium of  $\langle E \rangle$  is not known!)

#### 2. Anharmonic quantum oscillator 1D (see Fig. 2)

(a) Consider also an anharmonic part in the potential, i.e.  $V(x) = x^2/2 + bx^4$ . Set for instance b = 1/8, make a plot of V(x). Use the first order perturbation theory to calculate the changes at the lowest order in energy of the ground state due to the anharmonic term. Choose a reasonable form for the trial wavefunction, e.g. (1.b), and calculate  $\langle E \rangle$  with VMC. Compare the result obtained with the one obtained using the perturbation theory.

#### 3. Hydrogen atom. (Optional)

- (a) We want to find numerically the ground state of the H atom. We want to find numerically the ground state. The hamiltonian is:  $\mathcal{H} = p^2/(2m) e^2/r$ ; It is convenient to use atomic units  $(h = 1, m_e = 1/2, e^2 = 2, \text{ and therefore to measure all length in terms of Bohr radius, <math>a_0 = \hbar^2/(me^2)$ , the energies in Rydberg,  $Ry = me^4/(2\hbar^2)$ . Consider the trial wavefunction  $\psi(\mathbf{r}) = \psi(r) = e^{-r/a}$ , where a is a variational parameter. calculate the optimal value of ak and the corresponding energy. Hints:
  - 1) you may reduce the problem (spherical part) to a 1D problem. Pay attention that

$$< E_L > = \frac{\int \psi^2(r) E_L(r) d\mathbf{r}}{\psi^2(r) d\mathbf{r}} = \frac{\int \psi^2(r) E_L(r) 4\pi r^2 dr}{\int \psi^2(r) 4\pi r^2 dr}$$

and therefore the sampling probability is  $r^2\psi^2(r)$  and not just  $\psi^2(r)$ .

- 2) Pay attention close to the origin!
- (b) Approach the problem keeping a 3D formulation, considering the isotropy of the trial move (The displacement is a vector!)

```
! metropolis_gaussian.f90
! METROPOLIS sampling of several physical observables for the
! hamiltonian:
              h = -1/2 \quad h = -1/2 \quad 1/2 \quad x^2
! comparison exact expected results with numerical results
! on psi^2(x), with psi(x) = exp(-x^2/(4 sigma^2))
! \sigma=1 => psi^2(x) = costant * standard gaussian
P(x) = \exp(-x**2/(2*sigma**2))/sqrt(2*pi*sigma**2)
program metropolis_gaussian
 implicit none
 integer, parameter :: dp=selected_real_kind(13)
 integer :: i,n
 real(kind=dp):: sigma,etot,ekin,epot,rnd,ekinL,epotL,etot2
 real (kind=dp) :: pigr,pi2b,var,beta,var_th
 real(kind=dp):: x,x1,x2,xp,delta,expx,expxp,p,acc
 character(len=13), save :: format1 = (a7,2x,2f9.5)"
 open(unit=7,file='e_var_gauss.dat',position='append')
 pigr = 2*asin(1.0_dp)
 acc = 0.0_dp
 x1 = 0.0_dp
 x2 = 0.0_dp
 ekin = 0.0_dp
 epot = 0.0_dp
 etot2= 0.0_dp
 print*, "n, sigma (remember: beta = 1 / (4*sigma**2)), x0, delta"
 read*, n,sigma,x,delta
 beta = 1 / (4*sigma**2)
! call random_seed(put=seed)
 do i=1,n
    ekinL = -0.5_dp * ((x/(2*sigma**2))**2 - 1/(2*sigma**2))
    epotL = 0.5_dp * x**2
    ekin = ekin + ekinL
    epot = epot + epotL
    etot = ekin + epot
    etot2 = etot2 + (ekinL + epotL)**2
    x1 = x1 + x
    x2 = x2 + x**2
    !ccccccccccccccccccccccc
    expx = -x**2/(2*sigma**2)!
    call random_number(rnd)
    xp = x + delta * (rnd-0.5_dp) !
```

```
expxp = - xp**2 /(2*sigma**2) !
                                        metropolis
    p = exp (expxp-expx)
                                         algorithm
     call random_number(rnd)
     if (p > rnd) then
       x = xp
     !ccccccccccccccccccccccc
       acc=acc+1.0_dp
     endif
  enddo
 var_th = 1._dp/(32*beta**2)+beta**2/2-1._dp/4
 write(unit=*,fmt=*)"acceptance ratio = ",acc/n
 write(unit=*,fmt=*)"# Results (simulation vs. exact results):"
 write(unit=*,fmt=format1)"etot = ",etot/n,1.0_dp/(8.0_dp*sigma**2)&
       +0.5_dp*sigma**2
 \label{lem:write} write(unit=*,fmt=format1)"ekin = ",ekin/n,1.0_dp/(8.0_dp*sigma**2)
 write(unit=*,fmt=format1)"epot = ",epot/n,0.5_dp*sigma**2
 write(unit=*,fmt=format1)"evar = ",etot2/n-(etot/n)**2,var_th
 write(unit=*,fmt=format1)"<x> = ",x1/n,0.0_dp
 write(unit=*,fmt=format1)"<x^2>= ",x2/n,sigma**2
  write (7,*) sigma, etot/n, sqrt(abs(etot2/n-(etot/n)**2)), etot2/n-(etot/n)**2) \\
close(7)
end program metropolis_gaussian
```

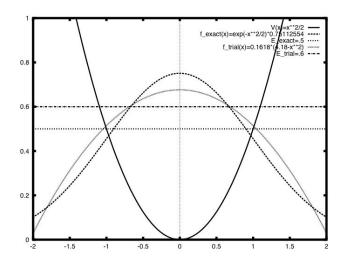


Figure 1: Harmonic oscillator in 1D with VMC (ex. 1): Ground state Eigenvalue and Eigenstate with two different trial wavefunctions.

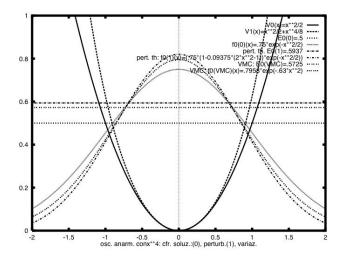


Figure 2: Anharmonic oscillator in 1D with VMC (ex. 2): Ground state Eigenstate and eigenvalue with two different trial wavefunctions, and comparison with the analytic solution obtained within the first order perturbation theory.