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# The simple harmonic oscillator ground state using a variational Monte Carlo method

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**Abstract.** A Monte Carlo method is used to evaluate the ground-state energy of a quantum particle in a harmonic oscillator potential. The use of a trial wavefunction illustrates the process by means of which the Monte Carlo method approximates with great accuracy the well known ground-state energy of a quantum mechanical harmonic oscillator. A FORTRAN program incorporating the numerical approach that is suitable for a personal computer is available in the online edition.

## 1. Introduction

In the case of a few idealized scenarios, the Schrödinger equation may be solved analytically in order to describe the phenomenon of a quantum particle. For other systems the behaviour of the quantum particle can become so complex that numerical techniques must be used in order to solve the Schrödinger equation and obtain its eigenfunctions and eigenvalues. The Monte Carlo method provides a convenient way to solve the Schrödinger equation because of its success in obtaining a probability distribution [1].

The Monte Carlo method is commonly used in physics to simulate complex systems that are of a random nature in statistical physics [2], semiconductor devices and material properties [3], charge transport in semiconductor devices [4], nanocrystals [5], and quantum dot scenarios [6]. Because of the widespread use of this this method, it is important to understand the simple process by which this numerical method describes these systems. We will explain the algorithm involved in solving the Schrödinger equation for the ground-state energy of a quantum particle in a simple harmonic oscillator potential and show the accuracy of this method. This numerical method can provide a basis on which the ground-state energy of any system of quantum particles in any potential may be described.

The ground-state energy of a quantum particle may be obtained analytically by solving the Schrödinger equation if the problem is simple enough for this to be possible. Alternatively, using a variational wavefunction for the quantum particle, the Schrödinger equation can be solved numerically within a Monte Carlo method. The Monte Carlo method makes use of an initial probability distribution to estimate the ground-state energy of the quantum particle. The exact minimum energy of the quantum particle is found by varying the trial wavefunction. The minimum ground-state energy as a function of the variational parameter identifies the ground state as well as the system's eigenstate. The minimum of the energy must be accompanied by a minimum in the standard deviation.

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## 2. Theory

Because of its popularity, a quantum particle in a quadratic potential is an attractive scenario in which the variational Monte Carlo method may be used to solve for the ground-state energy of the particle. Thus the standard wave equation

$$H\Psi = E\Psi \tag{2.1}$$

with the Hamiltonian $H = -(\hbar/2m)\nabla_D^2 + V(r_D)$ and the harmonic potential $V(r_D) = \frac{1}{2}m\omega^2 r_D^2$, where $E$ is the eigenvalue corresponding to an eigenstate $\Psi$ of the system and $m$ and $\omega$ are respectively the mass and rotational frequency of the particle, will be solved numerically. The differential operator used here for one, two and three dimensions, respectively, is

$$\nabla_D^2 = \begin{cases} \partial^2/\partial x^2 & D=1 \\ \partial^2/\partial x^2 + \partial^2/\partial y^2 & D=2 \\ \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2 & D=3 \end{cases}$$

where, similarly,

$$r_D^2 = \begin{cases} x^2 & D=1 \\ x^2+y^2 & D=2 \\ x^2+y^2+z^2 & D=3. \end{cases}$$

One way to obtain the exact ground-state energy is to assume a wavefunction of the form

$$\Psi(x) = \exp(-\alpha r_D^2) \tag{2.2}$$

which when substituted in the Schrödinger equation, equation (2.1), gives

$$4\alpha^2 = \left(\frac{m\omega}{\hbar}\right)^2 \tag{2.3}$$

and

$$2D\alpha = \frac{2m}{\hbar^2}E \tag{2.4}$$

for the harmonic potential, where $D = 1, 2, 3$ for one, two and three dimensions, respectively. Therefore $\alpha = m\omega/2\hbar$, and

$$E = \tfrac{1}{2}\hbar\omega D. \tag{2.5}$$

There are many versions of the Monte Carlo method used to solve the Schrödinger equation for the ground-state energy of a quantum particle. One method, for example, is the diffusion Monte Carlo method [7], which is used to solve the time-dependent Schrödinger equation. Another method is the fixed-phase Monte Carlo method [6], which is used for wave equations that consider a magnetic field. Below we will show how it is possible to adapt a Monte Carlo scheme [1] to approximate these exact ground-state energies given a trial wavefunction. The ground-state energy of the system is found by defining a local energy, $E_{\mathrm{L}}$, which from (2.1) is written as

$$E_{\mathrm{L}} = \frac{H\Psi}{\Psi}. \tag{2.6}$$

Using the wavefunction of (2.2) the local energy becomes, in units of $\hbar\omega$,

$$E_{\mathrm{L}} = D\alpha + (\tfrac{1}{2} + 2\alpha^2)r_D^2. \tag{2.7}$$

For a set of $\alpha$, $\{\alpha\}$, we define the following energy:

$$\langle E_{\mathrm{L}}\rangle_{\Psi^2} = \frac{\int_{-\infty}^{\infty}\Psi^2(\boldsymbol{x})E_{\mathrm{L}}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}}{\int_{-\infty}^{\infty}\Psi^2(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}} \tag{2.8}$$

where $\boldsymbol{x}$ represents random positions in corresponding $D$ dimensions. A minimum gives the eigenvalue, in addition to isolating an $\alpha$ in $\{\alpha\}$ which yields the ground state of the system [2].

The weighted average of (2.8) is conveniently evaluated in any dimension using its Monte Carlo estimate. This estimate of the energy makes use of random numbers sampled from the probability density

$$P(\boldsymbol{x}) = \frac{\Psi^2(\boldsymbol{x})}{\int_{-\infty}^{\infty} \Psi^2(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}}. \tag{2.9}$$

The random numbers, $\boldsymbol{x}_{ij}$, obtained are used to calculate the Monte Carlo average energy

$$\langle E_{\mathrm{L}} \rangle_{\Psi^2} = \lim_{N\to\infty} \lim_{M\to\infty} \frac{1}{N} \frac{1}{M} \sum_{j=1}^{N} \sum_{i=1}^{M} E_{\mathrm{L}}(\boldsymbol{x}_{ij}) \tag{2.10}$$

where $M$ is the ensemble size of random numbers $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_i, \ldots, \boldsymbol{x}_M\}$ and $N$ is the number of ensembles. Each ensemble uses a different set $\{\boldsymbol{x}\}$ of random numbers, in accordance with (2.9) in an importance sampling context [3].

## 3. Importance sampling

To evaluate $\langle E_{\mathrm{L}} \rangle$ using ensembles of random numbers from the probability distribution $P(\boldsymbol{x})$, the ensembles so generated must reflect the distribution function itself. A given ensemble is chosen according to the Metropolis method [8]. This method uses an acceptance and rejection process of random numbers that have a frequency probability distribution like $\Psi^2$ [3, 9]. The acceptance and rejection method is due to the work of von Neumann [10] and is performed by obtaining a random number from the probability distribution, $P(\boldsymbol{x})$, then testing its value to determine if it will be acceptable for use in the approximation of the local energy [11]. Random numbers may be generated using a variety of methods [12–15].

A step process of our algorithm is given in appendix A. After an ensemble of random numbers is generated, the acceptance criterion is such that the probability of moving from an initial random number of the ensemble, $\boldsymbol{x}_i$, to a new random number, $\boldsymbol{x}_k$, is defined as

$$A = \frac{\Psi^2(\boldsymbol{x}_k)}{\Psi^2(\boldsymbol{x}_i)} \tag{3.1}$$

restricted, however, to have a maximum value of unity. These moves are done to broaden subsequent ensembles for a wider sampling range. Thus each new $\boldsymbol{x}_k$ that is a member of the next ensemble is accepted according to whether $A$ obeys the inequality $A \geqslant R$, where $R$ is a random number between 0 and 1. Five of the 50 individual ensembles are shown in figure 1 compared with the Gaussian curve used in figure 2 for illustrative purposes. As mentioned earlier, each ensemble is broader than the previous ensemble (histograms 1–5), in order to achieve a wider sampling range. The initial random number, $\boldsymbol{x}_i$, is kept in the accepted ensemble if the above inequality is not true. This process is repeated for each member of an ensemble, as indicated by the algorithm in appendix A. A histogram in figure 2 shows the frequency of random numbers from an average of 50 typical accepted ensembles that were used to evaluate the energy, $E_{\mathrm{L}}$, in (2.10). The ensemble averaged has the property that it obeys a Gaussian shape. In figure 2 a Gaussian fit was carried out to illustrate this property. We expect that in the limit as $N \to \infty$ and $M \to \infty$ the accepted ensembles used to evaluate the Monte Carlo estimate for the average energy will yield the ground state of the system according to (2.10).

In the program, given in appendix B, the broadening of the ensemble is achieved through the line

$$Y = X(K) + DELTA * (RAN\,0(SEED) - 0.5). \tag{3.2}$$

(Appendix B is not printed in the paper edition, but is available in, and may be downloaded from, the online edition of the journal: see `http://www.iop.org`.)

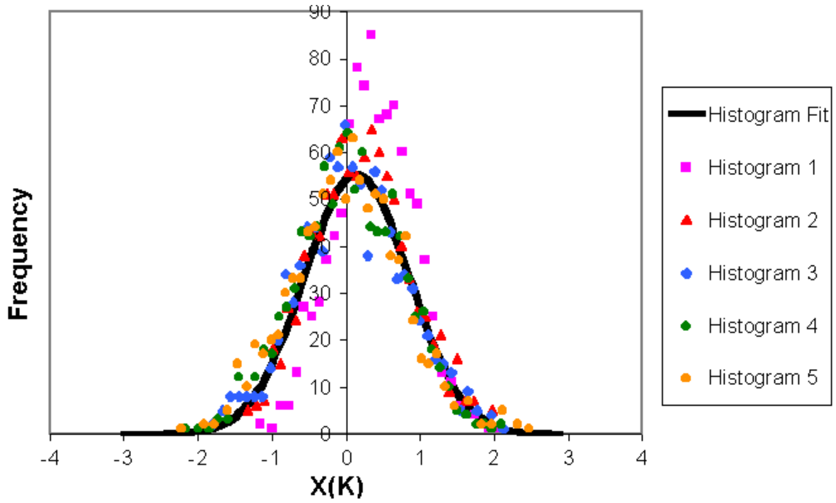


**Figure 1.** Five of the 50 histograms used in the average histogram shown in figure 2. The solid Gaussian line from figure 2 is shown here for comparison.

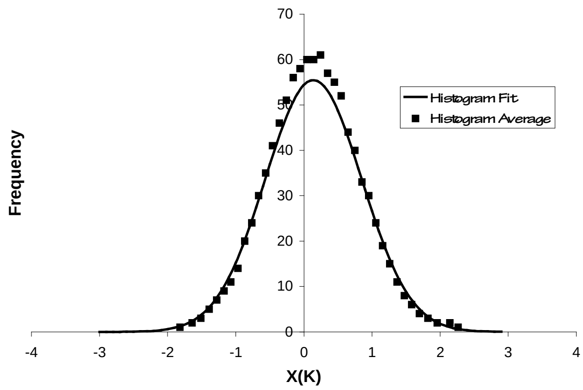


**Figure 2.** Average of 50 typical ensembles (dots) fitted by a Gaussian curve (solid line).

Here $Y$ is the new value $x_f$ to be tested and $X(K)$ is the value $x_i$ of a previously accepted ensemble for $K = i$ . The range width is determined by *DELTA*, adjusted to suit particular needs, and the value 0.5 ensures the availability of negative numbers. The random number generator only produces numbers between 0 and 1, so there will be an initial maximum random value and an initial minimum random value. These maximum and minimum values in the new accepted ensemble, $\{X(K)\}$, are kept as subsequent ensembles grow in range. The number of ensembles used is adjusted by *NSTEP*.

When evaluating the energy of the system it is important to calculate the standard deviation

$$\sigma = \sqrt{\frac{\left(\langle E_{\mathrm{L}}^2\rangle_{\Psi^2} - \langle E_{\mathrm{L}}\rangle_{\Psi^2}^2\right)}{\left(M(N-1)\right)}}$$

of this energy. Since $\langle E_{\mathrm{L}}\rangle_{\Psi^2}$ will be exact when an exact trial wavefunction is used, then the standard deviation of the local energy will be zero for this case [6]. Thus in the Monte Carlo method, the minimum of $\langle E_L \rangle_{\Psi^2}$ should coincide with a minimum in the standard deviation.

A full implementation of the algorithm in appendix A, using code suitable for a personal computer, is incorporated, for the case of one dimension, into the program of appendix B.

## 4. Results

The Monte Carlo process described here has been employed for the one-, two- and three-dimensional cases of the simple harmonic oscillator. Figures 3–5 respectively give the energies obtained for each dimension. The minimum energy for each dimension is accompanied by a minimum in the standard deviation shown as an inset in each figure. The energy minima are in agreement with what is expected analytically, $E = D/2$ in units of $\hbar\omega$, $\alpha = \frac{1}{2}$ in units of $m\omega/\hbar$, and $D = 1, 2, 3$ for each dimension, respectively.

Finally, in one dimension, we have studied a family of curves using the exponential

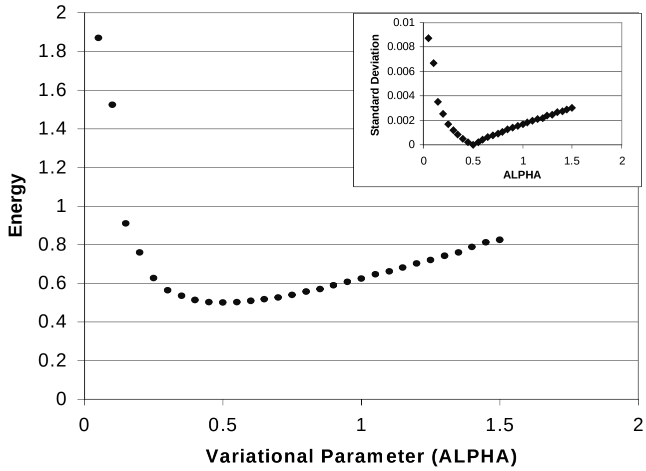


**Figure 3.** One-dimensional results for the energy using 50 ensembles each with 500 random points. The inset shows the standard deviation. Both minima occur at $\alpha = 0.5$.

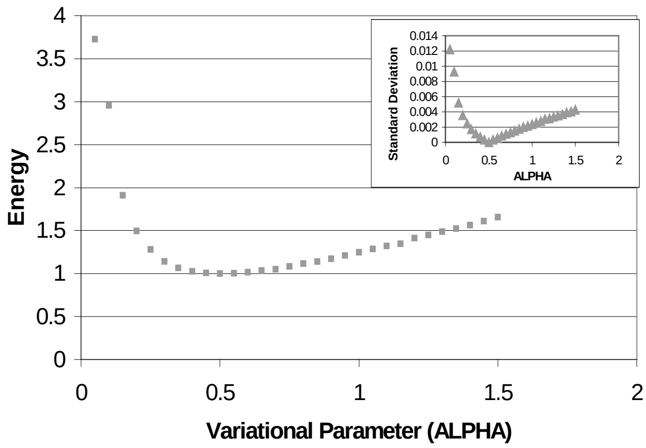


**Figure 4.** Two-dimensional results for the energy using 50 ensembles each with 500 random points. The inset shows the standard deviation.

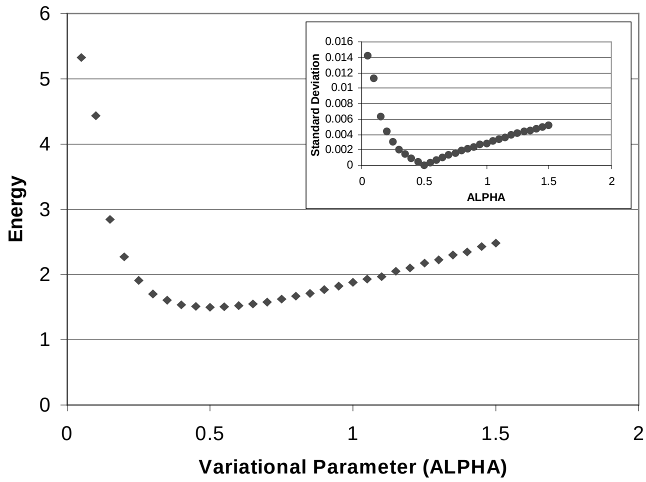


**Figure 5.** Three-dimensional results for the energy using 50 ensembles each with 500 random points. The inset shows the standard deviation.

function $\Psi(x) = \exp(-\alpha x^n)$ for $n = 4$ and 6 (even values of $n$) for comparison with the $n = 2$ case. We also included in this study the function $\Psi(x) = \cos(\pi x/2\alpha)$, $-\alpha < x < \alpha$, for completeness. Our results are summarized in table 1. The results are consistent with our conclusions, i.e. the variational Monte Carlo method indicates that $\Psi(x) = \exp(-\alpha x^2)$ is the correct wavefunction because for a given $\alpha$ a minimum of energy, $E_{\min}$, is achieved along with a simultaneous minimum in $\sigma$. None of the non-exact wavefunctions give such conclusive results.

## 5. Summary

A variational Monte Carlo method (VMC) has been used to obtain the numerical ground-state energies of the one-, two- and three-dimensional versions of the simple harmonic oscillator. In our example a variational wavefunction was used that is similar to the exact ground state. In figures 3–5, a minimum in the energy is accompanied with a minimum in the standard deviation for the one-, two- and three-dimensional cases, which together showed that the numerical results are in very good agreement with the exact analytical results. It is expected

**Table 1.** Minimum values for the energy, $E$, standard deviation, $\sigma$, and variational parameter, $\alpha$, are shown for the exact wavefunction and three non-exact wavefunctions. There are two types of values indicated: an $\alpha$ and a $\sigma$ that correspond to a minimum energy, $E_{\min}$. Also there is an $\alpha$ and an $E$ that correspond to a minimum standard deviation, $\sigma_{\min}$. For the case where $n = 2$ an $E_{\min}$ and a $\sigma_{\min}$ are both found at the same value of $\alpha$. This is due to the fact that $\Psi(x) = \exp(-\alpha x^2)$ happens to be the exact wavefunction.

| Case | | $\alpha_{E_{\min}}$ | $E_{\min}$ | $\sigma_{E_{\min}}$ | $\alpha_{\sigma_{\min}}$ | $E_{\sigma_{\min}}$ | $\sigma_{\min}$ |
|---|---|---|---|---|---|---|---|
| $\Psi(x) = \exp(-\alpha x^n)$ | $n = 2$ | 0.5 | 0.5 | 0 | 0.5 | 0.5 | 0 |
| | $n = 4$ | 0.15 | 0.583 6 | 0.000 624 | 0.5 | 0.694 511 | 0.000 63 |
| | $n = 6$ | 0.045 | 0.693 572 | 0.001 083 | 0.015 | 0.751 23 | 0.000 902 |
| $\Psi(x) = \cos\left(\frac{\pi x}{2\alpha}\right)$ $-\alpha < x < \alpha$ | | 2.2 | 0.563 042 | 0.001 165 | [a] | [a] | [a] |

[a] Here the cosine function does not yield a minimum $\sigma$ for which we can find a corresponding value of $E$.

that for cases in which the exact wavefunction is not known the minimum energy can still be identified with a minimum in the standard deviation. In fact the results summarized in table 1 as discussed in the previous section strengthen this capability of the variational Monte Carlo method. We hope to apply this general numerical method to obtain ground-state energies in more complex systems in the future.

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## Appendix A

Ground-state energy of a quantum harmonic oscillator algorithm using a variational Monte Carlo method.

Output: Ground-state energy, $E(\alpha)$, standard deviation, $\sigma$, acceptance ratio, *ARATIO*.

Modifiable parameters: $M$, $P$, $N$, *DELTA*, *NSTEP*, and the *ALPHA* iteration range.

STEP 1. Create the array of random numbers $X(M, N, P)$.

STEP 2. Initialize *EAVE*, *ESQU* and *ACCEPT* to zero.

STEP 3. Evaluate $PSIX = \exp(-ALPHA * X^2)$ with $X(M, N, P)$.
Evaluate $PSIY = \exp(-ALPHA * X^2)$ with
$Y = X(M, N, P) + DELTA * (RAND(0) - 0.5)$.
Evaluate the probability ratio $A = (PSIY)^2/(PSIX)^2$.
If $A > 1$, then $A = 1$.

STEP 4. If $A \geqslant RAND(0)$, then
$X(M, N, P) = Y$
$ACCEPT = ACCEPT + 1/P$.

STEP 5. Evaluate the local energy, $E_L$, $EAVE = EAVE + E_L$, $ESQU = ESQU + E_L$.

STEP 6. For $K = 1, \ldots, M$, repeat STEP 3–5 until $K = M$.

STEP 7. For $ISTEP = 1, \ldots, NSTEP$, repeat STEP 3–5 until $ISTEP = NSTEP$.

STEP 8. Evaluate $ARATIO = ACCEPT/(M * NSTEP)$,
$EMEAN = EAVE/(M * NSTEP)$,
$ESQUMEAN = ESQU/(M * NSTEP)$,

$$ESIGMA = \frac{\sqrt{(EMEAN)^2 - ESQUMEAN}}{M * NSTEP - 1}.$$

Output *EMEAN*, *ESIGMA*, *ARATIO*.

STEP 9. $ALPHA = ALPHA + 0.05$.
For $I = 1, \ldots, 20$, repeat STEP 2–8.
STOP.

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## Online supplement

This item does not appear in the paper edition.

### Appendix B

The program below is a full implementation of the algorithm in appendix A, for the case of one dimension, using code suitable for a personal computer.

```
C OSC1DPC.FOR
C      Variational Monte Carlo method for the ground state energy
C of a one dimensional simple harmonic oscillator.
C X(M,P,N) is a random number where M is the ensemble size, P is
C the dimension of the wave function (let P=1), and N is the
C number of electrons in the system (let N=1).  In this case, N
C and P may be omitted because their loops are not needed in this
C program, so that the random number array is X(M,1,1) or X(M).
C The function RAND returns a uniform random number between 0 and
C 1, and is a nonintrinsic function.
C Problems.  Contact Shawn Pottorf (stu596@westga.edu) or
C J.E. Hasbun (jhasbun@westga.edu).
C Code tested on an 80486 IBM compatible personal computer.

C-------------------------------Declarations---------------------------------
      CHARACTER*14 FILEN1, FILEN2
      PARAMETER(M=500)
      COMMON SEED
      INTEGER NSTEP, ACCEPT, SEED
      DOUBLE PRECISION ALPHA,DELTA,EAVE,ESQU,EX,ARATIO,EMEAN
      DOUBLE PRECISION ESIGMA,PSIX,PSIY,Y,A,X(M)

C----------------------------------Constants----------------------------------
      ALPHA=0.
      DELTA=0.9
      SEED=57721566.
      NSTEP=50

C---------------------------------Main Program-------------------------------
      FILEN1='E1'
      FILEN2='E2'
 14 FORMAT(A14)
      OPEN(UNIT=15,FILE=FILEN1)
      OPEN(UNIT=16,FILE=FILEN2)

C Initial random ensemble - X(K)
      DO 10 K=1,M
      X(K)=RAND(0)
 10 CONTINUE
```

```
C Variational parameter (ALPHA) loop.
      DO 210 I=1,20
      ALPHA=ALPHA+0.05
      EAVE=0.
      ESQU=0.
      ACCEPT=0.

C NSTEP - the number of loops to average the ground state energy.
C PSIX - the initial wave function.
C The move Y=X + DELTA*RAND is proposed.
C PSIY - the test wave function using Y.
C EX - the local energy.
C The K loop does the energy integral.
C The value A should not exceed unity.
      DO 20 ISTEP=1,NSTEP
        DO 30 K=1,M
          PSIX=DEXP(-ALPHA*X(K)*X(K))
          Y=X(K)+DELTA*(RAND(0)-.5)
          PSIY=DEXP(-ALPHA*Y*Y)
          A=DMIN1((PSIY*PSIY)/(PSIX*PSIX),DBLE(1.))
          IF (A.GE.RAND(0)) THEN
            X(K)=Y
            ACCEPT=ACCEPT+1
          END IF
          EX=ALPHA+(0.5-2.*ALPHA*ALPHA)*X(K)*X(K)
          EAVE=EAVE+EX
          ESQU=ESQU+EX*EX
   30   CONTINUE
   20 CONTINUE

C Acceptance ratio, mean local energy, and standard deviation.
C EPSI - known analytic result for the 1D harmonic oscillator.
      ARATIO=1.*ACCEPT/M/NSTEP
      EMEAN=EAVE/M/NSTEP
      ESIGMA=EMEAN*DSQRT(DABS(ESQU/M/NSTEP/EMEAN-1.))
      TEXTSIGMA=ESIGMA/DSQRT(DBLE(1.*M*NSTEP-1.))
      EPSI=0.5*ALPHA+1./8./ALPHA

C-----------------------------------Output---------------------------------------
       WRITE(6,*)'   EMEAN            ESIGMA           ARATIO  '
       WRITE(6,100) EMEAN, ESIGMA, ARATIO
       WRITE(15,100) ALPHA, EMEAN, EPSI
       WRITE(16,100) ALPHA, ESIGMA, TEXTSIGMA
210 CONTINUE
100 FORMAT(3F15.10)
110 FORMAT(4F15.10)
120 FORMAT(F15.10)
130 FORMAT(2F15.10)
```

```
140 FORMAT(F15.10,I10)
       STOP
       END

C ===================== RAND ======================
      FUNCTION RAND(X)
      COMMON SEED
      DATA A,C,P/3141592621.,2718281829.,10000000000./
      R=A*SEED+C
      SEED=MOD(R,P)
      RAND=SEED/P+X
      RETURN
      END
```