Monte Carlo methods for accelerating barrier crossing: Anti-force-bias and variable step algorithms

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For computer simulations of systems in which particles must cross large potential energy barriers, slow convergence is a problem. Basically there are two very disparate time scales: one characterizing motion in the potential wells and one characterizing the rare jumps from one stable well to another. Multiple time scale problems like this sorely test computer resources, and stand in the way of progress on simulations of chain folding, glass transitions, nucleation phenomena, activated barrier crossing, and quantum tunneling processes. Here several new methods are developed and tested on classical and quantum barrier crossings in double well problems. These new methods, called the anti-force-bias and variable step methods, lead to much faster convergence than standard methods. Convergence is tested by studying the deviation in the mean of the cumulative spatial distribution function from the exact distribution function.

I. INTRODUCTION

The simulation of system with rare events continues to be a thorny problem in the computer simulation of physical systems.[1] A paradigm for this problem is a particle moving in a double well potential with a large energy barrier separating the stable states. In Metropolis Monte Carlo sampling, the particle will very rarely cross the barrier, and the system will take an enormously long time to equilibrate. There are two time scales characterizing this problem: the time it takes the particle to sample one of the potential wells, and the time it takes the particle to cross the barrier. The first time scale is analogous to vibrational relaxation and the second time scale is analogous to the mean first passage time for barrier crossing in dynamical systems. For very large barriers, the barrier crossing time will be exponentially longer than the vibrational relaxation time by the inverse Arrhenius factor $\exp[E/kT]$, where E is the activation energy. Although a quantum particle moving on a double well potential can tunnel through the barrier, the tunneling period also increases dramatically with barrier height, leading to very slow convergence for quantum problems. To simulate barrier crossing one must therefore invent new rapidly converging sampling methods.

In this paper we present methods for treating problems of this kind. Building on techniques developed several years ago, namely, force-bias (FB) and smart Monte Carlo (SMC) methods,[2–5] it is possible to achieve rapid convergence in such problems. We call the new method the anti-force-bias (AFB) method. A special case of this method is a variable step Monte Carlo algorithm that is very promising for simple problems. Although these methods can be applied to a wide variety of problems in physics and chemistry, here they are applied to the simple problem of equilibration in a double well for illustrative purposes. For both classical activated barrier crossing and quantum barrier tunneling it is shown that these methods are far superior to standard methods.

II. FORCE-BIAS, ANTI-FORCE-BIAS, AND VARIABLE STEP ALGORITHMS

The basic idea in this paper is to choose a sampling function for a Monte Carlo move,

$$T(\mathbf{x}_f|\mathbf{x}_i) = \left[\frac{1}{4\pi A_i}\right]^{3/2} \exp - \frac{[\mathbf{x}_f - \mathbf{x}_i - \beta\lambda_i A_i \mathbf{F}_i]^2}{4A_i}, \tag{2.1}$$

where $\mathbf{x}_i$ is the initial position of the particle, $\mathbf{x}_f$ is the new position after a step, $\mathbf{F}_i$ is the force acting on the particle initially, A_i is a parameter to be defined later which depends on the initial position, $\beta = 1/kT$. The parameter λ_i depends upon the method used. In the force-bias method (FB), $\lambda_i = 1$; for the anti-force-bias technique (AFB),

$$\lambda_i = \frac{V''(\mathbf{x}_i)}{|V''(\mathbf{x}_i)|} \tag{2.2}$$

is the sign of the second derivative of the potential energy function at the initial position of the particle.

If no biasing is used, then $\lambda_i = 0$ and the force term is ignored in Eq. (2.1). The sampling function becomes

$$T(\mathbf{x}_f|\mathbf{x}_i) = \left[\frac{1}{4\pi A_i}\right]^{3/2} \exp - \frac{[\mathbf{x}_f - \mathbf{x}_i]^2}{4A_i}. \tag{2.3}$$

This sampling function allows for variable step size moves as discussed later.

The move is sampled from Eq. (2.1) [or Eq. (2.3)] and accepted or rejected according to the usual Monte Carlo prescription; that is, the move to $\mathbf{x}_f$ is accepted with probability

$$p = \min\{1, q(\mathbf{x}_f|\mathbf{x}_i)\}, \tag{2.4}$$

where

$$q(\mathbf{x}_f|\mathbf{x}_i) = \frac{T(\mathbf{x}_i|\mathbf{x}_f)P(\mathbf{x}_f)}{T(\mathbf{x}_f|\mathbf{x}_i)P(\mathbf{x}_I)} \tag{2.5}$$

and $P(\mathbf{x}) = Z^{-1} \exp - \beta V(\mathbf{x})$ is the Boltzmann distribution function.

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The sampling distribution given by Eq. (2.1) produces a biasing of the moves such that

$$\langle(\mathbf{x}_f - \mathbf{x}_i)\rangle = \beta\lambda_i A_i \mathbf{F}_i \tag{2.6}$$

and

$$\langle(\mathbf{x}_f - \mathbf{x}_i)^2\rangle = 6A_i + \beta^2 A_i^2 \mathbf{F}_i^2. \tag{2.7}$$

In the FB method, $\lambda_i = 1$, this procedure would bias the moves such that there would be a drift in the direction of the initial force and a spreading of the distribution that would depend on the square foot of the force. Thus in the double well problem the drift would be towards the local well minimum. If, however, λ_i is determine from Eq. (2.2), the AFB method, the drift will be anti-parallel to $\mathbf{F}_i$ for initial positions above the inflection point of the potential, and parallel to $\mathbf{F}$ otherwise. The effect should be enhanced barrier penetration.

In addition to invoking antiforce biasing it is possible to superpose a variable step size on the Monte Carlo walk by taking A_i to depend in the initial position. Even when the force term in Eqs. (2.1), (2.6), and (2.7) is neglected (λ_i), this variable step size; that is, taking A_i to depend on the initial state, may well lead to more rapid barrier crossings than would be found with a constant step size algorithm. One simple choice for this is

$$\sqrt{A_i} = \Delta x \frac{c\beta V(\mathbf{x}_i) + 1}{\beta V(\mathbf{x}_i) + 1}, \tag{2.8}$$

where V_i is the potential energy at the initial position, c is a parameter that defines the variability of the step size, and Δx is a constant step parameter. This rule allows the step size to vary between a lower bound of Δx at low energies, and a maximum of $c\Delta x$ at high energies. Clearly there are many possible functional forms for the variable step size. Goldman[6] has discussed another variable step procedure for treating fluids. In his method the step is uniformly sampled between $-\Delta/2$ and $+\Delta/2$, where Δ is chosen to depend on the deviation of the particles energy from the average energy of a particle. After correcting for problems with detailed balance, Goldman applied his algorithm to simulations of simple liquids and concluded that it did not accelerate convergence of these systems over what could be attained using ordinary Metropolis sampling. Here we show that a different implementation of a variable step algorithm based on the above leads to greatly accelerated convergence for barrier crossing.

All of the foregoing can be summarized by defining λ_i as,

$$\lambda_i = \begin{cases} 0 & \text{no force-bias} \\ 1 & \text{force-bias} \\ \dfrac{V(\mathbf{x}_i)''}{|V(\mathbf{x}_i)''|} & \text{anit-force-bias} \end{cases}. \tag{2.9}$$

Although the foregoing is formulated in terms of a continuous function Eq. (2.1) as in SMC, it is possible to implement this in the original force-bias formulation. The only difference is that instead of sampling Gaussians one would sample square mound distributions. One must be careful in using the variable step idea in this way to guarantee detailed balance because otherwise one runs into the same problem encountered by Goldman.[6]

In this paper we compare no force-bias, force-bias, and anti-force-bias algorithms with and without variable steps with respect to the rapidity of convergence of classical and quantum double well problems. Quantum double well problems involve tunneling through the barrier. In the path integral simulation of tunneling one studies the motion of isomorphic chain polymers. The quantum barrier crossing problem requires more computer time than the corresponding classical problem. Moreover, there is the fundamental problem of instanton relaxation. The anti-force-bias method with variable step size allows this problem to be treated very effectively.

In order to compare these methods it is necessary to define criteria for convergence. Usually one studies the time required for the convergence of the cumulative averages of various observables to converge to equilibrium. We find it useful to study the time dependence of χ where

$$\chi^2(t) = \int_{-\infty}^{\infty} d\mathbf{x}[\rho(\mathbf{x},t) - \rho_{\text{exact}}(\mathbf{x})]^2, \tag{2.10}$$

where $\rho(\mathbf{x},t)$ is the cumulative normalized spatial probability distribution function (or diagonal density matrix in the position representation). The decay constants of $\chi(t)$ give a good indication of the rate of convergence of the algorithm. The exact function, $\rho_{\text{exact}}(\mathbf{x})$, is known to be Z^{-1} $\exp -\beta V(\mathbf{x})$ for classical systems, and Z^{-1} $\langle\mathbf{x}|\exp -\beta H|\mathbf{x}\rangle$ for quantum systems. The latter can be determined using NMM.

III. RESULTS

The methods presented in the preceding section are tested on the following simple symmetric double well potential:

$$V(x) = \frac{(x^2 - a^2)^2}{2a^2}, \tag{3.1}$$

where units are chosen such that $\hbar = 1$ and a is a constant. The two potential minima ($V = 0$) are located at $\mathbf{x} = \mathbf{a}$ and $\mathbf{x} = -\mathbf{a}$ and the local potential maximum ($V = a^2/2$) is located at $x = 0$. The parameters are taken as $m = 1.0$, $\beta = 1.0$, and $a = 4.0$, and the step size Δx of Eq. (2.8) is adjusted to give an acceptance rate of 50%. To compare the speed of convergence of different algorithms, the time dependence of $\chi(t)$, defined in Eq. (2.10), is plotted vs the number of passes t. It suffices for our purpose to determine $\chi(t)$ over 10^5 passes.

A. Barrier crossing in classical systems

The variable step algorithm without FB or AFB ($\lambda_i = 0$) in Eq. (2.9) is first investigated. The step variation is defined in Eq. (2.8). The three curves corresponding to (a) $c = 1.0$, (b) $c = 2.0$, (c) $c = 5.0$ in Fig. 1 clearly show that the variable step method converges much more rapidly than the standard constant step MC algorithm.

The biasing algorithms, for which $\lambda_i \neq 0$ in Eq. (2.1), are next considered. In Fig. 2 we compare (a) FB with constant step size ($\lambda_i = 1$, $c = 1.0$), (b) AFB with constant step size [$\lambda_i = V''(x_i)/|V''(x_i)|$, $c = 1.0$], and (c) AFB

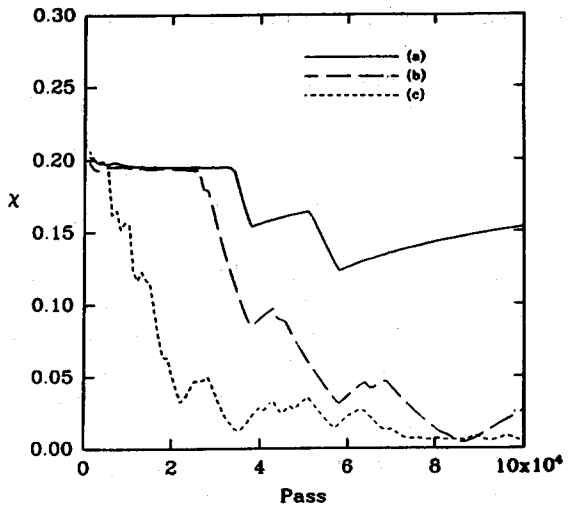

FIG. 1. A plot of χ vs the number of passes. The three curves are for the variable step Monte Carlo simulations of the classical double-well potential defined in the text. No FB or AFB is used [$\lambda_i = 0$ in Eq. (2.9)]. The step variation is determined using Eq. (2.8). The three curves correspond to (a) $c = 1$, $\Delta x = 1.5$, (b) $c = 2$, $\Delta x = 1.2$, and (c) $c = 5$, $\Delta x = 0.7$. Δx is the constant step size parameter appearing in Eq. (2.8).

with variable step size [$\lambda_i = V''(x_i)/|V''(x_i)|$, $c = 2.0$]. Because in the FB method the force tends to draw the particle towards the well minima and away from the barrier, it is expected that this method will lead to slower convergence for multiple-well potentials than does standard Monte Carlo methods. Because the AFB algorithm often pushes the particle into the barrier it corrects for this shortcoming and should accelerate the convergence in barrier crossing simulations. When AFB is combined with variable step size the convergence should be more rapid than for AFB with constant step size. These expectations are corroborated in Fig. 2.

In Figs. 3 and 4 the no-bias constant step algorithm ($\lambda_i = 0$, $c = 1.0$) and the AFB with variable step size [$\lambda_i = V''(x_i)/|V''(x_i)|$, $c = 2.0$] are presented. Each figure consists of three curves. The topmost curve shows the position as a function of the time. Each run starts in the left well ($x \sim -4.0$) and the coordinate samples this well and then jumps over the barrier, ($x = 0$) samples the right well ($x \sim +4.0$) and jumps again *ad infinitum*. The middle curve shows how the corresponding $\chi(t)$ decays with time. The bottom plate shows how the cumulative distribution builds up after (b) 1×10^4 passes, (c) 4×10^4 passes, and (d) 10^5 passes compare to the exact distribution for the potential function of Eq. (3.1) given by curve (a). Comparison of Figs. 3 and 4 clearly shows that the AFB with variable step size generates many more independent barrier crossings and much more rapid convergence than the constant step size method.

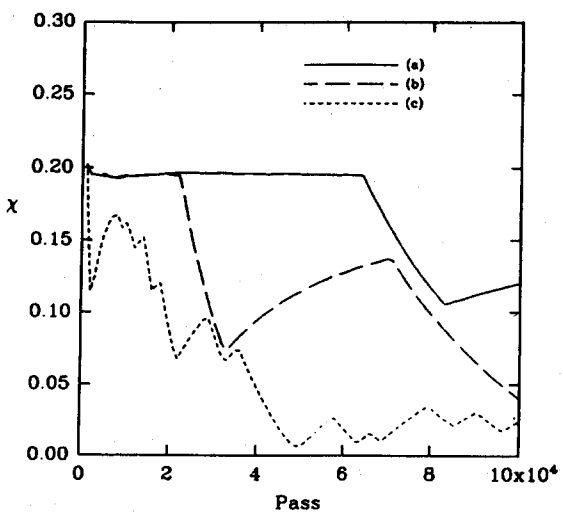

FIG. 2. A plot of χ vs the number of passes. Again, the three curves are various Monte Carlo simulations for the same classical double-well potential. The three curves correspond to (a) FB with constant step size ($\lambda_i = 1$, $c = 1$, $\Delta x = 1.5$), (b) AFB with constant step size [$\lambda_i = V''(x_i)/|V''(x_i)|$, $c = 1$, $\Delta x = 1.5$], and (c) AFB with variable step size [$\lambda_i = V''(x_i)/|V''(x_i)|$, $c = 2.0$, $\Delta x = 1.2$].

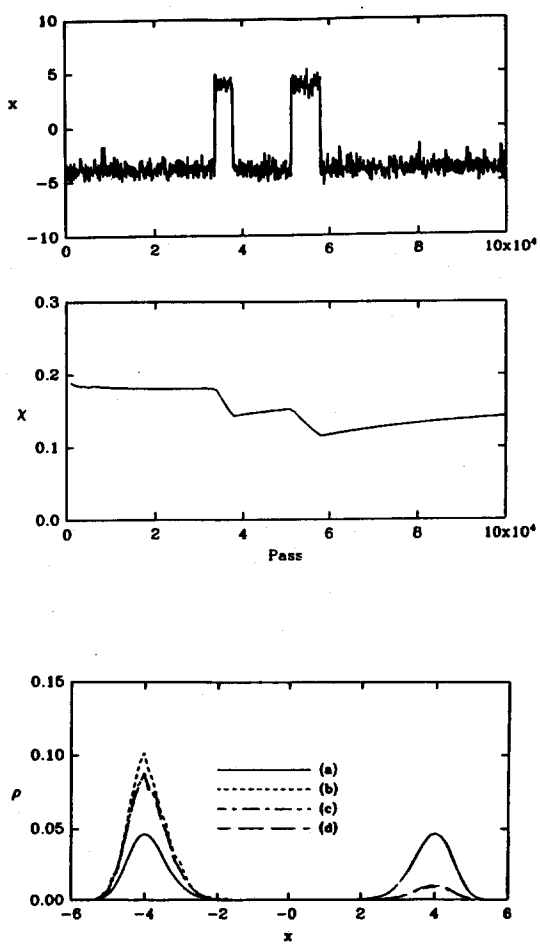

FIG. 3. This figure is a simulation of a classical activated barrier crossing using a constant step size algorithms without biasing ($\lambda_i = 0$, $c = 1$, $\Delta x = 1.5$). The top curve gives the position versus the number of passes. The middle curve gives χ vs the number of passes. The bottom plate shows how the cumulative distribution builds up after (b) 1×10^4, (c) 4×10^4, and (d) 10^5 passes. Curve (a) gives the exact distribution.

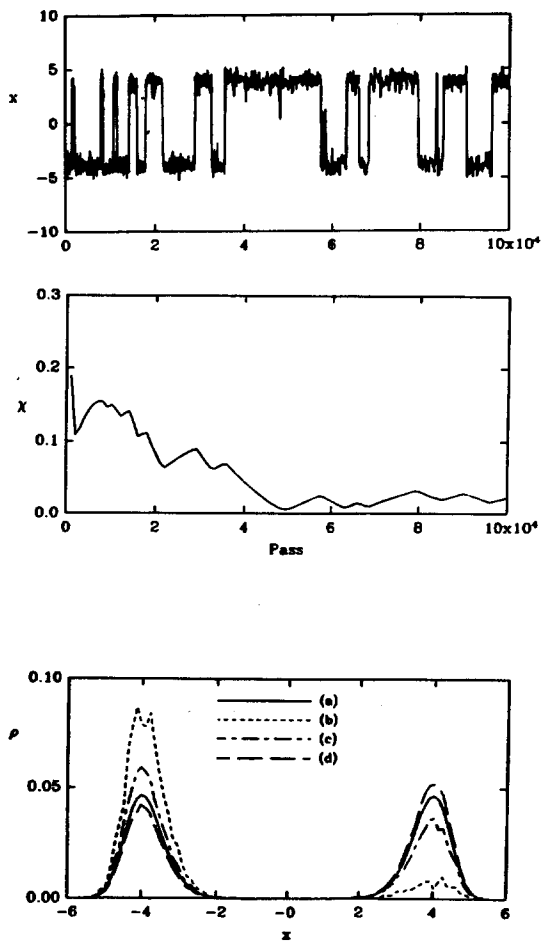

FIG. 4. This figure is the same as Fig. 3 except that a variable step size AFB algorithm is used [$\lambda_i = V''(x_i)/|V''(x_i)|$, $c = 2.0$, $\Delta x = 1.2$].

The variable step size algorithm defined by Eq. (2.8) is only one of many possible choices. An alternative function for A_i is

$$\sqrt{A_i} = \max[1, 1 + c\beta(V_i - \langle V \rangle)], \tag{3.2}$$

where $\langle V \rangle$ is the running average of the potential energy, and c is a constant which determines the linear growth rate. This form allows for a large step when the potential exceeds the average potential energy but does not give an upper bound on the step size. Although we do not present the data for this case, it is worth mentioning that it also displays rapid convergence.

B. Barrier crossing in quantum systems

It is of considerable interest to study the tunneling of a quantum particle in a multiple well potential. For simplicity we investigate the tunneling of a particle moving in the symmetric double well potential defined in Eq. (3.1). The same strategy used on the classical particle can be applied to the quantum particle using the path integral Monte Carlo method[7] where, as usual, the quantum particle is represented by a classical isomorphic chain polymer consisting of P beads, in which each bead is harmonically coupled to its nearest neighbors with force constant ($mP/2\beta^2\hbar^2$) and moves in the potential defined in Eq. (3.1) attenuated by a factor $1/P$. This isomorphic classical system is described by the potential energy function

$$V(x_1, x_2, \ldots, x_P) = V_1(x_1, x_2, \ldots x_P) + V_2(x_1, x_2, \ldots, x_P), \tag{3.3}$$

where

$$V_1(x_1, x_2, \ldots, x_P) = \left(\frac{mP}{2\beta^2\hbar^2}\right) \sum_{t=1}^{P} (x_t - x_{t+1})^2 \tag{3.4}$$

and

$$V_2(x_1, x_2, \ldots x_P) = \frac{1}{P} \sum_{t=1}^{P} V(x_t). \tag{3.5}$$

Here x_t is the position of bead t, and V_1 and V_2 spring, respectively, from the kinetic and potential energy parts of the Hamiltonian for the quantum particle. Monte Carlo methods are easily applied to the study of this problem. The standard approach is to uniformly sample a trial move for each bead which is then accepted or rejected according to the usual Metropolis algorithm. One pass consists of trial moves for all the P beads. This method involves a constant maximum step size. One of the problems with this approach is that for P sufficiently large, the chain becomes very stiff and the beads can only be moved by very small amounts. Then it will take an enormous amount of time to sample all regions of the double well potential. One way to speed up convergence is to augment the moves such that after every pass the center of mass of the chain is moved and the move is accepted or rejected by a Metropolis criterion.[8] Another approach is to transform to the normal modes[9] of the quadratic part of the potential, V_1, defined in Eq. (3.4). One of these modes corresponds to translation of the center of mass (c.m.) of the chain. The remaining modes correspond to various collective vibrations of the chain. The normal modes can be directly sampled using a Box–Mueller technique[10] such that the low frequency modes are moved through much larger displacements than the high frequency modes. This method allows for large excursions of the chain with a concommitant rapid equilibration rate.

One can apply the variable step, the FB and the AFB methods to the Monte Carlo simulation of tunneling using direct sampling of $\{x_t\}$ or normal mode sampling. These are now compared.

First we consider MC based on the primitive algorithm consisting of two kinds of moves. In the first kind, a move for each bead is sampled from Eq. (2.1) and accepted or rejected on the basis of Eq. (2.4). In the second, the average force on the c.m., $\Sigma_{t=1}^{P} F_2(x_t)/P$, is computed and a move of the c.m. of the chain is sampled from Eq. (2.1) with this force and accepted or rejected on the basis of Eq. (2.4). If the move is accepted, this displacement is added to the positions of each of the beads. Note that in the biasing algorithms it is the force corresponding to V_2, the double well part, that is used; otherwise, because the quadratic part V_1 is very stiff, it would dominate the biasing and would not accelerate barrier crossing. Figure 5 shows the results of several simulations based on this mode of sampling. Curve (a) corresponds to no-biasing with constant step size moves ($\lambda = 0$, $c = 1.0$) for both the individual bead moves and for the c.m. moves. Curve (b) corresponds to no-biasing with a constant step

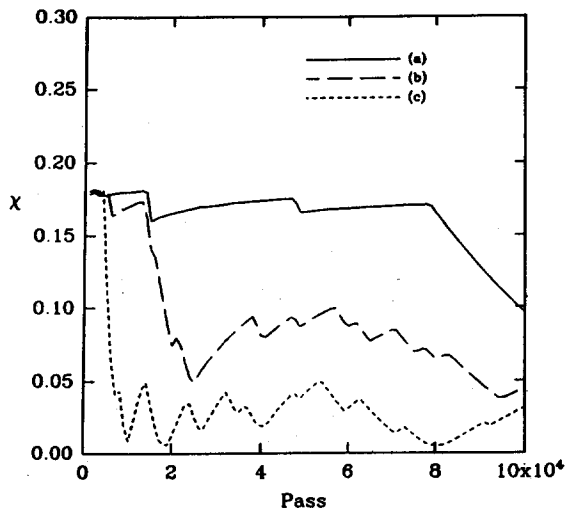

FIG. 5. χ vs the number of passes for the primitive path integral Monte Carlo simulation of a quantum particle moving in the potential defined in the text. The AFB and the variable step size methods are based only on V_2 in Eq. (3.5). And we treat individual beads and center of mass differently. The number of beads is 10. The exact normalized distribution $\rho_{\text{exact}}(x)$ in the calculation of χ is determined from NMM with $P=10$. The three curves correspond to (a) no-biasing with constant step size for individual bead moves ($\lambda_i=0, c=1.0, \Delta x=0.15$) and no-biasing with a constant step for c.m. move ($\lambda_i=0, c=1.0, \Delta x=1.5$); (b) no-biasing with a constant step size for individual bead moves ($\lambda_i=0, c=1.0, \Delta x=0.15$) and no-biasing with the variable step size for c.m. move ($\lambda_i=0, c=2.0, \Delta x=1.2$); (c) AFB with a constant step size for individual bead moves $[\lambda_i=V''(x_i)/|V''(x_i)|, c=1.0, \Delta x=0.15]$ and AFB with the variable step size for c.m. move $[\lambda_i=V''(x_i)/|V''(x_i)|, c=2.0, \Delta x=1.2]$.

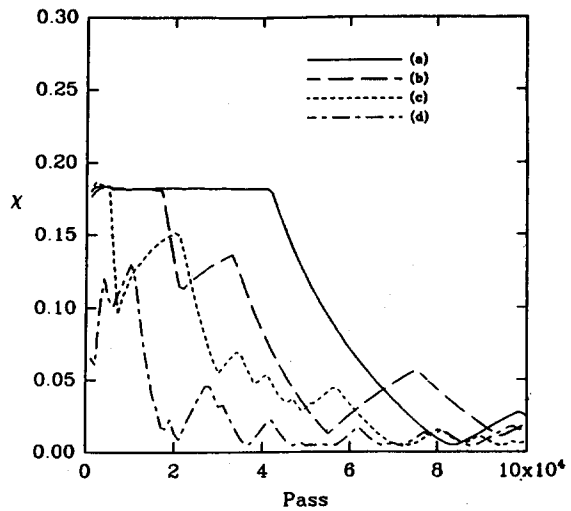

FIG. 6. χ vs the number of passes for the normal-mode path integral Monte Carlo simulation of a quantum particle moving into the potential defined in the text. The AFB and the variable step size method are used to sample the translation move of the whole chain. The number of beads is 10. The exact normalized distribution $\rho_{\text{exact}}(x)$ in the calculations of χ is determined from NMM with $P=10$. The four curves correspond to (a) no-biasing and constant step size $[\lambda_i=0, c=1.0, \Delta x=1.5]$, (b) AFB and constantstep size $[\lambda_i=V''(x_i)/|V''(x_i)|, c=1.0, \Delta x=1.5]$, (c) no-biasing and variable step size $[\lambda_i=0, c=2.0, \Delta x=1.2]$, and (d) AFB and variable step size $[\lambda_i=V''(x_i)/|V''(x_i)|, c=2.0, \Delta x=1.2]$.

size for the individual bead moves ($\lambda=0, c=1.0$), and no biasing with variable step size for the c.m. moves ($\lambda_{\text{c.m.}}=0$, $c=2.0$). Curve (c), on the other hand, corresponds to AFB with a constant step size for the individual bead moves $[\lambda_t=V_2''(x_t/|V_2''(x_t)|, c=1.0]$, and AFB with variable step size for the c.m. moves $(\lambda_{\text{c.m}}=V_2''(x_{\text{c.m}})/|V_2''(x_{\text{c.m}})|$, $c=2.0$). It is clear from this figure that the anti-force-bias technique is superior to no biasing and when combined with the variable step size method results in a very powerful method for studying tunneling phenomena.

Next we turn to normal mode techniques.[9] Here the real coordinates of the beads $\{x_t\}$ are tranformed to

$$x_t = x_0 + \left[\frac{2}{P}\right]^{1/2} \sum_k \sin(\pi k t/P) Q_k. \tag{3.6}$$

After tranformation to normal modes Eq. (3.1) is becomes

$$V_1 = \left(\frac{mP}{2\beta^2\hbar^2}\right) \sum_k \left\{2\left[1-\cos\left(\frac{\pi k}{P}\right)\right]\right\} Q_k^2 \tag{3.7}$$

and

$$V_2 = \frac{1}{P}\sum_{t=1}^{P} V(x_t(\{Q_k\})). \tag{3.8}$$

New steps are generated by Box–Mueller sampling of Q_k from the Gaussian distribution, $\exp[-\beta V_1]$, where V_1 is defined in Eq. (3.7). The c.m. position x_0 is sampled using biasing and constant and variable step moves as before. Figure 6 gives a summary of results using the normal mode tranformation. Here the force on the c.m. coordinate, $\Sigma_{t=1}^{P} F_2(x_t)/P$, is computed and a move of the c.m. of the chain is sampled from Eq. (2.1) with this force and accepted or rejected on the basis of Eq. (2.4). If the move is accepted this displacement is added to the positions of each of the beads. Curve (a) corresponds to no biasing and constant step size ($\lambda=0, c=1.0$), curve (b) corresponds to AFB and constant step size $(\lambda_{\text{c.m.}}=V_2''(x_{\text{c.m}})/|V_2''(x_{\text{c.m}})|$, $c=1.0$), curve (c) corresponds to no biasing and variable step size ($\lambda=0, c=2.0$), and curve (d) corresponds to AFB and variable step size $(\lambda_{\text{c.m.}}=V_2''(x_{\text{c.m}})/|V_2''(x_{\text{c.m}})|$, $c=2.0$). Once again we see that AFB with variable step size is more rapidly convergent, but here the no-biasing algorithm with variable step size is not bad.

IV. CONCLUSION

The aim of this paper is to present a simple method for accelerating the sampling of potential wells separated by large barriers. Standard MC or MD methods converge so slowly that they are impractical. Of course it is a simple matter to use umbrella sampling technique when the dealing with a simple analytical form of the multiple well potential function; however, in most problems of interest the wells and barriers result from the superposition of two-body potential functions and a simple analytic form is not available. If this is the case the reference potential used in the umbrella sampling is an almost uniform potential. In that case the same

time is spent sampling the improbable regions as the probable regions which is wasteful. Moreover, we have found that umbrella sampling when applied to the determination of the potential of mean force for the dihedral angle of butane dissolved in Lennard-Jonesium, and the ST2 water gives extremely slow convergence.[11] The methods outlined in this paper can be applied to these many-body problems, for which umbrella sampling techniques are not adequate.

Variable step sampling has been tried before on classical simulations of Lennard-Jonesium, albeit with a different sampling function, where it did not accelerate the sampling of the Boltzmann distribution function.[12] Because of this problem it has not been used much in the literature. Here we have shown that variable step methods are quite useful for simulations involving barrier crossing, because the steps made are large enough to allow the new position to be on the other side of the barrier with an acceptable potential energy change. It is very likely that other algorithms for the variable step size would give even better results than ours.

Force-bias methods have been used before with considerable success, especially on aqueous systems.[2-5] These methods are very simple and rapidly convergent. It is even possible to go beyond force-bias and to include biasing using the second derivatives of the potential energy function. We show here that the FB method tends to move the particle towards the minimum of the well it starts from and therefore does not lead to rapid barrier crossings. In unpublished work of 10 years ago, we also found that the higher order biasing algorithms using V'' do not do any better. In fact, the usual constant step MC method often leads to faster convergence than do these biasing techniques.

In this paper we proposed an anti-force-bias technique that biases the move to be in a direction antiparallel to the instantaneous force, whenever the sign of V'' is negative. This method generates moves into the barrier region and leads to a much larger number of uncorrelated barrier crossings than the standard and FB methods produce. When a variable step size is used in conjunction with this AFB method, it achieves rapid convergence in double well and multiple well problems.

Path integral MC methods for studying localization phenomena often involve bottlenecks arising from the slow time scale connected with barrier crossings. The methods described here are quite useful in accelerating convergence of such problems. We have chosen to study only the simplest algorithm such as primitive and normal mode sampling. There are, of course, other methods. For example, following Barker's lead,[13] Ceperley and Pollack[14] have shown that staging with drift terms gives a rapidly convergent method for studying many-body problems such as the properties of quantum liquids. Sprik *et al.* have devised a different kind of staging algorithm. Do these methods accelerate barrier crossing? We have applied the Ceperley staging algorithm to the systems studied in this paper and find that it performs as badly as the constant step MC. The Sprik staging method,[15] although not studied here, should perform even worse.

We conclude that the AFB technique with variable step size leads to a significant acceleration of equilibration in multiple well problems. In the future we plan to apply this method to many-body problems involving large energy barriers. Clearly the search for improved methods should not stop here.

ACKNOWLEDGMENT

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