Stochastic calculation of tunneling in systems with many degrees of freedom

C. Alexandrou* and J. W. Negele
Center for Theoretical Physics, Laboratory for Nuclear Science, and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
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A new method is presented for the stochastic solution of tunneling problems in quantum many-body systems. The primary practical problem of trapping in local minima of the action is overcome by extending the standard implementation of the Metropolis algorithm to include collective updates motivated by semiclassical instanton solutions. We demonstrate the accuracy of our method in the case of tunneling in one degree of freedom and apply it to a model many-fermion system in one spatial dimension which undergoes spontaneous symmetric fission.

I. INTRODUCTION

Tunneling phenomena in quantum many-particle systems pose a challenging problem in the microscopic theory of collective motion. This present work is motivated by phenomena in nuclear physics such as spontaneous and induced fission, sub-barrier heavy ion reactions, and exotic radioactivity. Analogous problems, for which the ideas developed here are equally applicable, also arise in many other disciplines including tunneling in solid state devices, the contribution of cyclic permutations to the ground state energy of solid ^{3}He, systems with multiply degenerate vacua in field theory, and a rich variety of molecular and biological systems.

Traditional approximations are of limited value in obtaining a quantitative understanding of the nature of the collective path, the coupling of collective variables to other degrees of freedom, and the physics of preformation factors. One common approach, which is difficult to make systematic, is reduction to an effective one-body problem with an effective mass and collective potential. Such a reduction necessarily involves some prescription for the collective variable, and ultimately includes some average effects of other degrees of freedom without direct coupling to them.

Path integrals provide a natural and convenient framework for addressing tunneling in systems with many degrees of freedom. A great deal of physical insight into this tunneling may be obtained by application of the stationary phase approximation to an appropriately formulated path integral. The basic idea developed by Langer,[1] Polyakov[2] and Coleman[3] is to find the appropriate stationary path, referred to as a "bubble," "instanton," or "bounce," which connects the two relevant classically allowed regimes. In the case of the eigenvalues for a particle in a one-dimensional symmetric double well, evaluation of the Fourier transform of the trace of the evolution operator $\int dT\, e^{iET} \mathrm{tr} e^{-iHT}$ yields stationary solutions in the classically forbidden region in which the time parameter in the equation of motion is purely imaginary. Since the equation is second order in time, the solution corresponds to the classical periodic motion in the inverted potential. In the case of nuclear fission, the stationary-phase approximation may be applied to a functional integral over an auxiliary field or an overcomplete set of Slater determinants to obtain analogous mean-field solutions in an inverted well.[4] Although this mean-field theory yields physical insight and may provide a useful approximation, it is subject to significant conceptual and practical limitations. In the case of nuclear physics, there is no explicit small parameter, so the stationary-phase approximation is uncontrolled. Furthermore, since no two-body correlations are included in the theory, the bare two-body interaction must be replaced by an effective interaction. Although it is practical to solve the self-consistent periodic time-dependent mean field equations, evaluation of the determinant appearing in the pre-multiplying factor is, in general, impractical, and terms beyond the quadratic corrections are completely hopeless.

As an alternative to these approximations, this work explores the use of stochastic methods to evaluate path integrals for tunneling problems. The basic approach will be to express tunneling observables in terms of an appropriate path integral, which is then evaluated exactly with the Monte Carlo method, subject only to statistical sampling errors which can be made as small as desired. However, the Monte Carlo method for evaluating an integral has two distinct limitations which must be avoided. The first is that the integrand must be dominantly positive. Otherwise, if the integrals of the positive and negative regions are separately much larger in magnitude than their sum, then the stochastic noise will hide the signal for all practical numbers of samples. The second is that we must assure that the probability distribution is sampled independently over its complete domain. Although there are general theorems governing the convergence of Markov processes and other methods used to sample distributions, there is generally little or no control over the rate of convergence. In particular, the possibility of becoming trapped in some region which is not representative of the entire space is a crucial concern for tunneling problems. In the present application to tunneling, it turns out to be crucial to exploit the freedom in formulat-

ing the path integral and stochastic method so as to utilize physical insight to overcome these limitations.

This work specifically addresses the fission lifetime of a model nucleus, and is organized as follows. Section II treats the problem of expressing the lifetime in terms of observables which can be evaluated with Euclidean path integrals. For the high barriers of interest in nuclear physics, it is shown that the lifetime can be related to the splitting of the two lowest energy levels of an appropriately defined double well, constructed by defining a hard wall boundary condition in a collective variable in the outer asymptotic regime. The problem is thereby reduced to the general problem of calculating energy splittings between low lying states in systems with degenerate, or nearly degenerate, vacua. Section III develops and quantitatively tests the essential ideas for the calculations of the energy splitting and lifetime in the special case of a single degree of freedom. It is shown that for high barriers, the paths generated by sampling the Feynman path integral with standard sequential updates become trapped in a single well and fail to generate the multiple instanton configurations required to describe tunneling. The relevant configurations are included in the calculation by generalizing the algorithm to offer correlated updates corresponding to semiclassical instanton solutions. It is also shown that the Euclidean correlation function normally used to calculate excitation energies is ineffective for measuring the energy splitting for high barriers, and that a new observable measuring matrix elements between the left and right wells is the appropriate quantity to efficiently measure the contribution of instanton configurations to the energy splitting. These ideas are generalized to the many-body problem in Sec. IV, where, because of the minus signs arising from antisymmetry for fermions in more than one dimension, we solve a model nuclear system in one spatial dimension. Section V summarizes our principal results and conclusions.

II. RELATION OF THE LIFETIME TO THE ENERGY SPLITTING

The objective of this section is to relate the lifetime Γ of a metastable state to an energy splitting for an appropriately defined double well which can be calculated by averaging over Euclidean paths. The basic ideas are demonstrated by considering the one-dimensional barrier sketched at the top of Fig. 1. The lowest eigenstate of $V(x)$ has a node at $x=a$ and energy E. This corresponds to a scattering solution of energy $E(a)$ with a node at $x=a$ in the absence of the hard wall. Since E specifies the momentum k and a specifies the phase shift δ, calculating the energy $E^{(1)}(a)$ of the lowest eigenfunction as a function of the wall position a, in principle, specifies $\delta(k)$ and thus the lifetime through the familiar expression for a Breit-Wigner resonance

$$\delta(k)=\delta_0+kb+\tan^{-1}\frac{\gamma}{k_0-k}\ , \tag{2.1}$$

where $\gamma=m\Gamma/2k_0$. Since this expression for $\delta(k)$ assumes a narrow resonance, the definition of the lifetime γ is only meaningful to order (γ/k_0), and we shall thus work to leading order in (γ/k_0). The constant b in (2.1) corresponds approximately to the distance from the origin to the barrier.

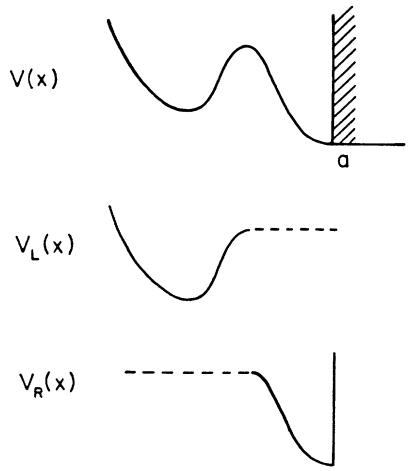

FIG. 1. Potential $V(x)$ for a metastable state in one dimension, and its decomposition into inner and outer wells, $V_L(x)$ and $V_R(x)$.

For the high barriers of interest in this work, it is impractical to calculate γ directly from $\delta(k)$, so it is preferable to relate γ to the energy splitting between two degenerate states. The equation for the bound states of $V(x)$ with the wall at $x=a$ is given by

$$\delta(k)=n\pi-ka,\quad n=1,2,\ldots\ . \tag{2.2}$$

Solution of (2.2) for the two lowest states k_1 and k_2 in the limit $\gamma\ll|k_0-k_1|$ and $\gamma\ll|k_0-k_2|$, which is justified *a posteriori,* yields

$$k_1-k_2=\left[\left[k_0+\frac{\pi-\delta_0}{a+b}\right]-4\frac{k_0(\pi-\delta_0)-\gamma}{a+b}\right]^{1/2} \tag{2.3a}$$

and

$$k_1+k_2=k_0+\frac{\pi-\delta_0}{a+b}\ . \tag{2.3b}$$

Minimizing $(k_1-k_2)^2$ with respect to a and keeping the leading order terms in γ/k_0, we obtain

$$\gamma=\left[\frac{a+b}{8}\right]\left[\frac{m}{E_0}\right](E_2-E_1)^2\left[1+\mathcal{O}\left[\frac{\gamma}{k_0}\right]\right]\Bigg|_{a=a_m}\ , \tag{2.4}$$

where $E_0=k_0^2/2m$ and $(E_2-E_1)|_{a_m}$ is the minimum energy splitting which occurs for a_m satisfying $(\partial/\partial a)(k_1-k_2)^2|_{a_m}=0$. Here we note that for $a=a_m$ the approximation

$$\tan^{-1}\frac{\gamma}{k-k_0}\Bigg|_{a_m}\sim\frac{\gamma}{k-k_0}\Bigg|_{a_m}$$

is consistent to the order we are working.

We now show that this minimum energy splitting occurs for a special condition on the inner and outer wells. We decompose $V(x)$ into inner and outer wells $V_L(x)$ and $V_R(x)$, respectively, as shown in the lower part of Fig. 1. For $V_R(x)$ the phase shift δ_R is given by

$$\delta_R(k_R)=\delta_0+bk_R \ , \tag{2.5}$$

where δ_0 and b are the same constants that appear in (2.1). For the ground state, k_R is given by

$$k_R=\frac{\pi-\delta_0}{a+b} \ . \tag{2.6}$$

Comparing (2.6) and (2.3a) we obtain

$$k_R \mid_{a_m}=k_0+\mathcal{O}\left[\frac{\gamma}{k_0}\right] \ . \tag{2.7}$$

Combining this result with the fact[4,5] that for the ground states of V_L,

$$k_L=k_0+\mathcal{O}\left[\frac{\gamma}{k_0}\right] \ , \tag{2.8}$$

we obtain the familiar result that resonances occur to leading order at energies corresponding to the energy levels of the inner well. Therefore we conclude that the minimum energy splitting, $(E_2-E_1)\mid_{a_m}$ to order (γ/k_0) occurs when the inner and outer wells are degenerate. The coefficient a_m+b can be obtained by differentiating (2.7) with respect to a, and (2.4) becomes

$$\gamma=\left[-\frac{m}{4\left[\frac{dE_R}{da}\right]}(E_2-E_1)^2\right]\Bigg|_{E_L=E_R}\left[1+\mathcal{O}\left[\frac{\gamma}{k_0}\right]\right] \ . \tag{2.9}$$

Note that this result has the form expected from the Fermi golden rule of a transition matrix element squared (since $\Delta E\sim\langle\phi_L\mid\Delta v\mid\phi_R\rangle$) times a density of states [related to $(dE/da)^{-1}$]. Therefore, the task of calculating the lifetime is reduced to that of calculating the energy splitting for an appropriately constructed double well. An independent confirmation of the same result is obtained using the Kohn variational principle.[5]

This result is straightforwardly generalized to the lifetime of a fissile nucleus. The solution in the inner well is the metastable ground state of the parent nucleus and the solution in the outer well corresponds to the metastable state of the two daughter nuclei in the vicinity of the scission point with a hard wall boundary condition on the relative coordinate. Since the derivation used the asymptotic behavior of the wave function, the mass which enters into the lifetime is the reduced mass of the two fission fragments. The only physical assumption is that the interaction between the fragments is negligible at the exterior wall. This implies that the fragments are in their ground states and there is no potential acting on the relative coordinate. While the derivation could be extended to take into account a residual interaction between the fragments, it is not obvious how to generalize it to take into account excitation of the fragments. We have also tacitly assumed that there is no coupling between decay channels, and therefore do not address the case in which the system can tunnel from one decay channel to another.

III. STOCHASTIC CALCULATION OF TUNNELING WITH ONE DEGREE OF FREEDOM

The essential difficulties encountered in stochastic calculation of tunneling for systems with degenerate vacua separated by barriers, as well as their remedies, may be illustrated for the case of the symmetric quartic double well

$$\left[\frac{-1}{2m}\frac{d^2}{dx^2}+(x^2-1)^2\right]\psi(x)=E\psi(x) \ . \tag{3.1}$$

The x coordinate has been scaled so that the minima occur at $x=\pm1$, and the energy such that the barrier height is 1, so the mass m is the only free parameter. High values of m characterize impenetrable barriers. For $m=4$, the exact ground state energy is $E_1=0.57$ as compared to 0.71 using the harmonic approximation about $x=\pm1$, and the energy splitting is $\Delta E=0.116$, which is of the same order as E_1. Such a barrier is much more penetrable than those of interest in fission, and tunneling is appreciable. For $m=12$ the exact energy $E_1=0.38$ is comparable to the harmonic approximation 0.41 and the energy splitting is 7×10^{-3}. Therefore, $m=12$ corresponds to highly impenetrable barriers characteristic of nuclear phenomena.

Quantum tunneling is governed to leading order in a semiclassical expansion by the zero energy instanton solutions to the classical equation of motion in Euclidean time. The trajectory as a function of imaginary time τ for the quartic well is $x(\tau)=\tanh\gamma\tau$ with $\gamma=\sqrt{2/m}$ leading to an approximate splitting $\Delta E=2\mathcal{K}e^{-S_0}$ where $S_0=\frac{4}{3}\sqrt{2m}$ and $\mathcal{K}=8(2/m)^{1/4}/\sqrt{\pi}$. In the dilute instanton approximation[3] the probability of having n instantons is

$$p(n)=\frac{1}{n!}\frac{(\beta K)^n e^{-nS_0}}{\mathcal{N}} \ ,$$

where β is the time interval and $\mathcal{N}$ is an appropriately defined norm. There are two principal options for evaluating the Feynman path integral

$$\langle x_N \mid e^{-\beta H} \mid x_0 \rangle = \int dx_{N-1} \cdots dx_1 \prod_{i=1}^{N} \exp\left[-\frac{m(x_i - x_{i-1})^2}{2\epsilon} - \frac{V(x_i)+V(x_{i-1})}{2}\epsilon \right] . \tag{3.2}$$

One possibility, which we pursue in this work, is to use the algorithm of Metropolis *et al.*[6] for sampling the action and to use the resulting trajectories to evaluate $\mathrm{Tr} e^{-\beta H}\mathcal{O}(\tau)\mathcal{O}(0)$ or $\langle \phi_L \mid e^{-\beta H} \mid \phi_R \rangle$. Alternatively, trajectories may be generated by evolution of an initial value diffusion equation and used to calculate $\langle \phi_L \mid e^{-\beta H} \mid \phi_R \rangle$ as discussed in Refs. 5–8. In either case, the algorithm must allow one to study the limit $\epsilon \to 0$ to reliably evaluate observables. A quantitative indication of the range of ϵ which must be studied is provided by the analytic solution of the harmonic oscillator, which has the original frequency ω replaced by an effective frequency ω_ϵ defined

$$\omega_\epsilon^2 \equiv \omega^2 \left[1 + \left[\frac{\epsilon\omega}{2} \right]^2 \right] .$$

Hence, at the very least, one must be able to study $\epsilon \ll 2/\omega \sim \sqrt{m/2}$ in the present model.

A. Collective updates in the Metropolis algorithm

In the Metropolis algorithm, the probability distribution,

$$P(x_1, \ldots, x_N) \equiv P(\mathbf{x}) = \frac{e^{-S(\mathbf{x})}}{\int \prod_i dx_i e^{-S(\mathbf{x})}} , \tag{3.3}$$

where

$$S(x_1, \ldots, x_N) = \frac{\epsilon}{2} \sum_n \left[(x_n - x_{n-1})^2 \frac{m}{\epsilon^2} + [V(x_n) + V(x_{n-1})] \right]$$

is sampled by a Markov process. The transition probability for each step in the Markov chain may be written

$$W(\mathbf{x};\mathbf{x}') = p(\mathbf{x};\mathbf{x}')[\theta(-\Delta S) + \theta(\Delta S) e^{-\Delta S}] + \prod_i \delta(x_i - x_i') \int \left[\prod_i dx_i'' \right] p(\mathbf{x};\mathbf{x}'') \theta(\Delta S) \times (1 - e^{-\Delta S}) , \tag{3.4a}$$

where

$$\Delta S = S(\mathbf{x}') - S(\mathbf{x}) \tag{3.4b}$$

and the probability p is symmetric,

$$p(\mathbf{x};\mathbf{x}') = p(\mathbf{x}';\mathbf{x}) . \tag{3.4c}$$

This transition probability satisfies the microreversibility condition $e^{-S(\mathbf{x})} W(\mathbf{x};\mathbf{x}') = e^{-S(\mathbf{x}')} W(\mathbf{x}';\mathbf{x})$ and if $p(\mathbf{x},\mathbf{x}')$ accesses all states of the system, the Markov process samples $P(\mathbf{x})$. In practice, given a configuration $\{\mathbf{x}\}$, a tentative configuration $\{\mathbf{x}'\}$ is first generated randomly according to the chosen probability density $p(\mathbf{x};\mathbf{x}')$; if $\Delta S < 0$, then $\{\mathbf{x}'\}$ is accepted as the new configuration. If $\Delta S > 0$, then either $\{\mathbf{x}'\}$ is accepted as the new configuration with probability $e^{-\Delta S}$ or otherwise the new configuration is defined to be the original configuration $\{\mathbf{x}\}$.

The Metropolis method is normally implemented by sequential updates of individual coordinates, that is, by taking $W(x_1, \ldots, x_N; x_1', \ldots, x_N')$ to be a convolution of single step transition probabilities:

$$W = W^1 \circ W^2 \circ \cdots W^{N-1} \circ W^N ,$$

$$W \circ W' \equiv \int \left[\prod_{i=1}^{N} dx_i'' \right] W(\mathbf{x};\mathbf{x}'') W'(\mathbf{x}'';\mathbf{x}') , \tag{3.5a}$$

where W^i is given by (3.4a) with

$$p^i(\mathbf{x};\mathbf{x}') = p(x_i;x_i') \prod_{j \neq i} \delta(x_j' - x_j) . \tag{3.5b}$$

A common choice for $p(x_i;x_i')$ is a uniform distribution

$$p(x_i;x_i') = \frac{\theta(x_i - x_i' + \xi) - \theta(x_i - x_i' - \xi)}{2\xi} ,$$

with the width ξ selected such that on the average approximately half of the trial configurations are accepted.

Now consider how an instanton can be created from a configuration where all $\{x_i\}$ begin in one well. Since we change one site x_i at a time, a section of the trajectory must be dragged over the barrier and into the other minimum. An extreme case which is easy to analyze is to switch one x_i from one well to the other. The change in the action for this single move is $4m/\epsilon$. Once x has crossed the barrier, there is no additional cost for each sequential variable to cross and therefore the probability that an instanton is created in this way is $\sim(\beta/\epsilon)e^{-4m/\epsilon}$ compared to the physical probability $p^{(1)}/p^{(0)} = K\beta e^{-4\sqrt{2m}/3}$. For extremely large values of the time step, $\epsilon \gtrsim \sqrt{m}$, there is no problem and the standard sequential update is able to create the correct number of instantons. This is the case, for example, in Ref. 9 where $m = 4$ and $\epsilon = 4$ were used. However, for $\epsilon \ll \sqrt{m/2}$, as required to approach the continuum limit for this problem, the formation of instantons in a single step is exponentially inhibited. A particularly clear indication of the problem is the result of using sequential updates to calculate the Euclidean time correlation function,

$$C(\tau) = \frac{\mathrm{Tr}\left[T\mathcal{O}(\tau)\mathcal{O}(0) \exp\left[-\int_0^\beta d\tau H \right] \right]}{\mathrm{Tr}\left[T \exp\left[-\int_0^\beta d\tau H \right] \right]} = \frac{\sum_{\alpha\gamma} e^{-E_\alpha(\beta-\tau)} e^{-E_\gamma \tau} \mid \langle \alpha \mid \mathcal{O} \mid \gamma \rangle \mid^2}{\sum_\alpha e^{-\beta E_\alpha}} , \tag{3.6a}$$

where T denotes ordering in imaginary time. For the special case of a symmetric double well, with $\mathcal{O}=x$,

$$C(\tau) \underset{\tau(E_2-E_0)\gg 1}{\rightarrow} \frac{|\langle 0|x|1\rangle|^2 e^{-\tau\Delta E}(1+e^{-(\beta-2\tau)\Delta E})}{(1+e^{-\beta\Delta E})}$$

$$\underset{\substack{\tau(E_2-E_0)\gg 1 \\ \beta\Delta E\gg 1}}{\rightarrow} |\langle 0|x|1\rangle|^2 e^{-\tau\Delta E}, \tag{3.6b}$$

and thus should decay exponentially at large τ with a slope given by the energy splitting. As seen in Fig. 2(a), the lack of instanton configurations in the Monte Carlo calculation with only sequential updates gives totally incorrect behavior. It is important to note that this problem is not unique to the Metropolis algorithm. It will occur with any microreversible method implemented using sequential updates.

Within a sector of specific instanton number, sequential updating efficiently sums fluctuations around the classical path, even when higher than quadratic terms are important. Typical results are shown in Fig. 3. Note particularly that although the average behavior of the trajectories closely follows the instanton in the classically forbidden region, the average is displaced away from the minima in the rest of the space reflecting significant contributions of anharmonic terms. Thus, we conclude that sequential updates are good at summing local fluctuations around stationary paths, but may fail in producing the global changes required to sample all sectors of the trajectory space.

Once the essential problem with sequential updates has been recognized, it is possible to introduce several generalizations to include instanton physics. One alternative for the symmetric function $p(\mathbf{x};\mathbf{x}')$ is to define the following correlated additive trial move for the entire trajectory

$$p(\mathbf{x};\mathbf{x}')=\prod_i \delta(x_i'-x_i-\sigma f_i), \quad \sigma=\pm 1 . \tag{3.7}$$

Here, f_i is some global change defined on all the time slices and σ is a random variable with value ± 1. In order to make the move reversible, f must be randomly added and subtracted, with the disadvantage that half the moves are thereby sure to be rejected. A physical choice for f in calculating the trace in a double well is the two instanton configuration sketched in Fig. 4, $f_i=\tanh\gamma(\tau_i-\tau_s)+\tanh\gamma(\tau_l-\tau_i)$. The cost in action for such a global change is distributed around the classical result as shown in Fig. 5, thus assuring that the equilibrium distribution of instantons is built up. Note that if the positions t_s and t_l are also picked randomly, subsequent updates will change the instanton number by ± 2

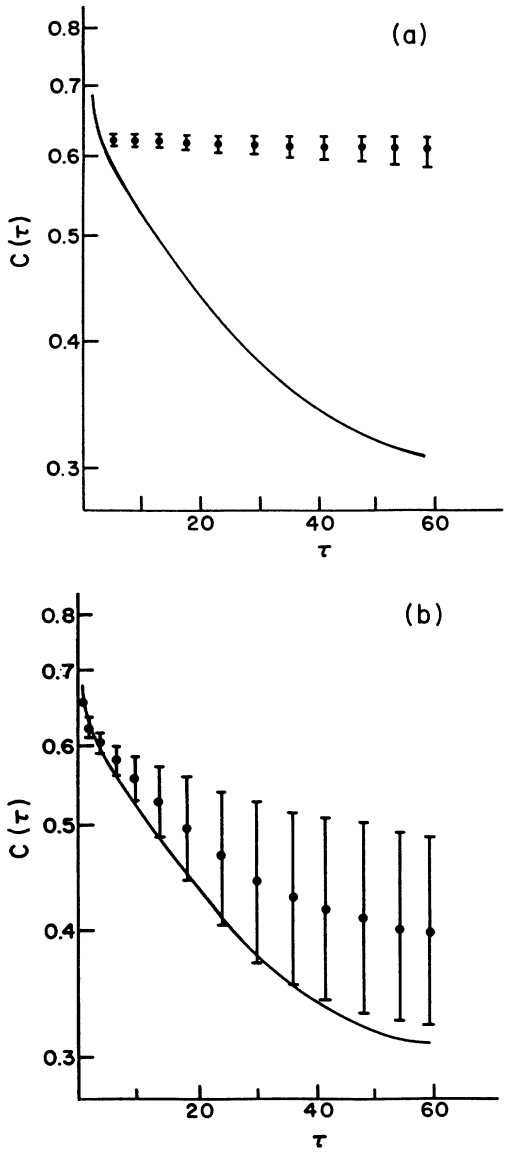

FIG. 2. The time dependence of the Euclidean correlation function $\langle x(0)x(t)\rangle$ for the one-dimensional quartic double well for $m=12$ and $\epsilon=0.6$. The solid curve denotes the exact result and the error bars show the result of a Monte Carlo calculation with 10^6 events. In part (a) only sequential updates are used, whereas collective instanton updates are included in addition to the sequential updates in part (b).

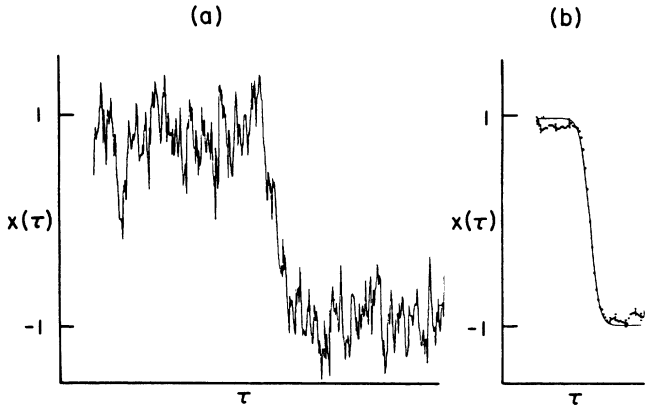

FIG. 3. Trajectories in the one-instanton sector for the quartic double well with $m=12$ and $\epsilon=0.6$. Panel (a) shows a typical trajectory containing one instanton. Panel (b) compares the average over many such trajectories in the frame of the instanton (open circles), with the classical instanton (solid curve).

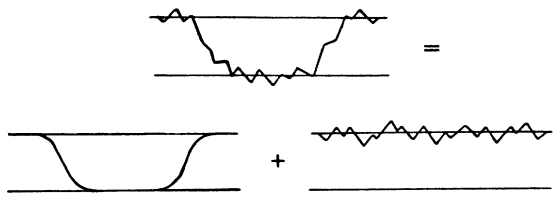

FIG. 4. The effect of adding a two-instanton trial move to a trajectory localized in a single well.

and distribute the instantons randomly.

A second option for $p(\mathbf{x};\mathbf{x}')$ is scaling of the variables by some arbitrary function α_i of the sites, so that the proposed new values are $x_i'=x_i[\alpha(i)]^\nu$ with ν a random variable. For our purpose we need only consider ν with values ± 1. For this case,

$$p(\mathbf{x};\mathbf{x}')=\frac{1}{1+\prod_{i=1}^{N}|\alpha_i|}\left[\prod_{i=1}^{N}\delta\left[x_i'-\frac{x_i}{\alpha_i}\right]+\prod_{i=1}^{N}|\alpha_i|\,\delta(x_i'-\alpha_i x_i)\right], \tag{3.8}$$

where the weight factors are required for symmetry. Intuitively, the reason for these weights is clear; $p(\mathbf{x};\mathbf{x}')$ must sample points $x_i=x_i+\delta_i$ and $x_i=x_i-\delta_i$ with equal probabilities. For scaling this means that the intervals $[x_i,x_i(\alpha_i)]$ and $[x_i,x_i/\alpha_i]$ must be sampled with probabilities proportional to the ratio of their volumes which is what the factor $|\alpha_i|$ represents. A simple choice for $p(\mathbf{x};\mathbf{x}')$ which takes one configuration from one well to the other is $\alpha_i=-1$, for all i. Such a global change will not affect the number of instantons but it will help ensure the correct value for $\langle x\rangle$ which stochastically can be non-zero even for low barriers, such as $m=4$, $\epsilon=0.56$. By changing the sign for only part of the configuration, one can create instantons. For high barriers one must interpolate with a smooth function across the barrier. This prescription is computationally faster since S is invariant under sign change and therefore ΔS only needs to be calculated for a few time steps.

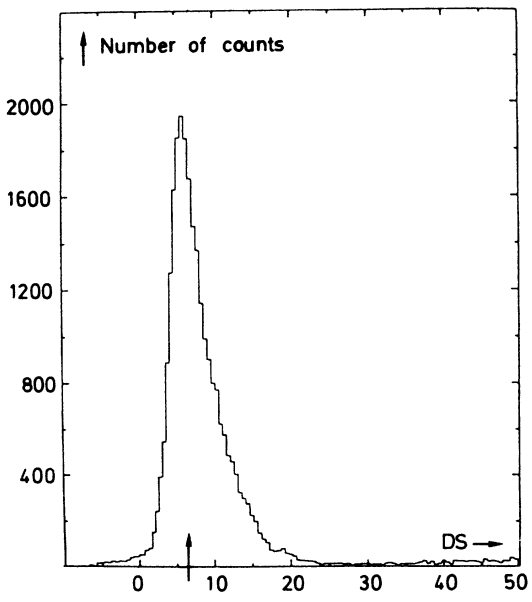

FIG. 5. The distribution of the change in action, ΔS, for the collective instanton updates. The value of the classical action, $S_0=\frac{4}{3}\sqrt{2m}$ for one instanton is indicated by the arrow.

Several comments concerning collective updates are appropriate. Note that each one of the collective changes described cannot by itself satisfy egodicity; to access all possible states of the system we must combine them with other moves, for example, sequential updates, so that a total of N independent changes are offered. Furthermore, one is always free to combine arbitrary sequences of updates, since each step is separately microreversible. Finally, in contrast to guided random walks[7,8] in which an unphysical trial function can introduce systematic bias, unphysical updates never introduce bias. At worst, they can only be rejected and not influence the outcome.

Finally, in addition to the introduction of collective moves, one always has the option of using importance sampling. We define a function $N(\mathbf{x})$ which counts the number of instantons in a configuration and write the tautology

$$\int d\mathbf{x}\,\mathcal{O}(\mathbf{x})e^{-S(\mathbf{x})}=\int d\mathbf{x}[\mathcal{O}(\mathbf{x})e^{-\eta N(\mathbf{x})}]e^{-[S(\mathbf{x})-\eta N(\mathbf{x})]}. \tag{3.9}$$

By adjusting η, one can make the acceptance of instantons in the Metropolis updates arbitrarily desirable and thus control the average number of instantons. Although the extraneous factor is exactly divided out in evaluating observables, if the quantity of interest is dominated by multi-instanton configuration, the technique lives up to its name by preferentially sampling the space in the "important" regime. Note also that the definition of an instanton does not need to be absolutely precise: As long as $N(\mathbf{x})$ counts configurations in the desired sector, it will introduce configurations in this sector which subsequently properly equilibrate.

The effectiveness of sequential updates of the form (3.7) is demonstrated in Fig. 2 where Monte Carlo calculations of the time correlation functions are shown for the case of a high barrier, $m=12$. The time correlation function $C(\tau)$ involves delicate cancellations and thus poses a stringent test. The essential result is that although the calculation with sequential updates appears to have converged with small error bars, it yields totally erroneous results because the trajectories are trapped in a single well. In contrast, the collective updates yield the correct qualitative behavior, and produce realistic error bars reflecting the true sensitivity of the calculation.

Another application in which collective updates are useful is in the global equilibration of a ground state solution, which becomes particularly important for systems with many degrees of freedom. The essential idea can be

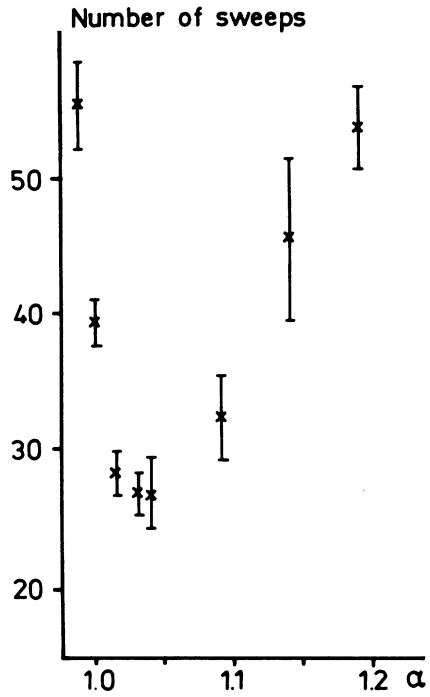

FIG. 6. Number of sweeps for equilibration as a function of the scaling parameter α, for the harmonic oscillator potential $2x^2$ and for $m=1$. The initial configuration was distributed about $x \sim 6.5$.

illustrated for a single particle in the harmonic oscillator potential $(\omega/2)x^2$, with $\omega=4$ and $m=1$, where the initial configuration is systematically chosen to have x_i too large. Since the kinetic term in the action will inhibit sequential updates from allowing large decreases of x_i relative to $x_{i\pm1}$, a large number of sweeps will be required to reduce all the x_i's to the appropriate equilibrium distribution. If, in addition to the sequential updates we also offer global scaling of all $\{x\}$ using (3.8) with $\alpha_i=\alpha$, the spatial extent of the solution can equilibrate rapidly. The energy converges to its equilibration value approximately exponentially with the number of sweeps and we may therefore define an average equilibration time to be the number of sweeps at which the energy falls to $1/e$ of its initial value. This equilibration time as a function of α is shown in Fig. 6, from which we observe that equilibrium can be reached twice as fast by choosing an optimum value for the scaling parameter α. This optimum value occurs when the acceptance ratio for these moves is about $\frac{1}{2}$. Once equilibrium is reached, scaling has no other effect on the observables.

B. Evaluation of the energy splitting

As the penetrability of the barrier is decreased, instanton configurations are exponentially suppressed relative to configurations localized in one of the potential minima. Therefore, it becomes increasingly important to calculate the energy splitting ΔE, using an observable which is dominated by instanton configurations and is minimally influenced by the trajectories localized in the potential minima.

An example of an inappropriate observable for measuring ΔE in this limit is the Euclidean time correlation function defined in Eq. (3.6a). The expectation value $\langle x(\tau)x(0)\rangle$ can only decrease exponentially by virtue of cancellations between products of coordinates on opposite sides of the barrier, produced by instantons, and products of coordinates on the same side of the barrier, produced by the localized trajectories. As shown in Fig. 3(b), even when the correct density of instantons is present in the calculation, the error bars are extremely large as a result of the sensitivity of the cancellation to statistical fluctuations.

To avoid this cancellation, it is desirable to express ΔE in terms of the expectation value of an operator which does not receive contributions from zero instanton configurations. This may be accomplished by calculating the matrix element of the evolution operator between a state $|\tilde{\phi}_R\rangle$ localized in the right-hand well and a state $\langle\tilde{\phi}_L|$ localized in the left-hand well, which clearly only receives contributions from trajectories with odd numbers of instantons. Since $\tilde{\phi}_L$ and $\tilde{\phi}_R$ are arbitrary, subject only to this requirement of having reasonably large overlap with the lowest two eigenstates, their contribution is eliminated by calculating the following ratio:

$$R=\frac{\langle\tilde{\phi}_L|e^{-\beta H}|\tilde{\phi}_R\rangle}{(\langle\tilde{\phi}_R|e^{-\beta H}|\tilde{\phi}_R\rangle\langle\tilde{\phi}_L|e^{-\beta H}|\tilde{\phi}_L\rangle)^{1/2}}\ . \tag{3.10}$$

Defining

$$\alpha_{R,L}=\frac{\langle 1|\tilde{\phi}_{R,L}\rangle}{\langle 0|\tilde{\phi}_{R,L}\rangle}\ ,$$

where $|0\rangle$ and $|1\rangle$ denote the lowest, nearly degenerate eigenstates and expanding in $(\alpha_L+\alpha_R)$, which is small because $\alpha_L\sim-\alpha_R$, we obtain the general result

$$R\underset{(E_3-E_1)\beta\gg1}{\rightarrow}\tanh\left[\frac{\beta}{2}\left[\Delta E-\frac{1}{\beta}\ln|\alpha_R\alpha_L|\right]\right]\times\left[1-\frac{1}{2}\frac{(\alpha_R+\alpha_L)^2e^{-\beta\Delta E}}{(1+|\alpha_L\alpha_R|e^{-\beta\Delta E})}+\cdots\right]. \tag{3.11}$$

For the special case of a symmetric double well, taking $\tilde{\phi}_R(x)=\tilde{\phi}_L(-x)$ gives $\alpha_L=-\alpha_R=\alpha$ and all the correction terms vanish to yield the exact result

$$\Delta E_{\text{eff}}(\beta)\equiv\frac{2}{\beta}\tanh^{-1}(R)\underset{(E_3-E_1)\beta\gg1}{\rightarrow}\Delta E-\frac{\ln\alpha}{\beta} \tag{3.12}$$

from which ΔE can be obtained by calculating $\Delta E_{\text{eff}}(\beta)$ at several values of β. For the asymmetric double well with a high barrier, $\alpha_R+\alpha_L$ is small, and therefore the dominant contribution is given by the tanh in (3.11). The correction term of order $(\alpha_R+\alpha_L)^2$ can be calculated stochastically[5] and provides a consistency check. In the same Monte Carlo calculation in which R is calculated, one can simultaneously measure ΔE_{eff} at $\beta/2$ by calculating

$$R_{1/2}=\frac{(\langle\tilde{\phi}_R\mid e^{-\beta H/2}\mid\tilde{\phi}_R\rangle\langle\tilde{\phi}_R\mid e^{-\beta H/2}\mid\tilde{\phi}_L\rangle)(\langle\tilde{\phi}_L\mid e^{-\beta H/2}\mid\tilde{\phi}_L\rangle\langle\tilde{\phi}_L\mid e^{-\beta H/2}\mid\tilde{\phi}_R\rangle)}{(\langle\tilde{\phi}_R\mid e^{-\beta H/2}\mid\tilde{\phi}_R\rangle\langle\tilde{\phi}_R\mid e^{-\beta H/2}\mid\tilde{\phi}_R\rangle)(\langle\tilde{\phi}_L\mid e^{-\beta H/2}\mid\tilde{\phi}_L\rangle\langle\tilde{\phi}_L\mid e^{-\beta H/2}\mid\tilde{\phi}_L\rangle)}\ , \tag{3.13}$$

which is a significant advantage in calculating the β dependence which determines ΔE. The statistical accuracy may be further improved by using importance sampling, Eq. (3.9), with η adjusted such that on average we have equal numbers of zero and one instanton configurations, since these are the dominant contributions to R.

C. Lifetime of a metastable state

Having solved the tunneling problem in a symmetric double well, we now address the steps required to calculate the lifetime of a metastable state in a potential of the form shown in Fig. 1. First, we must adjust the boundary a to render V_L and V_R degenerate.

Because difference expressions for the kinetic energy are subject to large variance, it is preferable to use the virial theorem to replace $\langle T\rangle$ by a local expression. Retaining the surface terms arising from the non-hermiticity of the boundary condition, we obtain, for an arbitrary x_0,

$$\begin{aligned} i\langle\psi\mid[H,p(x-x_0)]\mid\psi\rangle&=2\langle T\rangle-\langle(x-x_0)V'(x)\rangle\\ &=\frac{\hbar^2}{2m}(x-x_0)\mid\psi'\mid^2\mid_{-\infty}^{a}\ . \end{aligned} \tag{3.14}$$

Hence, the presence of a single hard wall may be accommodated by selecting $x_0=a$ and the energy may be written

$$E=\langle V+\tfrac{1}{2}(x-a)V'\rangle\ . \tag{3.15}$$

The derivative dE/da is needed for two reasons: to improve the precision of determination of a and to determine the density of states factor contributing to γ. An infinitesimal rescaling of the Schrödinger equation of the form $y=ax/(a+\delta_a)$ yields

$$\left\{-\frac{1}{2m\left[1+\frac{\delta_a}{a}\right]^2}\frac{\partial^2}{\partial y^2}+V\left[\left[1+\frac{\delta_a}{a}\right]y\right]\right\}\psi =E(a+\delta_a)\psi\ , \tag{3.16}$$

so that, expanding to first order in δ_a and using the virial theorem,

$$\frac{dE}{da}=\frac{1}{a}\langle -2T+xV'(x)\rangle=\langle V'(x)\rangle\ . \tag{3.17}$$

Finally, it is desirable to incorporate the hard wall boundary condition in the path integral to the same accuracy in ϵ as the rest of the approximations. Although for smooth potentials, the infinitesimal evolution operator

$$\exp\left[-\frac{m}{2\epsilon}(x_n-x_{n-1})^2-\epsilon\left[\frac{V(x_{n-1})+V(x_n)}{2}\right]\right]$$

produces errors in observables of order ϵ^2, for a hard wall the wave function is of order $\sqrt{\epsilon}$ at the boundary leading to order $\sqrt{\epsilon}$ errors in observables. The cure is to generate the path integral using states that are odd about $x=a$, with the result

$$\begin{aligned}&(\langle x_n\mid-\langle 2a-x_n\mid)e^{-\epsilon H}\mid x_{n-1}\rangle\\ &\quad=\left[\frac{2m\pi}{\epsilon}\right]^{1/2}\exp\left[-\frac{m}{2\epsilon}(x_n-x_{n-1})^2\right]\\ &\qquad\times\exp\left[-\frac{\epsilon}{2}[V(x_n)+V(x_{n-1})]\right]\\ &\qquad\times\left[1-\exp\left[-\frac{2m}{\epsilon}(a-x_n)(a-x_{n-1})\right]\right]\ . \end{aligned}$$

This antisymmetrization just subtracts off the Green's function corresponding to the first image across the boundary, and one can explicitly verify for the first odd state of the harmonic oscillator that the leading error is $\mathcal{O}(\epsilon^2)$ when images are included.

Finally, all these results may be combined to determine the lifetime of a metastable state. A test problem of the form shown in Fig. 1 was defined by

$$V=\begin{cases}[(1-y)^2+V_0]\left[1-\dfrac{y}{y_0}\right], & y\le y_0\\ 0, & y>y_0\end{cases} \tag{3.18}$$

with $y_0=4$, $V_0=0.05$, and mass $m=16$.

After fixing the wall to make the two wells degenerate, the energy splitting is obtained from $\Delta E_{\rm eff}(\beta)$ as shown in Fig. 7. Using a sample size of $N\sim 10^4$ and performing a

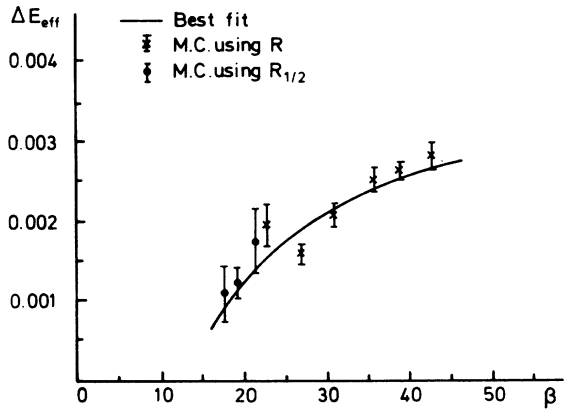

FIG. 7. Monte Carlo calculation of the effective energy gap $\Delta E_{\rm eff}(\beta)$ giving the energy splitting for the evaluation of the lifetime of a metastable state. The crosses and circles refer to Eqs. (3.10) and (3.13), respectively, and the exact result is denoted by the solid line for comparison.

least squares fit to the data with the function (3.12) yields $\Delta E_{mc}=(3.85\pm0.22)\times10^{-3}$ in excellent agreement with the exact result of 3.82×10^{-3}. Combining this with the factor dE/da yields a lifetime $\gamma_{mc}=(3.4\pm0.41)\times10^{-4}$ as compared to the exact value of 3.32×10^{-4}. The correction term proportional to $(a_L+a_R)^2$ in (3.11) was computed stochastically to be $(2.72\pm2.96)\times10^{-2}$ and can safely be neglected while the expansion parameter γ/k_0 is of the order of 10^{-4} assuring an unambiguous definition of the lifetime.

IV. TUNNELING IN MANY DEGREES OF FREEDOM

Having developed the techniques to calculate tunneling in one degree of freedom we shall now use them, with the necessary generalizations, to study tunneling for a quantum many-body system.

In choosing a model system to study, we must recognize the serious practical problems associated with fermions in more than one spatial dimension. Since $\mathrm{Tr}e^{-\beta H}$ has no restriction on the symmetry of states, it is dominated at low temperature by the lowest state of any symmetry. For the usual forces, the lowest state is symmetric and corresponds to bosons. Any attempt to calculate the fermion ground state is thus subject to the problem that the exponentially favored boson ground state will dominate the calculation unless it is exactly projected out.

Antisymmetrization of the coordinate states in a Feynman path integral in more than one spatial dimension is not satisfactory since the projection only occurs stochastically through the approximate cancellation of very large positive and negative contributions, and the stochastic noise from the incomplete projection of the bosonic solution becomes exponentially large compared to the physical fermion signal. The case of one dimension is special because the nodal surfaces are just the points specified by antisymmetry. By working in the ordered subspace $x_1<x_2<\cdots x_A$ with the boundary condition that the wave function vanish whenever any two adjacent coordinates are equal, one can make each contribution to the path integral positive. Thus, one option is to study a many-fermion model in one spatial dimension. In this case, there is no restriction on the form of the potential, and we may use a potential with the strong short-range repulsion and intermediate range attraction characteristic of realistic nuclear forces.

Another possibility is to put fermion field operators on a lattice and to use the Hubbard-Stratonovich transformation to write a functional integral over an auxiliary field of an action which contains a fermionic determinant.[10] Unfortunately, the conditions on the interaction required to obtain a convergent real integral and a positive integrand rule out realistic interactions. Even if some clever trick enabled one to treat a more realistic interaction, the spatial mesh spacing of 0.2 fm required to represent a nuclear force over a region of 20 fm to contain a heavy nucleus dictates a prohibitively large lattice of size 100^3.

The last alternative is to consider a boson system, such as drops of liquid ^{4}He, which could be made to fission by adding a fictitious, Coulomb-like long-range interaction. Of these alternatives, for this initial investigation we have chosen to study fermions in one spatial dimension, where we are unencumbered with spatial lattices, and can study the interplay of dynamics at two very different physical scales—the short-range correlations characteristic of the range of the repulsive core and collective motion characteristic of the size of the nucleus.

The Feynman path integral is restricted to the ordered subspace $x_1<x_2<x_3<\cdots<x_A$ by imposing hard wall boundary conditions at $x_i=x_{i+1}$ using images as before with the result that the one-body path integral (3.3) is replaced by

$$P(x_1^1,\ldots,x_A^n)=\lim_{\epsilon\to0}\frac{1}{Z}\exp\left[-\frac{m}{2\epsilon}\sum_{i,n}(x_i^n-x_i^{n-1})^2-\frac{\epsilon}{2}\sum_n\sum_{i>j}V(|x_i^n-x_j^n|)+V(|x_i^{n-1}-x_j^{n-1}|)\right]$$
$$\times\exp\left[\ln\left\{\prod_{\substack{n,\\ A}}^{i=2}\left[1-\exp\left[-\frac{m}{2\epsilon}(x_i^n-x_{i-1}^n)(x_i^{n-1}-x_{i-1}^{n-1})\right]\right]\right\}\right], \tag{4.1}$$

where subscripts denote particle labels and superscripts denote time labels.

A. One-dimensional model

In order to construct a one-dimensional model as relevant as possible to nuclear physics, it is desirable to define a saturating system interacting with a two-body potential exhibiting the qualitative behavior of the nuclear force. To define the potential quantitatively, it is useful to require that relevant dimensionless ratios be comparable in one and three dimensions. The fundamental length scale in a saturating system is specified by the saturation density ρ_0, so that denoting the dimension by D, we define $l_0=\rho_0^{-1/D}=1.89$ fm in three dimensions. To within unintersting geometrical constants, l_0 specifies the characteristic distance between particles. The Schrödinger equation may then be reduced to dimensionless form by measuring all lengths in units of l_0 and energies in units of $E_0=\hbar^2/ml_0^2=11.6$ MeV such that the scaled binding energy per particle, $(E/A)/E_0$, fermi gas kinetic energy per particle, $(T/A)/E_0$, core radius,

r_0/l_0, and maximum attraction, $V_{\max}/E_0$, are roughly comparable to the three-dimensional values. It has the form

$$V_N(x)=\sum_{i=1}^{2}\frac{V_i}{\gamma_i\sqrt{\pi}}e^{-x_i^2/\gamma_i^2} \tag{4.2}$$

with strengths $V_1=12$, $V_2=-12$ and widths $\gamma_1=0.2$, $\gamma_2=0.8$ and is graphed in Fig. 8.

A crucial consideration for a practical calculation is the choice of the time step ϵ. Although all the observables are accurate to order ϵ^2, the scale of ϵ is set by the scale of variation of the short-range component of the nuclear force $\Delta x\sim 0.2$ and the relation $\epsilon\sim\Delta x^2$, so that we expect convergence to set in for $\epsilon\sim 0.04$. Calculations of nuclear matter[7] and a four-particle nucleus[5] verify that quadratic convergence in the energy sets in at $\epsilon\sim 0.05$, where the fractional error in the binding energy is of order of 5%. Although, in principle, we would prefer to use a smaller value of ϵ, in order to calculate the fission lifetime, it is necessary to eliminate the effect of low-lying single-particle states by using $\beta=15$, which requires 300 time steps for $\epsilon=0.05$. This is a manifestation of the interplay between the very different energy scales governing short-range correlations and low-energy collective motion. We believe that the absolute error in binding energy, which is extremely sensitive to the cancellation between the repulsive core and the long-range attraction, will not significantly affect fission dynamics, because the energies of all the relevant configurations will experience essentially the same overall shift.

The ground states of nuclei from 4 to 16 particles were calculated for $\epsilon=0.05$. The binding energies are well reproduced by the expected one-dimensional semiempirical mass formula $BE(A)\sim E_V A-E_S$, where E_V is the binding energy of bulk nuclear matter at saturation density, ~ -1.06, and E_S is the surface energy, ~ 1.7.

The ground-state density distributions are shown for two nuclei in Fig. 9. As expected, they have an average interior density in agreement with the saturation density of bulk matter $\rho_0=1.2$.

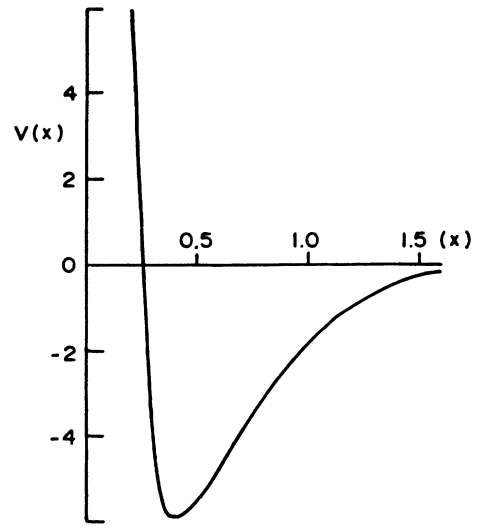

FIG. 8. Two-body potential for the one-dimensional nuclear model.

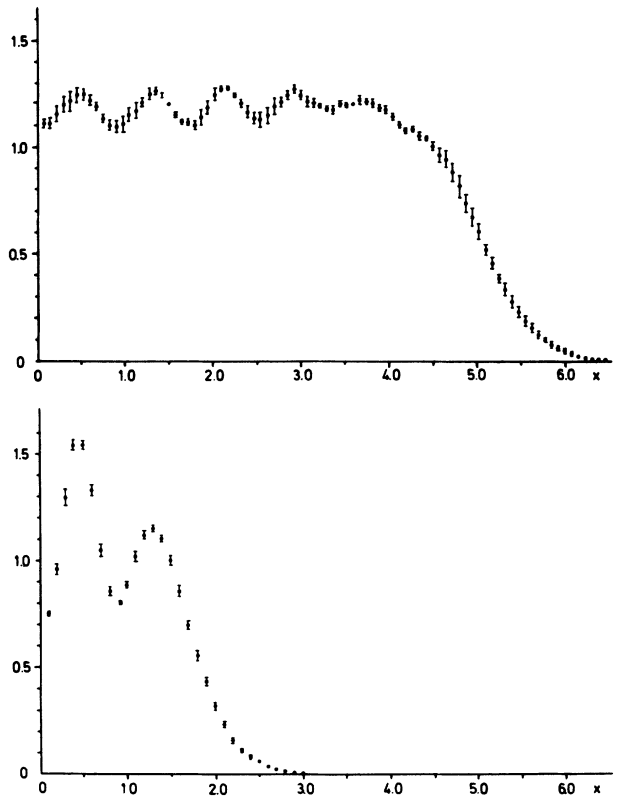

FIG. 9. The one-body density for 4- and 12-particle systems for the nuclear potential $V_N(x)$.

In these calculations we found that initial equilibration is accelerated using dilation updates of the form given in (3.8). The scaling parameter was the same for all particles and all times so the nucleus is uniformly expanded or contracted.

Our model is completely defined by including a Coulomb-like force in order to produce spontaneous fission. The barrier height for the symmetric fission of a 16-particle system was maximized in our model by using the following trapezoidal shape:

$$V_c(x)=\begin{cases} V_c, & x<a \\ \dfrac{(x-b)}{(a-b)}V_c, & a<x<b \\ 0, & x>b\ , \end{cases} \tag{4.3}$$

where $V_c=0.09$, $a=8.0$, and $b=8.56$. We have verified that this interaction produces a sensible barrier by calculating the effective barrier in the constrained Hartree-Fock approximation, using a Skyrme-like effective interaction which reproduces the correct binding energy and surface energy. Solving the Schrödinger equation in this constrained barrier with a reduced mass $\mu=A/2=8$ yields $\gamma/k_0\sim 10^{-3}$, which places the model in the regime of physical interest.

A collective fission variable must be identified for two reasons: To obtain the lifetime from the phase shift in the fission fragment channel, a hard wall forcing a node in the relative wave function must be introduced as in the one-dimensional example. In addition, it is required to offer instanton configurations. The ambiguity, in principle, in defining a collective fission variable is no problem, since any definition must reduce to the relative fragment separation at the outer boundary and any reasonable definition which connects the inner and outer local minima suffices to sample all multiple instanton sectors. For the present calculation it is sufficient to use

$$r=\frac{1}{8}\left[\sum_{i=9}^{16} x_i-\sum_{i=1}^{8} x_i\right], \tag{4.4}$$

which is well defined in the ordered subspace in which we are working. As with the one-particle model problem, the meaningful quantity is the energy splitting. However, since we have a large Coulomb barrier it is again useful to speak separately of inner and outer wells. Therefore, there are again three main parts to the calculations of Γ: the calculation of the ground state energy of the parent nucleus, the calculation of the ground state energy of the two fragments as a function of the position of the hard wall, and the calculation of the energy splitting. We proceed now to give the essential generalizations needed for these calculations.

The hard wall conditions at each hyperplane $x_i=x_{i-1}$ effectively introduced by particle antisymmetry and the hard wall at $r=a$ create a completely bounded $(A-1)$-dimensional domain of relative coordinates. The surface terms at the walls can no longer be made to vanish. In the Appendix it is shown that the virial theorem now reads

$$\langle T\rangle=\left\langle\frac{1}{2}\sum_{i>j}\left[|x_i-x_j|-(\alpha_i-\alpha_j)\frac{a}{2}\mathrm{sgn}(x_i-x_j)\right]\times V'(|x_i-x_j|)+\frac{S}{2i}\right\rangle, \tag{4.5}$$

with

$$S=\frac{ia}{m}\int dy_1\cdots dy_7 dy_9\cdots dy_{15}\left|\frac{\partial\tilde{\psi}}{\partial\tilde{r}}\right|^2_{\tilde{r}=0},$$

where $y_i=x_{i+1}-x_i$, $\tilde{r}=x_9-x_8$, $\tilde{\psi}$ is the intrinsic eigenfunction with the center of mass integrated out, $\alpha_i=-1$ for $i\leq 8$ and $+1$ for $i>8$, and integration is over the hypersurface at $\tilde{r}=0$. The correction S is small because, in addition to the hard core in V_N, the Coulomb barrier keeps the two fragments separated and makes $\tilde{\psi}$ have almost vanishing derivative near $\tilde{r}=0$. Note that for the calculation of the energy of the parent nucleus, the surface term can be made to vanish, since there is no outer wall in r. Although S can be calculated stochastically[5] it has a different ϵ dependence and for $\epsilon=0.05$, for which our calculation is done, can only be used as an estimate for the correction to the virial theorem. As long as it is small compared to the other terms in (4.5) it can safely be neglected.

The equilibration of the parent nucleus is facilitated by offering dilation moves which leave the center of mass invariant

$$x_j^{n'}=x_j^n+j\alpha+c,\quad c=-\left[\frac{A+1}{2}\right]\alpha=-\frac{17\alpha}{2}. \tag{4.6}$$

Internal equilibration of each fragment is aided by offering dilation moves which expand or contract each fragment keeping their distance constant

$$x_j^{n'}=\begin{cases}x_j^n+j\alpha+c', & j\leq 8\quad c'=-\dfrac{9\alpha}{2}\\ x_j^n+(j-8)\alpha+c', & j>8,\end{cases} \tag{4.7}$$

For the many-Fermion system, in addition to symmetric fission, other asymmetric decay channels with energies very close to the energy of symmetric fission are present. Since we have focused on treatment of single-channel decay, we work in a symmetric space, defined by requiring

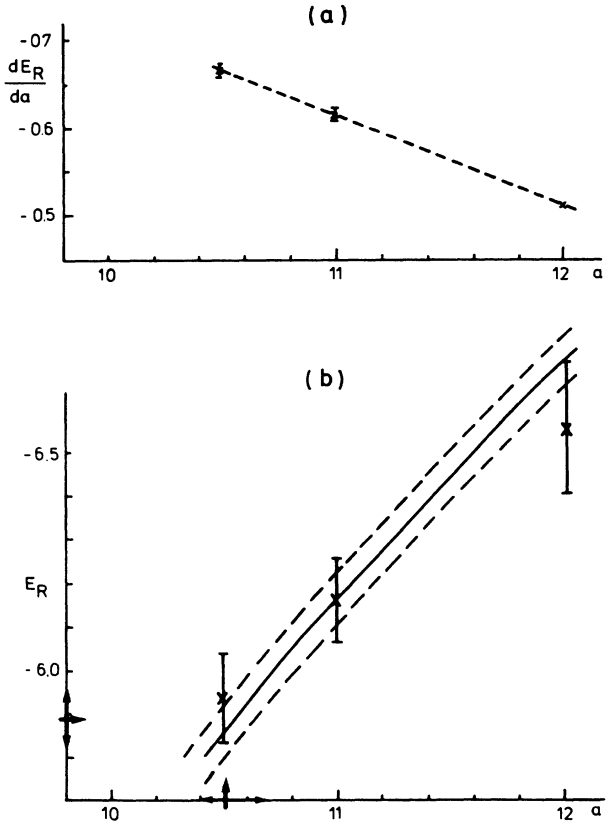

FIG. 10. Determination of boundary position using both E_R and dE_R/da. Part (a) shows the derivative of the energy of the two fragments in the outer well, dE_R/da, as a function of the boundary, a. Part (b) shows Monte Carlo calculations of E_R (error bars) as well as the best simultaneous parabolic least squares fit to E_R and dE_R/da (solid line). The dashed curves show the one standard deviation error envelope. The arrows on the vertical axis indicate the energy of the parent nucleus and the associated error and those on the horizontal axis show the position of the hard wall and the associated error.

that all states be symmetric with respect to reflection about the center of mass. This is accomplished by generating a random walk using coordinate eigenstates.

$$|\chi^n\rangle = |x_1^n,\ldots,x_{16}^n\rangle_A + |2R - x_{16}^n,\ldots,2R - x_1^n\rangle_A \ , \tag{4.8}$$

where $R = \frac{1}{16}\sum_{i=1}^{16} x_i$ and the subscript A on the ket denotes antisymmetrized states with respect to particle interchange.

The collective variable r is sequentially updated at each time step, that is, we move the two fragments toward or away from each other, keeping fixed the distances of particles within each fragment and the center of mass. This introduces changes in r large enough to explore the relevant domain of r in a much smaller number of steps than would be necessary if only moves in the single-particle coordinates x_i were offered.

The results of calculations of the energies and densities of the parent nucleus and of the two fragments calculated using $\sim 10^5$ events are shown in Figs. 10 and 11. Figure 10 shows how the position of the boundary a was determined making use of Monte Carlo calculations of both $E_R(a)$ and $dE_R(a)/da$. The density distributions of the solutions in the degenerate inner and outer wells are shown in Fig. 11. One observes that the eight-particle fragment in the outer well is well separated from the other fragment and very close to a "noninteracting" eight-particle ground state.

For the calculation of the matrix element $\langle \tilde{\phi}_R | e^{-\beta H} | \tilde{\phi}_L \rangle$ in the double well we offer instantons in r. The shape of the instanton is estimated by using the constrained Hartree-Fock potential as an effective one-body potential. Importance sampling of the instanton sectors is included in the same way as for the one-dimensional problem. In Fig. 12 we show a many-body instanton configuration contributing to $\langle \tilde{\phi}_L | e^{-\beta H} | \tilde{\phi}_R \rangle$ which clearly exhibits breakup of the parent nucleus into two fission fragments. The corresponding r trajectory connecting the parent and fission fragments has the same behavior as the instanton of the one-dimensional double well.

These results provide all the necessary ingredients for the calculation of the lifetime. In addition to establishing the methodology for a class of interesting tunneling problems, we hope that this calculation will also provide the basis for a subsequent quantitative test of the imaginary-time mean field approximation[11] applied to this same model.

V. SUMMARY AND CONCLUSIONS

This study of tunneling highlights both the danger and promise of Monte Carlo calculations. The danger is that inappropriate algorithms may yield trapping in local minima. To make matters worse, the problem may not even be apparent for unreasonably large ϵ, and when trapping occurs, the statistical behavior of the results may not reveal the fact that they are completely wrong. The promise is the fact that the freedom in formulating the path integral and the stochastic method may be exploited to include known physics. If the essential physics is included, the Monte Carlo method provides a powerful tool for calculating fluctuation corrections to path integrals which cannot be handled any other way.

In this work, we have demonstrated that collective updates explicitly build into the algorithm the instanton configurations and make the calculation of tunneling in one and many degrees of freedom feasible. We have also learned how to use stochastic techniques to go beyond the calculation of static properties and start to investigate observables which directly depend on nuclear dynamics. We explicitly calculated the lifetime of a metastable state for one degree of freedom using stochastic techniques and obtained excellent agreement with the exact result. We showed that our method is applicable to a nucleus by directly applying it to a model 16-particle system which undergoes spontaneous fission. Although, at present, limited to fermions in one-spatial dimension, we have shown how within a carefully constructed model one may investigate the interplay between short range correlations characterized by a large energy scale and collective phe-

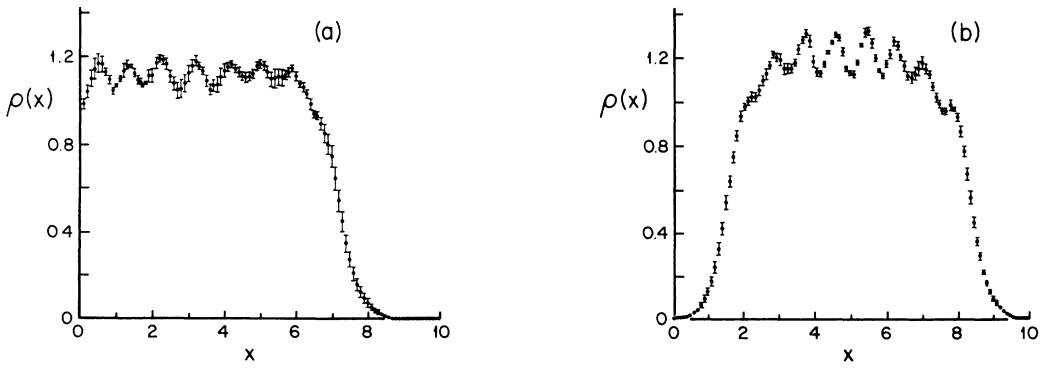

FIG. 11. The one-body density distribution for a 16-particle system is shown for the inner well [part (a)] and for two 8-particle fragments in the degenerate outer well [part (b)].

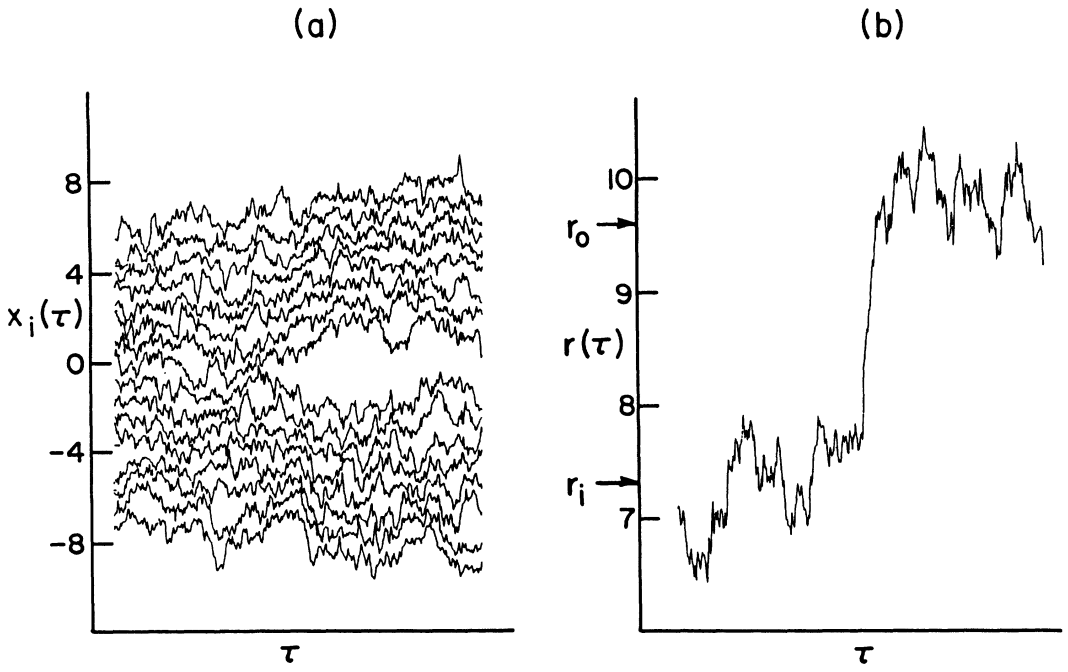

FIG. 12. Typical trajectories of the 16-particle system in the one-instanton sector. Part (a) shows the coordinates of each of the 16 particles on 400 time slices and part (b) shows the corresponding trajectory of the collective coordinate.

nomena characterized by a low energy scale, both of which are very relevant to the realistic problem.

ACKNOWLEDGMENT

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APPENDIX

In this appendix we show how to apply the virial theorem in the presence of more than one hard wall. The expectation value of the commutator $[(x-x_0)p,H]$ in an eigenstate of H for some arbitrary x_0 gives for the kinetic energy

$$\langle T\rangle=\langle\psi\,|\,\tfrac{1}{2}(x-x_0)V'\,|\,\psi\rangle+\frac{1}{4m}\left[(x-x_0)\left|\frac{\partial\psi}{\partial x}\right|^2\right]_a^b . \tag{A1}$$

It is clear that if both endpoints are finite we can no longer eliminate the surface term by an appropriate choice of x_0.

In the many-particle case, while the geometry of the problem is more complicated, essentially the same procedure can be followed. We now look at the expectation value of $[\sum_{i=1}^{A}(x_i+f_i)p_i,H]$ on eigenstates of H, with constants f_i to be fixed later. The Hamiltonian H is translationally invariant and therefore the wave function factorizes into a center of mass part and a relative part in which we are interested. We thus take expectation values in the relative wave functions. The domain of relative coordinates is bounded in all directions by the requirements that the x_i's be ordered and that the coordinate $r=2(\sum_{i=1+A/2}^{A}x_i-\sum_{i=1}^{A/2}x_i)/A$ be less than some value r_0, where A is number of fermions. The integration region is thus an $(A-1)$-dimensional simplex having as its surfaces the $(A-1)$ hyperplanes $x_i=x_{i-1}$ and the hyperplane $r=r_0$. This region is shown in Fig. 13 for the special case of four particles. The generalized virial theorem now reads

$$\langle T\rangle_{\rm rel}=\langle\psi_{\rm rel}\,|\,\tfrac{1}{2}\sum_i(x_i+f_i)\partial_i V\,|\,\psi_{\rm rel}\rangle + \frac{1}{4m}\int d^{N-1}x_{\rm rel} \times\sum_i\frac{\partial}{\partial x_i}\left[\frac{\partial\psi_{\rm rel}}{\partial x_i}\sum_j(x_j+f_j)\frac{\partial\psi_{\rm rel}}{\partial x_j}\right], \tag{A2}$$

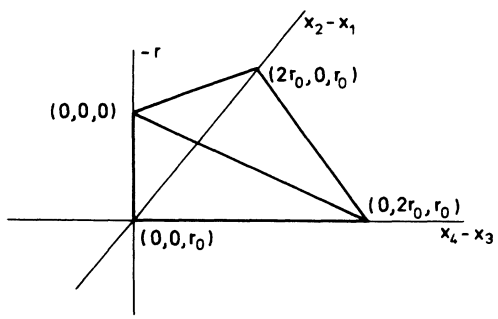

FIG. 13. Integration region for the special case of four particles.

where the last term, being a total derivative, becomes an integral over each of the surfaces of the simplex, and can no longer be made to vanish by the choice of the f_i's. We want to arrange it so that the wall at $r=r_0$ does not contribute, since on the rest of the surfaces $|\partial\psi/\partial x|$ is expected to be small due to the hard core. In fact, we can eliminate simultaneously all surface terms except for the one at $y_{A/2}=x_{A/2+1}-x_{A/2}=0$ by the choice

$$f_i=-\frac{r_0}{2},\quad i>\frac{A}{2} \tag{A3}$$

and

$$f_i=\frac{r_0}{2},\quad i\le\frac{A}{2}\ .$$

[One might be puzzled at this stage by the fact that the choice to work in an ordered subspace, which might be considered as placing artificial walls on our domain, results in contributions to the virial theorem from these walls. The point here is that different orderings require different definitions of r, the fragment separation, and therefore different permuted values of f_i to cancel the surface terms at $r=r_0$. Then the operator $\sum_i (x_i+f_i)p_i$ becomes discontinuous at $x_j=x_{j-1}$ and contributes a surface term.] Using

$$\left[\frac{\partial}{\partial x_i}-\frac{\partial}{\partial x_{i-1}}\right]\psi\,|_{x_i=x_{i-1}}=0\ ,\qquad \frac{\partial\psi}{\partial x_j}\bigg|_{x_i=x_{i-1}}=0\quad (i\neq j\neq i-1) \tag{A4a}$$

and

$$\frac{\partial\psi}{\partial x_1}\bigg|_{r=r_0}=\cdots=\frac{\partial\psi}{\partial x_{A/2}}\bigg|_{r=r_0}=-\frac{\partial\psi}{\partial x_{A/2+1}}\bigg|_{r=r_0}=\cdots=-\frac{\partial\psi}{\partial x_A}\bigg|_{r=r_0}\ , \tag{A4b}$$

we verify that the only surface contribution is

$$\langle T\rangle_{\rm rel}=\left\langle\psi_{\rm rel}\left|\frac{1}{2}\sum_i (f_i+x_i)\partial_i V\right|\psi_{\rm rel}\right\rangle+\frac{r_0}{2m}\int_{y_{A/2}=0}\prod_{i=1}^{A-1}{}'\,dy_i\left|\frac{\partial\psi_{\rm rel}}{\partial y_{A/2}}\right|^2\ , \tag{A5}$$

where we have defined relative coordinates $y_i=x_{i+1}-x_i$, $i=1,\ldots,A-1$. The integral is over the $(A-2)$-dimensional surface $y_{A/2}=0$ and the prime on $\prod$ signifies omission of $dy_{A/2}$. This establishes Eq. (4.5).

*Present address: Institut für Theoretische Physik III, Universität Erlangen-Nürnberg, Glückstrasse 6, 8520 Erlangen, Federal Republic of Germany.

[1]J. Langer, Ann. Phys. (N.Y.) **54**, 258 (1969).
[2]A. M. Polyakov, Nucl. Phys. B **121**, 429 (1977).
[3]S. Coleman, in *The Whys of Subnuclear Physics,* edited by A. Zichichi (Plenum, New York, 1977), p. 805.
[4]J. W. Negele, Rev. Mod. Phys. **54**, 913 (1982).
[5]C. Alexandrou, Ph.D. thesis, Massachusetts Institute of Technology, 1985.
[6]N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).
[7]J. W. Negele, in *Proceedings of the International Symposium on Time-Dependent Hartree-Fock and Beyond,* Vol. 71 of *Lecture Notes in Physics,* edited by K. Goeke and P. G. Reinhard (Springer-Verlag, New York, 1982); J. Stat. Phys. **31**, 991 (1986).
[8]J. W. Negele and H. Orland, *Quantum Many-Particle Systems* (Addison-Wesley, Reading, MA, 1987).
[9]M. Creutz and B. Freedman, Ann. Phys. (N.Y.) **132**, 427 (1981).
[10]G. Sugiyama and S. E. Koonin, Ann. Phys. (N.Y.) **168**, 1 (1986).
[11]S. Levit, J. W. Negele, and Z. Paltiel, Phys. Rev. C **22**, 1979 (1980).