

## Monte Carlo calculation of quantum tunneling in the dilute instanton limit

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A new approach for estimating small quantum tunneling rates by Monte Carlo calculation is proposed and demonstrated on a simple one-dimensional model. The application to many-body situations such as atomic exchange in solid  $^3\text{He}$  is discussed.

The instanton picture of quantum tunneling<sup>1</sup> and the associated path-integral formulation provides a natural approach to calculating slow decay rates via tunneling through barriers or the small splitting of otherwise degenerate states connected by tunneling. In the semiclassical limit (small  $\hbar$ ) a steepest descent evaluation of the instanton configuration leads to the familiar Wentzel-Kramers-Brillouin (WKB) expression for the tunneling rate. Away from the semiclassical limit Monte Carlo methods have been used<sup>2</sup> to estimate the appropriate weights of instanton configurations. However, the algorithm used, where the Monte Carlo updates themselves generate instantons (tunneling events) from zero instanton configurations (path remaining in one well), becomes inefficient for small tunneling rates or in high-dimensional (i.e., many-body) situations.

I propose a method that eliminates this difficulty by evaluating separately the weights of one-instanton and zero-instanton configurations produced by appropriate initial conditions. The cost of this approach is that we are left with a task equivalent to evaluating by Monte Carlo calculation the partition function of a classical system—well known to be a difficult problem.<sup>3</sup> One approach, which leads to an intuitively appealing scheme, is to integrate over a range of system parameters. For example, the thermodynamic identity between the free energy  $F$  and energy  $E$

$$\frac{F(T)}{T} = \frac{F(T_0)}{T_0} + \int_{T_0}^T \frac{E(T')}{T'^2} dT', \quad (1)$$

with  $T$  the temperature of our equivalent classical system maps, in the original tunneling problem, to investigating the tunneling over a range of  $\hbar$ . The small  $\hbar$ , semiclassical limit is then effectively used to normalize the Monte Carlo probability distribution.

This method should work well for systems that can be

$$\begin{aligned} \rho_h(\beta, \hbar) &= \int dx_1 \cdots \int dx_{N-1} \rho(x_0, x_1, \beta/N, \hbar) \rho(x_1, x_2, \beta/N, \hbar) \times \cdots \times \rho(x_{N-1}, P x_0, \beta/N, \hbar), \\ &\approx A \int dx_1 \cdots \int dx_{N-1} \exp \left[ -\hbar^{-1} \left[ \sum_{i=1}^{N-1} \frac{m}{2\eta} (x_i - x_{i-1})^2 + \eta V(x_i) \right] \right], \end{aligned} \quad (4)$$

where  $N\eta = U = \beta\hbar$ , and we have made a lowest-order (high-temperature) approximation to  $\rho(x, x', \beta/N, \hbar)$  for large  $N$ . (The normalization constant  $A$  drops out below.) With this approximation the right-hand side of Eq. (4) can be interpreted as the partition function  $\exp[-F_h(T)/T]$  of  $N-1$  classical particles, joined by springs of stiffness

transformed continuously to the semiclassical limit. This is not always the case. An example is the atomic exchange in solid  $^3\text{He}$ ,<sup>4</sup> which motivated this study. Here, at low pressures, the atomic lattice sites are at a maximum of the potential, albeit very weak; decreasing  $\hbar$  yields an *unstable* classical limit.<sup>5</sup> In this case we may have to study the tunneling as a function of other parameters, e.g., specific volume, or seek a different way to evaluate the equivalent classical free energy.

I envision applying the method to problems where the tunneling rate is small compared with the frequency  $\omega_0$  within each well, so that conventional (e.g., variational) methods are inadequate, but where the semiclassical limit does not apply. Atomic exchange in solid  $^3\text{He}$  falls into this class, since quantum effects are large,<sup>4</sup> but the tunneling rate measured by the exchange splitting  $J$  of the spin degeneracy is small:  $J/\omega_0 \sim 10^{-4}$ . Other examples might be where quantum internal degrees of freedom are important, e.g., nuclear fission.

Here I describe the method and demonstrate its use on a simple one-dimensional model that has been addressed previously,<sup>2</sup> namely, tunneling in the symmetric well given by

$$\mathcal{H}\psi = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = \epsilon\psi; \quad V(x) = (x^2 - 1)^2. \quad (2)$$

I will estimate the tunneling splitting  $\delta = \epsilon_1 - \epsilon_0$  between the lowest two states. At the end I discuss the merits of the method in realistic many-body application.

A direct measure of the tunneling rate is the “hop” amplitude

$$\rho_h(\beta, \hbar) = \rho(x_0, P x_0, \beta, \hbar) = \langle x_0 | e^{-\beta\mathcal{H}} | P x_0 \rangle, \quad (3)$$

with  $\beta$  the inverse temperature.<sup>6</sup> Here  $x_0$  is the position of the potential minimum in the left well and  $P x_0$  the symmetry related point in the right well. A discrete approximation to the Feynman path integral is generated by writing

$m/\eta$  and acted on by the potential  $\eta V(x)$ , connecting  $x_0$  to  $P x_0$  at an effective<sup>7</sup> “classical” temperature  $T$  given by  $\hbar$  in the original problem. The effective classical Hamiltonian  $H$  is the quantity in the large parentheses in the exponent in Eq. (4).

Now dividing by the amplitude for starting and ending

at the same minimum  $\rho_0(\beta, \hbar) = \rho(x_0, x_0, \beta \hbar)$ , we have

$$\frac{\rho_h(\beta, \hbar)}{\rho_0(\beta, \hbar)} \approx \exp(-T^{-1}\Delta F), \quad (5)$$

with  $\Delta F = F_h - F_0$  the difference in the classical free energies of the particles with the hop and one-well boundary conditions at the effective temperature  $T = \hbar$ . The left-hand side is evaluated by inserting the complete set of exact eigenstates of energies  $\epsilon_i$ . For

$$\omega_0^{-1} \ll \beta \hbar = U \ll (\delta/\hbar)^{-1} \quad (6)$$

we find

$$\rho_h/\rho_0 \approx \frac{1}{2}(1 - |\langle x_0 | 1 \rangle|^2 / |\langle x_0 | 0 \rangle|^2) + U\delta/2\hbar, \quad (7)$$

with  $|0\rangle$  the (even) ground state and  $|1\rangle$  the (odd) first excited state.<sup>8</sup> Equations (5-7) lead to the central result

$$\frac{\delta}{\hbar} \rightarrow \frac{2}{U} \exp[-T^{-1}\Delta F(T)]_{T=\hbar} + O\left(\frac{1}{U}\right), \quad (8)$$

where the leading order  $U$  independent part for large  $U$  in the range given by Eq. (6) is to be extracted.<sup>9</sup> Progress from here on depends on suitable Monte Carlo algorithms for considering the classical free energy  $\Delta F(T)$  or its derivatives.

The length-scale Grüneisen constant for the exchange splitting may be estimated by taking the logarithmic derivative of Eq. (8). For the one-dimensional problem

$$\frac{\partial \ln \delta}{\partial L} = -T^{-1}\Delta P, \quad (9)$$

where each "pressure" is given by the length-derivative of the free energy and may be sampled directly by the Monte Carlo:<sup>3</sup> for Eq.(2) with  $V(x) = (x^2/L^2 - 1)^2$  we have at  $L = 1$

$$P = \left\langle \sum_{i=1}^{N-1} \frac{m}{\eta} (x_i - x_{i-1})^2 \right\rangle, \quad (10)$$

where the  $\langle \rangle$  denote averaging with the classical Boltzmann weight  $\exp(-T^{-1}H)$  and the appropriate endpoints. This type of result, generalized to higher dimension, will give us, by Monte Carlo sampling at one volume, the volume Grüneisen constant for exchange in solid <sup>3</sup>He—a quantity of direct experimental interest. Note that  $\Delta P$  will be dominated by contributions from the instanton regions of the hop paths, so that the algorithm focuses on the important regions of phase space.

For systems varying continuously to the semiclassical limit Eq. (1) may be used to give

$$\delta(\hbar) = \delta(\hbar_0) \exp\left[-\int_{\hbar_0}^{\hbar} dT T^{-2}\Delta E(T)\right] + O(U^{-1}), \quad (11)$$

with  $\Delta E = \langle H_h \rangle - \langle H_0 \rangle$ , the difference in the average classical energies, which is easily estimated by the Monte Carlo. Typically  $\hbar_0$  may be chosen small enough that  $\delta(\hbar_0)$  may be evaluated semiclassically. Note for small  $T$  we expect

$$\Delta E(T) \approx S_0 - \frac{1}{2}T + \dots, \quad (12)$$

where the second term comes from the single zero-energy translation mode in the hop configuration that reduces the number of modes contributing  $\frac{1}{2}T$  (by equipartition) to the specific heat. This leads to

$$\delta(\hbar) \sim \hbar^{1/2} \exp(-S_0/\hbar)[1 + O(\hbar)], \quad (13)$$

so that  $S_0$  corresponds to the classical action and the prefactor dependence of the semiclassical expressions<sup>1</sup> is reproduced. Note that Eqs. (8) and (11) provide a very appealing formulation of the exchange splitting, giving directly a sampling of the exponent.

I have chosen to illustrate the application of the method and Eq. (11), in particular by investigating the *corrections* to the semiclassical WKB result for Eq. (2), i.e., to<sup>2</sup>

$$\delta_{sc} = \frac{16}{\sqrt{\pi}} \left(\frac{2}{m}\right)^{1/4} \hbar^{1/2} \exp(-\frac{4}{3}\sqrt{2m}/\hbar), \quad (14)$$

for  $\hbar = 1$ ,  $m = 12$  (for which  $\delta/\omega_0 \approx 0.0084$ ).

The most troubling aspect turned out to be eliminating the  $O(U^{-1})$  "end effects" in Eq. (11). Direct elimination by extrapolation proved costly in computer time: At the large  $U, N$  required to establish the  $U^{-1}$  dependence the difference  $\Delta E$  is small compared to  $E_h$  or  $E_0$  separately, and becomes difficult to extract above the statistical fluctuations. Instead a method suggested by the classical analogy was used. Note that at  $T = 0$  we expect only exponentially small [ $\sim \exp(-\omega_0/U)$ ] corrections due to the tails of the instanton configuration. At  $T \neq 0$  the important finite length ( $U$ ) corrections to  $E_h - E_0$  come from members of the ensemble where the instanton approaches either end. To eliminate these members a procedure is included in the Monte Carlo update to maintain the instanton near the center of the path. Specifically, add  $S$  particles with coordinate  $x_m$  between  $x_{N-1}$  and  $x_N$  ( $x_0$  and  $x_1$ ) and eliminate  $S$  particles  $x_1$  to  $x_{S+1}$  ( $x_{N-S-1}$  to  $x_{N-1}$ ) and relabel to move the center of the instanton  $S$  particles to the left (right) towards the center when necessary.<sup>10</sup> The particles are added at the position of the potential minimum. Systematic errors in  $E_h - E_0$  are reduced by updating the hop and one-well configurations simultaneously, and performing the same shift operation (redundant of course for the one-well configuration). The  $U \rightarrow \infty$  values estimated in this way from a finite system with  $U = 15$  are compared with the extrapolation of finite  $U$  (with no shift) estimates in Fig. 1. Good consistency is obtained, although the latter method is less precise. Using the shifting algorithm for  $U = 20$  produced the same results within the statistical uncertainty.

In Fig. 2,  $I(T) = T^{-2}[\Delta E(T) - \Delta E(0) + \frac{1}{2}T]$ , the quantity to be integrated to give the *correction* to the semiclassical expression Eq. (14), is plotted for  $U = 15$ ,  $N = 31$ . [ $\Delta E(0)$  was evaluated by direct numerical solution with the same discretization, not by Monte Carlo calculation.] The integral was done by integrating a straight-line fit through the points, to give

$$\delta/\delta_{sc} = 0.824 \pm 0.01. \quad (15)$$

Negele and Alexandrou<sup>2</sup> give the value calculated by direct numerical solution to be 0.82. We have checked for

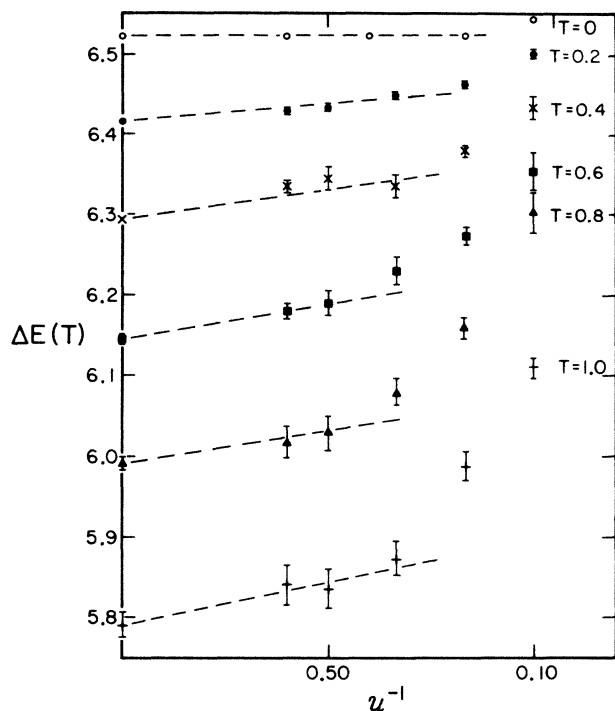


FIG. 1. Comparison between  $\Delta E(T)$  for various  $U^{-1}$  and the value (plotted at  $U^{-1}=0$ ) given by keeping the instanton towards the center (for  $U=15$ ) at various temperatures  $T$  as labeled. The error bars are the standard deviations of repeated runs. Parameters were  $m=12$ ,  $\eta=0.5$ .

any residual dependence on  $U$  and  $N$  as tabulated in Table I.

These results show that tunneling splittings of less than  $10^{-2}$  can be reasonably calculated to an accuracy of about 1%. (The correction to the semiclassical estimate is accurate to about 5%.) The data used for the estimate (i.e., in Fig. 2) took 16 hours of Ridge-32 CPU time, corresponding to a total of  $4 \times 10^6$  sweeps through the two sets of 29 dynamic particles.

I certainly do not claim that this approach is the best (or even the best Monte Carlo) way to attack the one-dimensional problem: The example was chosen to be a problem that could be trivially integrated directly for com-

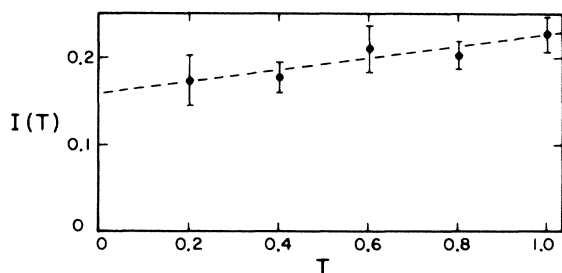


FIG. 2.  $I(T) = T^{-2}[\Delta E(T) - \Delta E(0) + \frac{1}{2}T]$  as a function of  $T$ , for the  $U=15$  data (with shift) of Fig. 1. The straight-line fit is  $I(T) = 1.60 + 0.67T$ .

TABLE I. Values of the energy splitting  $\delta$  for various choices of  $U$  (all with the instanton-shift procedure) and  $N$ .

$U$	$N$	$\delta/\delta_{sc}$
15	31	$0.824 \pm 0.01$
20	41	$0.825 \pm 0.01$
15	45	$0.819 \pm 0.01$

parison. Also, since the system is near the semiclassical limit, a Monte Carlo method sampling with the *known* semiclassical weight would directly give the exchange splitting without integrating over a range of  $\hbar$ . In fact, using such a method when approaching small  $\hbar$  in a more realistic problem would save considerable computing effort. However, the method does look very promising for more complex problems where direct integration is, of course, impossible. Competing methods are similar instanton path-integral approaches, but where instantons are generated by (or fed to) the Monte Carlo updating procedure,<sup>2</sup> or particle-diffusion approaches, using guided random walks.<sup>2,11</sup> The former method becomes inefficient for small tunneling rates, and in complex many-body situations where the structure of the instanton to be offered to the Monte Carlo is not *a priori* known. In either case the acceptance of the instanton configurations would be anticipated to become very small. The guided random-walk approach is attractive, since much of the quantum structure can be built in using variational wave functions to guide the walks. However, the basic algorithm, corresponding to starting random "walkers" in the left-hand well and counting the number that appear in the right-hand well, becomes increasingly subject to fluctuations, as the number of degrees of freedom increases.<sup>11</sup> On the other hand, in the present approach the number of sweeps required to maintain a given precision should only grow linearly with the number of degrees of freedom.<sup>12,13</sup>

There is considerable flexibility in applying the method. Higher-order expansions of  $\rho(x, x', \beta/N, \hbar)$  may be used to give more rapid convergence with  $N^{-1}$ . This is probably necessary in <sup>3</sup>He, where the interaction potential involves rapid spatial variation. Here the next order analytic term or the numerical pair-approximation form of Pollock and Ceperley<sup>14</sup> may be useful. For hard spheres the pair-wise image approximation of Barker<sup>15</sup> may be appropriate. Various derivatives of the exchange rate may be sampled. Also, instead of varying towards the analytic semiclassical limit, the highly quantum limit may be approached, where a conventional variational calculation of the larger exchange rate may be adequate to normalize the result. The implementation of these ideas in many-body situations is in process.

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- <sup>1</sup>S. Coleman, in *Proceeding of the 1977 International School of Subnuclear Physics, Erice, Italy, 1977*, edited by A. Zichichi (Plenum, New York, 1979).
- <sup>2</sup>C. Alexandrou, Ph.D. thesis, Massachusetts Institute of Technology, 1985 (unpublished); J. W. Negele, in *Proceedings of Frontiers of Quantum Monte Carlo, Los Alamos, 1985* [J. Stat. Phys. **43**, 911 (1986)].
- <sup>3</sup>K. Binder and D. Stauffer, in *Applications of the Monte Carlo Method in Statistical Physics*, Topics in Current Physics, Vol. 36 (Springer, Berlin, 1984), p. 1.
- <sup>4</sup>For a review, see M. C. Cross and D. S. Fisher, *Rev. Mod. Phys.* **57**, 881 (1985).
- <sup>5</sup>This is not too surprising since the other more classical inert gases do not form stable bcc phases.
- <sup>6</sup>This development closely follows that of Ref. 2. The relationship between the density matrix and the exchange gap in <sup>3</sup>He was previously considered by M. Roger, *Phys. Rev. B* **30**, 6432 (1984).
- <sup>7</sup>Not that  $T$  is *not* related to  $\beta$  in Eq. (4).
- <sup>8</sup>It is useful to formulate the comparison in terms of the (imaginary) time  $U$ , since the characteristic frequency  $\omega_0$  is independent of  $\hbar$  for small  $\hbar$ .
- <sup>9</sup>For  $U$  in the range of Eq. (6) only zero or one instanton will be present, depending on the end-point conditions. Keeping the full exponential dependences (cf. Eq. 3.4 of Ref. 2) instead of the expansion in Eq. (7) then corresponds to summing over re-

peated, well isolated tunneling events (Ref. 1). Note that we are making a "dilute instanton" approximation, justified by the small  $\delta$ , but are not assuming small Gaussian fluctuations about the classical path for each instanton.

- <sup>10</sup>This was typically done after 25 sweeps whenever the number of particles with  $x > 0$  exceeded  $(N-1)/2$  by  $S_{\min} = 2$ .
- <sup>11</sup>E. L. Pollock and D. M. Ceperley, *Phys. Rev. B* **30**, 2555 (1984).
- <sup>12</sup>This can be seen [M. W. Wilkinson (private communication)] by considering  $M$  transverse harmonic degrees of freedom added to the one-dimensional problem. In the guided-walk approach each extra degree of freedom gives a multiplicative fluctuating component corresponding to the sampling of the transverse wave functions. Thus the *logarithm* of the fluctuations should grow as  $\sqrt{M}$ . A rapid growth of fluctuations with  $M$  was indeed found in a straightforward implementation of this approach [M. W. Wilkinson (unpublished)]. The fluctuations would be reduced by a sufficiently accurate guiding wave function.
- <sup>13</sup>Uncoupled extra degrees of freedom are eliminated by the joint updating.
- <sup>14</sup>In  $\rho(x, x', \Delta\beta, \hbar)$  make the replacement  $V(x) \rightarrow V(x) + (\hbar^2/12m)\Delta\beta V''(x)$  (Ref. 11). Note that for the model problem the correction is small for  $\eta = 0.5$ ,  $m = 12$ ,  $\hbar = 1$ .
- <sup>15</sup>J. A. Barker, *J. Chem. Phys.* **70**, 2914 (1979).