



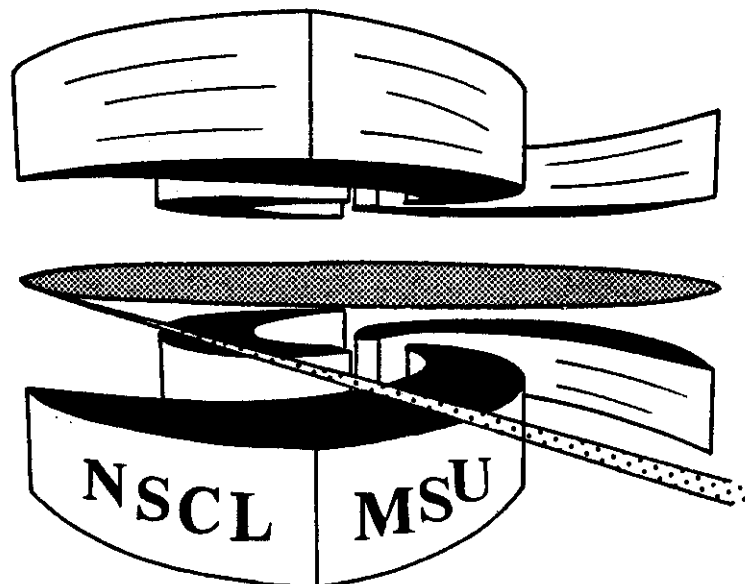
Michigan State University

National Superconducting Cyclotron Laboratory

**CHAOS → ERGODICITY → ISOTHERMAL DYNAMICS**

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## ABSTRACT

We present a cursory review of the new developments of the finite temperature molecular dynamics approach along with some selected applications.

## ISOTHERMAL MOLECULAR DYNAMICS

In recent years molecular dynamics (MD) techniques have been improved and applied to a wide range of physical systems: fluids, gases, molecular systems, atomic clusters and in some cases lattice gauge calculations. The extension of these methods to non-equilibrium phenomena is an unbeatable advantage of molecular dynamics methods over other existing approaches. One can safely say that MD techniques are on the rise and their potential has not yet been fully exploited and explored. We shall not try to present a review of what was already done in this field, but instead we shall concentrate on presenting our recent developments in isothermal MD.

In 1984 **Nosé**<sup>1</sup> presented a very elegant method of simulating the coupling of a classical system with  $N$  degrees of freedom to a thermal bath. He showed that, by adding only one additional degree of freedom to the system under study, one can emulate the action of an infinite number of degrees of freedom of the thermostat. Subsequently, Hoover<sup>2</sup> simplified the approach by replacing the additional coordinate and momentum introduced by **Nosé** with a single pseudofriction coefficient, thus and eliminating a rather unintuitive method of time sampling of the phase space. **Jellinek**<sup>3</sup> pointed to some other potentially interesting ways to generalize **Nosé's** initial scheme. However, in all these formulations of the isothermal MD scheme it was assumed that the resulting equations of motion generate an ergodic trajectory in the enlarged phase space, not merely a chaotic one. Ergodicity implies that the integral over the phase space, with the appropriate **Boltzmann** factor in the measure, is identical to a time average over the trajectory followed by the system. This is just the opposite of what the forefathers of statistical mechanics told us to do. The absence of ergodicity in some relatively simple cases was observed almost right **away**<sup>2</sup>, but ways to cure this **undesireable** feature were only found **recently**<sup>4,5</sup>.

In **Refs. 4,5** we proposed the following equations of motion in order to study

a system coupled with a thermostat at temperature  $T$

$$\dot{q}_i = \frac{\partial H(p, q)}{\partial p_i} - h_2(\xi)F_i(q, p), \quad \dot{p}_i = -\frac{\partial H(p, q)}{\partial q_i} - h_1(\zeta)G_i(q, p), \quad (1a, b)$$

$$\dot{\zeta} = \alpha \sum_{i=1}^N \left[ \frac{\partial H(p, q)}{\partial p_i} G_i(p, q) - T \frac{\partial G_i(p, q)}{\partial p_i} \right], \quad (2a)$$

$$\dot{\xi} = \beta \sum_{i=1}^N \left[ \frac{\partial H(p, q)}{\partial q_i} F_i(p, q) - T \frac{\partial F_i(p, q)}{\partial q_i} \right], \quad (2b)$$

where  $H(p, q)$  is the Hamiltonian of the envisaged system,  $G_i(p, q)$ ,  $F_i(p, q)$ ,  $h_1(\zeta)$ ,  $h_2(\xi)$  are some arbitrary functions,  $\alpha$ ,  $\beta$  are constants and  $T$  is the absolute temperature at which one is interested in studying the system. We shall call the extra variables  $\zeta$  and  $\xi$  pseudofriction coefficients and their introduction into the equations of motion is aimed at simulating the coupling to the thermostat.

It can be shown that in the extended phase space  $(q_1, \dots, q_N, p_1, \dots, p_N, \zeta, \xi)$  the equations of motion (1,2) are compatible with the existence of the following invariant measure

$$d\mu = \mathcal{N} \exp \left\{ -\frac{1}{T} \left[ H(p, q) + \frac{1}{\alpha} g_1(\zeta) + \frac{1}{\beta} g_2(\xi) \right] \right\} dq_1 \dots dq_N dp_1 \dots dp_N d\zeta d\xi, \quad (3)$$

where  $dg_1(\zeta)/d\zeta = h_1(\zeta)$  and  $dg_2(\xi)/d\xi = h_2(\xi)$  and  $\mathcal{N}$  is a normalization constant. Consequently, if Eqs. (1,2) generate an ergodic trajectory, one can replace the phase space integral over the measure (3) with a time average integral.

The equations of motion (1-2) have a rather unexpected structure. First of all, the symplectic structure has been lost in the augmented phase space  $(q_1, \dots, q_N, p_1, \dots, p_N, \zeta, \xi)$  or, in other words, the equations of motion no longer have a Hamiltonian character. As a consequence, the phase space volume is not conserved, since

$$\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} \neq 0, \quad (i = 1, \dots, N). \quad (4)$$

However, the time or phase space average of the r.h.s. of Eq. (4) vanishes. Consequently, under the influence of the thermostat the phase space "breathes". The additional terms in Eqs. (1) are referred to as pseudofriction for a simple reason. A friction force has a dissipative character, it leads to a loss of energy of the system. The pseudofriction terms have the same formal appearance as a dissipative force. However, since the pseudofriction variables  $\zeta, \xi$  take both positive and negative values as functions of time, energy is either extracted or given to the system in such a way as to achieve thermalization, and the motion never ceases. On this augmented phase space one can introduce a phase space probability<sup>2</sup>  $f(q_1, \dots, q_N, p_1, \dots, p_N, \zeta, \xi, t)$  which can be easily shown to satisfy the following generalized Liouville equation

$$\frac{\partial f}{\partial t} + \sum_{i=1}^N \left[ \frac{\partial(f\dot{q}_i)}{\partial q_i} + \frac{\partial(f\dot{p}_i)}{\partial p_i} \right] + \frac{\partial(f\dot{\zeta})}{\partial \zeta} + \frac{\partial(f\dot{\xi})}{\partial \xi} = 0. \quad (5)$$

It can be easily checked that the weight of the measure  $d\mu$  (3) is a stationary solution of Eq. (5). This is the only time-independent solution of the generalized Liouville equation (5) if and only if the system described by Eqs. (1-2) is ergodic. Neither the form nor the number of the pseudofriction terms is unique or prescribed by "theory". This should be looked upon as an advantage, allowing the possibility of modeling different types of couplings to a thermostat. The rate of energy exchange between the system and the thermostat can also be controlled in this way. The rather particular and to some extent peculiar type of coupling we have chosen in Eqs. (1) is to some extent accidental. Since at equilibrium the distribution of coordinates and momenta are uncorrelated, we have chosen this form of coupling to the thermal bath merely to achieve thermalization as quickly as possible. If someone is interested in dynamical properties of a thermalized system (e.g. autocorrelation functions for different quantities) the specific form of the coupling might be crucial. We shall not dwell anymore on these questions here and refer the reader to Ref. 5 for a detailed discussion of this.

## SHORT DESCRIPTION OF SEVERAL APPLICATIONS

As a simple illustration of the effectiveness of this approach we present in Fig. 1 the time evolution of the relative deviations of the computed distributions for variables  $(q, p, \zeta, \xi)$  for the case of a simple 1D harmonic oscillator  $H(q, p) = (p^2 + q^2)/2$  coupled to a thermal bath. This example is important for several reasons: it is one of the simplest examples in which nonergodicity of the Nosé-Hoover scheme was observed; at low temperatures essentially every system can be approximately described by coupled harmonic oscillators; the harmonic oscillator is in a way "very regular" and relatively hard to make chaotic; numerical simulations can be easily compared to exact results. We describe the coupling to the thermostat most of the time by the following functions (or slight modifications of these):

$$h_1(\zeta) = \zeta^3, \quad g_1(\zeta) = \zeta^4/4, \quad h_2(\xi) = \xi, \quad g_2(\xi) = \xi^2/2, \quad (6a)$$

$$F_i(q, p) = q_i^3, \quad G_i(q, p) = p_i, \quad (i = 1, \dots, N). \quad (6b)$$

We link the ability of this type of approach to generate canonical distributions with the high degree of chaoticity of the trajectories. In Fig. 2 we present the time evolution of a circle in the phase space  $(q, p)$  for a 1D harmonic oscillator using the present approach as well as the earlier Nosé-Hoover scheme. The calculated Lyapunov exponents<sup>5</sup> are rather big, which fact ensures a rapid exploration of the phase space, starting essentially from any point in the phase space. The fact that the motion is chaotic (positive Lyapunov exponents) is in itself not a sufficient property of this scheme to describe a system in thermal equilibrium. Ergodicity implies chaoticity but the reverse is generally not true. It can be shown as well that the equations of motion (1-2) do not have stable fix points.

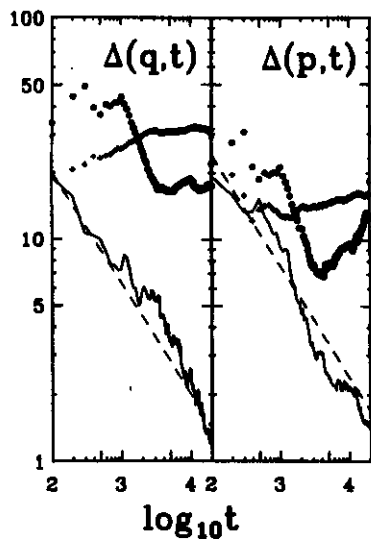


Fig. 1. The time evolution of the integrated absolute difference between the computed and the exact thermal distribution (solid) for the specified variables,  $\Delta(\phi, t)$ , ( $\phi = q, p$ ). Circles and crosses are results from the Nosé-Hoover scheme<sup>2</sup>. The dashed line corresponds to  $\Delta(\phi, t) = \text{const}/t^{1/2}$ .

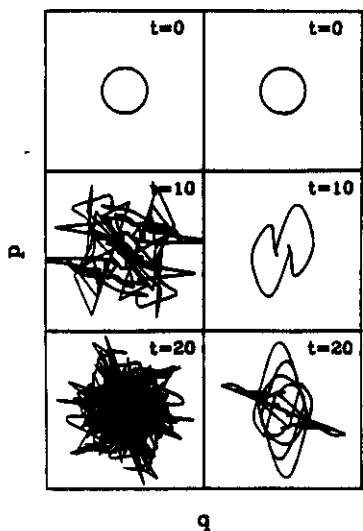


Fig. 2. Time evolution of a circular set of 1000 initial points using the couplings of Eqs. (6) (left) compared to Nosé-Hoover<sup>2</sup> for a 1D harmonic oscillator.

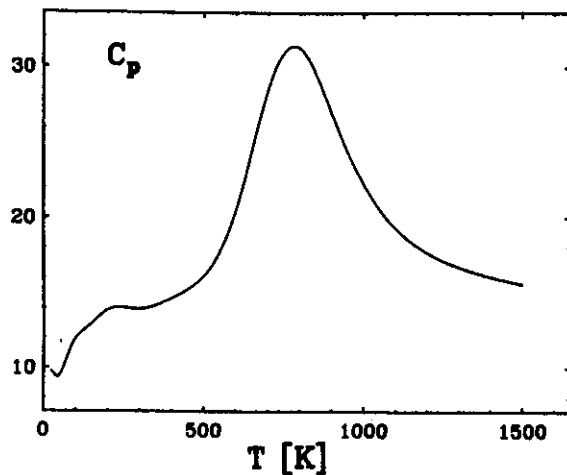


Fig. 3. Specific heat for the potential energy for a  $Na_8$  microcluster.

Recently<sup>6</sup>, we have applied this technique to the study of thermal properties of  $Na$  microclusters. One can treat the interaction among the ions and the effect of valence electrons in a  $Na$  microcluster by some suitably defined effective many-particle (not two-body) interactions among atoms only. In the range of temperatures we were interested in, the motion of the atoms can be treated fairly well at the classical level and consequently the procedure we sketched above can be applied in a straightforward manner. We have computed a wide range of properties, such as shape, bond lengths, momenta of inertia, rotational, vibrational and potential energies, density of states, specific heats, etc. in order to fully characterize the behaviour of the microcluster upon changing the temperature. We shall limit ourselves here to displaying only a couple of them. In this case we have introduced six pseudofriction coefficients, three for coordinates and three for the momenta (one for each cartesian direction). The motivation for this is to ensure that both the total angular momentum and its direction are not conserved quantities, and a sufficiently high randomness was induced. Also the couplings (6) were slightly modified in such a way as not to affect the center of mass coordinate and total momentum of the system, since we were only interested in the intrinsic properties of the cluster. The equations of motion in this case read (only for the  $x$ -components here)

$$\dot{x}_i = \frac{p_{xi}}{m} - \xi_x \left[ x_i^3 - \frac{1}{N} \sum_{k=1}^N x_k^3 \right], \quad \dot{p}_{xi} = -\frac{\partial H}{\partial x_i} - \zeta_x^3 \left[ p_{xi} - \frac{1}{N} \sum_{k=1}^N p_{xk} \right], \quad (7a, b)$$

$$\dot{\xi}_x = \beta \sum_{i=1}^N \left[ \frac{\partial H}{\partial x_i} x_i^3 - 3 \frac{N-1}{N} T x_i^2 \right], \quad \dot{\zeta}_x = \alpha \left[ \sum_{i=1}^N p_{xi}^2 - (N-1)T \right]. \quad (7c, d)$$

In spite of the relatively small number of particles in a microcluster its properties are rather complex. One of the most spectacular features is the coexistence of liquid and solid phases and the occurrence of phase transitions. In Fig. 3 the specific heat (for the potential energy  $U$  only) for a  $Na_8$  cluster is shown. One can see the presence of two peaks, a smaller, less defined one around 200 K, corresponding to a transition to a "molten" or "glassy" state, and a bigger one around 700-1000 K, corresponding to the "melting" of the cluster. From the runs at about ten different temperatures, ranging from 25 to 1500 K we extracted the density of states (here for the potential energy only) in a rather wide range of excitation energies of the cluster, see Fig. 4. In each run we had  $10^6$  "measurements" (the total time of the trajectory between 200 psec for high  $T$  and 2000 psec for low  $T$ ). Using the fact that the distribution of the potential energy in a canonical ensemble is  $P(U, T) = \rho(U) \exp(-U/T) / Z(T)$ , where  $\rho(U)$  is the density of states and  $Z(T)$  is the partition function (for potential energy only) one can easily "measure"  $\rho(U)$  in a run, up to an arbitrary multiplication factor. One can fix the normalization of the density of states in several ways if that is required as well. One million configurations allowed us to define the density of states over essentially twelve orders of magnitude, in an energy interval around

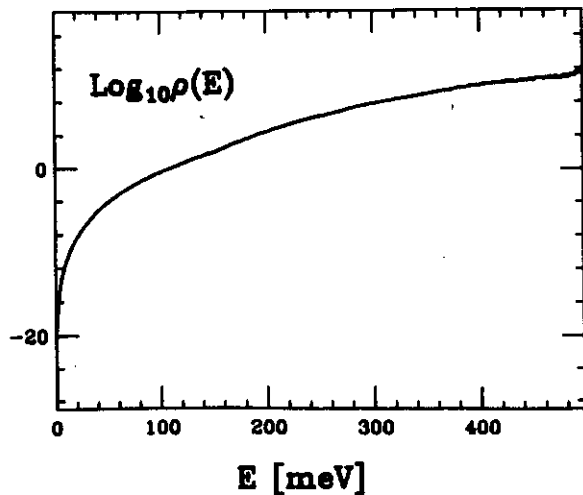


Fig. 4. The unnormalized density of states (potential energy only) for a  $Na_8$  microcluster as extracted from isothermal MD. At energies near 150 meV the logarithm of  $\rho(E)$  has a slight negative curvature. This is responsible for the occurrence of the phase transition.

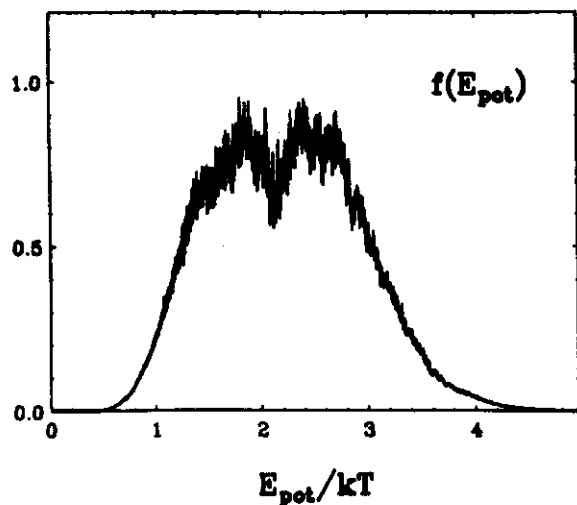


Fig. 5. The distribution of the potential energy at  $T = 820 K$  for  $Na_8$ . This type of double-humped structure is characteristic of the phase transition in microclusters and corresponds to the coexistence of a liquid and a solid phase.

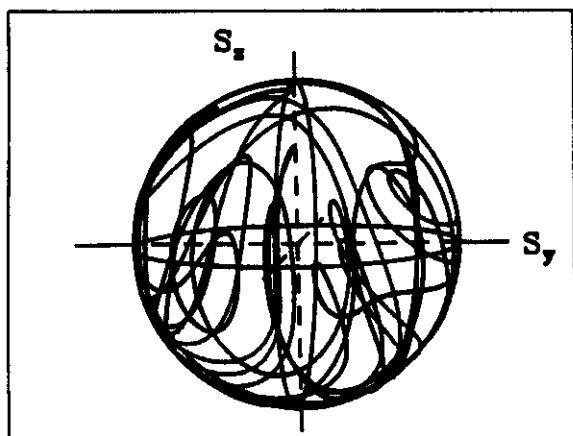


Fig. 6. Chaotic trajectory of a classical spin ( $SU(2)$ ) coupled to a thermal bath on the sphere  $S_2$ .

the average  $U(T)$ . By piecing together different portions of  $\rho(U)$  we defined the density of states with quite high accuracy for over more than 20 orders of magnitude. The same thing can be done rather accurately actually using only about half of these runs, over the same range of temperatures and of the same length. The knowledge of the density of states allows one to predict the thermal behaviour of the system. In contradistinction to an infinite system, the phase transitions are not sharp, however, they are quite well defined and amenable to observation. The distribution of (potential) energy can have a double-humped structure at temperatures around the phase transition, see Fig. 5.

In Refs. 4,10 we presented a generalization of the isothermal MD method to systems characterized by a compact phase space (e.g. classical limit of Lie algebras). The classical mechanics formalism in this case looks a bit unusual, there are "topological conserved" quantities, the Poisson brackets have the structure of Dirac brackets and the theory has a beautiful gauge structure. In spite of their exotic character, compact phase spaces appear quite often in different physical situations. In particular quantum mechanics can be cast into such a framework and this has proved extremely useful in some circumstances (e.g. large amplitude nuclear collective motion). In the case of a compact phase space one cannot define canonical variables globally, but instead one has to use different atlases. A naive attempt to directly apply the Nosé-Hoover scheme or our generalization of it to this case, by using local canonical variables, failed. Instead we have chosen a slightly different route<sup>2,10</sup> and managed to describe thermal properties of classical SU(2), SU(3) algebras and classical spin chains in this way. One possible form of the equations of motion which we investigated is

$$\dot{X}_i = J_{ij}(X) \left[ \frac{\partial H(X)}{\partial X_j} - h(\zeta) D_j(X) \right], \quad (i = 1, \dots, N), \quad (8a)$$

$$\dot{\zeta} = \alpha J_{ij}(X) \left[ \frac{\partial H(X)}{\partial X_i} D_j(X) - T \frac{\partial D_j(X)}{\partial X_i} \right], \quad (8b)$$

where  $X_i$  are the (noncanonical) phase space variables,  $J_{ij}(X)$  is the Poisson tensor, which defines the Poisson brackets,  $H(X)$  is the Hamiltonian of the system. The functions  $D_i(X)$  satisfy the constraints

$$\frac{\partial \dot{X}_i}{\partial X_i} = -h(\zeta) J_{ij}(X) \frac{\partial D_j(X)}{\partial X_i} \neq 0. \quad (9)$$

These equation of motion are compatible with the conservation of the following measure on the augmented phase space  $(X_1, \dots, X_N, \zeta)$

$$f(X, \zeta) = \mathcal{N} \exp \left\{ -\frac{1}{T} \left[ H(X) + \frac{g(\zeta)}{\alpha} \right] \right\}, \quad (10)$$

where  $h(\zeta) = dg(\zeta)/d\zeta$ . We display in Fig. 6 the chaotic trajectory of a classical spin, coupled to a thermal bath, on a  $S_2$  sphere. The time average of this trajectory reproduces the expected canonical distribution. As before, the number of



pseudofriction coefficients is arbitrary and should be chosen in such a way as to ensure ergodicity. However, the number of pseudofriction coefficients can influence rather strongly the convergence properties of the method. In Fig. 7 we have plotted the average internal energy as a function of the time of the simulation for an SU(3) Hamiltonian for the case of two and three pseudofriction coefficients. The scheme with three pseudofriction coefficients leads to a significantly quicker thermalization of the system.

The so-called XY-model is a spin lattice model and has been studied quite often in the past<sup>7</sup>. The potential energy for the XY-model is

$$V(\theta) = - \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j), \quad (11)$$

where  $\theta_i$  is the angle made by the spin  $i$  with some arbitrary direction in the plane and the sum is over all nearest-neighbor pairs on a square lattice with periodic boundary conditions. The equations of motion describing the isothermal dynamics in this case are here we have introduce a simple redefinition of  $\zeta, \xi$

$$\dot{\theta}_i = p_i - \frac{\beta}{NT} \xi \sin^3 \theta_i, \quad \dot{p}_i = - \frac{\partial V(\theta)}{\partial \theta_i} - \frac{\alpha}{NT} \zeta^3 p_i, \quad (12a, b)$$

$$\dot{\zeta} = \alpha \left[ \frac{1}{NT} \sum_i p_i^2 - 1 \right], \quad \dot{\xi} = \frac{\beta}{N} \left[ \frac{1}{T} \sum_i \frac{\partial V(\theta)}{\partial \theta_i} \sin^3 \theta_i - \sum_i 3 \sin^2 \theta_i \cos \theta_i \right]. \quad (12c, d)$$

In the case when  $\alpha, \beta \simeq O(1)$  the frequency of motion of the pseudofriction coefficients is comparable with the with the highest frequency mode of the spin system. We have investigated the cases  $\alpha, \beta \simeq O(1), O(\sqrt{N})$  and  $O(N)$ , where  $N$  is the total number of spins for  $16 \times 16$  and  $64 \times 64$  lattices. The algorithm described above was slightly modified by introducing a refreshing of the momenta every  $t = 64$  for the  $64 \times 64$  lattice<sup>9</sup>. The main reason for us to do this was the fact that in this particular type of coupling to the thermal bath the zeroth mode is not thermalized properly and one should modify the Eqs. (12) in the same spirit as we have done for the Na microclusters<sup>6</sup>, see Eqs. (7). We compared the results of the isothermal MD with standard hybrid Monte Carlo calculations<sup>8a</sup>. In Fig. 9 we present the autocorrelation function for the total magnetization at a temperature  $T = 1/4$ , below the phase transition, for the standard hybrid Monte Carlo method and the isothermal MD. The autocorrelation time versus the correlation length for the  $64 \times 64$  lattice for the total magnetization (Fig. 9) and one isolated spin (Fig. 10) were computed for the same two approaches. As one can judge from the presented results, the isothermal MD approach seems to perform extremely well. We also intend to compare these results with the improved hybrid Monte Carlo algorithm suggested in Ref. 8b.

One extension of these methods to real quantum problems is straightforward. In the summer of 1990, two undergraduate students worked under our supervision on the applicability of isothermal MD to the finite temperature path integral

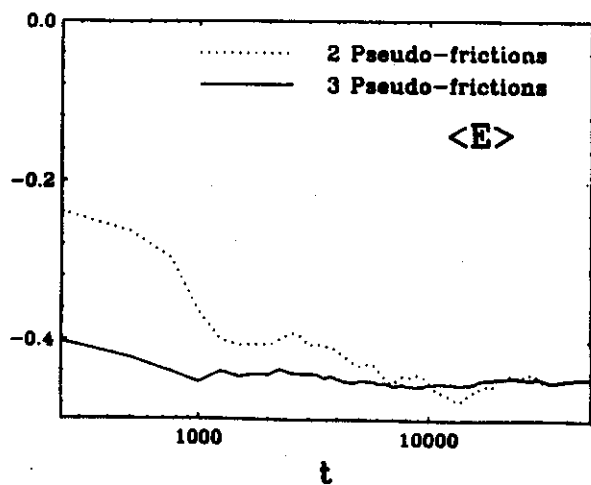


Fig. 7. Time evolution of the average energy  $\langle E \rangle$  for an  $SU(3)$  Hamiltonian using two (dots) and three (solid) pseudo-frictions. In general, convergence to the canonical ensemble can be achieved much sooner by using additional pseudo-frictions.

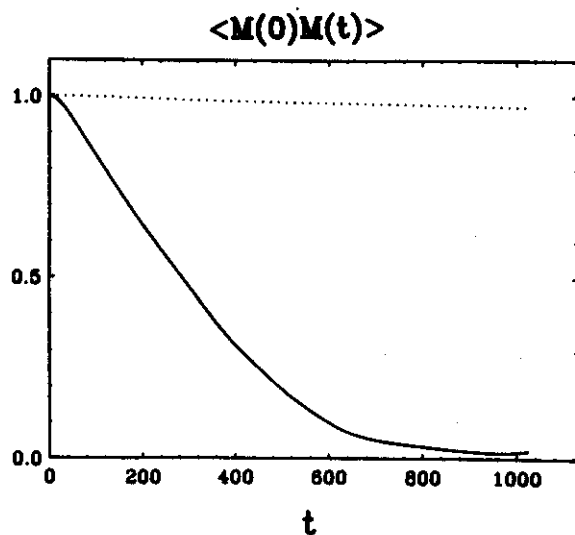


Fig. 8. XY-model auto-correlation function for the total magnetization using isothermal MD (solid) and standard hybrid Monte Carlo (dots). These results are for  $\beta = 4$  on a  $64^2$  lattice with 160K statistics.

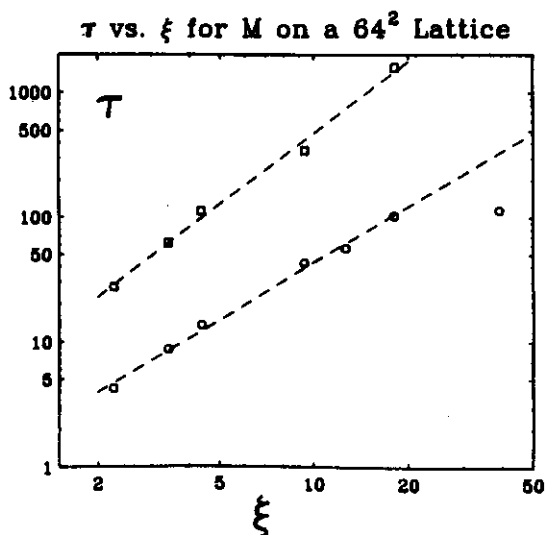


Fig. 9. Auto-correlation time versus correlation length for a  $64^2$  lattice. Isothermal MD (circles) methods have a noticeably smaller critical exponent and prefactor than standard hybrid Monte Carlo methods (boxes). (Results are preliminary, see Ref. 9 for details.)

description of the properties of a simple  $\text{Ne}_2$  system<sup>11</sup>. Quantum propagators expressed through a Feynman path integral become equivalent to a many-body classical partition function, and consequently the above methods can be applied without any modifications. It is likely that one can devise a completely different approach as well, by modifying the time dependent Schrödinger equation through the addition of a properly chosen “random” field and/or making it nonlinear and/or relinquishing the hermiticity of the Hamiltonian. These modifications of the Schrödinger equation are in the same spirit as the modifications of the classical Hamilton equations of motion we described earlier.

We did not discuss another extremely interesting extension of the MD techniques, namely the study of non-equilibrium phenomena. We shall only present an extension of the present ideology to the study of Brownian motion<sup>12</sup>. Almost anyone is familiar with the phenomenology of the Brownian motion in the Langevin description. The Newton equation of motion is modified by adding a dissipative term (friction) and a random force (usually white noise). Both these additional terms lead to an irreversible time evolution. There is a long standing argument on whether the equation of motion for a Brownian particle should have a dissipative and irreversible character; it does not seem that there is a consensus yet. In a way the presence of the two additional terms looks like overdoing things. The random force should account for whatever the surrounding molecules do to the Brownian particle and the friction term looks a bit superfluous. MD ideology should in principle be able to describe Brownian motion as well, especially if one intends to study transport and nonequilibrium phenomena. In Ref. 12 we have shown that one can develop a deterministic and time-reversal invariant description for a Brownian particle. Instead of the celebrated Langevin equation, we introduced the following equations of motion for a one-dimensional Brownian particle (unit mass  $m = 1$ )

$$\dot{q} = p, \quad \dot{p} = -\alpha\zeta^3 p - \beta\xi(p^2 - a) - \gamma\epsilon p^3, \quad (13)$$

$$\dot{\zeta} = p^2 - T, \quad \dot{\xi} = p(p^2 - a) - 2Tp, \quad \dot{\epsilon} = p^4 - 3Tp^2, \quad (14)$$

where, as before,  $T$  is the absolute temperature in energetic units and  $a, \alpha, \beta, \gamma$  are some arbitrary constants. These equations display a time-reversal invariance if the phase space coordinates change as  $q, p, \zeta, \xi, \epsilon \rightarrow q, -p, -\zeta, \xi, -\epsilon$  when  $t \rightarrow -t$ . The right hand side of the equation for the momentum can be interpreted as the “thermal” force exerted by the medium on the particle. In Fig. 11 we show a characteristic time dependence of this force. As one can see, it looks pretty random. Namely this feature ensures that the rms radius of a particle (initially at the origin) behaves like  $1/\sqrt{t}$  over long periods of time, see Fig. 12. At the same time, the momentum has an Boltzmann distribution as expected for a Brownian particle. We find it remarkable that a diffusion process can be described without any recourse to dissipation (time irreversibility) and/or random noise (non-deterministic element).

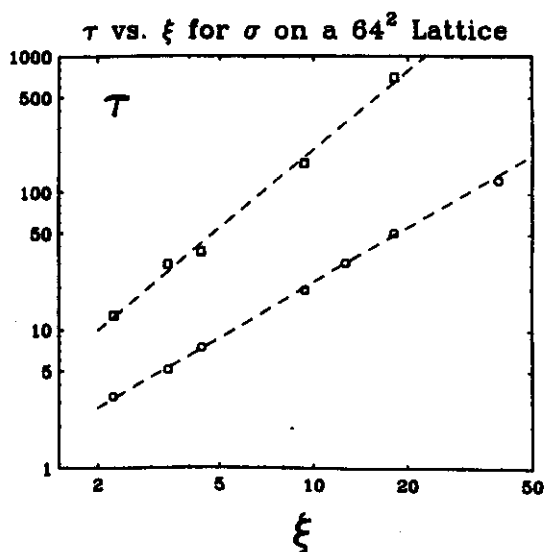


Fig. 10. Same as figure 9, except that auto-correlation times  $\tau$  are extracted from the single-spin auto-correlation function. As before, Isothermal MD (circles) methods have a noticeably smaller critical exponent and prefactor than standard hybrid Monte Carlo methods (boxes). (Results are preliminary, see Ref. 9 for details.)

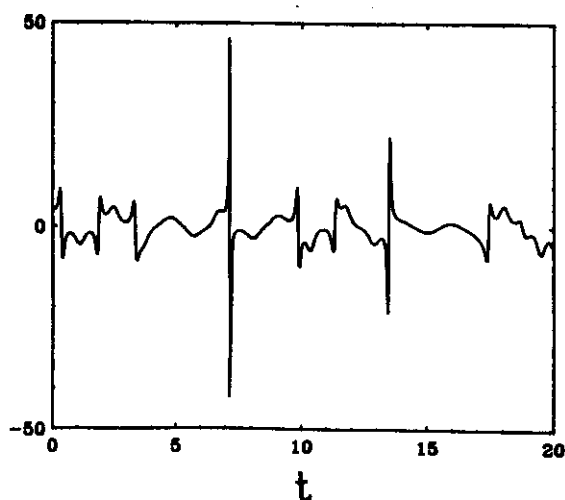


Fig. 11. Characteristic behavior of the (deterministic) friction force  $\dot{p} = F(t)$  for a Brownian particle, using equations (13).

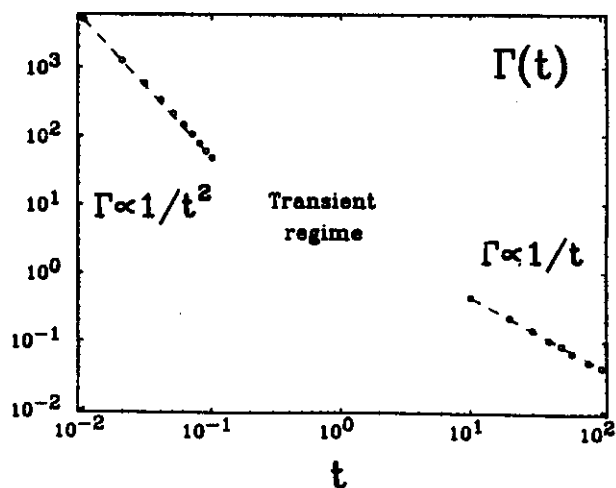


Fig. 12. Time dependence of the inverse width of the distribution  $f(q, t) = \sqrt{\Gamma(t)/\pi} \exp[-\Gamma(t)q^2]$  obtained by fitting to spatial distributions at selected times. The mean spreading velocity reaches its asymptotic behavior  $\sim \sqrt{t}$  for long times, characteristic for the Brownian particle.

We hope that our extremely short exposure of the isothermal MD techniques, gave the reader an idea about the huge potential of the MD techniques.

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