Hybrid Stochastic Differential Equations Applied to Quantum Chromodynamics

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(Received 18 October 1985)

Hybrid stochastic differential equations are applied to the thermodynamics of lattice gauge theory with dynamical fermions. The tuned algorithm is much more efficient than pure Langevin or molecular-dynamics equations. The method is applied to quantum chromodynamics and the abrupt finite-temperature crossover between hadronic matter and the quark-gluon plasma is elucidated.

PACS numbers: 11.15.Ha, 05.50.+q, 12.35.Cn

Among the most challenging problems in computer-simulation techniques are those involving dynamical fermions. Naive Monte Carlo simulation methods are not able to handle fermionic problems because they do not respect the antisymmetric character of fermion wave functions in a practical fashion. However, several new algorithms have been suggested for systems with dynamical fermions which appear to be practical in three and four dimensions. Two of those methods, the molecular-dynamics[1] and the Langevin equations,[2] are particularly promising since their convergence properties and errors, both systematic and statistical, can be understood in examples and can be monitored in large-scale simulations. It has recently been pointed out that there is a simple connection between these two algorithms and that hybrid algorithms exist which have superior properties to both original methods.[3]

The motivation for the hybrid algorithms is based on several simple observations. Consider a problem of one stochastic Bose degree of freedom q, an action $S(q)$, and ensemble averages

$$\langle F(q)\rangle = Z^{-1}\int dq\, F(q)\exp[-S(q)]. \tag{1}$$

Such averages are computed in a Langevin approach through the stochastic differential equation in a new "time" variable τ,

$$\dot{q}(\tau) = -\partial S/\partial q + \eta(\tau), \tag{2a}$$

where $\eta(\tau)$ is white noise,

$$\langle \eta(\tau)\eta(\tau')\rangle = 2\delta(\tau-\tau'), \tag{2b}$$

and $\langle\ \rangle$ indicates a time average. The expectation value of Eq. (1) is computed in this scheme as a time average,

$$\langle F(q)\rangle = \lim_{T\to\infty} T^{-1}\int_0^T F(q(\tau))\, dt. \tag{3}$$

In a numerical simulation Eq. (2) is evolved in time through discrete steps,

$$q_{n+1} = q_n + \Delta\xi_n - \tfrac{1}{2}\Delta^2 S(q_n), \tag{4a}$$

with

$$\xi_n\xi_{n'} = \delta_{nn'}, \quad \tau_{n+1}-\tau_n = \tfrac{1}{2}\Delta^2. \tag{4b}$$

The strength of the Langevin method is that the appearance of noise in the evolution equation guarantees that its long-time properties are correct; i.e., the path eventually covers all of phase space with the appropriate Boltzmann weight. Its problem is that the noise term $\Delta\xi_n$ tends to dominate the short-time evolution of the equation, so that the trajectory explores phase space slowly.

Another way to study the original system is through the molecular-dynamics algorithm of its microcanonical ensemble.[1] The equation of motion is purely deterministic,

$$\ddot{q}(\tau) = -\partial S/\partial q, \tag{5}$$

and Eq. (3) is employed again to calculate expectation values of observables. For discrete time steps, Eq. (5) becomes

$$q_{n+1} = 2q_n - q_{n-1} - \Delta^2 S'(q_n), \tag{6}$$

with $\tau_{n+1}-\tau_n = \Delta$. The strength of the molecular-dynamics approach is that for small times the trajectory samples phase space very efficiently since $q(\tau)$ follows the equation of motion deterministically. Its weakness lies in the fact that for long times $q(\tau)$ might fail to cover uniformly the energy shell of the microcanonical ensemble because of hidden conservation laws or the failure of the ergodic hypothesis.

Since the strengths of the Langevin and molecular-dynamics algorithms are complementary, it is sensible to seek a hybrid method.[3] If one rewrites Eq. (6) as

$$q_{n+1} = q_n + \tfrac{1}{2}(q_{n+1}-q_{n-1}) - \tfrac{1}{2}\Delta^2 S'(q_n), \tag{7}$$

then we note the following correspondences:

Langevin		Molecular dynamics
noise	$\leftrightarrow$	velocity
$\tau_{n+1}-\tau_n = \frac{1}{2}\Delta^2$	$\leftrightarrow$	$\tau_{n+1}-\tau_{n-1} = \Delta$

This correspondence suggests a one-parameter family of algorithms. In this "hybrid" scheme a time step will be executed by either the Langevin algorithm or the molecular-dynamics algorithm with a probability $p\Delta$,

$$q_{n+1}=q_n+\Delta v_n-\tfrac{1}{2}\Delta^2 S'(q_n), \tag{8a}$$

with

$$v_n=\begin{cases}(q_{n+1}-q_{n-1})/2\Delta, & \text{probability } p\Delta,\\ \xi_n, & \text{otherwise,}\end{cases} \tag{8b}$$

$$\tau_{n+1}-\tau_n=\Delta.$$

The algorithm can be optimized by a tuning of p so that the short-time evolution of the trajectory has the speed of the molecular-dynamics algorithm, while the long-time evolution has explicit randomness in it to insure the breaking of any hidden conservation laws and the validity of the erdogic hypothesis. A study of the Fokker-Planck equation yields a proof that Eq. (8) simulates the path integral Eq. (1) as long as $p\Delta\neq 1$.[3,4] For free fields, one can prove that the optimal $p\Delta$ is twice the characteristic frequency of the system.[3] For nontrivial systems, $p\Delta$ can be determined "experimentally" by a study of the time correlations of the observable of interest.

Recall the molecular-dynamics Lagrangean for lattice gauge theory with fermions,

$$L=\tfrac{1}{2}\sum_{n,\mu}\dot{U}_\mu^\dagger(n)\hat{P}\dot{U}_\mu(n)+\sum_{ij}\dot{\phi}_i^\dagger[A^\dagger(U)A(U)]_{ij}\dot{\phi}_j-\omega^2\sum_i\phi_i^\dagger\phi_i-\beta\sum(\mathrm{tr}UUUU+\mathrm{H.c.}), \tag{9}$$

where $A(U)$ is the hopping matrix of staggered fermions, $\hat{P}=\mathrm{diag}(1,1,0)$, and ϕ_i is a complex field residing on every other lattice site. The field ϕ_i and its kinetic energy involving $A^\dagger(U)A(U)$ were invented such that the molecular dynamics of L is that of SU(3) gauge fields coupled to four identical species of colored quarks which obey Fermi statistics.[1]

To implement the hybrid algorithm on Eq. (9), we use the fact that $\dot{U}$, $\dot{\phi}$, and ϕ appear in three quadratic terms. Therefore, at any time step in the evolution of the molecular-dynamics equations one can replace the $\dot{U}$ fields, say, by a completely new field configuration in the Boltzmann distribution $\exp(-\frac{1}{2}\sum\dot{U}\hat{P}\dot{U})$ by standard formulas. Similarly, $\dot{\phi}$ and ϕ can be replaced by new random fields in the appropriate distributions at chosen intervals. Some care must be exercised with $\dot{\phi}$ because of the matrix character of the second term in Eq. (9). Details such as these will be presented at length elsewhere.[4] Extensive tests and algorithm tuning on small asymmetric lattices which simulate finite temperatures were made. The expectation value of the pure-gauge-field action (the plaquette), the Wilson line (the exponential of the negative of the excess free energy for a heavy quark in the vacuum), $\langle\bar{\psi}\psi\rangle$ (the chiral-symmetry order parameter), and quark and gluon energy densities were measured. In Fig. 1 we show the time-correlation data for the Wilson line. The hybrid algorithm was run with a discrete time step $dt=0.02$ for 10000 sweeps on a 2×4^3 lattice, and noise was applied at regular intervals ranging from every step (Langevin) to every 1000 sweeps. Figure 1 shows that the minimum correlation time occurs when noise is applied every 50 ± 20 sweeps. Since $dt=0.02$, this corresponds to a "physical time" of 1 ± 0.4 unit. Note that the hybrid algorithm is more than 3.3 times as efficient as the Langevin limit. In fact, the correlation times for all the matrix elements could be reduced to 2 or 3 time units by application of noise to the system at intervals of 0.5–2 time units. This favorable result was also found on larger lattices, 4×8^3 and 6×10^3.

Next the algorithm was applied to the thermodynamics of quantum chromodynamics. The lattice theory was simulated on a 4×8^3 lattice with bare quark masses of 0.10, 0.075, and 0.050 so that zero-mass extrapolations could be done. Typically, 5000–15000 sweeps were made at each coupling β in the vicinity of the interesting phase transition. We expect a fluctuation-induced chiral-symmetry–restoring transi-

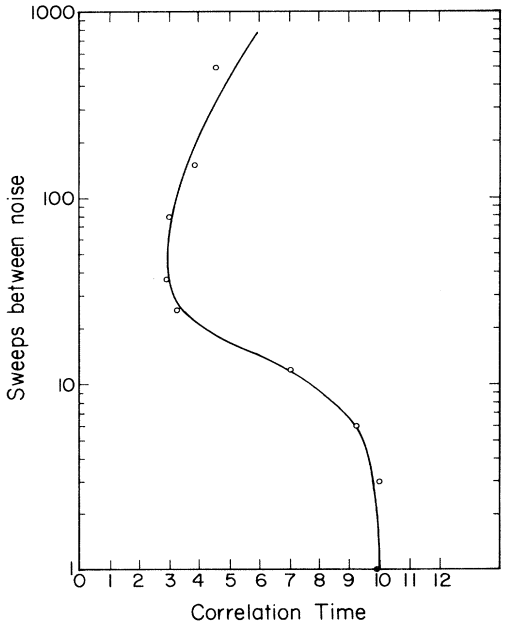

FIG. 1. Correlation time of the Wilson line vs the interval between Langevin steps.

tion in the continuum limit.[5] However, although the pure gauge field has a first-order deconfining phase transition signaled by a discontinuous Wilson line, that behavior should not persist in the theory with dynamical quarks because quark pairs screen long-range color forces at all temperatures. However, the chiral-symmetry–restoring transition could result in a discontinuous change in the dynamically generated quark mass which could affect the thermodynamics of the system dramatically. We located the critical couplings β for both the pure gauge theory and the full theory with light quarks. The pure gauge theory showed a clear first-order deconfining transition at $\beta = 5.725 \pm 0.025$, and the full theory with a bare quark mass of $m = 0.050$ had a chiral-symmetry–restoring transition at $\beta = 5.000 \pm 0.025$. The character of these transitions were compared by a search for metastable states as shown in Fig. 2. In Fig. 2(a) we show the time history of the Wilson line for the pure gauge theory at $\beta = 5.725$ for both a confined and an unconfined initial configuration. 10 000 sweeps of the algorithm were run with $dt = 0.02$ with noise applied every 0.75 time unit to the $\dot{U}$ fields. The two-state signal in Fig. 2(a) is clear evidence for a first-order transition. The same procedure was followed for the theory with light fermions at $\beta = 5.025$, and the evidence for a hard first-order transition is lost, as shown in Fig. 2(b). However, as shown in Fig. 3, the transition between the hadronic and quark-gluon phases is very abrupt—the energy density ϵ/T^4, for example, changes from 0.00 ± 5.00 to 42 ± 4.0 as β changes from 5.000 to 5.025. If asymptotic freedom applies to these data, the fractional change of the physical temperature over this β interval is only 3.8%. In an extended publication the simulation data at $m = 0.10$ and 0.075 will be used to extrapolate these curves to zero mass.[6] The statistics accumulated and the resolution in β are far superior to earlier simulations,[7] and they strengthen the controversial result that the finite-temperature transition in quantum chromodynamics is abrupt.

Clearly there is much room for further algorithm development and applications. The algorithm may be improved by acceleration of the time development of its infrared modes.[8] In addition, asymptotic freedom should be verified for lattice gauge theory with light fermions.

The authors thank D. K. Sinclair and J. Polonyi for

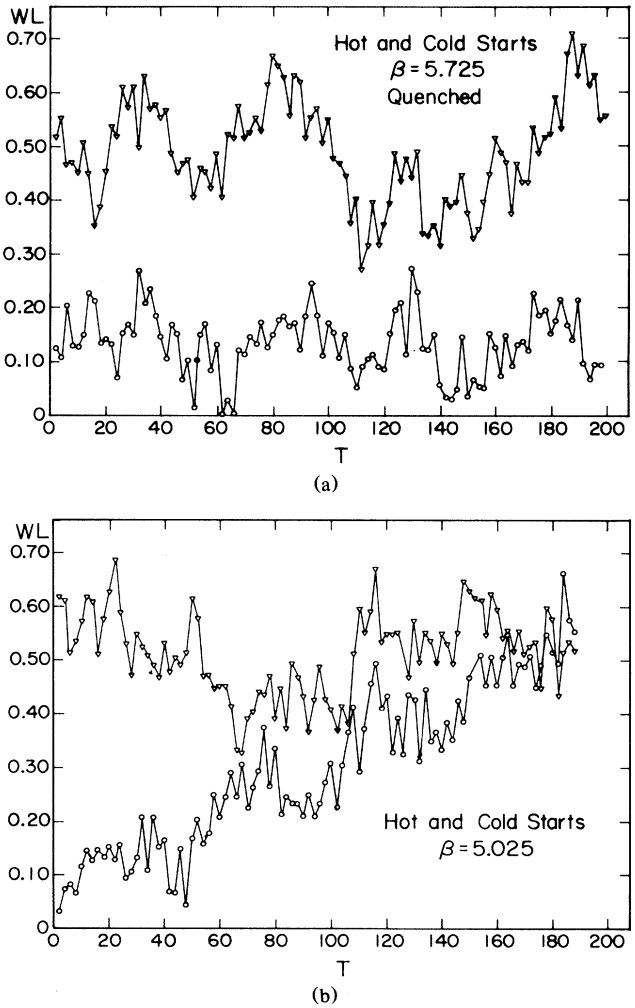

FIG. 2. (a) Coexistence of states at the deconfining phase transition in the pure gluon theory. (b) Same as (a) but with dynamical fermions having bare mass 0.050.

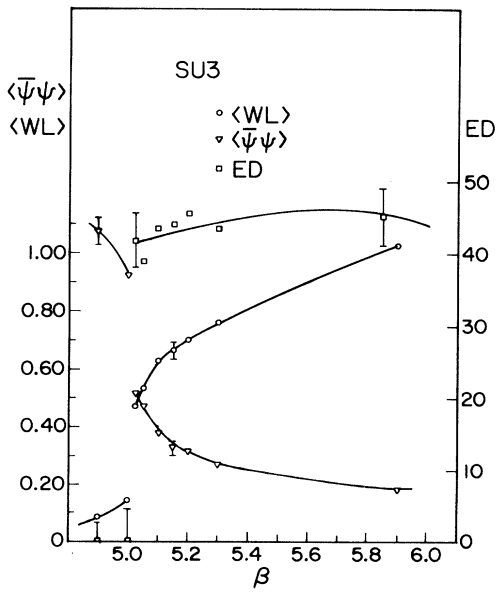

FIG. 3. Chiral-symmetry–restoring phase transition at finite temperature. The bare fermion mass is 0.050, and the Wilson line, $\langle\bar{\psi}\psi\rangle$, and total energy density ϵ/T^4 are plotted.

helpful conversations. The computer simulations described here were done at the National Center for Supercomputing Applications at the University of Illinois. One of us (J.B.K.) thanks the administrators and staff of this new facility for this opportunity and for their dedicated help. This work was supported in part by the National Science Foundation under Grant No. PHY82-01948.

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