Spin dynamics for the Lebwohl-Lasher model

Michael P. Allen

Department of Physics and Centre for Scientific Computing, University of Warwick, Coventry CV4 7AL, United Kingdom
(Received 21 May 2005; published 14 September 2005)

A spin dynamics algorithm, combining checkerboard updating and a rotation algorithm based on the local second-rank ordering field, is developed for the Lebwohl-Lasher model of liquid crystals. The method is shown to conserve energy well and to generate simulation averages that are consistent with those obtained by Monte Carlo simulation. However, care must be taken to avoid the undesirable effects of director rotation, and a method for doing this is proposed.

Many physical systems may be represented by the highly idealized model of a set of interacting classical spin vectors located on a regular, often cubic, lattice [1]. This paper considers a classical Hamiltonian of the form

$$H = \sum_{\langle j,k \rangle} h(\mathbf{s}_j \cdot \mathbf{s}_k) = \tfrac{1}{2} \sum_j \sum_{k \in N_j} h(\mathbf{s}_j \cdot \mathbf{s}_k), \qquad (1)$$

where the interaction energy is given by

$$h(\mathbf{s}_j \cdot \mathbf{s}_k) = -J\left(\tfrac{3}{2}(\mathbf{s}_j \cdot \mathbf{s}_k)^2 - \tfrac{1}{2}\right). \qquad (2)$$

In Eq. (1), the notation $\Sigma_{\langle j,k \rangle}$ indicates a sum over all nearest neighbor lattice sites j, k, considering each neighbor pair only once. Correspondingly, $\Sigma_{k \in N_j}$ denotes a sum over sites k that constitute the set N_j of nearest neighbors of j. Full periodic boundary conditions are assumed. The spins $\mathbf{s}_j$ are three-dimensional vectors of unit length, and the pair interaction has the form of a simple function h of the scalar product of the corresponding vectors. The case $h(\mathbf{s}_j \cdot \mathbf{s}_k) = -J\mathbf{s}_j \cdot \mathbf{s}_k$ is the well-studied classical Heisenberg model, which, for $J > 0$, exhibits a ferromagnetic ground state. Our interest lies in the model defined by Eq. (2), originally proposed by Lebwohl and Lasher [2,3] to represent the ordering in nematic liquid crystals. This model has been extensively studied by Monte Carlo simulations [1] in the canonical ensemble [4–6]. At high-temperature T, the system is disordered, while for $J > 0$ the low-temperature phase has aligned spins; the definition of an order parameter will be given below. The phase transition is known to be weakly first order. Brownian or Langevin dynamics have also been applied to this model [7–10]; here the approach of spin dynamics is considered.

The spin-dynamics equations of motion take the form [11]

$$\dot{\mathbf{s}}_j = \gamma \frac{\partial H}{\partial \mathbf{s}_j} \times \mathbf{s}_j \equiv \mathbf{\Omega}_j \times \mathbf{s}_j; \qquad (3)$$

the dot denotes time differentiation and $\times$ is the vector product. The local field $\partial H / \partial \mathbf{s}_j$ at spin j defines an instantaneous angular velocity of precession, $\mathbf{\Omega}_j$. The gyromagnetic factor γ, which converts energies into frequency units, will henceforth be set to unity. This dynamics conserves the individual spin lengths, as may be seen by considering the time derivative of $|\mathbf{s}_j|^2$,

$$\frac{d}{dt}|\mathbf{s}_j|^2 = 2\dot{\mathbf{s}}_j \cdot \mathbf{s}_j = 2(\mathbf{\Omega}_j \times \mathbf{s}_j) \cdot \mathbf{s}_j = 0.$$

The Hamiltonian is also conserved,

$$\dot{H} = \sum_j \frac{\partial H}{\partial \mathbf{s}_j} \cdot \dot{\mathbf{s}}_j = \sum_j \mathbf{\Omega}_j \cdot (\mathbf{\Omega}_j \times \mathbf{s}_j) = 0.$$

Finally, for the class of Hamiltonians of Eq. (1), the total magnetization $\mathbf{S} = \Sigma_j \mathbf{s}_j$ is also conserved,

$$\dot{\mathbf{S}} = \sum_j \dot{\mathbf{s}}_j = \sum_j \frac{\partial H}{\partial \mathbf{s}_j} \times \mathbf{s}_j = \sum_j \sum_{k \in N_j} h'(\mathbf{s}_j \cdot \mathbf{s}_k)\mathbf{s}_k \times \mathbf{s}_j = \mathbf{0}.$$

Here h' stands for the derivative of h with respect to its argument, and the right-hand side vanishes because every pair interaction is included twice: once as (j,k) and once as (k,j), and these cancel because $\mathbf{s}_k \times \mathbf{s}_j = -\mathbf{s}_j \times \mathbf{s}_k$.

An algorithm to simulate the spin dynamics of the Heisenberg model was developed independently by Frank *et al.* [12] and Krech *et al.* [13]. The set of all spins $\mathbf{s} \equiv \{\mathbf{s}_j\}$ is subdivided into two sublattices, A and B, in a checkerboard fashion. All spins on sublattice A interact only with their nearest neighbors, which are all on sublattice B, and *vice versa*. Formally, the generator of infinitesimal rotations of the whole set of spins may be decomposed into separate, noncommuting, matrices or operators that act on the corresponding sublattices. A time-reversible approximation to the full rotation operator acting over a finite time step may be formally written as

$$\mathbf{s}(\Delta t) \approx \mathcal{B}\left(\tfrac{1}{2}\Delta t\right)\mathcal{A}(\Delta t)\mathcal{B}\left(\tfrac{1}{2}\Delta t\right)\mathbf{s} + \mathcal{O}(\Delta t^3). \qquad (4)$$

The operator $\mathcal{A}(\Delta t)$ represents the rotation of the A spins in an external field caused by the neighboring fixed B spins, during a period Δt; similarly for $\mathcal{B}$. The algorithm proceeds in an alternating fashion: first, solving the dynamics of the spins on one sublattice, with the other sublattice spins held fixed; then *vice versa*, and so on. For the detailed justification of this algorithm, see [12,13].

For the Heisenberg model, this decomposition is especially convenient, since $\mathbf{\Omega}_j$ does not depend on $\mathbf{s}_j$, and the motion of spins on a sublattice $\dot{\mathbf{s}}_j = \mathbf{\Omega}_j \times \mathbf{s}_j$ with constant $\mathbf{\Omega}_j$ may be solved *exactly*. Set $\Omega_j = |\mathbf{\Omega}_j|$, and $\hat{\mathbf{\Omega}}_j = \mathbf{\Omega}_j / \Omega_j$ in the finite rotation formula [14] to give

$$\mathbf{s}_j(\Delta t) = (\hat{\mathbf{\Omega}}_j \cdot \mathbf{s}_j)\hat{\mathbf{\Omega}}_j + \sin(\Omega_j \Delta t)\hat{\mathbf{\Omega}}_j \times \mathbf{s}_j + \cos(\Omega_j \Delta t)[\mathbf{s}_j$$
$$- (\hat{\mathbf{\Omega}}_j \cdot \mathbf{s}_j)\hat{\mathbf{\Omega}}_j]. \tag{5}$$

This represents the practical implementation of one of the $\mathcal{A}$ or $\mathcal{B}$ substeps in Eq. (4).

For the Lebwohl-Lasher model of Eq. (2),

$$\mathbf{\Omega}_j = -3J \sum_{k \in N_j} (\mathbf{s}_j \cdot \mathbf{s}_k)\mathbf{s}_k,$$

the motion during one time step is no longer a simple rotation, because although the neighboring spins $\mathbf{s}_k$ are fixed, the moving spin $\mathbf{s}_j$ appears on the right. Krech *et al.* [13] propose an iterative approach to this problem; here a different method is adopted. The equation of motion of each spin is conveniently written as

$$\dot{\mathbf{s}}_j = \mathbf{\Omega}_j \times \mathbf{s}_j = -3J \sum_{k \in N_j} (\mathbf{s}_j \cdot \mathbf{s}_k)\mathbf{s}_k \times \mathbf{s}_j \equiv \mathbf{s}_j \cdot \mathbf{F}_j \times \mathbf{s}_j,$$

defining a tensor field at each lattice site due to the neighboring spins,

$$\mathbf{F}_j = -3J \sum_{k \in N_j} \left(\mathbf{s}_k \otimes \mathbf{s}_k - \tfrac{1}{3}\mathbf{1}\right).$$

A term $\frac{1}{3}\mathbf{1}$, where $\mathbf{1}$ is the unit tensor, is subtracted to make $\mathbf{F}_j$ traceless: this has no effect on the equations of motion since $\mathbf{s}_j \cdot \mathbf{1} \times \mathbf{s}_j = \mathbf{s}_j \times \mathbf{s}_j = \mathbf{0}$.

The above equation is well known in another context: the torque-free time evolution of the angular velocity of a rigid body, expressed in the frame of reference of the inertia tensor of the body itself [14]. The symmetric tensor $\mathbf{F}_j$ plays the role of the inertia, but it arises from a different mechanism here. A method for integrating this over a time step has been proposed [15]. It is convenient to resolve all the vectors in the principal axis system of $\mathbf{F}_j$. Denote the eigenvalues, in order $F_{j1} > F_{j2} > F_{j3}$, and the corresponding eigenvectors $\mathbf{1}_j, \mathbf{2}_j, \mathbf{3}_j$. These are taken to be mutually perpendicular and of unit length, and all the following vector and matrix expressions are expressed in this frame. It should be noted that the algorithm is independent of the sign ambiguity associated with these eigenvectors. $\mathbf{F}_j$ becomes diagonal, and the instantaneous angular velocity takes a simple form,

$$\mathbf{F}_j = \begin{pmatrix} F_{j1} & 0 & 0 \\ 0 & F_{j2} & 0 \\ 0 & 0 & F_{j3} \end{pmatrix}, \quad \Rightarrow \mathbf{\Omega}_j = \begin{pmatrix} s_{j1}F_{j1} \\ s_{j2}F_{j2} \\ s_{j3}F_{j3} \end{pmatrix}.$$

The equations of motion $\dot{\mathbf{s}}_j = \mathbf{\Omega}_j \times \mathbf{s}_j$ become

$$\dot{s}_{j1} = (F_{j2} - F_{j3})s_{j2}s_{j3}, \quad \text{and cyclic permutations.}$$

Consider the component involving F_{j1}, generating rotations about the $\mathbf{1}_j$ axis (the others are similar),

$$\dot{s}_{j1} = 0, \quad \dot{s}_{j2} = -F_{j1}s_{j1}s_{j3}, \quad \dot{s}_{j3} = F_{j1}s_{j1}s_{j2}.$$

During the action of this part of the field, the component s_{j1} remains constant, and the other two components are rotated about the $\mathbf{1}_j$ direction at an angular velocity $\Omega_{j1} = F_{j1}s_{j1}$. Suppose the generator of this infinitesimal rotation, for the A sublattice, is represented by the operator $\mathcal{A}_1$. This is com-

bined with the generators of rotations about the other two axes, and approximated over a finite interval in the following symmetric decomposition [15]:

$$\mathbf{s}(\Delta t) \approx \mathcal{A}_3\left(\tfrac{1}{2}\Delta t\right)\mathcal{A}_2\left(\tfrac{1}{2}\Delta t\right)\mathcal{A}_1(\Delta t)\mathcal{A}_2\left(\tfrac{1}{2}\Delta t\right)\mathcal{A}_3\left(\tfrac{1}{2}\Delta t\right)\mathbf{s}$$
$$+ O(\Delta t^3). \tag{6}$$

A similar approach is applied to the B-lattice updates. Each separate rotation is implemented with the finite rotation formula (5). In the above equation, the rotation $\mathcal{A}_1$ associated with the largest eigenvalue F_{j1} is centrally placed, and for brevity this is denoted the **32123** sequence; an empirical comparison with an alternative **12321** sequence is presented below.

Ordering in this model is measured by the symmetric and traceless second-rank tensor,

$$\mathbf{Q} = \frac{1}{N}\sum_{j=1}^{N} \left(\tfrac{3}{2}\mathbf{s}_j \otimes \mathbf{s}_j - \tfrac{1}{2}\mathbf{1}\right).$$

Note that this, like the Hamiltonian of Eqs. (1) and (2), is invariant to all spin flips $\mathbf{s}_j \rightarrow -\mathbf{s}_j$. The largest eigenvalue of $\mathbf{Q}$ is conventionally taken to be the order parameter Q, and the corresponding eigenvector $\mathbf{n}$ is the director.

A comparison with Monte Carlo simulations is facilitated by evaluating the "configurational temperature" introduced by Rugh [16], and specifically derived for orientational degrees of freedom by Chialvo *et al.* [17]. The relevant expression, in our notation, is

$$k_B T = \frac{\sum_j \langle |\hat{\mathbf{\nabla}}_j H|^2 \rangle}{\sum_j \langle \hat{\nabla}_j^2 H \rangle} = -\frac{1}{12}\frac{\sum_j \langle |\dot{\mathbf{s}}_j|^2 \rangle}{\langle H \rangle},$$

where $\hat{\mathbf{\nabla}}_j$ is the angular gradient, and $\hat{\nabla}_j^2$ the angular Laplacian, with respect to the orientation of spin j. The second expression above is specific to the Lebwohl-Lasher potential, and is easily obtained from Eq. (2). In the results reported below, Boltzmann's constant k_B, and the strength parameter J, are chosen to be unity.

In Fig. 1 simulation averages generated by the spin dynamics algorithm are compared with those produced by conventional Monte Carlo. A system size of $8 \times 8 \times 8$ spins is employed, which is sufficient to show interesting behavior in the phase transition region, while being economical. It is worth emphasizing that the aim is not to properly characterize the transition, for which much larger systems are required [4–6]. Spin dynamics runs of 20000 steps, each of length $\Delta t = 0.01$, starting from equilibrated Monte Carlo configurations, were carried out. Good agreement, within the statistical errors, is obtained with the Monte Carlo curves. This suggests that the sampling of the constant-energy hypersurface by spin dynamics generates satisfactory averages (but see later). Three state points, at $T \approx 1.5, 1.1, 0.7$, with order parameters $Q \approx 0.0, 0.5, 0.8$, representative of the disordered, transitional, and ordered states, respectively, were selected for further illustration.

The accuracy of the algorithm, as measured by the root-mean-squared fluctuation of the energy,
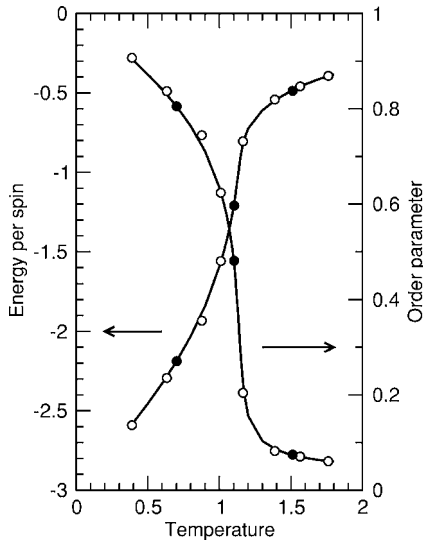
FIG. 1. Energy per spin, and nematic order parameter, as functions of temperature. Lines: Monte Carlo simulations. Circles: spin dynamics. Statistical errors are smaller than the plotting symbols. Filled symbols indicate state points studied in more detail below.

$$\Delta E_{\text{rms}} = \sqrt{\langle E^2 \rangle - \langle E \rangle^2},$$

is presented in Fig. 2: $\Delta E_{\text{rms}} \propto \Delta t^2$ over a wide range of Δt. For the largest time steps there is some drift in the energy (which is removed in the calculation of ΔE_{rms}). Within each sublattice rotation step, there are several choices for the se-
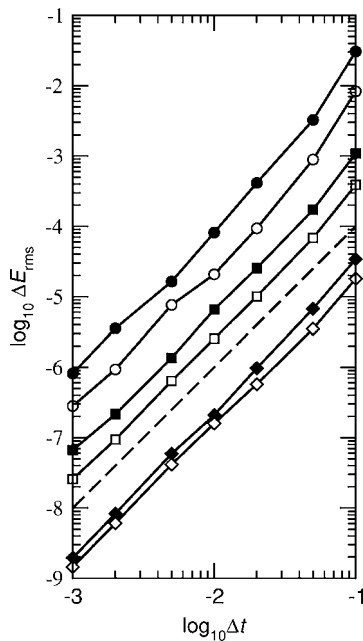

FIG. 2. Root-mean-squared energy fluctuations, plotted against the time step, on logarithmic scales. Circles: $T \approx 0.7$, $Q \approx 0.8$. Squares: $T \approx 1.1$, $Q \approx 0.5$ (displaced down by a factor of 10 for clarity). Diamonds: $T \approx 1.5$, $Q \approx 0$ (displaced down by a factor of 100 for clarity). Open symbols correspond to the rotation sequence **32123**; filled symbols to the sequence **12321** (see the text). The dashed line has gradient 2 for reference.
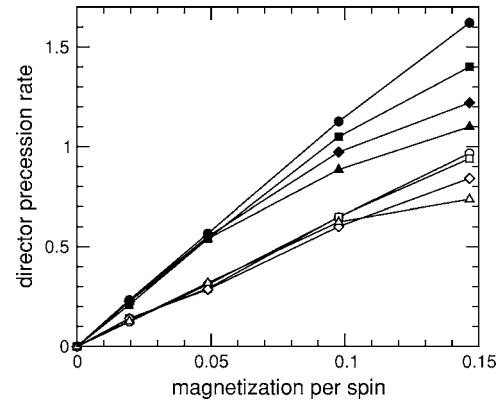

FIG. 3. Director rotation as a function of net magnetization per spin. Filled symbols: $T \approx 0.7$, $Q \approx 0.8$. Open symbols: $T \approx 1.1$, $Q \approx 0.5$. The director is inclined with respect to the magnetization vector by 30° (circles), 45° (squares), 60° (diamonds), and 90° (triangles).

quence of axes about which to carry out the rotations. The figure shows that the sequence **12321** (in which the axis corresponding to the *smallest* eigenvalue of $\mathbf{F}_j$ is placed centrally) is worse than the sequence **32123** of Eq. (6) (in which the *largest* eigenvalue is central) by a factor 2–3. Also, the low-temperature ordered state point exhibits worse energy conservation than the high-temperature, disordered state point, reflecting the larger torques resulting from the local field.

There are some caveats associated with spin dynamics applied to this model. First, as noted, the total magnetization is conserved exactly by the dynamics, and asymptotically by the algorithm as $\Delta t \to 0$. This is an artificial, physically meaningless, conservation law for the present model. The Hamiltonian, and the order parameter defined above, are invariant under all spin flips $\mathbf{s}_j \to -\mathbf{s}_j$, reflecting the symmetry of the nematic phase. However, the dynamics is not. If a spin is flipped, it will begin to rotate in the physically opposite direction. Macroscopic consequences come from this: in the ordered phase, the director rotates systematically about the fixed overall magnetization vector, if $\mathbf{S} = \Sigma_j \mathbf{s}_j$ is nonzero. This regular precession is superimposed on a general tendency of the director to become aligned with the magnetization vector: this happens slowly in the ordered phase, and more rapidly in the transition region. The rate of precession is shown in Fig. 3, for both the state points, and for a range of tilt angles of the director relative to the magnetization, at a range of net magnetizations obtained simply by flipping spins in an equilibrated Monte Carlo configuration. The precession rate is essentially independent of the tilt angle, and is proportional to both the order parameter Q and to the net magnetization per spin, as would be expected by considering the interaction between a typical spin and the local field.

This effect is a potential pitfall in simulations of these systems by spin dynamics. In a typical configuration of N spins, the net magnetization per spin will statistically be of order $1/\sqrt{N}$: this will produce a long-lived slow rotation of the director, which, if uncorrected, will dominate measured dynamical properties. If the magnetization is, for any reason, substantial, the fast director precession distorts the measured

simulation averages, such as configurational temperature. However, the solution to this problem seems relatively straighforward. Since the statistical properties of the Lebwohl-Lasher model are invariant to spin flips, it should be satisfactory to fix the system magnetization at the minimum possible magnitude, by flipping spins, at the start of a simulation run. In addition, once the director is aligned with the magnetization, the effects seem to be minimal.

In this paper, an algorithm for simulating the Lebwohl-Lasher model by spin dynamics has been presented. It remains to be seen whether this approach will lead to the determination of interesting "dynamical" properties of this model, and related models, and possibly to accelerated sampling of the transition region.

ACKNOWLEDGMENTS

[1] D. P. Landau and K. Binder, *A Guide to Monte Carlo Simulations in Statistical Physics* (Cambridge University Press, Cambridge, 2000), ISBN 0521653665.

[2] P. A. Lebwohl and G. Lasher, Phys. Rev. A **6**, 426 (1972).

[3] P. A. Lebwohl and G. Lasher, Phys. Rev. A **7**, 2222 (1973).

[4] G. R. Luckhurst and P. Simpson, Mol. Phys. **47**, 251 (1982).

[5] U. Fabbri and C. Zannoni, Mol. Phys. **58**, 763 (1986).

[6] Z. Zhang, M. J. Zuckermann, and O. G. Mouritsen, Mol. Phys. **80**, 1195 (1993).

[7] J. D. Ding and Y. L. Yang, Polymer **37**, 5301 (1996).

[8] Z. Bradač, S. Kralj, and S. Žumer, Phys. Rev. E **58**, 7447 (1998).

[9] C. Goze, R. Paredes, C. Vasquez, E. Medina, and A. Hasmy, Phys. Rev. E **63**, 042701 (2001).

[10] M. Svetec, Z. Bradač, S. Kralj, and S. Žumer, Mol. Cryst. Liq. Cryst. **413**, 43 (2004).

[11] S. H. Tsai, H. K. Lee, and D. P. Landau, Am. J. Phys. **73**, 615 (2005).

[12] J. Frank, W. Huang, and B. Leimkuhler, J. Comput. Phys. **133**, 160 (1997).

[13] M. Krech, A. Bunker, and D. P. Landau, Comput. Phys. Commun. **111**, 1 (1998).

[14] H. Goldstein, *Classical Mechanics* (Addison Wesley, Reading, MA, 1980), 2nd ed.

[15] A. Dullweber, B. Leimkuhler, and R. McLachlan, J. Chem. Phys. **107**, 5840 (1997).

[16] H. H. Rugh, Phys. Rev. Lett. **78**, 772 (1997).

[17] A. A. Chialvo, J. M. Simonson, P. T. Cummings, and P. G. Kusalik, J. Chem. Phys. **114**, 6514 (2001).