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Monte Carlo Molecular Dynamics Simulations for Two-Dimensional Magnets

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A combined Monte Carlo molecular dynamics simulation technique is used to study the *dynamic* structure factor on a square lattice for isotropic Heisenberg and planar classical ferromagnetic spin Hamiltonians.

KEY WORDS: Monte Carlo molecular dynamics; dynamic structure factor; Kosterlitz–Thouless transition, two-dimensional ferromagnets.

We have implemented[1] a *two*-dimensional version of a Monte Carlo molecular dynamics scheme previously used for classical one-dimensional spin systems. The Monte Carlo (MC) procedure is used for thermally equilibrated random initial spin configurations, and molecular dynamics is then applied to the equilibrated configurations to determine *dynamic* response functions, $S(\vec{q}, \omega)$ ($\vec{q}$ and ω are wave vector and frequency, respectively). In the preliminary work reported here we have used up to 32×32 size lattices, but much larger systems are now possible. For a 16×16 lattice we have typically used 10^4 MCS per spin, and a 4th order Runge–Kutta scheme for the molecular dynamics with time step 0.05 and total time 512×0.05. Averaging over 10 ensembles yielded acceptable statistics. For the MC, random numbers were generated[2] by the hardware (memory register) of our large-scale general purpose computer. We obtained excellent statistical tests of the random numbers with respect to uniformity, correlation, and period. This hardware-based scheme was approximately twice as fact as calling library software subroutines. In the future we hope that very high-speed computers will be purpose-designed to generate random numbers by the central processing unit.

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Dynamic simulations for *two*-dimensional spin models are currently very interesting because of the recent emergence of high quality quasi-two-dimensional magnetic materials, and particularly inelastic neutron scattering measurements for several of those materials. Systems include layered compounds (e.g., K_2CuF_4,[3] Rb_2CrCl_4,[4] and several $BaM_2(XO_4)_2$ compounds),[5] surfaces (e.g., lipid layers[6] or epitaxial systems), and magnetically intercalated graphites.[7] The dynamics is expected to be rich because of the intrinsic nonlinearity of the coupled spins, leading (depending on symmetry) to domain walls, topological vortex-like structures, and other strongly nonlinear excitations. For instance, in two-dimensional *easy-plane* symmetry ferromagnets a "topological" (Kosterlitz–Thouless, KT) phase transition is predicted at which vortex–antivortex pairs become unbound.[8] There is considerable evidence for such a transition from static thermodynamic measurements on quasi-two-dimensional magnets as well as mathematically equivalent physical problems (surface melting, superfluid helium films, etc.). However, the *dynamics* at such transitions has generally been elusive, even though we can anticipate extremely interesting influences from the nonlinear excitations—somewhat analogous to intrinsic mechanisms for soft modes and central peaks at structural phase transitions.[9]

As a preliminary application we have studied the Hamiltonian

$$\mathcal{H} = \sum_{(ij)} \{ S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z \} \tag{1}$$

where, with conventional notation, $\lambda = 0, 1$ corrsponds to planar (XY) and isotropic Heisenberg (H) limits, respectively. $\lambda = 1$ should show no KT behavior, whereas $\lambda = 0$ exhibits[10] a topological transition at T (temperature) $= T_{KT} \simeq 0.8$. Our simulations show a spin-wave dispersion for H consistent with $\omega \sim q^2$, whereas for XY, $\omega \sim q$ for $T \lesssim T_{KT}$. In the XY model we find strong evidence for a rapid spin-wave softening to $\omega \simeq 0$, as $T \to T_{KT}$ with spin-wave broadening for $T \gtrsim T_{KT}$. In the H limit there is no dramatic softening. Most interestingly, in the XY model for $S = S_{xx}$ or S_{yy}, there is no central weight observed for $T \lesssim T_{KT}$ but *above* the transition temperature at small finite $\vec{q}$, data fits suggest a "central peak" comprising an incompletely softened spinwave and a separate contribution centered at $\omega \simeq 0$ (cf the inelastic neutron scattering data reported in Ref. (4)).

Complete details of these and related results are given elsewhere,[1,11] together with a discussion of theoretical models and relevant experimental data.

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