Monte Carlo Simulations of Spin-Diffusion in a 2-D Heisenberg Paramagnet

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We study spin diffusion and spin waves in paramagnetic quantum crystals (solid $^3$He, for example) by direct simulation of a square lattice of atoms interacting via a nearest-neighbor Heisenberg exchange Hamiltonian. Recently, Cowan and Mullin have used a moments method to study spin transport at arbitrary polarizations. We test their analytic results by calculating the statistical spin correlation function from molecular dynamics simulations using a Monte Carlo algorithm to average over initial spin configurations. Since it is not practical to diagonalize the $S = \frac{1}{2}$ exchange Hamiltonian for a lattice which is of sufficient size to study long-wavelength (hydrodynamic) fluctuations, we instead study the $S \to \infty$ limit and treat each spin as a vector with a classical equation of motion. We compare our simulations with the assumptions of the moments method regarding the short-time behavior and the long exponential tail of the correlation function. We also present our numerical results for the polarization dependence of the longitudinal spin diffusion coefficient and the complex transverse spin diffusion coefficient.

1. INTRODUCTION

The Leggett-Rice (LR) equation was originally derived for paramagnetic Fermi fluids, but it has been shown that it applies to the spin dynamics of any polarized system interacting via quantum exchange. In the linear regime, the LR equation describes conventional diffusion of longitudinal Fourier modes $S^z \propto e^{i\mathbf{q}\cdot\mathbf{r}-D_\parallel q^2 t}$, where $D_\parallel$ is the longitudinal diffusion coefficient, as well as damped transverse spin waves $S^+ \equiv S^x + i S^y \propto e^{i\mathbf{q}\cdot\mathbf{r}-D^+ q^2 t}$, characterized by a complex diffusion coefficient $D^+$. The transverse diffusion coefficient can be written in terms of a bare diffusion coefficient as
\[ D^+ = \frac{D_\perp}{1 - i\mu M} \]  

where \( D_\perp \) is real and the denominator takes into account the precession of the spin current about the molecular field with quality factor \( \mu M = \text{Im}D^+/\text{Re}D^+ \).

Cowan and Mullin et al. (CM) have applied this description to the spin dynamics of paramagnetic \(^3\text{He}\) in its hcp phase, with a nearest-neighbor pair exchange Hamiltonian, and have used a moments method, originally due to Redfield and deGennes, to calculate the polarization dependence of the transport coefficients. At zero polarization \( P = 0 \) they found ordinary spin diffusion \((\mu M = 0, D_\perp = D_\parallel \sim \omega a^2)\), where \( \omega \) is the exchange frequency and \( a \) is the lattice spacing. For \( P \to 1 \) they found that all the transport coefficients diverge, but with \( D_\perp/\mu M \) finite, as one would expect for undamped spin waves. Over a wide range of \( P \) they found \( D_\perp \approx D_\parallel \), although the two diverge differently as \( P \to 1 \).

In order to test this picture we carried out a numerical study of spin diffusion on a 2d square lattice with the Hamiltonian

\[ H = -\sum_i BS_i^z - \sum_{i,j} JS_i \cdot S_j \]  

where the second sum is over nearest neighbors. We shall restrict our attention to the weakly paramagnetic case, with \( J/T \to 0 \) but \( B/T \) remaining finite. Since a lattice of \( N \) spins involves \( 2^N \) quantum states, it is not practical to diagonalize the \( S = \frac{1}{2} \) exchange Hamiltonian for a lattice which is of sufficient size to study long-wavelength (hydrodynamic) fluctuations. We instead study the \( S \to \infty \) limit and treat each spin as a vector \( S(r) \) with a classical equation of motion,

\[ \frac{d}{dt} S(r) = \omega \sum_{r'} S(r) \times S(r') \]  

where the sum is over nearest neighbors. For convenience, we have moved to the Larmor frame, and we set the exchange frequency \( \omega = J/\hbar \) and the vector magnitude of the spins \( |S| \) equal to 1. The longitudinal diffusion coefficient was calculated by simulating the motion of a hydrodynamic \((q \to 0)\) fluctuation \( S_q^z(t) \). We define the correlation function

\[ G_q^z(t) = \langle S_q^z(t)S_q^{z*}(0) \rangle \]  

which is assumed to have an exponential decay \( \propto e^{-D_q q^2 t} \) as \( t \to \infty \). The brackets indicate an average over initial conditions sampled from an equilibrium ensemble.
Fig. 1. Log plot of the longitudinal spin correlation function $G^z_q(t)$ at zero polarization. The slope is equal to $-D_\| q^2$ from which a value of $D_\| = 0.51 \pm 0.01$ (in units of $\omega \alpha^2$) is obtained. To the right, the short time behaviors of the first and second derivatives are also shown. For comparison, the dashed line in the $G''$ plot is the Gaussian ansatz used by CM.

2. NUMERICAL SIMULATIONS

We shall outline the procedure for calculating $D_\|$. First, an initial spin configuration was obtained by generating a lattice of randomly oriented spins $S_i$ with a Boltzmann distribution $e^{(B/T)S_i}$. The exchange energy was neglected in the Boltzmann factor, since in a weakly paramagnetic system the spins are basically uncorrelated, although their motion is not. The spin configuration was then allowed to evolve according to Eq.3 and the spin correlation function $G^z_q(t)$ was calculated from the definition Eq.4. The average was then performed over $N$ initial configurations were $N = 1000$ was typical. The size of the lattice was $L_x \times L_y = 64 \times 8$ spins with periodic boundary conditions. The length $L_x$ of the lattice was chosen so that the wave number $q = 2\pi/L_x = 0.098$ was small. To insure that the lattice was a 2-d system, $L_y$ was chosen so that the mean free time $\tau \equiv D_\|/(\omega \alpha)^2$ was shorter than the time $L_y^2/(D_\| \pi^2)$ to diffuse across the width of the lattice. The equation of motion was integrated with a second-order modified Euler method, with time step $\Delta t = 0.01$. The typical motion of a spin in a time step was half a degree or so. The conserved quantities such as the total energy, the polarization, and the individual spin magnitudes were found to be constant to a high degree of accuracy.

In Fig.1 the correlation function $G^z_q(t)$ is shown for $P = 0$. A similar
procedure was used to calculate $D_\perp$ and the quality factor $\mu M$ from $S_q^\perp$. Some typical results are shown in Fig. 2 for $P = 0.673$.

3. RESULTS AND DISCUSSION

The polarization dependence of the transport coefficients are shown in Fig.3-4. The results are very similar to results of CM obtained with a moments method. As expected, all the transport coefficients diverge as $P \to 1$, although $D_\perp/\mu M$ remains finite. There was no indication of anisotropy in the diffusion coefficients for $P < 0.8$. At higher polarizations the divergence of $D_\parallel$ required prohibitively large lattices and calculation times. This was not a problem in the transverse case, since $\text{Re}D^+ \to 0$ as $P \to 1$. Some disagreement with CM is expected since they considered a 3d spin-1/2 system using a mean field approximation. When our transport coefficients are plotted vs. $1 - P^2$ on a log-log plot the resulting curve fits are linear and indicate a divergence $\propto (1 - P^2)^{3.0\pm0.3}$. This disagrees with CM who found an exponent of $-1$ for the transverse coefficients and $-1/2$ for $D_\parallel$.

However, there is remarkable agreement at low polarization. For example, at zero polarization CM obtained $D_\parallel = D_\perp = 0.79$ for a 2d square lattice. This is higher than our value of 0.51, but when comparing classical and quantum results one should make the substitution $S^2 \to S(S + 1)$ with
Fig. 3. Polarization dependence of $D_{\parallel}$ (squares) and $D_{\perp}$ (triangles). The error bars are smaller than the size of the symbols, except for the two $D_{\parallel}$ points at $P > 0.8$. The inset shows $D_{\parallel}$ and the effective transverse diffusion coefficient $\text{Re}D^+$ for comparison with Fig.1 of Ref.5.

Fig. 4. Polarization dependence of the quality factor. The inset shows $\text{Im}D^+$. Obviously, $\text{Im}D^+ \approx P\omega a^2$. Since the spin wave frequency is $\text{Im}D^+ q^2$, this supports the notion of a molecular precessional field. It also agrees with the mean field results of CM, and agrees with the exact solution at $P = 1$. 

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$S = 1/2$. We omit the details of the analysis here, but this increases our value by a factor of $\sqrt{3}$ to 0.87. Also, for 3d hcp they obtain $\mu M/P = 2.3$ as $P \to 0$ which is higher than our value of 1.5. The quantum correction above cancels for this quantity, but from connectivity arguments, one would expect the molecular field in a 3d system to be stronger by a factor $\sqrt{3}$, which would increase our value to 2.3, in perfect agreement with CM.

Finally, our simulations with classical spin vectors support some of the assumptions of the moments method. For long times, hydrodynamic fluctuations were found to decay exponentially. For short times, the second derivative of the correlation function was well-described by a Gaussian ansatz and decayed on a time scale $\tau \equiv D_{\parallel}/(\omega a)^2$ (See Fig.1).

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