magnitude smaller than D_{param}. This fact has already been recognized qualitatively by Hirst and Kaplan.[14] Moreover, the sign of D_{ferro} is negative. This is so because there are two effects which contribute to the diffusion constant, as they do also to the stiffness parameter.[13] The first of these effects is the kinetic energy it costs to create a spatially dependent spin polarization. This effect gives rise to the second term in Eq. (27). The second effect is that the exchange interactions partially tend to compensate the change in kinetic energy. The first term in Eq. (27) is due to the latter effect. In a ferromagnet, the first effect dominates the second, thus making D_{ferro} negative. The following alternative argument also shows that the ferromagnetic diffusion constant is negative. Suppose that at a certain time the static ferromagnetic spin polarization is in the z direction at nearly every point in space, save for a small spatial region where it makes an angle θ with the z direction. Then, in the absence of a static magnetic field and additional relaxation mechanisms (i.e., described by T_2), the spin polarization will eventually make an angle θ with the z direction at every point in space due to diffusion and ferromagnetic exchange interactions.[15]

After this paper was submitted for publication, an article by Fulde and Luther appeared, where independently a similar problem was treated—however, from a different point of view.[16] Because of the fact that different approximations were used, a direct comparison with the work of these authors is not feasible.

[14] L. L. Hirst, Phys. Rev. **141**, 503 (1966); J. I. Kaplan, *ibid.* **143**, 351 (1966).

[15] For our theory to remain valid, we must require that the total effective relaxation time $T_2/(1+T_2Dq^2)$ be positive. This is satisfied under the usual experimental conditions.

[16] P. Fulde and A. Luther, Phys. Rev. **175**, 337 (1968).

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Spin and Energy Transport in Anisotropic Magnetic Chains with $S=\frac{1}{2}$*

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Spin and energy transport in spin-$\frac{1}{2}$ anisotropic magnetic chains with nearest-neighbor interactions are studied in the high-temperature limit. The analysis is based on a calculation of the zeroth, second, and fourth moments of the Fourier transforms of the spin and energy density correlation functions. Spin diffusion is predicted for sufficiently small values of the wave vector, except in the XY limit. Energy transport is nondiffusive for all values of the wave vector. Energy diffusion is predicted for chains with isotropic nearest-neighbor interactions and spin greater than $\frac{1}{2}$ as well as for spin-$\frac{1}{2}$ two-dimensional square lattices and three-dimensional simple and body-centered cubic lattices having isotropic nearest-neighbor interactions.

RECENTLY there has been considerable interest in the dynamical properties of spin-$\frac{1}{2}$ magnetic chains in the high-temperature limit.[1,2] This interest has been stimulated partly by the availability of computer calculations by Carboni and Richards[3] for isotropic systems with up to 10 spins and partly by the fact that the Hamiltonian in the XY limit (see below) can be transformed into that of a system of noninteracting fermions whose dynamical properties are easily analyzed.[4]

For the most part the calculations reported to date have focused on spin transport. It is known that spin transport is diffusive for small values of the wave vector k for an isotropic interaction.[1] The emphasis in this paper is on the complementary phenomenon of energy transport.[5] We will show that the energy transport remains nondiffusive in the $k\to 0$ limit. On the other hand, energy diffusion is present in chains with $S>\frac{1}{2}$ and in two- and three-dimensional lattices with $S=\frac{1}{2}$.

Our analysis is based on the Hamiltonian with nearest-neighbor interactions and periodic boundary conditions

$$\mathcal{H}(\alpha,\gamma)=\alpha\sum_{n=1}^{N}(S_x{}^nS_x{}^{n+1}+S_y{}^nS_y{}^{n+1})+\gamma\sum_{n=1}^{N}S_z{}^nS_z{}^{n+1}, \tag{1}$$

where the sum is over the N spins in the chain. $H(\alpha,0)$ is the Hamiltonian for the XY model, while $H(\alpha,\alpha)$ is the isotropic (Heisenberg) Hamiltonian. In the high-temperature region the dynamical behavior is most conveniently analyzed in terms of the spin and energy correlation functions $f_S{}^k(t)$ and $f_E{}^k(t)$, which are defined as follows:

$$f_{S,E}{}^k(t)=\frac{\mathrm{Tr}[A_{S,E}(-k)\exp(i\mathcal{H}t)A_{S,E}(k)\exp(-i\mathcal{H}t)]}{\mathrm{Tr}[A_{S,E}(-k)A_{S,E}(k)]}. \tag{2}$$

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[1] J. F. Fernandez and H. A. Gersch, Phys. Rev. **172**, 341 (1968).

[2] R. A. Tahir-Kheli and D. G. McFadden, Phys. Rev. **178**, 800 (1969).

[3] F. Carboni and P. M. Richards, Phys. Rev. **177**, 889 (1969).

[4] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N. Y.) **16**, 407 (1961).

[5] A. G. Redfield and W. N. Yu, Phys. Rev. **169**, 443 (1968).

Here Tr signifies the trace operation and the $A_{S,E}(k)$ are defined by the equations

$$A_S(k)=\sum_{n=1}^{N} e^{ikx_n}S_z^n, \tag{3}$$

$$A_E(k)=\tfrac{1}{2}\sum_{n=1}^{N} e^{ikx_n}[\alpha(S_x^nS_x^{n+1}+S_y^nS_y^{n+1}+S_x^nS_x^{n-1}+S_y^nS_y^{n-1})+\gamma(S_z^nS_z^{n+1}+S_z^nS_z^{n-1})]. \tag{4}$$

It is seen that $A_S(k)$ and $A_E(k)$ are the Fourier transforms of the spin and energy density operators, respectively.

We introduce the Fourier time transforms of $f_{S,E}^k(t)$ by means of the equation

$$f_{S,E}^k(t)=\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t}F_{S,E}(k,\omega). \tag{5}$$

The dynamical behavior is reflected in the moments of $F_{S,E}(k,\omega)$

$$\langle\omega^{2n}\rangle_{S,E}^k=\int_{-\infty}^{\infty} d\omega\, \omega^{2n}F_{S,E}(k,\omega). \tag{6}$$

The moments of $F_S(k,\omega)$ are easily calculated from equations given in Ref. 5:

$$\langle\omega^0\rangle_S^k=1, \tag{7}$$

$$\langle\omega^2\rangle_S^k=2\alpha^2\sin^2(\tfrac{1}{2}ka), \tag{8}$$

$$\langle\omega^4\rangle_S^k=6\alpha^4\sin^4(\tfrac{1}{2}ka)+\alpha^2\gamma^2\sin^2(\tfrac{1}{2}ka), \tag{9}$$

where a is the lattice parameter. The calculation of the moments of the energy density function is tedious but straightforward. The results are

$$\langle\omega^0\rangle_E^k=1, \tag{10}$$

$$\langle\omega^2\rangle_E^k=\frac{2\alpha^2(\alpha^2+2\gamma^2)}{2\alpha^2+\gamma^2}\sin^2(\tfrac{1}{2}ka), \tag{11}$$

$$\langle\omega^4\rangle_E^k=\frac{4\alpha^2(\alpha^4+4\alpha^2\gamma^2+\gamma^4)}{2\alpha^2+\gamma^2}\sin^4(\tfrac{1}{2}ka). \tag{12}$$

The relation of the moments to the dynamical behavior is displayed in the moment fluctuation ratios $R_{S,E}(k)$,[6]

$$R_{S,E}(k)=(\langle\omega^2\rangle_{S,E}^k)^2/[\langle\omega^4\rangle_{S,E}^k-(\langle\omega^2\rangle_{S,E}^k)^2]. \tag{13}$$

When $R_{S,E}(k)\ll 1$, the transport is diffusive, and when $R_{S,E}(k)\gg 1$, weakly damped wave propagation predominates. The appropriate ratios are

$$R_S(k)=\frac{4\sin^2(\tfrac{1}{2}ka)}{2\sin^2(\tfrac{1}{2}ka)+(\gamma/\alpha)^2}, \tag{14}$$

$$R_E(k)=\frac{\alpha^2(\alpha^2+2\gamma^2)^2}{\alpha^6+5\alpha^4\gamma^2+2\alpha^2\gamma^4+\gamma^6}. \tag{15}$$

For $\gamma\neq 0$, $R_S(k)\approx 0$ when $ka\ll|\gamma/\alpha|$, indicating diffusive behavior in the long-wavelength limit; and $R_S(k)\approx 4/[2+(\gamma/\alpha)^2]$ for $ka\approx\pi$, indicating a more complex transport process on a shorter spatial scale. For $\gamma=0$, $R_S(k)=2$, so that there are no diffuse modes for any value of k, as is to be expected for a gas of noninteracting particles.[7] On the other hand, $R_E(k)$ is independent of k and has the same value, 1, for $\gamma=0$ as it has for $\gamma=\alpha$. These two features together point to the absence of diffusion.[8]

The absence of energy diffusion appears to be limited to the spin-$\frac{1}{2}$ chain. We have calculated $R_E(k)$ for the two-dimensional square lattice and three-dimensional simple and body-centered cubic lattices with isotropic nearest-neighbor interactions and $S=\frac{1}{2}$ and have found that $R_E(k)\to 0$ as $k\to 0$. The moments for the chain with isotropic nearest-neighbor interactions and arbitrary spin have also been calculated. The moment fluctuation ratio has the value

$$R_E(k)=\frac{\sin^2(\tfrac{1}{2}ka)}{\sin^2(\tfrac{1}{2}ka)+\{\tfrac{1}{4}-\tfrac{3}{16}/[S(S+1)]\}}, \tag{16}$$

indicating diffuse propagation for $(ka)^2\ll 1-3/[4S(S+1)]$.

[6] H. S. Bennett, Phys. Rev. **174**, 629 (1968).

[7] K. Kawasaki, Ann. Phys. (N. Y.) **37**, 142 (1966).

[8] The function $F_E(k,\omega)$ can be computed in closed form for $\gamma=0$:

$$F_E(k,\omega)=[\pi|\alpha\sin(\tfrac{1}{2}ka)|]^{-1}[1-\omega^2/4\alpha^2\sin^2(\tfrac{1}{2}ka)]^{1/2},\quad |\omega|\le 2|\alpha\sin(\tfrac{1}{2}ka)|$$

$$F_E(k,\omega)=0,\quad |\omega|>2|\alpha\sin(\tfrac{1}{2}ka)|.$$