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Simulation of spin systems with Langevin dynamics

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Abstract. We propose a new method for the simulation of spin dynamics based on the Langevin equations and apply it to an anisotropic ferromagnet on the square lattice. Our method reproduces the temperature dependence of the magnetisation in the Monte Carlo method. The dynamical transverse susceptibility $G(\boldsymbol{q}, \omega)$ is calculated and the dispersion relation is obtained from the peak position of Im $G(\boldsymbol{q}, \omega)$. The dispersion relation at the lowest temperature follows the results in the linearised spin-wave theory. We also investigate the temperature dependence of the dispersion relation.

1. Introduction

Recently, many investigations for spin systems with competing interactions have been performed, and work using the Monte Carlo (MC) simulation has played an important role in combining theoretical suggestions and experimental results. However, only a few studies on the basis of dynamic simulation for spin systems have been reported (Walker and Walstedt 1977, Fujimoto *et al* 1987) and almost all of these are restricted to investigations at very low temperatures.

Here we devise a dynamic simulation for spin systems at a finite temperature using Langevin equations. In section 2, we present a method for numerical integrations of the Langevin equations. In section 3, we apply it to an anisotropic ferromagnet on the square lattice. We firstly show that the method reproduces well known results by other methods and then demonstrate that it is applicable to spin dynamics at finite temperatures. Section 4 is devoted to conclusions.

2. Method

We consider a classical Heisenberg model with anisotropic interactions:

$$H = -\sum_{\langle ij \rangle}[J_{ij}^{\parallel}\sigma_{iz}\sigma_{jz} + J_{ij}^{\perp}(\sigma_{ix}\sigma_{jx} + \sigma_{iy}\sigma_{jy})] - \sum_{i} \boldsymbol{\sigma}_i \cdot \boldsymbol{h}_i \tag{1}$$

where $|\boldsymbol{\sigma}_i| = 1$ and $\boldsymbol{h}$ is an external magnetic field which will vary in time and space. Now we start with the following Langevin equations:

$$\mathrm{d}\sigma_{il}(t)/\mathrm{d}t = \{H_{\mathrm{eff}}, \sigma_{il}\} - \Gamma_0\, \delta H_{\mathrm{eff}}/\delta\sigma_{il} + \zeta_{il}(t) \tag{2}$$

where σ_{il} is the lth component of a classical spin at site i and ζ_{il} is a Gaussian white noise with the following mean and variance:

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$$\langle \zeta_{il}(t) \rangle_\zeta = 0$$
$$\langle \zeta_{il}(t) \zeta_{jl'}(t') \rangle_\zeta = 2\tau\Gamma_0 \delta_{ij} \delta_{ll'} \delta(t - t') \tag{3}$$

where $\tau = k_B T$ (T and k_B are the absolute temperature and the Boltzmann constant, which is chosen as $k_B = 1$ hereafter, respectively) and random noise averages are expressed by $\langle \cdots \rangle_\zeta$. The $\{\cdot, \cdot\}$ means the Poisson bracket and $\{\sigma_{ix}, \sigma_{jy}\} = \gamma\sigma_{iz}\delta_{ij}$, $\{\sigma_{iy}, \sigma_{jz}\} = \gamma\sigma_{ix}\delta_{ij}$ and $\{\sigma_{iz}, \sigma_{jx}\} = \gamma\sigma_{iy}\delta_{ij}$, where γ is the magnetomechanical ratio.

We can readily show (Ma 1976) that (2) with the noise of (3) leads to the Boltzmann distribution of $P(\{\boldsymbol{\sigma}_i\}) \propto \exp(-H_{\text{eff}}/\tau)$ in the stationary limit, where $P(\{\boldsymbol{\sigma}_i\}; t)$ is the probability of finding a spin configuration of $\{\boldsymbol{\sigma}_i\}$ at time t and

$$P(\{\boldsymbol{\sigma}_i\}) = \lim_{t \to \infty} P(\{\boldsymbol{\sigma}_i\}; t).$$

However, (2) does not assure the constraint $|\boldsymbol{\sigma}_i(t)| = 1$ for all i and t. Here, instead of the correct constraint, we impose a rather weak constraint:

$$\langle |\boldsymbol{\sigma}_i| \rangle = 1 \qquad \text{for all } i \tag{4}$$

where $\langle \cdots \rangle$ means a long-time average. To ensure the constraint, a weight function W is added to the original Hamiltonian. Now the Hamiltonian used in our simulation is expressed as

$$H_{\text{eff}} = H + W \tag{5}$$

with

$$W = \sum_i (\tfrac{1}{2} r |\boldsymbol{\sigma}_i|^2 + \tfrac{1}{8} u |\boldsymbol{\sigma}_i|^4). \tag{6}$$

Therefore in this model there are fluctuations of the magnitudes of individual spins. We choose u as a positive constant. The larger u is chosen to be, the smaller the fluctuations which result. It is seen, however, that there is an upper limit of u determined from the magnitude of the discreteness of time for numerical integrations, as mentioned later. We consider r as a chemical potential for $\Sigma_i |\boldsymbol{\sigma}_i|^2$ and determine it so as to satisfy the condition

$$\left\langle \sum_i |\boldsymbol{\sigma}_i|^2 \right\rangle = N. \tag{7}$$

Since we do not know *a priori* the value of r, we simultaneously determine it while numerical integrations of (2) are performed. To do this, we change r according to the following equation:

$$\frac{1}{\Gamma_0} \frac{\mathrm{d}r}{\mathrm{d}t} = \frac{1}{N} \sum_i |\boldsymbol{\sigma}_i|^2 - 1. \tag{8}$$

Next we proceed to the details of numerical integrations. Using equations (1) and (6), each term in (2) is expressed as follows:

$$\{H_{\text{eff}}, \sigma_{il}\} = \gamma [\boldsymbol{\sigma}_i \times \boldsymbol{h}_{i\text{eff}}]_l \tag{9}$$

$$-\frac{\delta H_{\text{eff}}}{\delta \sigma_{il}} = \sum_j J_{ij}^l \boldsymbol{\sigma}_{jl} + h_{il} - r\boldsymbol{\sigma}_{il} - \tfrac{1}{2} u |\boldsymbol{\sigma}_i|^2 \sigma_{il} \tag{10}$$

where $\boldsymbol{h}_{i\text{eff}} = (\Sigma_j J_{ij}^{\perp} \sigma_{jx} + h_{ix}, \Sigma_j J_{ij}^{\perp} \sigma_{jy} + h_{iy}, \Sigma_j J_{ij}^{\parallel} \sigma_{jz} + h_{iz})$, $J_{ij}^x = J_{ij}^y = J_{ij}^{\perp}$, $J_{ij}^z = J_{ij}^{\parallel}$ and $\{W, \boldsymbol{\sigma}_i\} = 0$ for exterior products between parallel vectors.

First we perform numerical integrations using the Euler difference equations. Replacing $d\sigma_{il}/dt$ by $[\sigma_{il}(t+\Delta t)-\sigma_{il}(t)]/\Delta t$, (2) and (3) are rewritten as follows:

$$\sigma_{il}(t+\Delta t)=\sigma_{il}(t)+\Gamma_0\,\Delta t\,[(\gamma/\Gamma_0)(\boldsymbol{\sigma}_i\times\boldsymbol{h}_{i\mathrm{eff}})_l-\delta H_{\mathrm{eff}}/\delta\sigma_{il}+\xi_{il}(t)] \tag{11}$$

$$\langle\xi_{il}(k\,\Delta t)\rangle_\xi=0 \tag{12}$$

$$\langle\xi_{il}(k\,\Delta t)\xi_{jl'}(k'\,\Delta t)\rangle_\xi=[2\tau/(\Gamma_0\,\Delta t)]\delta_{ij}\delta_{ll'}\delta_{kk'}$$

where $\xi_{il}(t)\equiv\zeta_{il}(t)/\Gamma_0$ and we put

$$\delta(k\,\Delta t-k'\,\Delta t)\to\delta_{kk'}/\Delta t.$$

Similarly (8) is replaced by

$$r(t+\Delta t)=r(t)+\Gamma_0\,\Delta t\left(\frac{1}{N}\sum_i|\boldsymbol{\sigma}_i|^2-1\right). \tag{13}$$

From (11)–(13), we can perform numerical integrations using Gaussian random numbers with variance $2\tau/(\Gamma_0\,\Delta t)$ for $\xi_{il}(t)$-values with given values $\Gamma_0\,\Delta t$, γ/Γ_0 and u. We see from experience that there exists an upper limit of u for a given $\Gamma_0\,\Delta t$; unless $u\lesssim J/(2\Gamma_0\,\Delta t)$, numerical integrations become divergent where $J=\max\{J_{ij}^l\}$. In this paper, we mainly chose the following values for the parameters:

$$\Gamma_0\,\Delta t=1/100\qquad\gamma/\Gamma_0=10\qquad u=40\,J.$$

To see the validity of the method, we firstly calculate the magnetisation (versus T) of an anisotropic ferromagnet on the square lattice and compare it with that in the MC method. (We performed a MC simulation following Binder and Landau (1976).) The results are very different from the MC result. It is to be noted, however, that, if we drop the $\{H_{\mathrm{eff}},\sigma_{il}\}$ terms in (2), good agreement is obtained. Therefore a higher-order approximation is required in order to treat the precession terms $\{H_{\mathrm{eff}},\sigma_{il}\}$ precisely. Instead of the Euler difference, we use the simple Runge–Kutta method. Replacing $\sigma_{il}(t+\Delta t)$ in (11) by $\hat{\sigma}_{il}(t+\Delta t)$, $\sigma_{il}(t+\Delta t)$ in the simple Runge–Kutta method is obtained from

$$\sigma_{il}(t+\Delta t)=\sigma_{il}(t)+(\Delta t/2)[(\mathrm{d}\sigma_{il}/\mathrm{d}t)_{\{\sigma(t)\}}+(\mathrm{d}\sigma_{il}/\mathrm{d}t)_{\{\hat{\sigma}(t+\Delta t)\}}]. \tag{14}$$

The result in this method is in good agreement with the MC result (figure 1(*a*) later). Therefore we use (14) instead of (11). We see by experience that the condition for convergence $u\lesssim J/(2\Gamma_0\,\Delta t)$ in the Euler method is relaxed as $u\lesssim J/(\Gamma_0\,\Delta t)$ in the simple Runge–Kutta method.

3. Application to an anisotropic ferromagnet

We apply the method to a ferromagnet with anisotropic interactions ($J_{ij}^{\parallel}=J$, $J_{ij}^{\perp}=0.6J$, $J>0$, for nearest-neighbour pairs) on the square lattice with periodic boundary conditions. Hereafter r/J and u/J are simply described as r and u, respectively.

To examine the reliability of the method, we firstly calculate the magnetisations, the fluctuations of the magnitude of spins and the average value of r:

$$M_z\equiv\frac{1}{N}\left\langle\sum_i\sigma_{iz}\right\rangle\qquad M_x\equiv\frac{1}{N}\left\langle\sum_i\sigma_{ix}\right\rangle\qquad M_y\equiv\frac{1}{N}\left\langle\sum_i\sigma_{iy}\right\rangle$$

$$\mathrm{LSF}\equiv\frac{1}{N}\left\langle\sum_i(|\boldsymbol{\sigma}_i|^2-1)^2\right\rangle\qquad\mathrm{TSF}\equiv\left\langle\left(\frac{1}{N}\sum_i|\boldsymbol{\sigma}_i|^2-1\right)^2\right\rangle$$

$$\bar{r}=\langle r\rangle$$

for a lattice with $N = 20 \times 20$ and show these plotted against T in figure 1. The initial state is chosen to be $\boldsymbol{\sigma}_i = (1, 1, 1)/\sqrt{3}$ (for all i) and the temperature is gradually decreased from $1.2J$. At each temperature, after n_i steps per spin are discarded, data for $n_f - n_i$ steps per spin are used to average the physical quantities. We choose $n_i = 1500$ and $n_f = 3000$ for $u = 40$, and $n_i = 3000$ and $n_f = 4000$ for $u = 80$. Comparing the results with those for a smaller lattice, we find no remarkable size dependence at low temperatures, except for TSF. It seems that TSF is inversely proportional to N. The results for the two cases $u = 40$ and $u = 80$ are compared in figure 1 when the other parameters are fixed such as $\Gamma_0 \Delta t = 1/100$ and $\gamma/\Gamma_0 = 10$. As expected, the LSF becomes smaller when u becomes larger. Irrespective of the value of u, the LSF and TSF become smaller as the temperature is decreased. This is because the fluctuation becomes smaller as the temperature is reduced.

Now we investigate the spin-wave excitations at finite temperatures on the lattice with $N = 20 \times 20$. Here we use the parameters $\Gamma_0 \Delta t = 1/100$, $\gamma/\Gamma_0 = 10$ and $u = 40$. We tried two methods to extract the spin excitations, i.e. the dynamical transverse susceptibility $G(\boldsymbol{q}, \omega)$: one is to calculate the space–time Fourier transforms of spin–spin correlation functions obtained by the simulation; the other is to measure the response of a system against an external field. It turned out that, within the same computational time, scatterings of the results are smaller in the latter method than in the former method. Therefore we use the latter method and explain it in the following.

An external field which depends on space and time and is given by

$$\begin{aligned} h_{ix}(t) &= \delta h \cos(\boldsymbol{k} \cdot \boldsymbol{r}_i - \omega t) \\ h_{iy}(t) &= \delta h \sin(\boldsymbol{k} \cdot \boldsymbol{r}_i - \omega t)\, \mathrm{sgn}(M_z) \end{aligned} \qquad \text{for all } i \tag{15}$$

is applied, where $\boldsymbol{r}_i$ is the position vector at site i. The spin components induced by this field may be written as

$$\sigma_{ix}(t) = \delta\sigma_{ic}(\boldsymbol{k}, \omega) \cos(\boldsymbol{k} \cdot \boldsymbol{r}_i - \omega t) - \delta\sigma_{is}(\boldsymbol{k}, \omega) \sin(\boldsymbol{k} \cdot \boldsymbol{r}_i - \omega t) + \ldots . \tag{16}$$

The response functions are given by

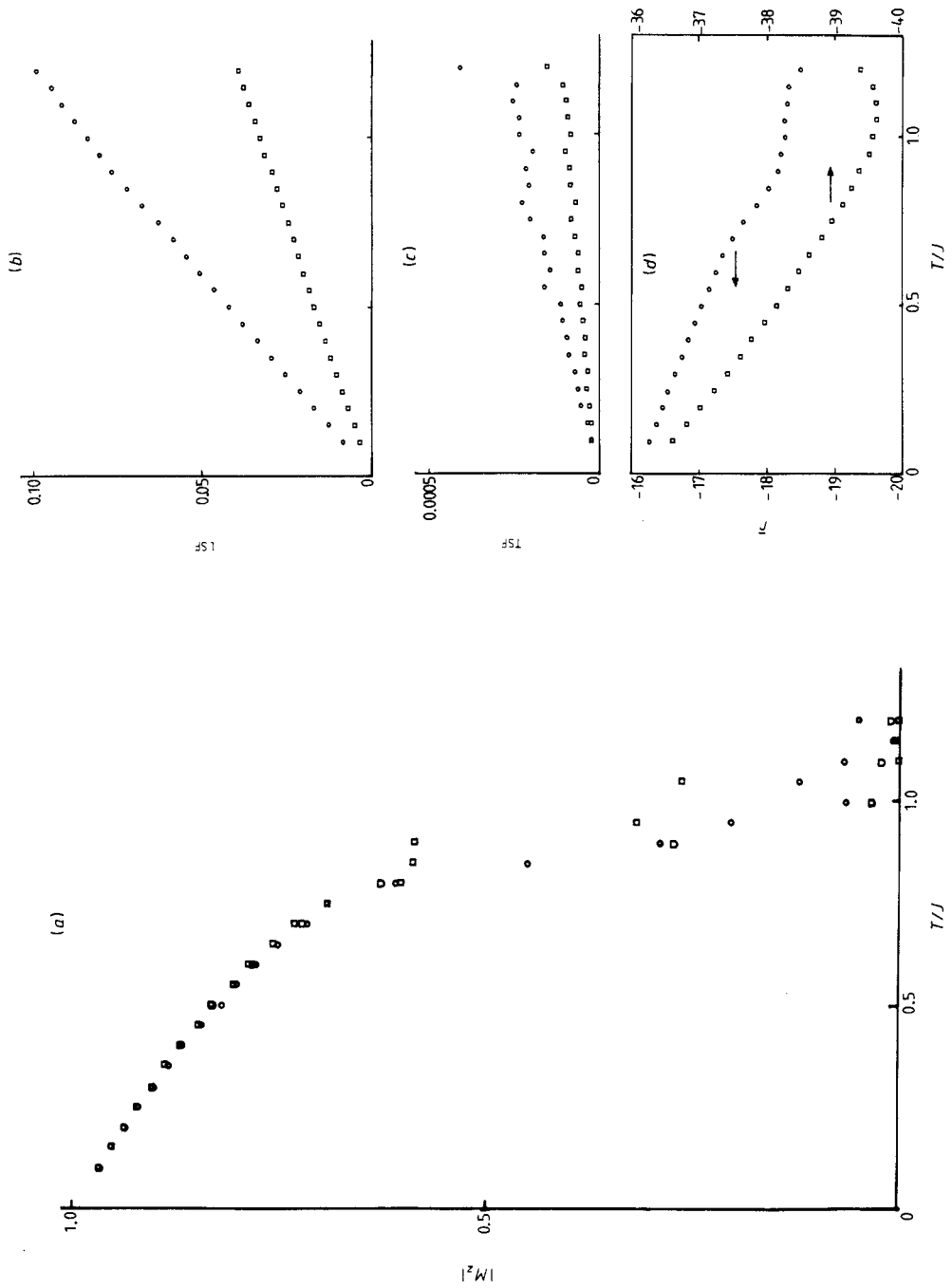
$$\begin{aligned} \mathrm{Re}\, G(\boldsymbol{k}, \omega) &= \frac{1}{N} \sum_i \frac{\langle \delta\sigma_{ic}(\boldsymbol{k}, \omega) \rangle}{\delta h} \\ \mathrm{Im}\, G(\boldsymbol{k}, \omega) &= \frac{1}{N} \sum_i \frac{\langle \delta\sigma_{is}(\boldsymbol{k}, \omega) \rangle}{\delta h}. \end{aligned} \tag{17}$$

The inverse participation rate (IPR) (Walker and Walstedt 1977), which is a measure of the extended or localised nature of the excitation, is defined by

$$\mathrm{IPR} = \sum_i \langle \delta\sigma_{is}(\boldsymbol{k}, \omega) \rangle^2 \Big/ \left(\sum_i |\langle \delta\sigma_{is}(\boldsymbol{k}, \omega) \rangle| \right)^2. \tag{18}$$

Values of IPR are O(1) and $O(N^{-1})$ for localised and extended modes, respectively.

Figure 1 (opposite). (*a*) The uniform magnetisation M_z, (*b*) LSF, (*c*) TSF and (*d*) $\bar{r}$ (versus T) in the two-dimensional anisotropic ferromagnet ($J_{ij}^{\parallel} = J$, $J_{ij}^{\perp} = 0.6J$ for the nearest-neighbour pairs). The results with $u = 40$ (○) and $u = 80$ (□) are shown with other parameters fixed as $N = 20 \times 20$, $\Gamma_0 \Delta t = 1/100$ and $\gamma/\Gamma_0 = 10$. In (*a*), the MC results ($N = 20 \times 20$) (∪) in the classical Heisenberg model are also shown.


(a)
(b)
(c)
(d)
$|M_z|$
LSF
TSF
T/J
1.0
0.5
0
0.10
0.05
0.0005
-16
-17
-18
-19
-20
-36
-37
-38
-39
-40

The calculation has been performed as follows: after the temperature has been decreased to the measured temperature, the field (15) is applied (δh was chosen to be $0.03J$ after several trials). The angular frequency of the field is chosen to be $\omega = 2\pi/(\Delta t\, n_{\rm cycl})$, where $n_{\rm cycl}$ is a positive integer. At each angular frequency, after $I_{\rm i} n_{\rm cycl}$ steps per spin are discarded to obtain a stationary state, data for $(I_{\rm f} - I_{\rm i})n_{\rm cycl}$ steps per spin are kept for Fourier analysis of (16).

The plots of Im G, Re G and IPR against ω/γ for several $\boldsymbol{k}$-values at $T = 0.05J$ and $0.65J$ are shown in figures 2 and 3. Even at the lowest temperature, Im G has a peak with a larger half-width for a larger $|\boldsymbol{k}|$, but this is understood by noting that $\delta H_{\rm eff}/\delta\sigma_{-kx} \simeq (c_1 + c_2|\boldsymbol{k}|^2)\sigma_{kx} + \cdots$, $c_1, c_2 > 0$, for $|\boldsymbol{k}| \ll 1$. The resonance frequencies $\omega_{\rm c}/\gamma$ are determined from the peak points of the values of Im G, or from the zero points of the values of Re G. At $T = 0.05J$, IPRs for all $\boldsymbol{k}$-values become $1/N\,(=0.0025)$ at $\omega = \omega_{\rm c}$. At higher temperatures, the decrease in IPR at $\omega = \omega_{\rm c}$ becomes smaller for larger $|\boldsymbol{k}|$. In figure 4, the values of $\omega_{ck}(T)/\omega_{ck}(0)$ for several $\boldsymbol{k}$-values are shown against T with the magnetisation curve, where $\omega_{ck}(0)$ is the resonance frequency of the linearised spin-wave theory, i.e. $\omega_{ck}(0)/\gamma = 4J[1 - \eta\hat{\gamma}(\boldsymbol{k})]$, $\hat{\gamma}(\boldsymbol{k}) \equiv [\cos(k_x a) + \cos(k_y a)]/2$, where a is a lattice constant. At the lowest temperature, our results are in good agreement with those of the spin-wave theory. As seen in figure 4, the temperature dependence of $\omega_{ck}(T)/\omega_{ck}(0)$ for $\boldsymbol{k} = ((2/5a)\pi, 0)$ is in agreement with that of the magnetisation for $T \lesssim 0.8J$. (We could not obtain clear results for $T \geqslant 0.95J$ within the same computational time as for $T \leqslant 0.80J$.) The values of $\omega_{ck}(T)/\omega_{ck}(0)$ for $\boldsymbol{k} = (0, 0)$ and $((4/5a)\pi, 0)$ are smaller and larger than that for $\boldsymbol{k} = ((2/5a)\pi, 0)$, respectively.

Theoretically, the RPA Green function method (Tyablikov 1959) predicted the dispersion relation $\omega_{ck}(T)/\gamma = 4JM_z[1 - \eta\hat{\gamma}(\boldsymbol{k})]$ at finite temperatures, but this result cannot explain our results of the $\boldsymbol{k}$-dependence of $\omega_{ck}(T)/\omega_{ck}(0)$. Lines (1971) insisted that the M_z in the above equation should be replaced by $\hat{\xi}_k(T) = (\langle\sigma_{iz}\sigma_{i+Rz}\rangle)^{1/2}$, $|\boldsymbol{R}| \simeq 2\pi/|\boldsymbol{k}|$. This qualitatively explains the $\boldsymbol{k}$-dependence of $\omega_{ck}(T)/\omega_{ck}(0)$, because $\hat{\xi}_k(T)$ increases as $|\boldsymbol{k}|$ increases. However, the Lines assumption does not agree with our results, because $\hat{\xi}_k(T) \to M_z$ for $|\boldsymbol{k}| \to 0$ in the Lines assumption, while $\omega_{ck=0}(T)/\omega_{ck=0}(0)$ in our simulations is obviously smaller than M_z.

4. Conclusions

We have proposed a new method of analysing the spin dynamics of the classical Heisenberg model. Our method is based on a Langevin equation of motion which contains both a dissipative term and a noise term representing thermal disturbances of spins. Thus the method is applicable to the system at finite temperatures. We have shown that the method reproduces the static magnetisation curve of the MC method fairly well.

Our method has been applied to the dynamics of an anisotropic ferromagnet on the square lattice. At a very low temperature, our results are in good agreement with those of the spin-wave theory. As the temperature is increased, the resonance frequency $\omega_{ck}(T)$ for every wavevector $\boldsymbol{k}$ decreases monotonically. This is consistent with a well known result of the RPA theory in which $\omega_{ck}(T)/\omega_{ck}(0) = M_z(T)$, where $M_z(T)$ is the magnetisation per lattice site. Our results predicted a $\boldsymbol{k}$-dependence of $\omega_{ck}(T)/\omega_{ck}(0)$ which is qualitatively in agreement with the Lines' suggestions in which $M_z(T)$ should be replaced by the square root of the two-spin correlation function $(\langle\sigma_{iz}\sigma_{i+Rz}\rangle)^{1/2}$, $|\boldsymbol{R}| \simeq 2\pi/|\boldsymbol{k}|$. Our results also predict a problem that $\omega_{ck}(T)/\omega_{ck}(0)$ for $|\boldsymbol{k}| = 0$ is smaller than $M_z(T)$ at finite temperatures.

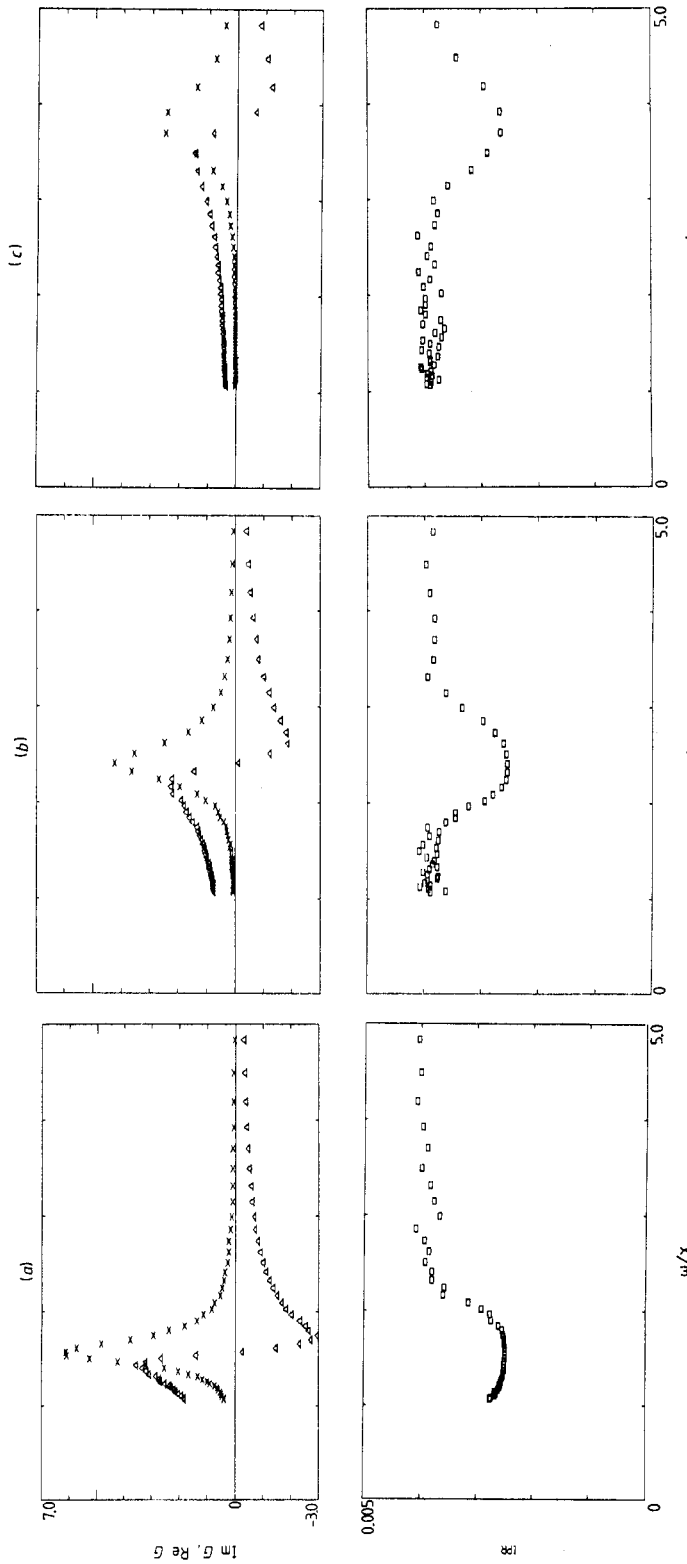


Figure 2. Im G (×), Re G (△) and IPR (□) against ω/γ (in units of J) at $T = 0.05J$ for (*a*) $\boldsymbol{k} = (0, 0)$, (*b*) $\boldsymbol{k} = ((2/5a)\pi, 0)$ and (*c*) $\boldsymbol{k} = ((4/5a)\pi, 0)$, and $I_i = I_f - I_i = 40$ for all n_{cycl}-values.

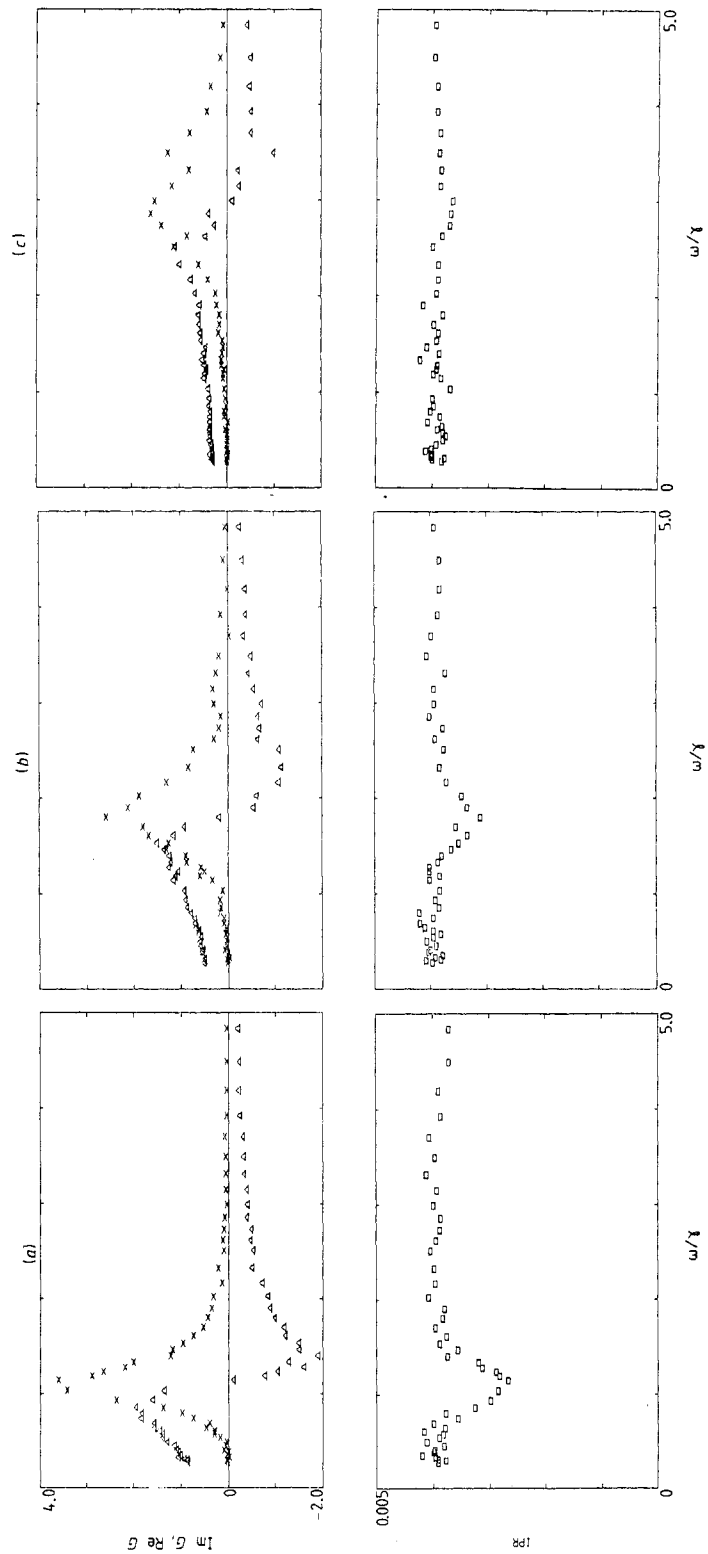


Figure 3. Im G (×), Re G (△) and IPR (□) against ω/γ (in units of J) at $T = 0.65J$ for (*a*) $\boldsymbol{k} = (0, 0)$, (*b*) $\boldsymbol{k} = ((2/5a).\pi, 0)$ and (*c*) $\boldsymbol{k} = ((4/5a).\pi, 0)$, and $(I_i, I_f - I_i) =$ (80, 120), (40, 60), (20, 30) and (10, 15) for $12 \leqslant n_{\text{cycl}} \leqslant 25$, $27 \leqslant n_{\text{cycl}} \leqslant 55$, $61 \leqslant n_{\text{cycl}} \leqslant 115$ and $127 \leqslant n_{\text{cycl}} \leqslant 223$, respectively.

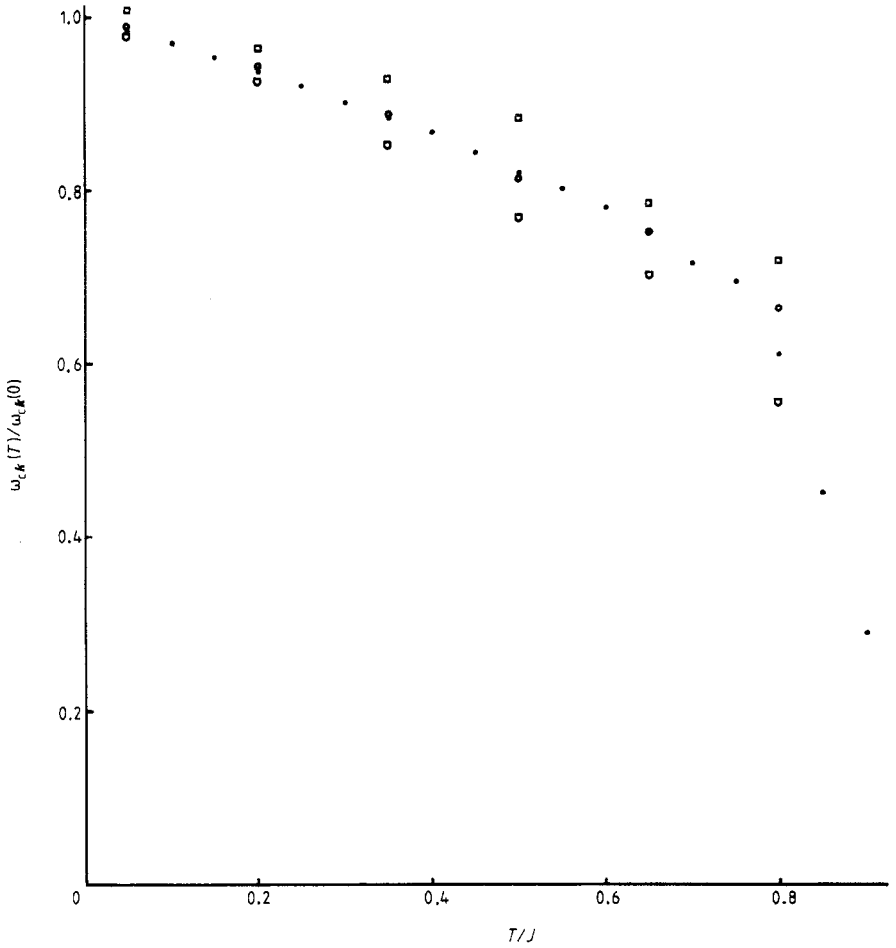


Figure 4. The temperature dependence of the resonance frequencies which are determined from zero points of the values of Re G, normalised by the zero-temperature values $\omega_{ck}(T)/\omega_{ck}(0)$ for $\boldsymbol{k} = (0, 0)$ (▽), $((2/5a)\pi, 0)$ (○) and $((4/5a)\pi, 0)$ (□), together with the magnetisations M_z (●).

We have used an effective Hamiltonian which contains additional parameters u and r. So far as we can see, the dependence of the results on u is not large, if u is large enough. We have shown that our method can reproduce the well established results of the magnetisation curve and the spin-wave resonance at $T \simeq 0$. We have also shown that the method can be successfully applied to the spin dynamics at finite temperatures. There are many applications of the method for the dynamics of more interesting and non-trivial models (e.g. a two-dimensional ferromagnet with an easy-plane anisotropy, random magnets). These will be reported in the near future.

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