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SOME EXACT CALCULATIONS ON A CHAIN OF SPINS $\frac{1}{2}$

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Synopsis

The X–Y model of a linear chain of spins $\frac{1}{2}$, introduced by Lieb, Schultz and Mattis[1]), is studied in the presence of a magnetic field h along the z axis. In section A the Hamiltonian is diagolalized in terms of fermion operators. In section B the magnetization along the z axis is calculated for arbitrary field and temperature. We find that there is no spontaneous magnetization and that only at zero temperature there is a phase transition of the second kind, the magnetic susceptibility being of the form $c \cdot \ln|h - h_c|$ in the neighbourhood of a critical field h_c. In section C we derive an expression for the time-dependent correlation function $\rho_R^z(\beta, t)$ of the z-components of spins separated by an arbitrary number R of lattice sites. Starting from this expression we will show that there is no long-range order of the z components of the spins in the absence of the field and that in the presence of a field the long-range order corresponds with the magnetization. Furthermore we discuss the time-dependent autocorrelation function of the z component of one single spin, of the total magnetization of the chain, and the possibility that Im $\rho_R^z(\beta, t)$ satisfies a kind of wave equation, for this special case, as has been proposed by Ruygrok[2]) for more general cases. In section D the isolated chain is assumed to be in thermal equilibrium in a certain magnetic field, after which the field is suddenly changed by an arbitrary amount, and an exact expression is derived for the temporal development of the z component of the magnetization, which is found to reach an equilibrium value as time goes to infinity. In section E this exact time development is compared with the exact solution of the Kubo formalism[3]) and it is proved analytically that the Kubo formula holds for high temperatures and small perturbation, but some numerical calculations show that the development into powers of the perturbation converge very slowly. We conclude with a short discussion of the approach of Mazur and Terwiel[4]) to the relaxation of more general spin systems, in connection with our exact results on the chain.

Introduction. In 1961 Lieb, Schultz and Mattis[1]) introduced a model for an antiferromagnetic linear chain of spins $\frac{1}{2}$, with nearest neighbour interaction, which they called the X–Y model. They considered a chain of N spins $\frac{1}{2}$, governed by the Hamiltonian:

$$H = 2J \sum_{j=1}^{N} [(1+\gamma)\, S_j^x S_{j+1}^x + (1-\gamma)\, S_j^y S_{j+1}^y], \qquad J > 0$$

where the operators S_j^i are half the Pauli spin matrices, and γ is a parameter characterizing the degree of anisotropy of the interaction in the xy plane.

In our case a magnetic field h along the z axis is added giving rise to an extra term

$$-2h \sum_{j=1}^{N} S_j^z$$

in the Hamiltonian. We will choose $0 \leqslant \gamma \leqslant 1$ and $J < 0$, and since we will only use the fact that J is greater than zero, we take $J = \frac{1}{2}$. Furthermore we will consider the chain to be cyclic, i.e. $S_{N+1}^i = S_1^i$.

It is possible to determine exactly some equilibrium and non-equilibrium properties of this system in the thermodynamic limit. In equilibrium one is interested in calculating the magnetization per spin in the z direction as a function of β, γ and h, ($\beta = 1/kT$), and in the correlation function $\langle S_1^i S_m^j(t)\rangle \beta = \rho_{l,m}^{ij}(\beta, t)$, where the shorthand $\langle A\rangle_\beta$ denotes

$$\frac{\mathrm{Tr}\, e^{-\beta H} A}{\mathrm{Tr}\, e^{-\beta H}}.$$

Because the Hamiltonian is invariant under translation by any number of lattice sites we have $\rho_{l,m} = \rho_{|l-m|}$. It is the function $\rho_m(\beta, t)$ which enters for example into calculations on the scattering of neutrons by spin systems. For $t = 0$, $\rho_m(\beta, 0)$ contains as special cases the so-called short- and long-range order, which are defined by:

$$\text{short-range order} \equiv \rho_1^{ii}(\beta, 0) = \rho_1^i(\beta, 0)$$

$$\text{long-range order} \equiv \lim_{n\to\infty} \rho_{2n}^{ii}(\beta, 0), \text{ if this limit exists.}$$

For arbitrary γ and $h = 0$ Lieb, Schultz and Mattis were able to derive exact expressions for $\rho_1^x(\beta, 0)$, $\rho_1^y(\beta, 0)$ and $\rho_1^z(\beta, 0)$. As to the long-range order they could prove for the special case $\gamma = 0$ and $h = 0$ that

$$\lim_{n\to\infty} \rho_{2n}^i(\beta, 0) = 0.$$

For $\gamma \neq 0$ their method yielded only very weak results.

In section A the Hamiltonian is diagonalized in terms of fermion operators. In section B the magnetization (per spin) in the z direction is calculated as a function of the field and the temperature: $\langle M^z(h)\rangle_\beta$. It is found that $\langle M^z(h)\rangle_\beta$ is a continuous function of β and h, but that at zero temperature the magnetic susceptibility $\chi^z(h)$ shows a singularity at a certain critical field h_c. In the neighbourhood of this point the susceptibility can be written as $\chi^z(h) = c \cdot \ln|h - h_c|$. The ground state shows no spontaneous magnetization. For $\gamma = 1$ the model reduces to the one-dimensional Ising chain in a perpendicular field, which has already been studied by Katsura[13]).

In section C the time-dependent correlation function $\rho_R^z(\beta, t) = \langle S_l^z S_{l+R}^z(t)\rangle_\beta$ of the z components of two spins separated by an arbitrary number R of lattice sites is calculated. From the result we show that when there is no magnetic field there is no long-range order and when there is a magnetic field, the long-range order corresponds with the magnetization. Furthermore the autocorrelation functions of the z components of one single spin and of the total magnetization of the chain are discussed, and the possibility that the imaginary part of $\rho_R^z(\beta, t)$ satisfies a king of wave equation is considered.

In section D the system is taken to be in equilibrium at temperature T and external field h_1 for $t < 0$. At $t = 0$ the field is suddenly changed to a different value h_2 and the temporal development of $\langle M^z(t)\rangle$ is calculated *exactly* for all values of t. It is shown that $\langle M^z(t)\rangle$ approaches a limit as t approaches infinity, but no exponential decay is found.

In section E it is proved analytically without making any assumptions that the usual way of treating relaxation phenomena, the Kubo formalism, holds, by developing the exact expression $\langle M^z(t)\rangle$ in powers of $(h_1 - h_2)$ and β and retaining only the first term. In order to get an idea how fast the series in β and $(h_1 - h_2)$ converge and to see whether there is an exponential decay of the magnetization the expressions for $\langle M^z(t)\rangle_{\text{exact}}$ and $\langle M^z(t)\rangle_{\text{Kubo}}$ were computed numerically for some cases. Both solutions behave like damped oscillations, of which only the first part can be described by an exponential, but the oscillations are not damped enough to permit the whole decay to be described by an exponential. It is shown that when the Kubo approximation is treated in the same way as Terwiel and Mazur[4]) recently treated more general spin systems, the use of the combination of their basic assumptions and the weak coupling limit yields an incorrect result and the possible reasons for this behaviour are indicated.

A. *Diagonalization of the Hamiltonian.* We consider a linear chain of N spins $\frac{1}{2}$ in an external magnetic field along the z axis, having only nearest neighbour interaction, governed by the Hamiltonian:

$$H = \sum_{j=1}^{N} [(1+\gamma)\, S_j^x S_{j+1}^x + (1-\gamma)\, S_j^y S_{j+1}^y - h S_j^z].$$

The S's are half the Pauli spin operators. By first performing the transformation

$$S_j^x = \frac{a_j^* + a_j}{2}, \quad S_j^y = \frac{a_j^* - a_j}{2i}, \quad S_j^z = a_j^* a_j - \tfrac{1}{2}$$

and then the transformation

$$a_j^* = \exp[i\pi \sum_{k=1}^{j-1} c_k^* c_k]\, c_j^* \qquad a_1^* = c_1^*$$

$$a_j = \exp[-i\pi \sum_{k=1}^{j-1} c_k^* c_k]\, c_j \qquad a_1 = c_1,$$

the Hamiltonian is transformed into

$$H = \tfrac{1}{2}Nh - h \sum_{j=1}^{N} c_j^* c_j + \tfrac{1}{2} \sum_{j=1}^{N} [(c_j^* c_{j+1} + \gamma c_j^* c_{j+1}^*) + \text{h.c.}] -$$
$$-\tfrac{1}{2}\{(c_N^* c_1 + \gamma c_N^* c_1) + \text{h.c.}\} \{\exp(i\pi \sum_{j=1}^{N} c_j^* c_j) + 1\}$$

where the c's are fermion operators, i.e. they satisfy anticommutation rules:

$$\{c_i, c_j\} = \{c_i^*, c_j^*\} = 0, \{c_i^*, c_j\} = \delta_{ij}$$

We have taken periodic boundary conditions, although the chain with free ends can also be solved exactly (see ref. 1, which we are following closely), and now we make use of the fact that for large systems the term proportional to

$$\{\exp(i\pi \sum_{j=1}^{N} c_j^* c_j) + 1\}$$

may be neglected, obtaining:

$$H = \tfrac{1}{2} \sum_{j=1}^{N} \{(c_j^* c_{j+1} + \gamma c_j^* c_{j+1}^*) + \text{h.c.}\} - h \sum_{j=1}^{n} c_j^* c_j + \tfrac{1}{2}Nh.$$

This Hamiltonian is of the form:

$$H = \sum_{i,j=1}^{N} [c_i^* A_{ij} c_j + \tfrac{1}{2}(c_i^* B_{ij} c_j^* + \text{h.c.})]$$

where A is a symmetric and B an anti-symmetric matrix, and the c's are fermion operators. As is shown in appendix A of ref. 1, a Hamiltonian of this kind can be diagonalized by the following canonical (i.e. the η operators are again fermion operators) transformation:

$$\eta_k^* = \sum_{i=1}^{N} g_{ki} c_i^* + h_{ki} c_i$$
$$\eta_k = \sum_{i=1}^{N} g_{ki} c_i + h_{ki} c_i^*$$

where the coefficients g_{ki} and k_{ki} are real numbers. This transformation sends H into the form:

$$H = \sum_{k=1}^{N} \Lambda_k \eta_k^* \eta_k + \text{constant}.$$

The coefficients g_{ki} and h_{ki} are determined by the matrices A and B through the following equations:

$$(A + B)\, \boldsymbol{\Phi}_k = \Lambda_k \boldsymbol{\Psi}_k$$
$$(A - B)\, \boldsymbol{\Psi}_k = \Lambda_k \boldsymbol{\Phi}_k$$

where the vectors $\boldsymbol{\Phi}_k$ and $\boldsymbol{\Psi}_k$ are defined by:

$$(\boldsymbol{\Phi}_k)_j = g_{kj} + h_{kj}$$
$$(\boldsymbol{\Psi}_k)_i = g_{kj} - h_{kj}.$$

The sets of vectors $\{\boldsymbol{\Phi}_k\}$ and $\{\boldsymbol{\Psi}_k\}$ can (and must) be chosen to be real and orthonormal. It is permitted to take all the $\Lambda_k's \geqslant 0$, this can only change the sign of $\boldsymbol{\Phi}_k$ or $\boldsymbol{\Psi}_k$ and it simplifies the definition of the ground state $|0\rangle$ as the state for which $\eta_k\,|0\rangle = 0$ for every k.

In our case the matrices A and B have the form:

$$A = \begin{Bmatrix} -h & \frac{1}{2} & & & \frac{1}{2} \\ \frac{1}{2} & -h & \ddots & 0 & \\ & \frac{1}{2} & \ddots & \ddots & \\ 0 & & \ddots & \ddots & \frac{1}{2} \\ \frac{1}{2} & & & \frac{1}{2} & -h \end{Bmatrix}, \quad B = \frac{1}{2}\begin{Bmatrix} 0 & \gamma & & & -\gamma \\ -\gamma & 0 & \gamma & 0 & \\ & -\gamma & \ddots & \ddots & \\ 0 & & \ddots & \ddots & \gamma \\ \gamma & & & -\gamma & 0 \end{Bmatrix}$$

Due to the fact that these matrices are cyclic, the transformation coefficients Φ_{kj} and Ψ_{kj} and the corresponding eigenvalues Λ_k are found rather easily. It is easy to verify that they are given by:

$$\Phi_{kj} = \sqrt{\frac{2}{N}} \cos\left(j\varphi_k - \lambda_k - \frac{\pi}{4}\right) \tag{1}$$

$$\Psi_{kj} = \sqrt{\frac{2}{N}} \cos\left(j\varphi_k + \lambda_k - \frac{\pi}{4}\right) \tag{2}$$

$$\Lambda_k = +\sqrt{(\cos\varphi_k - h)^2 + \gamma^2 \sin^2\varphi_k} \tag{3}$$

where

$$\varphi_k = k\,\frac{2\pi}{N}, \qquad k = 1, \ldots, N$$

and

$$\lambda_k = \tfrac{1}{2}\,\text{arctg}\left\{\frac{\gamma \sin\varphi_k}{\cos\varphi_k - h}\right\}. \tag{4}$$

In order to avoid ambiguity we define: $0 < \lambda_k \leqslant \pi$.

The Hamiltonian now has finally assumed the desired diagonal form:

$$H = \sum_{k=1}^{N} \Lambda_k \eta_k^* \eta_k - \tfrac{1}{2}\sum_{k=1}^{N} (\Lambda_k - h). \tag{5}$$

The operator M^z for the magnetization per spin in the z direction in terms of the c-operators is:

$$M^z = \frac{1}{N}\sum_{j=1}^{N} S_j^z = \frac{1}{N}\sum_{j=1}^{N} (a_j^* a_j - \tfrac{1}{2}) = \frac{1}{2N}\sum_{j=1}^{N} (c_j^* + c_j)(c_j - c_j^*).$$

Since Φ and Ψ are orthogonal matrices (where the k'th column of Φ is defined to be the vector $\boldsymbol{\Phi}_k$, and accordingly for Ψ), we can easily invert the relations:

$$\eta_k + \eta_k^* = \sum_{i=1}^{N} \Phi_{ki}(c_i + c_i^*)$$

$$\eta_k - \eta_k^* = \sum_{i=1}^{N} \Psi_{ki}(c_i - c_i^*)$$

to obtain:

$$c_i + c_i^* = \sum_{k=1}^{N} \Phi_{ki}(\eta_k + \eta_k^*)$$

$$c_i - c_i^* = \sum_{k=1}^{N} \Psi_{ki}(\eta_k - \eta_k^*)$$

so that M^z takes the form:

$$M^z = \frac{1}{2N} \sum_{c,m,n=1}^{N} \Phi_{mc}\Psi_{nc}(\eta_m^* + \eta_m)(\eta_n - \eta_n^*) \tag{6}$$

B. *Magnetization and susceptibility.* We are now ready to evaluate the magnetization as a function of β, γ and h, where $\beta = 1/kT$, in the canonical ensemble. This is most easily done not by differentiating the explicit expression for the free energy with respect to the external field, but by directly calculating $\langle M^z \rangle_\beta$, where we use the abbreviation

$$\langle M^z \rangle_\beta = \frac{\text{Tr } e^{-\beta H} M^z}{\text{Tr } e^{-\beta H}}.$$

Using formulae (5) and (6) this is:

$$\langle M^z \rangle_\beta =$$

$$= \frac{1}{2N} \frac{\text{Tr}[\exp -\beta\{\sum_{j=1}^{N} \Lambda_j \eta_j^* \eta_j + \frac{1}{2}(h - \Lambda_j\} \sum_{l,m,n,=1}^{N} \Phi_{ml}\Psi_{nl}(\eta_m^* + \eta_m)(\eta_n - \eta_n^*)]}{\text{Tr} \exp -\beta\{\sum_{j=1}^{N} \Lambda_j \eta_j^* \eta_j + \frac{1}{2}(h - \Lambda_j)\}} \tag{7}$$

Because of the simple form of the Hamiltonian, one easily verifies that:

$$\frac{\text{Tr } e^{-\beta H}(\eta_m^* + \eta_m)(\eta_n - \eta_n^*)}{\text{Tr } e^{-\beta H}} = -\text{tgh } \tfrac{1}{2}\beta\Lambda_m \, \delta_{mn}.$$

Inserting this into equation (7), one obtains:

$$\langle M^z(h) \rangle_\beta = -\frac{1}{2N} \sum_{l,m,n=1}^{N} \Phi_{ml}\Psi_{nl} \text{ tgh } \tfrac{1}{2}\beta\Lambda_m \, \delta_{mn}$$

$$= -\frac{1}{N^2} \sum_{l,m=1}^{N} \cos\left(l\varphi_m - \lambda_m - \frac{\pi}{4}\right) \cos\left(l\varphi_m + \lambda_m - \frac{\pi}{4}\right) \text{tgh } \tfrac{1}{2}\beta\Lambda_m \tag{7b}$$

The summation over l can be explicitly evaluated, and taking the thermodynamic limit, so that $\varphi_m = m(2\pi/N)$ becomes a continuous variable ranging from 0 to 2π, and the summation over m can be replaced by an integral, one finds:

$$\langle M^z(h)\rangle_\beta = -\frac{1}{4\pi}\int_0^{2\pi} \frac{\sin(N+1)\,\varphi \sin N\varphi}{\sin\varphi}\,\text{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi)\,\mathrm{d}\varphi - \\ -\frac{1}{4\pi}\int_0^{2\pi}\cos 2\lambda(\varphi)\,\text{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi)\,\mathrm{d}\varphi$$

The first integral is zero, since its integrand is an odd function of φ, so we have:

$$\langle M^z(h)\rangle_\beta = -\frac{1}{2\pi}\int_0^{\pi}\cos\left\{\text{arctg}\left(\frac{\gamma\sin\varphi}{\cos\varphi - h}\right)\right\}\text{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi)\,\mathrm{d}\varphi \tag{8}$$

One easily shows that

$$\lim_{h\to 0}\langle M^z(h)\rangle_\beta = 0$$

for all values of β so there is no spontaneous magnetization. Furthermore one sees from (8) that the magnetization is a continuous function of β and h. On differentiating the magnetization with respect to the field, we obtain the magnetic susceptibility, for $\gamma \neq 0$:

$$\chi_{\mathrm{T}}(h) = \chi_1 + \chi_2 =$$

$$= \frac{1}{2\pi}\int_0^{\pi}\left[\sin\left\{\text{arctg}\,\frac{\gamma\sin\varphi}{\cos\varphi - h}\right\}\frac{\gamma\sin\varphi\,\text{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi)}{(\cos\varphi - h)^2 + \gamma^2\sin^2\varphi}\right]\mathrm{d}\varphi +$$

$$+\frac{1}{2\pi}\int_0^{\pi}\left[\cos\left\{\text{arctg}\,\frac{\gamma\sin\varphi}{\cos\varphi - h}\right\}\frac{\beta(\cos\varphi - h)}{\cosh^2(\tfrac{1}{2}\beta\Lambda(\varphi)).2\Lambda(\varphi)}\right]\mathrm{d}\varphi.$$

For $T > 0$ both integrands are finite for all values of h, and $\chi(\beta, h)$ is a continuous function of both β and h. For $T = 0$, however, the integrand of χ_1 has a singularity when $h = 1$, since for $T = 0$ in the point $\varphi = 0$ the term $\sin\varphi/(\cos\varphi - h)^2$ is no longer compensated by the term tgh $\tfrac{1}{2}\beta\Lambda(\varphi)$. We will study $\chi_{1,T=0}$ a little closer near $h = 1$ and put $h = 1 + h'$, with $h' \geqslant 0$. Splitting the integration interval into two parts $[0, \delta]$ and $[\delta, \pi]$, where δ

is a small positive number, we can write:

$$\chi_{1,T=0}(h') = \chi' + \chi'' =$$

$$= \frac{1}{2\pi}\int_0^\delta \left[\sin\left\{\operatorname{arctg}\frac{\gamma\sin\varphi}{\cos\varphi - h' - 1}\right\}\frac{\gamma\sin\varphi}{(\cos\varphi - h' - 1)^2 + \gamma^2\sin\varphi^2}\right]d\varphi +$$

$$+ \frac{1}{2\pi}\int_\delta^0 \left[\sin\left\{\operatorname{arctg}\frac{\gamma\sin\varphi}{\cos\varphi - h' - 1}\right\}\frac{\gamma\sin\varphi}{(\cos\varphi - h' - 1)^2 + \gamma^2\sin^2\varphi}\right]d\varphi.$$

The integrand of χ'' is finite for every $\varphi = [\delta, \pi]$ and every h' so $\chi''(h')$ is a continuous function of h. Since δ is a small number we can write in the integrand of χ': $\sin\varphi = \varphi$ and $\cos\varphi = 1 - \frac{1}{2}\varphi^2$, obtaining:

$$\chi'_{T=0}(h') = \frac{\gamma^2}{2\pi}\int_0^\delta \frac{\varphi^2}{\left(1 + \frac{\gamma^2}{(\frac{1}{2}\varphi^2 + h')^2}\right)^{\frac{3}{2}}(\frac{1}{2}\varphi^2 + h')^3}\, d\varphi =$$

$$= \frac{\gamma^2}{2\pi}\int_0^\delta \frac{\varphi^2}{\{(\frac{1}{2}\varphi^2 + h')^2 + \gamma^2\varphi^2\}^{\frac{3}{2}}}\, d\varphi.$$

Since δ is small we can neglect φ^4 with respect to φ^2, obtaining

$$\chi'_{T=0}(h') = \frac{\gamma^2}{2\pi}\int_0^\delta \frac{\varphi^2}{\{h'^2 + (h'^2 + \gamma^2)\,\varphi^2\}^{\frac{3}{2}}}\, d\varphi$$

This integral is easily evaluated to yield:

$$\chi'_{T=0}(h') = \frac{\gamma^2}{2\pi}\frac{1}{(h'^2 + \gamma^2)^{\frac{3}{2}}}\left[-\frac{\delta}{\sqrt{\delta^2 + \frac{h'^2}{h'^2 + \gamma^2}}} + \right.$$

$$\left. + \log\left\{\delta + \sqrt{\delta^2 + \frac{h'^2}{h'^2 + \gamma^2}}\right\} - \frac{1}{2}\log\left(\frac{h'^2}{h'^2 + \gamma^2}\right)\right].$$

The last term of this expression is seen to equal

$$\frac{\gamma^2}{4\pi}\frac{1}{(h'^2 + \gamma^2)^{\frac{3}{2}}}\{2\log h' - \log(h'^2 + \gamma^2)\}$$

and diverges logarithmically as h' approaches zero, or h approaches the critical value $h_c = 1$, the asymptotic behaviour of $\chi'_{T=0}(h)$ being:

$$\chi'_{T=0}(h) \simeq -\frac{1}{2\pi\gamma} \log(|h-1|) \qquad \text{with} \qquad h \simeq 1.$$

The total susceptibility can be written as:

$$\chi'_{T=0}(h) = -\frac{1}{2\pi\gamma} \log(|h-1|) + f(h)$$

Where $f(h)$ is a continuous, finite function of h.

When h is large compared to 1, we can write the magnetization as:

$$\langle M^z(h)\rangle_\beta = \frac{1}{2\pi} \operatorname{tgh} \tfrac{1}{2}\beta h \int_0^\pi \frac{1}{\sqrt{1+\dfrac{\gamma^2}{h^2}\sin^2\varphi}} \, \mathrm{d}\varphi$$

$$= \frac{1}{\pi} \frac{1}{\sqrt{1+\gamma^2/h^2}} \operatorname{tgh} \tfrac{1}{2}\beta h \cdot K\left(\frac{\gamma^2}{\gamma^2+h^2}\right)$$

where K is the complete elliptic integral of the first kind. In fig. 1 the magnetization is plotted for $\gamma \neq 0$, $T = 0$ and $T > 0$, and in fig. 2 the susceptibility is plotted for $T = 0$.

This behaviour of $\chi_{T=0}(h)$ corresponds with a phase transition of the second kind at zero temperature. It can be considered as an extension to a spin system with anisotropic interaction of the so-called theorem of Jacob-

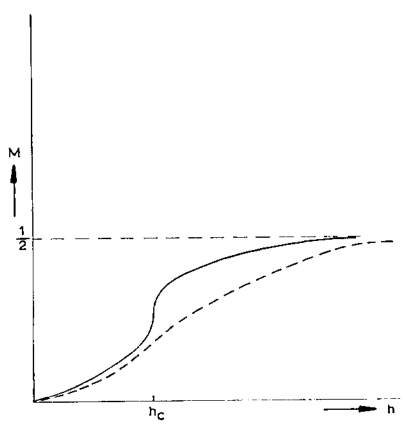

Fig. 1. $\langle M^z\rangle$ as function of h for $T = 0$ (solid line) and $T > 0$ (dashed line).

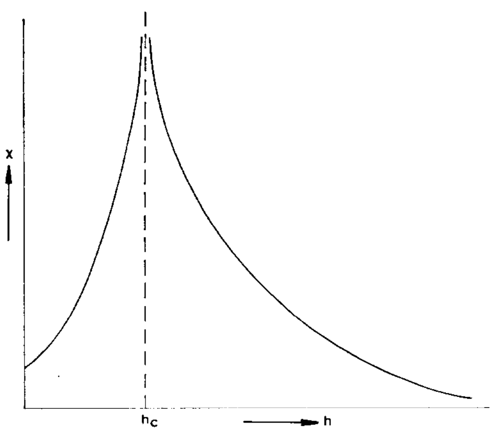

Fig. 2. $\chi^z(h)$ as function of h for $T = 0$.

sohn[11]), which states that a system of spins $\frac{1}{2}$ in an external magnetic field $\boldsymbol{h}$, governed by the Hamiltonian

$$H = \sum_{\substack{i=1 \\ j=\{z_i\}}}^{N} J \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \sum_{i=1}^{N} \boldsymbol{S}_i \cdot \boldsymbol{h}, \qquad J > 0,$$

where $\{z_i\}$ is the collection of neighbours of the i-th spin, has a discontinuity at zero temperature in either the magnetization or the magnetic susceptibility at a certain critical field. For $\gamma = 0$ the magnetization of the ground state is found to be

$$\langle M^z(h) \rangle_\infty = \begin{cases} \frac{1}{2} - \dfrac{1}{\pi} \arccos h & \text{for} \quad 0 \leqslant h \leqslant 1 \\ \frac{1}{2} & \text{for} \quad h \geqslant 1 \end{cases}$$

The magnetization and susceptibility of the ground state are sketched in fig. 3 and fig. 4:

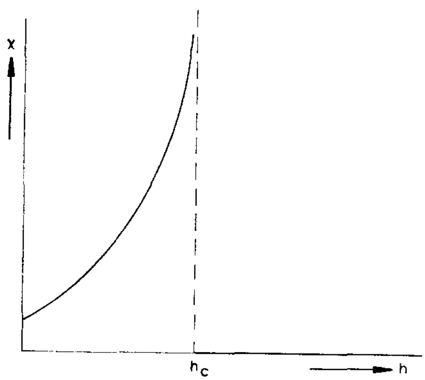

Fig. 3. Susceptibility of the ground state for $\gamma = 0$ as function of h.

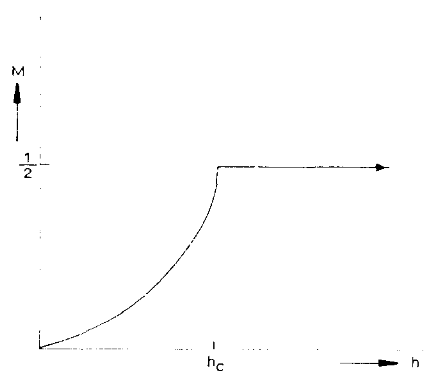

Fig. 4. Magnetization of the ground state as function of h for $\gamma = 0$.

The spins line up gradually when the field is increased, above the critical field $h_c = 1$ they are all parallel and the susceptibility again shows a discontinuity at h_c. The case of $\gamma = 1$ corresponds to the familiar antiferromagnetic Ising chain, but with a perpendicular field. Upon rotating the coordinate system the Hamiltonian becomes:

$$H = \sum_{j=1}^{N} [S_j^z S_{j+1}^z - h S_j^x]$$

whereas usually the case

$$H = \sum_{j=1}^{N} [S_j^z S_{j+1}^z - h S_j^z]$$

is considered. The transverse magnetization of the Ising chain has been calculated by Katsura[13]). It follows from the foregoing that this is

$$\langle M^x(h)\rangle_\beta =$$
$$= -\frac{1}{2\pi}\int_0^\pi \left[\cos\left\{\operatorname{arctg}\frac{\sin\varphi}{\cos\varphi - h}\right\} \operatorname{tgh} \tfrac{1}{2}\beta\sqrt{(\cos\varphi - h)^2 + \sin^2\varphi}\right] d\varphi \quad (10)$$

For $T = 0$ the magnetization and susceptibility in the x and z directions are plotted in figures 5 and 6:

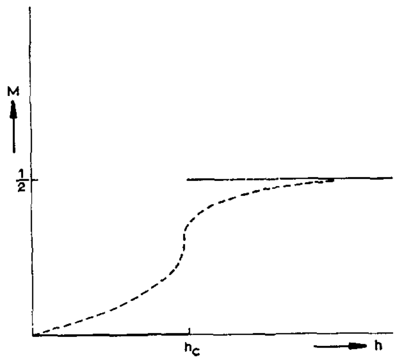

Fig. 5. Magnetization in the x and z direction of the Ising chain at $T = 0$, resp. dashed and solid line.

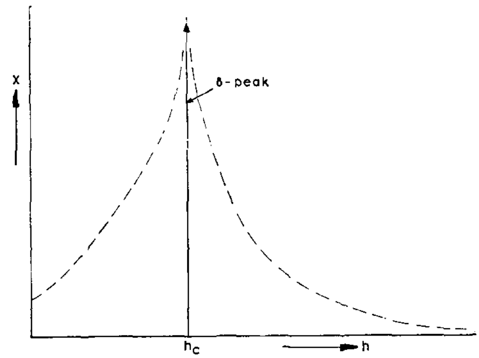

Fig. 6. Susceptibility in the x and y direction of the Ising chain at $T = 0$, resp. dashed and solid line.

For more practical purposes, if chains of this structure actually appear in nature, it is necessary not to work with dimensionless quantities, and we can indicate conditions under which the susceptibility behaves almost logarithmically as a function of the external field. If we had started from the Hamiltonian:

$$H = 2J\sum_{j=1}^{N}[(1+\gamma)\, S_j^x S_{j+1}^x + (1-\gamma)\, S_j^y S_{j+1}^y] - g_l\mu H \sum_j S_j^z$$

where J is the exchange energy, g_l the Landé-factor, μ the Bohr-magneton and H the external field, we would have found for the magnetization:

$$\langle M^z(H)\rangle_\beta = -\frac{1}{2\pi}\int_0^\pi \cos\left\{\operatorname{arctg}\frac{\gamma\sin\varphi}{\cos\varphi - 2g_l\mu H}\right\}\cdot$$
$$\operatorname{tgh}\frac{\beta J}{4}\sqrt{\left(\cos\varphi - \frac{2g_l\mu H}{J}\right)^2 + \gamma^2\sin^2\varphi}\cdot d\varphi$$

Introducing

$$H = \frac{J}{2g_l\mu}(1 + a)$$

this becomes

$$\langle M^z(a)\rangle_\beta = \frac{1}{2\pi}\int_0^\pi \cos\left\{\operatorname{arctg}\frac{\gamma\sin\varphi}{(\cos\varphi - 1 - a)}\right\}\cdot$$

$$\cdot\operatorname{tgh}\tfrac{1}{4}\beta J\sqrt{(\cos\varphi - 1 - a)^2 + \gamma^2\sin^2\varphi}\cdot d\varphi$$

For $0 < a \ll 1$ the larger part of the susceptibility again is given by:

$$\chi_1(a) \simeq \frac{1}{2\pi\gamma}\int_0^\delta \frac{\varphi^2}{[\varphi^2 + (a^2/\gamma^2)]^{\frac{3}{2}}}\operatorname{tgh}\frac{\beta J\gamma}{4}\sqrt{\varphi^2 + \frac{a^2}{\gamma^2}}\cdot d\varphi$$

where δ again is chosen to be a number so small that we could write $\sin\varphi \simeq \varphi$ and $\cos\varphi \simeq 1 - \frac{1}{2}\varphi^2$, so that

$$(\cos\varphi - 1 - a)^2 + \gamma^2\sin^2\varphi \simeq \gamma^2\varphi^2 + a^2.$$

Under the condition that $\beta Ja \gg 1$ we can write for all φ in this interval:

$$\operatorname{tgh}\frac{\beta J\gamma}{4}\sqrt{\varphi^2 + \frac{a^2}{\gamma^2}} \simeq \operatorname{tgh}\frac{\beta Ja}{4}$$

so

$$\chi_1(a) \simeq \operatorname{tgh}\frac{\beta Ja}{4}\frac{1}{8\pi\gamma}\int_0^\delta \frac{1}{[\varphi^2 + (a^2/\gamma^2)]^{\frac{3}{2}}}\cdot d\varphi$$

This is easily evaluated to be:

$$\chi_1(a) \simeq \operatorname{tgh}\frac{\beta Ja}{4}\left[-\frac{1}{8\pi\gamma}\log\frac{a}{\gamma} - \frac{1}{8\pi\gamma}\cdot\right.$$

$$\left.\cdot\left\{\frac{\delta}{\sqrt{\delta^2 + (a^2/\gamma^2)}} - \log\left(\delta + \sqrt{\delta^2 + \frac{a^2}{\gamma^2}}\right)\right\}\right].$$

Thus we have found that under the conditions

$$\beta Ja \gg 1 \quad \text{and} \quad 0 < a \ll 1$$

or

$$\beta J \gg 1 \quad \text{and} \quad 2g_l\mu H \simeq J$$

we can write for the susceptibility:

$$\chi(H) \simeq -\operatorname{tgh}\frac{\beta J}{4}\frac{(2g_l\mu H - 1)}{4}\log\left(\frac{2g_l\mu H}{J} - 1\right) + f'(H)$$

where $f'(H)$ again is a finite, continuous function of H.

C. *Correlation functions.* In this section we will study the time-dependent correlation function of the z components of spins on different places, of one single spin and of the magnetization. We will discuss the result and some related subjects. The time-dependent correlation function of the z component of two spins, respectively on lattice points l and $l + R$ is defined by:

$$\rho^z_{l,l+R}(\beta, t) = \langle S^z_l S^z_{l+R}(t)\rangle_\beta.$$

Since the Hamiltonian is invariant under translations, it turns out that it is easier to write:

$$\rho^z_R(\beta, t) = \frac{1}{N}\sum_{l=1}^{N} \langle S^z_l S^z_{l+R}(t)\rangle_\beta = \frac{1}{N}\sum_{l=1}^{N} \frac{\mathrm{Tr}\, e^{-\beta H}\, S^z_l\, e^{iHt}\, S^z_{l+R}\, e^{-iHt}}{\mathrm{Tr}\, e^{-\beta H}}$$

$$= \frac{1}{4N}\sum_{l,p,q,r,s=1}^{N} \Phi_{pl}\Psi_{ql}\Phi_{r,l+R}\Psi_{s,l+R}\langle\!\langle(\eta^*_p + \eta_p)(\eta_q - \eta^*_q)\, e^{iHt}\cdot$$

$$\cdot(\eta^*_r + \eta_r)(\eta_s - \eta^*_s)\, e^{-iHt}\rangle\!\rangle_\beta \tag{11}$$

Again on account of the simplicity of the Hamiltonian, the trace which occurs in this expression is found to be:

$$\langle\!\langle(\eta^*_p + \eta_p)(\eta_q - \eta^*_q)\, e^{iHt}(\eta^*_r + \eta_r)(\eta_s - \eta^*_s)\, e^{-iHt}\rangle\!\rangle_\beta =$$

$$= \mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda_p\, \mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda_r\delta_{pq}\delta_{rs} + f^+(\varphi_p)\, f^+(\varphi_q)\, \delta_{pr}\delta_{qs} -$$

$$- f^-(\varphi_p)\, f^-(\varphi_p)\, \delta_{ps}\delta_{qr} \tag{12}$$

where

$$f^+(\varphi) = \cos\Lambda(\varphi)\, t + i\sin\Lambda(\varphi)\, t\cdot\mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi)$$

and

$$f^-(\varphi) = i\sin\Lambda(\varphi)\, t + \cos\Lambda(\varphi)\, t\cdot\mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi) \tag{13}$$

Inserting this into equation (11) we get:

$$\rho^z_R(\beta, t) = \frac{1}{4N}\sum_{l,p,q=1}^{N} [\Phi_{pl}\Psi_{pl}\Phi_{q,l+R}\Psi_{q,l+R}\, \mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda_p\, \mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda_q +$$

$$+ \Phi_{pl}\Psi_{ql}\Phi_{p,l+R}\Psi_{q,l+R}\, f^+(\varphi_p)\, f^+(\varphi_q) - \Phi_{pl}\Psi_{ql}\Phi_{q,l+R}\Psi_{q,l+R} f^-(\varphi_p)\, f^-(\varphi_q)]$$

$$= \frac{1}{4N}\sum_{l,m,p,q=1}^{N} [\Phi_{pl}\Psi_{pl}\Phi_{qm}\Psi_{qm}\, \mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda_p\, \mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda_q +$$

$$+ \Phi_{pl}\Psi_{ql}\Phi_{qm}\Psi_{qm} f^+(\varphi_p)\, f^+(\varphi_q) - \Phi_{pl}\Psi_{ql}\Phi_{qm}\Psi_{qm} f^-(\varphi_p)\, f^-(\varphi_q)]\, \delta_{m-l,R} \tag{14}$$

For the Kronecker delta we can write:

$$\delta_{m-l,R} = \frac{1}{N}\sum_{k=1}^{N} e^{i\varphi_k(R+l-m)},\ \varphi_k = k\,\frac{2\pi}{N},\ k = 1, \ldots, N,$$

and introducing a matrix $B(\varphi_k)$ by

$$B_{ij}(\varphi_k) = \sum_{l=1}^{N} e^{il\varphi_k}\, \Psi_{il}\Phi_{ij} \tag{15}$$

we can rewrite (14) as:

$$\rho^z_R(\beta, t) = \frac{1}{4N^2} \sum_{k=1}^{N} e^{iR\varphi_k}[|\sum_{p=1}^{N} B_{pp}(\varphi_k) \operatorname{tgh} \tfrac{1}{2}\beta\Lambda_p|^2 + \\ \sum_{p,q=1}^{N} B_{pq}(\varphi_k)\, B^*_{pq}(\varphi_k)\, f^+(\varphi_p)\, f^+(\varphi_q) \\ - \sum_{p,q=1}^{N} B_{pq}(\varphi_k)\, B^*_{qp}(\varphi_k)\, f^-(\varphi_p)\, f^-(\varphi_q)] = I_1 + I_2 - I_3, \quad (16)$$

where the abbreviations are obvious. We will compute the functions I_1, I_2 and I_3 separately. In formula (15), inserting the values of Ψ_{il} and Φ_{jl}, the summation over l can again be performed explicitely, and introducing the abbreviations:

$$A = -\lambda_i + \lambda_j + \frac{N-1}{2}(\varphi - \varphi_i - \varphi_j), \quad B = \lambda_i - \lambda_j + \frac{N-1}{2}(\varphi + \varphi_i + \varphi_j)$$

$$C = \lambda_j + \lambda_j + \frac{N-1}{2}(\varphi + \varphi_i + \varphi_j), \quad D = -\lambda_i - \lambda_j + \frac{N-1}{2}(\varphi - \varphi_i + \varphi_j)$$

we can write for the matrix element $B_{ij}(\varphi)$:

$$B_{ij}(\varphi) = \frac{1}{2N}[\sin A \cdot S(\varphi - \varphi_i - \varphi_j) - \sin B \cdot S(\varphi + \varphi_i + \varphi_j) + \\ + \cos C \cdot S(\varphi + \varphi_i - \varphi_j) + \cos D \cdot S(\varphi - \varphi_i + \varphi_j)] \\ + \frac{i}{2N}[-\cos A \cdot S(\varphi - \varphi_i - \varphi_j) + \cos B \cdot S(\varphi + \varphi_i + \varphi_j) + \\ + \sin C \cdot S(\varphi + \varphi_i - \varphi_j) + \sin D \cdot S(\varphi - \varphi_i + \varphi_j)] \quad (17)$$

where

$$S(\varphi) = \frac{\sin \frac{N}{2}\varphi}{\sin \frac{1}{2}\varphi}$$

We can now deal with I_1. Inserting (15) into I_1 one has

$$I_1 = \frac{1}{4N^2} \sum_{k=1}^{N} e^{iR\varphi_k} |\sum_{j=1}^{N} B_{jj}(\varphi_k) \operatorname{tgh} \tfrac{1}{2}\beta\Lambda_j|^2 = \\ = \frac{1}{8N^3} \sum_{k=1}^{N} e^{iR\varphi_k} \sum_{j=1}^{N} \Big[\sin\left\{\frac{N-1}{2}(\varphi - 2\varphi_j)\right\} S(\varphi - 2\varphi_j) - \\ - \sin\left\{\frac{N-1}{2}(\varphi + 2\varphi_j)\right\} S(\varphi + 2\varphi_j) + \cos\left(2\lambda_j + \frac{N-1}{2}\varphi\right) S(\varphi) + \\ + \cos\left(-2\lambda_j + \frac{N-1}{2}\varphi\right) S(\varphi) - i\cos\left\{\frac{N-1}{2}(\varphi - 2\varphi_j)\right\} S(\varphi - 2\varphi_j) +$$

$$+ \cos\frac{N-1}{2}(\varphi + 2\varphi_j)\, S(\varphi + 2\varphi_j) + i\sin\left(2\lambda_j + \frac{N-1}{2}\varphi\right) S(\varphi) +$$

$$+ i\sin\left(-2\lambda_j + \frac{N-1}{2}\varphi\right) S(\varphi)\Big].$$

The first, second, fifth and sixth term change sign under the inversion $\varphi_j \to -\varphi_j$ and can be omitted. For large N the summations can be replaced by integrals:

$$I_1 = \frac{1}{2^6\pi^3}\int_{-\pi}^{\pi} e^{iR\varphi}\left|\int_{-\pi}^{\pi}\left[\cos\left(2\lambda_j + \frac{N-1}{2}\varphi\right) + \cos\left(-2\lambda_j + \frac{N-1}{2}\varphi\right) +\right.\right.$$

$$\left.\left. + i\sin\left(2\lambda_j + \frac{N+1}{2}\varphi\right) + i\sin\left(-2\lambda_j + \frac{N-1}{2}\varphi\right)\right]\cdot S(\varphi)\,\mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi_j)\,d\varphi_j\right|^2 d\varphi$$

$$= \frac{1}{2^4\pi^3}\int_{-\pi}^{\pi} e^{iR\varphi}\left|\int \cos 2\lambda_j\left\{\cos\frac{N-1}{2} + i\sin\frac{N-1}{2}\varphi\right\} S(\varphi)\,\mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi_j)\right|^2 d\varphi$$

$$= \left[\frac{1}{4\pi}\int_{-\pi}^{\pi}\cos 2\lambda(\varphi_j)\,\mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi_j)\,d\varphi\right]^2 \frac{1}{\pi}\int_{-\pi}^{\pi} e^{iR\varphi}\, S(\varphi)\,d\varphi = \langle M^z(h)\rangle_\beta^2,$$

where expression (8) has been used in the last step.

We can calculate I_2, using expression (17) for $B_{ij}(\varphi_k)$:

$$I_2 = \frac{1}{8N^4}\sum_{i,j,k=1}^{N} e^{iR\varphi_k}\,[\underline{\{\sin A\cdot S(\varphi - \varphi_i - \varphi_j) - \sin B\cdot S(\varphi + \varphi_i + \varphi_j)}$$

$$+ \cos C\cdot S(\varphi + \varphi_i + \varphi_j) + \cos D\cdot S(\varphi - \varphi_i - \varphi_j)\}^2$$

$$+ \{\underline{-\cos A\cdot S(\varphi - \varphi_i - \varphi_j) + \cos B\cdot S(\varphi + \varphi_i + \varphi_j)} +$$

$$+ \sin C\cdot S(\varphi + \varphi_i - \varphi_j) + \sin D\cdot S(\varphi - \varphi_i + \varphi_j)\}^2]\, f^+(\varphi_i)\, f^+(\varphi_j).$$

The underlined terms change sign under the inversion $\varphi_i \to -\varphi_i$, $\varphi_j \to -\varphi_j$, the other ones are invariant; so for large N we obtain:

$$I_2 = \frac{1}{2^6\pi^3 N}\int\int_{-\pi}^{\pi}\int e^{iR\varphi}[\{\sin A\cdot S(\varphi - \varphi_i - \varphi_j) - \sin B\cdot S(\varphi + \varphi_i + \varphi_j)\}^2$$

$$+ \{\cos C\cdot S(\varphi + \varphi_i - \varphi_j) + \cos D\cdot S(\varphi - \varphi_i + \varphi_j)\}^2$$

$$+ \{-\cos A\cdot S(\varphi - \varphi_i - \varphi_j) + \cos B\cdot S(\varphi + \varphi_i + \varphi_j)\}^2$$

$$+ \{\sin C\cdot S(\varphi + \varphi_i - \varphi_j) + \sin D\cdot S(\varphi - \varphi_i + \varphi_j)\}^2]\, f^+(\varphi_i)\, f^+(\varphi_j)$$

$$= \frac{1}{2^6\pi^3 N}\int\int_{-\pi}^{\pi}\int e^{iR\varphi}[S^2(\varphi - \varphi_i - \varphi_j) + S^2(\varphi + \varphi_i + \varphi_j) + S^2(\varphi - \varphi_i + \varphi_j) +$$

$+ S^2(\varphi + \varphi_i - \varphi_j) - \underline{2\cos(A - B)\, S(\varphi - \varphi_i - \varphi_j)\, S(\varphi + \varphi_i + \varphi_j) + 2\cos(C - D)\cdot}$
$\underline{\cdot S(\varphi + \varphi_i - \varphi_j)\, S(\varphi - \varphi_i + \varphi_j)}]\, f^+(\varphi_i)\, f^+(\varphi_j)\, d\varphi\, d\varphi_i\, d\varphi_j.$

The underlined term changes sign under the transformation $\varphi_i \to -\varphi_i$, and so:

$$I_2 = \frac{1}{2^4\pi^3} \int\int_{-\pi}^{\pi}\int e^{iR\varphi}\, \frac{S^2(\varphi - \varphi_i - \varphi_j)}{N}\, f^+(\varphi_i)\, f^+(\varphi_j)\, d\varphi\, d\varphi_i\, fd\varphi_j$$

Since the integrand is periodic in φ, we can extend the integration interval of φ from $[-\pi, \pi]$ to $[-2\pi, 2\pi]$, and introducing new variables $\psi_1 = \varphi_i + \varphi_j$ and $\psi_2 = \varphi_i - \varphi_j$ we obtain:

$$I_2 = \frac{1}{2^6\pi^3} \iiint_{-2\pi}^{2\pi} e^{iR\varphi}\, \frac{S^2(\varphi - \psi_1)}{N}\, f^+\left\{\frac{(\psi_1 + \psi_2)}{2}\right\} f^+\left\{\frac{(\psi_1 - \psi_2)}{2}\right\} d\varphi\, d\psi_1\, d\psi_2 \tag{18}$$

In the limit $N \to \infty$ the function $S^2(\theta)/N$ behaves like a delta function, the norm being determined by:

$$\int_0^{\pi} \frac{\sin^2 N\theta}{\sin^2\theta}\, d\theta = N\pi \qquad \text{(Fejér's integral).}$$

Inserting this into equation (18), and putting

$$\frac{\varphi + \psi_1}{2} = \theta_1 \text{ and } \frac{\varphi - \psi_1}{2} = \theta_2$$

we finally obtain:

$$I_2 = \frac{1}{2^6\pi^2} \int\int_{-2\pi}^{2\pi} e^{iR(\theta_1+\theta_2)}\, f^+(\theta_1)\, d\theta_1\, d\theta_2 = \left[\frac{1}{4\pi}\int_{-\pi}^{\pi} e^{iR\varphi}\, f^+(\varphi)\, d\varphi\right]^2 \tag{19}$$

In the same way we can deal with I_3. Introducing the abbreviations

$$\lambda_i - \lambda_j + \frac{N-1}{2}(\varphi - \varphi_i - \varphi_j) = A' \quad \lambda_i + \lambda_j + \frac{N-1}{2}(\varphi - \varphi_i + \varphi_j) = C'$$

$$-\lambda_i + \lambda_j + \frac{N-1}{2}(\varphi + \varphi_i + \varphi_j) = B' \quad -\lambda_i - \lambda_j + \frac{N-1}{2}(\varphi + \varphi_i - \varphi_j) = D'$$

we can write:

$$B_{ij}(\varphi)\, B^*_{ji}(\varphi) = \frac{1}{4N^2}\, [\{\underline{\sin A\cdot S(\varphi - \varphi_i - \varphi_j) - \sin B\cdot S(\varphi + \varphi_i + \varphi_j)} +$$

$$+ \cos C\cdot S(\varphi + \varphi_i - \varphi_j) + \cos D\cdot S(\varphi - \varphi_i + \varphi_j)\}$$

$$+ i\{\underline{-\cos A\cdot S(\varphi - \varphi_i - \varphi_j) + \cos B\cdot S(\varphi + \varphi_i + \varphi_j)} + \sin C\cdot S(\varphi + \varphi_i - \varphi_j) +$$

$$+ \sin D \cdot S(\varphi - \varphi_i + \varphi_j)\}] \cdot$$

$$\cdot [\{\underline{\sin A' \cdot S(\varphi - \varphi_i - \varphi_j) - \sin B' \cdot S(\varphi + \varphi_i + \varphi_j)} + \cos D' \cdot S(\varphi + \varphi_i - \varphi_j)$$

$$+ \cos C' \cdot S(\varphi - \varphi_i + \varphi_j)$$

$$-i\{\underline{-\cos A' \cdot S(\varphi - \varphi_i - \varphi_j) + \cos B' \cdot S(\varphi - \varphi_i - \varphi_j)} + \sin D' \cdot S(\varphi + \varphi_i - \varphi_j)$$

$$+ \sin D' \cdot S(\varphi - \varphi_i + \varphi_j)\}].$$

The underlined terms again change sign under the inversion $\varphi_i \to -\varphi_i$, $\varphi_j \to -\varphi_j$ and so we obtain, also using the fact that we need only retain the real part of $B_{ij}B_{ji}^*$:

$$B_{ij}B_{ji}^* = \frac{1}{4N^2} [\cos(A - A')\, S^2(\varphi - \varphi_i - \varphi_j) + \cos(B - B')\, S^2(\varphi + \varphi_i + \varphi_j)$$
$$+ \cos(C - D')\, S^2(\varphi + \varphi_i - \varphi_j) + \cos(D - C')\, S^2(\varphi - \varphi_i + \varphi_j) +$$
$$+ \{\cos(C - C') + \cos(D - D')\}\, S(\varphi - \varphi_i + \varphi_j)\, S(\varphi + \varphi_i - \varphi_j) +$$
$$+ \{\cos(A - B') + \cos(B - A')\}\, S(\varphi + \varphi_i + \varphi_j)\, S(\varphi - \varphi_i - \varphi_j)]$$

Under the transformation $\varphi_i \to -\varphi_i$, one finds that:

$$C \to \pi + A, \qquad C' \to \pi + B'$$
$$D \to \pi + B, \qquad D' \to \pi + A'$$

so the last two terms cancel each other and we obtain :

$$B_{ij}(\varphi)\, B_{ji}^*(\varphi) = \frac{1}{N^2} \cos(2\lambda(\varphi_i) + 2\lambda(\varphi_j))\, S^2(\varphi + \varphi_i - \varphi_j).$$

Inserting this into the expression for I_3 we obtain:

$$I_3 = \frac{1}{2^6\pi^3N} \int \int_{-\pi}^{\pi} \int e^{iR\varphi} \cos(2\lambda(\varphi_i + 2\lambda(\varphi_j))\, S^2(\varphi + \varphi_i - \varphi_j) \cdot$$
$$\cdot f^-(\varphi_i)\, f^-(\varphi_j)\, d\varphi\, d\varphi_i\, d\varphi_j$$

$$= \frac{1}{2^6\pi^3N} \int \int_{-\pi}^{\pi} \int e^{iR\varphi} \cos 2\lambda(\varphi_i) \cos 2\lambda(\varphi_j)\, S^2(\varphi + \varphi_i - \varphi_j) \cdot$$
$$\cdot f^-(\varphi_i)\, f^-(\varphi_j)\, d\varphi\, d\varphi_i\, d\varphi_j +$$

$$\frac{1}{2^6\pi^3N} \int \int_{-\pi}^{\pi} \int e^{iR\varphi} \sin 2\lambda(\varphi_i) \sin 2\lambda(\varphi_j)\, S^2(\varphi + \varphi_i - \varphi_j) \cdot$$
$$\cdot f^-(\varphi_i)\, f^-(\varphi_j)\, d\varphi\, d\varphi_i\, d\varphi_j,$$

which in the limit $N \to \infty$, analogous to I_2, reduces to:

$$I_3 = \left[\frac{1}{4\pi}\int_{-\pi}^{\pi} e^{iR\varphi} \cos 2\lambda(\varphi)\, f^-(\varphi)\, d\varphi\right]^2 + \left[\frac{1}{4\pi}\int_{-\pi}^{\pi} e^{iR\varphi} \sin 2\lambda(\varphi)\, f^-(\varphi)\, d\varphi\right]^2.$$

So we have found an explicit expression for the time-dependent correlation function of the z components of two spins in the chain that are separated by R lattice points:

$$\rho_R^z(\beta, t) = \langle M^z(h)\rangle_\beta^2 + \left[\frac{1}{4\pi}\int_{-\pi}^{\pi} e^{iR\varphi} f^+(\varphi)\, d\varphi\right]^2 -$$

$$-\left[\frac{1}{4\pi}\int_{-\pi}^{\pi} e^{iR\varphi} \cos 2\lambda(\varphi)\, f^-(\varphi)\, d\varphi\right]^2 - \left[\frac{1}{4\pi}\int_{-\pi}^{\pi} e^{iR\varphi} \sin 2\lambda(\varphi)\, f^-(\varphi)\, d\varphi\right]^2 \qquad (20)$$

Starting from this formula we will discuss the following subjects:

a. The long-range order

b. The time-dependent autocorrelation function of one spin

c. The autocorrelation function of the magnetization

d. The possibility that in $\rho_R^z(\beta, t)$ satisfies a wave equation.

a. The long-range order is usually defined in terms of sublattices, but since the Hamiltonian is invariant under translations, this is not useful in our case, and the quantity $\lim_{R\to\infty} \rho_{2R}^z(\beta, t)$ is used.

The well known theorem of Riemann-Lebesque[5]) states, that if the integral $\int_a^b f(x)\, dx$ exists and $f(x)$ has a limited total variation in the range (a, b), then, as $\lambda \to \infty$, one has

$$\lim_{\lambda\to\infty} \int_a^b f(x) \sin \lambda x\, dx = \lim_{\lambda\to\infty} \int_a^b f(x) \cos \lambda x\, dx = 0.$$

Since these conditions are clearly satisfied by the functions.

$$e^{iR\varphi} F^+(\varphi),\ e^{iR\varphi} \cos 2\lambda(\varphi)\, F^-(\varphi) \quad \text{and} \quad e^{iR\varphi} \sin 2\lambda(\varphi)\, f^-(\varphi),$$

we have:

$$\lim_{R\to\infty} \rho_R^z(\beta, t) = \langle M^z(h)\rangle_\beta^2. \qquad (21)$$

Since $\langle M^z(0)\rangle_\beta = 0$ there is no long-range order when there is no magnetic field. In the next section it will be shown that

$$\langle M^{z^2}(h)\rangle_\beta - \langle M^z(h)\rangle_\beta^2 = 0\,\frac{1}{N}$$

so we can write (20) as:

$$\lim_{r\to\infty} \rho_r^z(\beta, t) = \langle M^{z^2}(h)\rangle_\beta \qquad (22)$$

From (22) it can be seen that in this model the magnetization is the square root of the long-range order (in this way one also calculates the spontaneous magnetization of the two-dimensional Ising lattice), since in the expression

$$\langle M^z(h)\rangle_\beta^2 = \langle M^{z^2}(h)\rangle_\beta = \lim_{N\to\infty} \frac{1}{N^2} \sum_{i,j=1}^{N} \langle S_i^z S_j^z\rangle_\beta$$

$$= \lim_{N\to\infty} \frac{1}{N} \sum_{R=1}^{N} \rho_R^z(\beta, t)$$

the devision by N eliminates all except the long-range correlation.

b. For $R = 0$ the formula (20) reduces to the autocorrelation function of one arbitrary spin:

$$\rho^z(\beta, t) = \langle M^z(h)\rangle_\beta^2 + \left[\frac{1}{2\pi}\int_0^\pi \{\cos \Lambda t + i \sin \Lambda t \operatorname{tgh} \tfrac{1}{2}\beta\Lambda\}\, \mathrm{d}\varphi\right]^2$$

$$-\left[\frac{1}{2\pi}\int_0^\pi \cos 2\lambda(\varphi)\, \{i \sin \Lambda t + \cos \Lambda t \operatorname{tgh} \tfrac{1}{2}\beta\Lambda\}\, \mathrm{d}\varphi\right]^2. \tag{23}$$

Making use of the theorem of Riemann-Lebesque one sees that the last two terms vanish as t approaches infinity, so:

$$\lim_{t\to\infty} \langle S_l^z S_l^z(t)\rangle_\beta = \langle S_l^z\rangle^2.$$

Thus the correlation for one single spin is seen to vanish and the autocorrelation function simply goes over into the square of the expectation value of the operator S_l^z. This is an expression of the fact that the memory of one single spin is completely destroyed by the interaction with the rest of the chain, if this chain is infinite. Further on we will also consider the autocorrelation function $\langle M^z M^z(t)\rangle_\beta$; in this case there is a memory effect and the reason for this will be explained.

We want to study the time dependence of $\rho^z(\beta, t)$ a little better and consider the special case that there is no magnetic field. The integrands in expression (23) are even functions of φ, so the integration can be restricted to the interval $[0, \pi]$. Since

$$2\lambda(\varphi) = \operatorname{arctg} \frac{\gamma \sin \varphi}{\cos \varphi},$$

with $0 < \lambda \leqslant \pi$ by definition, we can now without ambiguity write

$$\cos 2\lambda(\varphi) = \frac{\cos \varphi}{\Lambda(\varphi)}$$

and so:

$$\rho^z(\beta, t) = \left[\frac{1}{2\pi}\int_0^\pi f^+(\varphi)\, \mathrm{d}\varphi\right]^2 - \left[\frac{1}{2\pi}\int_0^\pi \frac{\cos \varphi}{\Lambda(\varphi)}\, f^-(\varphi)\, \mathrm{d}\varphi\right]^2$$

For the case $h = 0$ we have $\Lambda(\varphi) = \Lambda(\pi - \varphi)$ and since $\cos(\pi - \varphi) = -\cos\varphi$ the second term is seen to vanish. Going over to Λ as integration variable in the first term we obtain:

$$\rho^z(\beta, t) = D^2(\beta, t)$$

with

$$D(\beta, t) = \frac{1}{\pi} \int_{\gamma}^{1} \frac{\Lambda \, \mathrm{d}\Lambda}{\sqrt{(\Lambda^2 - \gamma^2)(1 - \Lambda^2)}} \{\cos \Lambda t + i \sin \Lambda t \cdot \mathrm{tgh}\ \tfrac{1}{2}\beta\Lambda\} \tag{24}$$

As a check we easily verify that $D(\beta, 0) = \frac{1}{2}$, or $\rho^z(\beta, 0) = \frac{1}{4}$ as it should be. For high temperatures we need only to retain the term which is linear in β:

$$\begin{aligned} D(\beta, t) &= \frac{1}{\pi} \int_{\gamma}^{1} \frac{\Lambda \, \mathrm{d}\Lambda}{\sqrt{(\Lambda^2 - \gamma^2)(t - \Lambda^2)}} \left\{\cos \Lambda t + \frac{i\beta}{2} \sin \Lambda t\right\} \\ &= D_1 + D_2 \end{aligned}$$

where

$$D_1 = \frac{1}{\pi} \int_{\gamma}^{1} \frac{\Lambda \cos \Lambda t \cdot \mathrm{d}\lambda}{\sqrt{(\Lambda^2 - \gamma^2)(1 - \Lambda^2)}}, \quad D_2 = \frac{i\beta}{2\pi} \int_{\gamma}^{1} \frac{\Lambda^2 \sin \Lambda t \cdot \mathrm{d}\Lambda}{\sqrt{(\Lambda^2 - \gamma^2)(1 - \Lambda^2)}}$$

For the case $\gamma = 0$ these integrals reduce to:

$$D_1 = \frac{1}{\pi} \int_{0}^{1} \frac{\cos \Lambda t}{\sqrt{1 - \Lambda^2}} \, \mathrm{d}\Lambda = \tfrac{1}{2} J_0(t),$$

and

$$D_2 = \frac{i\beta}{2\pi} \int_{0}^{1} \frac{\Lambda \sin \Lambda t}{\sqrt{1 - \Lambda^2}} \cdot \mathrm{d}\Lambda = \frac{i\beta}{4} J_1(t)$$

where $J_0(t)$ and $J_1(t)$ are Bessel functions of the first kind, respectively of the order zero and one, so for $\gamma = 0$ one obtains for the high temperature limit and no external field:

$$\rho^z(\beta, t) = \left[\tfrac{1}{2} J_0(t) + \frac{i\beta}{4} J_1(t)\right]^2$$

Using the approximations for Bessel functions for small and large arguments

$$J_n(t) = (\tfrac{1}{2}t)^n / \Gamma(n + 1) \qquad \text{for} \quad t \ll 1$$

$$J_n(t) = \sqrt{\frac{2}{\pi t}} \cos\left\{t - \tfrac{1}{2}n\pi - \frac{\pi}{4}\right\} \qquad \text{for} \quad t \gg 1$$

we find for $\rho^z(\beta, t)$ for large or small times:

$$\rho^z(\beta, t) = \tfrac{1}{4}\left[1 + \frac{\beta t i}{4}\right]^2 \quad \text{for} \quad t \ll 1$$

$$\rho^z(\beta, t) = \frac{1}{2\pi t}\left[\cos\left\{t - \frac{\pi}{4}\right\} + \frac{i\beta}{4}\cos\left\{t - \frac{\pi}{2} - \frac{\pi}{4}\right\}\right]^2$$

$$= \frac{1}{2\pi t}\left[\cos\left(t - \frac{\pi}{4}\right) + \frac{i\beta}{4}\sin\left(t - \frac{\pi}{4}\right)\right]^2 \quad \text{for} \quad t \gg 1$$

If we had not made the Hamiltonian dimensionless but had kept the factor J in front, this would be:

$$\rho^z(\beta, t) = \tfrac{1}{4}\left[1 + \frac{i\beta J t}{z}\right]^2 \quad \text{for} \quad tJ \ll 1$$

$$\rho^z(\beta, t) = \frac{1}{4\pi J t}\left[\cos\left(2Jt - \frac{\pi}{4}\right) + \frac{i\beta}{4}\sin\left(2Jt - \frac{\pi}{4}\right)\right] \quad \text{for} \quad tJ \gg 1.$$

If $\gamma = 0$, we have

$$[\sum_{l=1}^{N} S_l^z, H] = 0, \quad \text{but} \quad [S_l^z, H] \neq 0,$$

and as a consequence one can see directly that $\rho^z(\beta, t)$ still depends on t, even when $\gamma = 0$.

For $\gamma \neq 0$ one can approximate the functions D_1 and D_2 for either small t, by expanding in powers of t and retaining only the linear part, or for large t, by using the stationary phase approximation, obtaining

$$\rho^z(\beta, t) \simeq \tfrac{1}{4}\left[1 + \frac{i\beta t}{\beta}(1 + \gamma^2)\right]^2 \quad \text{for} \quad t \ll 1$$

and

$$\rho^z(\beta, t) \simeq \frac{1}{4\pi t(1 - \gamma^2)}\left[(2\gamma)^{\frac{1}{2}}\cos\left(\gamma t - \frac{\pi}{4}\right) + \cos\left(t - \frac{\pi}{4}\right) + \right.$$
$$\left. + \frac{i\beta}{4}\left\{\gamma(2\gamma)^{\frac{1}{2}}\sin\left(\gamma t - \frac{\pi}{4}\right) + \sin\left(t - \frac{\pi}{4}\right)\right]^2 \quad \text{for} \quad t \gg 1$$

It is clear that $\rho^z(\beta, t)$ shows no exponential decay; except for the superimposed wiggles it is proportional to t^{-1} for large t.

For $\gamma = 0$ and $\beta \ll 1$ we can examine $\rho^z(\beta, t)$ a little better since then it is given by $\rho^z(\beta, t) = \frac{1}{4}J_0^2(t)$. On differentiating we obtain $d\rho^z/dt = -J_0(t)$. Since $J_0(t)$ and $J_1(t)$ are tabulated one easily checks, that $d\rho^z/dt$ is a negative decreasing function in the interval $0 \leqslant t \leqslant 1$, reaching a minimum for $t \simeq 1.1$. So in the interval $0 \leqslant t \leqslant 1.1$, where $\rho^z(t)$ drops almost exactly to half its initial value, we have $d^2\rho^z/dt^2 < 0$ and the behaviour of $\rho^z(t)$ can never be described by a linear combination of exponentials $\sum_j e^{-\tau_j t}$.

At $t = 2.4$ $\rho^z(t) = 0$ after which it rises again to a maximum $0.16\rho^z(0)$ at $t = 3.9$. The decay of $\rho^z(t)$ from its value at $t = 1$ to where it first takes on the value $0.16\ \rho^z(0)$ at $t \simeq 1.8$ can be rather well described by an exponential, namely $e^{-1.95(t-1)}$. At times later than $t \simeq 1.8$ this is of course impossible since $\rho^z(t = 1.8) = \rho^z(t = 3.9)$.

c. From formula (20) one can also calculate the time-dependent autocorrelation function of the z component of the magnetization. The quantity

$$\sum_{l, m=1}^{N} \rho^z_{l,m}(\beta, t)$$

will be of the order N^2, but in the Kubo-formula (34) we use

$$\sum_{l, m=1}^{N} \rho^z_{l,m}(\beta, t) - \langle \sum_{l=1}^{N} S^z_l \rangle^2_\beta$$

this quantity should be of the order N. So the function $R(\beta, t)$ defined by:

$$R(\beta, t) = \frac{1}{N} \{ \sum_{l, m=1}^{N} \rho^z_{l,m}(\beta, t) - \langle \sum_{l=1}^{N} S^z_l \rangle^2_\beta \} \tag{25}$$

should, on taking the limit $N \to \infty$, be a finite function of β and t, which it indeed turns out to be. By substituting (28) into (25) we find:

$$\begin{aligned} R(\beta, t) &= \frac{1}{4N^2} \sum_{R, i, j, =1}^{N} e^{iR(\varphi_i + \varphi_j)} f^+(\varphi_i)\ f^+(\varphi_i)\ f^+(\varphi_j) \\ &- \frac{1}{4N^2} \sum_{R, i, j=1}^{N} e^{iR(\varphi_i + \varphi_j)} \cos 2\lambda(\varphi_i) \cos 2\lambda(\varphi_j)\ f^-(\varphi_i)\ f^-(\varphi_j) \\ &- \frac{1}{4N^2} \sum_{R, i, j=1}^{N} e^{iR(\varphi_i + \varphi_j)} \sin 2\lambda(\varphi_i) \sin 2\lambda(\varphi_j)\ f^-(\varphi_i)\ f^-(\varphi_j) \\ &= \frac{1}{4\pi} \int_0^\pi [(f^+(\varphi))^2 - \{\cos^2 2\lambda(\varphi) - \sin^2 2\lambda(\varphi)\}\ (f^-(\varphi))^2]\ d\varphi \\ &= \frac{1}{4\pi} \int_0^\pi [(f^+(\varphi))^2 - (f^-(\varphi))^2 + 2 \sin^2 2\lambda(\varphi) (f^-(\varphi))^2]\ d\varphi \end{aligned}$$

One can split this autocorrelation function into a timedependent and a constant part as follows:

$$R(\beta, t) = \frac{1}{4\pi} \int_0^\pi \frac{\cos^2 2\lambda(\varphi)}{\cosh^2 \frac{1}{2}\beta\Lambda(\varphi)}\ d\varphi + \frac{1}{2\pi} \int_0^\pi \sin^2 2\lambda(\varphi) \operatorname{tgh} \tfrac{1}{2}\beta\Lambda(\varphi) \cdot$$

$$\cdot \left\{ i \sin 2\Lambda(\varphi)\ t + \frac{\cos 2\Lambda(\varphi)\ t}{\operatorname{tgh} \frac{1}{2}\beta\Lambda(\varphi)} \right\} d\varphi$$

For $\gamma = 0$ the time-dependent part is zero, since then $\sin 2\lambda(\varphi) = 0$. This agrees with the fact that for $\gamma = 0$ the operator for the magnetization in the z direction commutes with the Hamiltonian. The constant part is not equal to zero, not even when there is no external field. By means of the Riemann-Lebesgue theorem the time-dependent part of $R(\beta, t)$ is seen to go to zero as $t \to \infty$. The fact that the autocorrelation function reaches a non-zero value as $t \to \infty$ at first looks disturbing, but it turns out that (section E) it is actually necessary and due to the circumstance that we consider thermally completely isolated system.

In section E we will need the high-temperature limit of $R(\beta, t)$, i.e.

$$R(0, t) = \frac{1}{4\pi} \int_0^\pi \{1 - 2 \sin^2 2\lambda(\varphi) \sin^2 \Lambda(\varphi)t\} \, \mathrm{d}\varphi \tag{26}$$

We will not yet comment upon the way this function depends on time, this will be done in section E.

From the fact that the autocorrelation function is not of the form $a\mathrm{e}^{-ct} + b$ we may not conclude that, if the external field is changed a little, the change of the magnetization cannot be described by a Markoff process. We can conclude, however, that the change in the magnetization cannot be described by a Gaussian Markoff process, since one can prove that for such process the autocorrelation function is an exponential.

(For more general spin systems a master-equation, which governs the temporal behaviour of the magnetization, was constructed by Tjon[6]).

b. The possibility that $\mathrm{Im}\, \rho_R^z$ is determined by some kind of wave equation.

In an article on the quasi-elastic magnetic scattering of slow neutrons[2]), Th. W. Ruygrok has studied the function $\rho_R^{ij}(\beta, t)$, where the coefficients i and j may stand for the coordinates x, y and z respectively. He showed that $\mathrm{Im}\, \rho_R^{ij}(\beta, t)$ in a three-dimensional crystal, can be interpreted as the change in the j component of the local magnetic moment, at the time t and place R, due to the flashing on and off at time zero and place $R = 0$ of a neutron which is polarized in the i direction.

So, from the point of neutron scattering, it is important to know what kind of function $\mathrm{Im}\, \rho_R^{ij}(\beta, t)$ will be, or what kind of equation it satisfies. For the case of a ferromagnet, magnetized in the z direction, Van Hove[8]) derived exact expressions for $\rho_R^{ij}(\beta, t)$ in the spin wave approximation. From these Ruygrok showed that $\mathrm{Im}\, \rho_R^{xx}(\beta, t)$ satisfies the following "wave equation" in the spin wave approximation:

$$\frac{\partial^2}{\partial t^2} \mathrm{Im}\, \rho_R^{xx}(\beta, t) = -\left(\frac{2SJ}{\hbar}\right)^2 \sum_{\delta_1, \delta_2} \{\mathrm{Im}\, \rho_{R+\delta_1+\delta_2}^{xx}(\beta, t) - 2\, \mathrm{Im}\, \rho_{R+\delta_1}^{xx}(\beta, t) + \\ + \mathrm{Im} \rho_R^{xx}(\beta, t)\}$$

where the summations $\sum_\delta$ are over nearest neighbours. Considering only unmagnetized ferromagnetic, cubic materials, so that the full cubic symmetry is preserved, he argued that at higher temperatures than those at which the spin wave approximation is applicable, the lifetime of a spin wave is shortened. He tried to take this effect into account by adding a damping factor and postulated for $t > 0$ an equation of the form (putting $\rho^{ii} = \rho^{i}$):

$$\frac{\partial^2}{\partial t^2} \operatorname{Im} \rho^i_R(\beta, t) + \tau_1^{-1} \frac{\partial}{\partial t} \operatorname{Im} \rho^i_R(\beta, t) + \tau_2^{-2} \sum_{\delta_1, \delta_2} \{\operatorname{Im} \rho^i_{R+\delta_1+\delta_2}(\beta, t) - 2 \operatorname{Im} \rho^i_{R+\delta_1}(\beta, t) + \operatorname{Im} \rho^i_R(\beta, t)\} = 0,$$

where τ_1 and τ_2 are suitable parameters, and suitable boundary conditions are chosen.

In the case of the X-Y model, where we know $\operatorname{Im} \rho^z_R(\beta, t)$ exactly, it will be found that for the case that there is no external field we can write:

$$\operatorname{Im} \rho^z_R(\beta, t) = A_R(\beta, t) \cdot \sum_{\delta = \pm 1} \int_0^t A_{R+\delta}(\beta, \tau) \, d\tau$$

where $A_R(\beta, t)$ satisfies a "wave equation" for all temperatures if γ is small e.g. $\gamma < \frac{1}{10}$. From formula (19) one easily verifies that we have:

$$\operatorname{Im} \rho^z_R(\beta, t) = \frac{1}{2^3\pi^2} \int_{-\pi}^{\pi}\!\!\int \cos R\varphi \cdot \cos R\psi \cos \Lambda(\varphi)\, t \cdot \cos \Lambda(\psi)\, t \cdot$$

$$\cdot \operatorname{tgh} \tfrac{1}{2}\beta\Lambda(\varphi) \operatorname{tgh} \tfrac{1}{2}\beta\Lambda(\psi)\{1 - \cos 2\lambda(\varphi) \cos 2\lambda(\psi)\} \, d\varphi \, d\psi.$$

We will consider the case that R is an even number, for odd R one gets analogous results. Since $h = 0$ the second term between the curly brackets in the integrand is odd in φ and ψ and we obtain:

$$\operatorname{Im} \rho^z_R(\beta, t) = \frac{1}{2\pi^2} \int_0^{\pi} \cos R\varphi \cos \Lambda(\varphi)\, t \operatorname{tgh} \tfrac{1}{2}\beta\Lambda(\varphi) \, d\varphi \cdot$$

$$\cdot \int_0^{\pi} \cos R\psi \sin \Lambda(\psi) t \operatorname{tgh} \tfrac{1}{2}\beta\Lambda(\psi) \, d\psi.$$

Since γ is supposed to be small we can write $\cos \Lambda(\varphi)\, t \simeq \cos(|\cos \varphi|\, t)$ and $\sin \Lambda(\varphi)\, t \simeq \sin(|\cos \varphi|\, t)$, so:

$$\operatorname{Im} \rho^z_R(\beta. t) = A_R(\beta, t) \cdot B_R(\beta, t)$$

where we have introduced

$$A_R(\beta, t) = \frac{1}{\pi} \int_0^{\frac{1}{2}\pi} \cos R\varphi \cdot \cos\{(\cos \varphi)\, t\} \cdot \operatorname{tgh} \tfrac{1}{2}\beta\Lambda(\varphi) \, d\varphi$$

and

$$B_R(\beta, t) = \frac{2}{\pi} \int_0^{\frac{1}{2}\pi} \cos R\psi \cdot \sin\{(\cos \psi)\, t\} \cdot \mathrm{tgh}\, \tfrac{1}{2}\beta\Lambda(\psi)\, \mathrm{d}\psi.$$

Obviously one has:

$$\frac{\partial B_R(\beta, t)}{\partial t} = A_{R+1}(\beta, t) + A_{R-1}(\beta, t), \quad \text{with} \quad B_R(\beta, 0) = 0$$

so:

$$\mathrm{Im}\, \rho_R^z(\beta, t) = A_R(\beta, t) \cdot \int_0^t \{A_{R+1}(\beta, \tau) + A_{R-1}(\beta, \tau)\}\, \mathrm{d}\tau.$$

Thus for $h = 0$ and small γ, Im $\rho_R^z(\beta, t)$ can be expressed as a function of $A_R(\beta, t)$, and it is easily seen that it is this function which satisfies the following wave equation:

$$\frac{\partial^2 A_R(\beta, t)}{\partial t^2} + \tfrac{1}{4}[A_{R-2}(\beta, t) + 2A_R(\beta, t) + A_{R+2}(\beta, t)] = 0, \tag{26a}$$

In a certain sense equation (26*a*) can be considered to be an extension of equation (38) of ref. 2. We have found that Im $\rho_R^z(\beta, t)$ is completely determined by a function $A_R(\beta, t)$ which satisfies a wave equation like (38) in ref. 2, only in ref. 2 we have Im $\rho_R^i(\beta, t) = A_R(\beta, t)$. The fact that in our case we no longer have Im $\rho_R^z(\beta, t) = A_R(\beta, t)$ is probably due to the fact that the derivation of (38) of ref. 2 is heavily dependent on the isotropy of the Heisenberg interaction; the fact, however, that our wave equation is valid for all temperatures probably comes about because the diagonalization of the Hamiltonian of the chain is not dependent on temperature, whereas the diagonalization of the isotropic Heisenberg Hamiltonian to non-interacting magnons is only valid at very low temperatures. Still, the equations for $A_R(\beta, t)$ or Im $\rho_R^z(\beta, t)$ may radically change for larger values of γ.

D. *Behaviour of the model in a non-equilibrium case.* Due to the fact that the Hamiltonian of the model can still be diagonalized in the presence of an external magnetic field along the z axis, it is possible to solve exactly a non-equilibrium situation, which has been considered by many authors[12]) for more general spin systems, including for example dipole-dipole interaction. We will consider the following situation: let the chain be in thermal equilibrium at temperature T in an external magnetic field h_1 at time $t < 0$. Working in the Heisenberg representation we denote the canonical ensemble corresponding with this situation by the symbol $|E\rangle$. At $t = 0$ the external field h_1 is suddenly changed to h_2 and since the operator for the z component of the magnetization $M^z = \dfrac{1}{N} \sum_{l=1}^N S_l^z$ does not commute with the

Hamiltonian, the expectation value $\langle M^z(t)\rangle$ will be a function of time for $t > 0$, since in the Heisenberg picture $M^z(t)$ is a time dependent operator. In section A we have calculated the quantity $\langle M^z\rangle_\beta = \langle E\,|M^z|\,E\rangle$ for $t < 0$. We now propose to calculate the quantity:

$$\begin{aligned}\langle M^z(t)\rangle &= \langle E\,|M^z(t)|\,E\rangle \\ &= \langle E\,|e^{iHt}\,M^z\,e^{-iHt}|\,E\rangle \qquad \text{for} \quad t > 0 \qquad (27)\end{aligned}$$

to determine the time dependent behaviour. Since the Hamiltonian is given by:

$$H = \sum_{j=1}^{N} [(1+\gamma)\,S_j^x S_{j+1}^x + (1-\gamma)\,S_j^y S_{j+1}^y - h_1 S_j^z] \qquad \text{for} \quad t < 0$$

and

$$H' = \sum_{j=1}^{N} [(1+\gamma)\,S_j^x S_{j+1}^x + (1-\gamma)\,S_j^y S_{j+1}^y - h_2 S_j^z] \qquad \text{for} \quad t > 0,$$

the transformation coefficients needed to diagonalize the Hamiltonian for $t < 0$ will differ from those at $t > 0$, if $h_1 \neq h_2$. The coefficients Φ_{ij}, and Ψ_{ij}, the corresponding eigenvalues Λ_j amd the operators η_j etc., for the initial field h_1 will be denoted without a prime, those corresponding to the field h_2, will be denoted by a prime:

$$\begin{aligned}&H,\ \Phi_{ij},\ \Psi_{ij},\ \lambda_j,\ \Lambda_j,\ \eta_j \qquad \text{for} \quad t < 0,\ h = h_1 \\ &H',\ \Phi'_{ij},\ \Psi'_{ij},\ \lambda'_j,\ \Lambda'_j,\ \eta'_j \qquad \text{for} \quad t > 0,\ h = h_2\end{aligned}$$

So we have:

$$\langle M^z(t)\rangle = \begin{cases} \langle M^z(h_1)\rangle_\beta & \text{for} \quad t < 0 \\ \dfrac{\operatorname{Tr} e^{-\beta H}\, e^{iH't} \sum_{l=1}^{N} S_l^z\, e^{-iH't}}{\operatorname{Tr} e^{-\beta H}} & \text{for} \quad t > 0 \end{cases} \qquad (28)$$

We will follow the following procedure: first express the operator M^z in terms of the η' operators to determine the time dependence and next transform the η' operators, which appear in the matrix elements, into the η operators, via the M^z operator, in order to be able to calculate these matrix elements. In formulae this goes as follows:

$$\begin{aligned}\langle M^z(t)\rangle &= \left\langle E \left| e^{iH't}\,\frac{1}{N}\sum_{l=1}^{N} S_l^z\, e^{-iH't} \right| E \right\rangle \\ &= \frac{1}{2N}\sum_{l,m,n=1}^{N} \Phi'_{ml}\Psi'_{nl}\langle E\,|\{\exp it \sum_{j=1}^{N} \Lambda'_j \eta_j^{*\prime}\eta'_j\}\,(\eta_m'^{*} + \eta'_m) \\ &\quad (\eta'_n - \eta_n'^{*})\,\{\exp\ -it \sum_{j=1}^{N} \Lambda'_j \eta_j^{*\prime}\eta'_j\}|\,E\rangle\end{aligned}$$

Using the fact that for fermion operators one has

$$\{\exp it \sum_{j=1}^{N} \Lambda_j' \eta_j^{*\prime} \eta_j'\}\, \eta_k'^{*}\, \{\exp -it \sum_{j=1}^{N} \Lambda_j' \eta_j'^{*} \eta_j'\} = \eta_k'^{*} \exp it\Lambda_k'$$

and

$$\{\exp it \sum_{j=1}^{N} \Lambda_j' \eta_j^{*\prime} \eta_j'\}\, \eta_k'\, \{\exp -it \sum_{j=1}^{N} \Lambda_j' \eta_j^{*\prime} \eta_j'\} = \eta_k' \exp -it\Lambda_k'$$

we can take the time-dependent part out of the trace, and, introducing the abbreviation $t\Lambda_k' = \alpha_k$, we obtain:

$$\begin{aligned}\langle M^z(t)\rangle = \frac{1}{2N} \sum_{l,m,n=1}^{N} \Phi_{ml}' \Psi_{nl}' \,[&\cos \alpha_m \cos \alpha_n \,\langle E\, |(\eta_m'^{*} + \eta_m')(\eta_n' - \eta_n'^{*})|\, E\rangle \\ &+ \sin \alpha_m \sin \alpha_n \,\langle E\, |(\eta_m'^{*} - \eta_m')(\eta_n' + \eta_n'^{*})|\, E\rangle \\ &+ i \sin \alpha_m \cos \alpha_n \,\langle E\, |(\eta_m'^{*} - \eta_m')(\eta_n' - \eta_n'^{*})|\, E\rangle \\ &- i \cos \alpha_m \sin \alpha_n \,\langle E\, |(\eta_m'^{*} + \eta_m')(\eta_n' + \eta_n'^{*})|\, E\rangle]\end{aligned}$$

Upon transforming from the η' operators to the η operators by means of

$$\eta_m' + \eta_m'^{*} = \sum_{p=1}^{N} \Phi_{mp}'(c_p^{*} + c_p) = \sum_{p,q=1}^{N} \Phi_{mp}' \Phi_{qp}(\eta_q + \eta_q^{*})$$

$$\eta_n' - \eta_n'^{*} = \sum_{r=1}^{N} \Psi_{nr}'(c_r - c_r^{*}) = \sum_{r,s=1}^{N} \Psi_{nr}' \Psi_{sr}(\eta_s - \eta_s^{*})$$

and assuming that $\langle M^z(t)\rangle$ does not change discontinuously in the point $t = 0$, one gets:

$$\begin{aligned}\langle M^z(t)\rangle = -\frac{1}{2N} \sum_{\substack{l,m,n\\ p,q,r,s=1}}^{N} \;[&\cos \alpha_m \cos \alpha_n \Phi_{ml}' \Psi_{nl} \Phi_{mp}' \Phi_{qp} \Psi_{nr}' \Psi_{sr} \mathrm{tgh}\, \tfrac{1}{2}\beta\Lambda_q \cdot \delta_{qs} \\ &+ \sin \alpha_m \sin \alpha_n \Phi_{ml}' \Psi_{nl}' \Psi_{mp}' \Psi_{qp} \Phi_{nr} \Phi_{sr}\, \mathrm{tgh}\, \tfrac{1}{2}\beta\Lambda_q \cdot \delta_{qs} \\ &+ i \sin \alpha_m \cos \alpha_n \Phi_{ml}' \Psi_{nl}' \Psi_{mp}' \Psi_{qp} \Psi_{nr}' \Psi_{sr} \cdot \delta_{qs} \\ &- i \cos \alpha_m \sin \alpha_n \Phi_{ml}' \Psi_{nl}' \Phi_{mp}' \Phi_{qp} \Phi_{nr}' \Phi_{sr} \cdot \delta_{qs}].\end{aligned}$$

Using the orthogonality of the matrices Φ and Ψ the imaginary part of this expression is easily found to equal zero:

$$\sum_{\substack{l,m,n\\ p,q,r,s=1}}^{N} [\sin \alpha_m \cos \alpha_n \Phi_{ml}' \Psi_{nl}' \Psi_{mp}' \Psi_{qp} \Psi_{nr}' \Psi_{sr} \delta_{qs} - \cos \alpha_m \sin \alpha_n \Phi_{ml}' \Psi_{nl} \Phi_{mp}' \Phi_{qp} \Phi_{nr} \Phi_{sr} \delta_{qs}]$$

since

$$\sum_q \Psi_{qp} \Psi_{qr} = \delta_{pr} \quad \text{and} \quad \sum_q \Phi_{qp} \Phi_{qr} = \delta_{qr}$$

this expression reduces to zero:

$$\sum_{m,l,n=1}^{N} [\sin \alpha_m \cos \alpha_n \Phi_{ml}' \Psi_{nl}' \delta_{m,n} - \cos \alpha_m \sin \alpha_n \Phi_{ml}' \Psi_{nl}' \delta_{mn}] = 0$$

This should be the case of course, since $\langle M^z(t)\rangle$ is real. The expression for $\langle M^z(t)\rangle$ now simplifies to:

$$\langle M^z(t)\rangle = -\frac{1}{2N}\sum_{\substack{l,m,n\\p,q,r=1}}^{N}[\cos\alpha_m\cos\alpha_n\Phi'_{ml}\Psi'_{nl}\Phi'_{mp}\Psi_{qp}\Psi'_{nr}\Psi_{qr}\ \mathrm{tgh}\ \tfrac{1}{2}\beta\Lambda_q +$$
$$+\sin\alpha_m\sin\alpha_n\Phi'_{ml}\Psi'_{nl}\Psi'_{mp}\Psi_{qp}\Phi'_{nr}\Phi_{sr}\ \mathrm{tgh}\ \tfrac{1}{2}\beta\Lambda_q] \qquad (29)$$

The rest of this section consists mainly in showing that this sixfold sum reduces, as $N\to\infty$, to one single integral. Substituting the explicit form of the transformation coefficients we get

$$\langle M^z(t)\rangle = -\frac{4}{N^4}\sum_{\substack{l,m,n=1\\p,q,r}}^{N}\Bigg[\cos\alpha_m\cos\alpha_n\cos\left(l\varphi_m-\lambda'(\varphi_m)-\frac{\pi}{4}\right)$$
$$\cos\left(l\varphi_n+\lambda'(\varphi_n)-\frac{\pi}{4}\right)\cos\left(p\varphi_m-\lambda'(\varphi_n)-\frac{\pi}{4}\right)\cdot$$
$$\cdot\cos\left(p\varphi_q-\lambda(\varphi_q)-\frac{\pi}{4}\right)\cos\left(r\varphi_n+\lambda'(\varphi_n)-\frac{\pi}{4}\right)\cdot$$
$$\cdot\cos\left(r\varphi_q-\lambda(\varphi_q)-\frac{\pi}{4}\right)\ \mathrm{tgh}\ \tfrac{1}{2}\beta\Lambda_q$$
$$+\sin\alpha_m\sin\alpha_n\cos\left(l\varphi_m-\lambda'(\varphi_m)-\frac{\pi}{4}\right)$$
$$\cdot\cos\left(l\varphi_n+\lambda'(\varphi_n)-\frac{\pi}{4}\right)\cos\left(p\varphi_m+\lambda'(\varphi_m)-\frac{\pi}{4}\right)\cdot$$
$$\cdot\cos\left(p\varphi_q+\lambda(\varphi_q)-\frac{\pi}{4}\right)\cos\left(r\varphi_n-\lambda'(\varphi_n)-\frac{\pi}{4}\right)\cdot$$
$$\cdot\cos\left(r\varphi_q-\lambda(\varphi_q)-\frac{\pi}{4}\right)\mathrm{tgh}\ \tfrac{1}{2}\beta\Lambda_q\Bigg]$$

As in the former section the summations over l, p and r can be performed explicitly, and, on replacing the summations over m, n and q by integrations over φ_1, φ_2 and φ_3, ranging from 0 to 2π, we obtain:

$$\langle M^z(t)\rangle = -\frac{1}{2\pi^3N}\{L_1+L_2\}$$

where:

$$L_1 = \int\int_{-\pi}^{\pi}\int \mathrm{d}\varphi_1\,\mathrm{d}\varphi_2\,\mathrm{d}\varphi_3\cos\alpha(\varphi_1)\cos\alpha(\varphi_2)\ \mathrm{tgh}\ \tfrac{1}{2}\beta\Lambda(\varphi_3)\cdot$$
$$\cdot\Bigg[\sin\left\{\lambda'(\varphi_2)-\lambda'(\varphi_1)+\frac{N+1}{2}(\varphi_1+\varphi_2)\right\}S(\varphi_1+\varphi_2)+$$

$$\cos\left\{-\lambda'(\varphi_1) - \lambda'(\varphi_2) + \frac{N+1}{2}(\varphi_1 - \varphi_2)\right\} S(\varphi_1 - \varphi_2)\Big] \cdot$$

$$\cdot \Big[\sin\left\{-\lambda'(\varphi_1) - \lambda(\varphi_3) + \frac{N+1}{2}(\varphi_1 + \varphi_3)\right\} S(\varphi_1 + \varphi_3) +$$

$$\cos\left\{\lambda(\varphi_3) - \lambda'(\varphi_1) + \frac{N+1}{2}(\varphi_1 - \varphi_3)\right\} S(\varphi_1 - \varphi_3)\Big] \cdot$$

$$\cdot \Big[\sin\left\{\lambda'(\varphi_2) + \lambda(\varphi_3) + \frac{N+1}{2}(\varphi_2 + \varphi_3)\right\} S(\varphi_2 + \varphi_3) +$$

$$\cos\left\{\lambda'(\varphi_2) - \lambda(\varphi_3) + \frac{N+1}{2}(\varphi_2 - \varphi_3)\right\} S(\varphi_2 - \varphi_3)\Big]$$

and

$$L_2 = \int\int_{-\pi}^{\pi}\int \mathrm{d}\varphi_1\, \mathrm{d}\varphi_2\, \mathrm{d}\varphi_3 \sin\alpha(\varphi_1) \sin\alpha(\varphi_2)\, \mathrm{tgh}\, \tfrac{1}{2}\beta\Lambda(\varphi_3) \cdot$$

$$\cdot \Big[\sin\left\{-\lambda'(\varphi_1) + \lambda'(\varphi_2) + \frac{N+1}{2}(\varphi_1 + \varphi_2)\right\} S(\varphi_1 + \varphi_2) +$$

$$\cos\left\{-\lambda'(\varphi_1) - \lambda'(\varphi_2) + \frac{N+1}{2}(\varphi_1 - \varphi_2)\right\} S(\varphi_1 - \varphi_2)\Big]$$

$$\cdot \Big[\sin\left\{\lambda'(\varphi_1) + \lambda(\varphi_3) + \frac{N+1}{2}(\varphi_1 + \varphi_3)\right\} S(\varphi_1 + \varphi_3) +$$

$$\cos\left\{\lambda'(\varphi_1) - \lambda(\varphi_3) + \frac{N+1}{2}(\varphi_1 - \varphi_3)\right\} S(\varphi_1 - \varphi_3)\Big]$$

$$\cdot \Big[\sin\left\{-\lambda'(\varphi_2) - \lambda(\varphi_3) + \frac{N+1}{2}(\varphi_2 + \varphi_3)\right\} S(\varphi_2 + \varphi_3) +$$

$$\cos\left\{-\lambda'(\varphi_2) + \lambda(\varphi_3) + \frac{N+1}{2}(\varphi_2 - \varphi_3)\right\} S(\varphi_2 - \varphi_3)\Big]$$

Again the abbreviation

$$S(\varphi) = \frac{\sin\left(\dfrac{N}{2}\varphi\right)}{\sin\left(\dfrac{\varphi}{2}\right)}$$

has been used.

It turns out that the expressions for L_1 and L_2 can be greatly reduced, due to certain symmetry properties of the coefficients. Since by definition $0 < \lambda \leqslant \pi$, we have $\lambda(-\varphi) = \pi - \lambda(\varphi)$.

We will perform the reduction of L_1; L_2 can be treated in the same way.

Introducing the abbreviations:

$$-\lambda'(\varphi_1) - \lambda(\varphi_3) + \frac{N+1}{2}(\varphi_1 + \varphi_3) = A,$$

$$\lambda(\varphi_3) - \lambda'(\varphi_1) + \frac{N+1}{2}(\varphi_1 - \varphi_3) = B,$$

$$\lambda'(\varphi_2) + \lambda(\varphi_3) + \frac{N+1}{2}(\varphi_2 + \varphi_3) = C,$$

$$\lambda'(\varphi_2) - \lambda(\varphi_3) + \frac{N+1}{2}(\varphi_2 - \varphi_3) = D,$$

the part between the last two pairs of brackets of the integrand of L_1, which we will call X, becomes:

$$X = \sin A \sin C S(\varphi_1 + \varphi_3) S(\varphi_2 + \varphi_3) + \cos B \cos D S(\varphi_1 - \varphi_3) S(\varphi_2 - \varphi_3)$$
$$+ \sin A \cos D S(\varphi_1 + \varphi_3) S(\varphi_2 - \varphi_3) + \cos B \sin C S(\varphi_1 - \varphi_3) S(\varphi_2 + \varphi_3).$$

In the second and fourth term of this expression we now perform the transformation $\varphi_3 \to -\varphi_3$, this has the effect that

$$B \to A + \pi,\ C \to \pi + D,\ D \to C - \pi$$

yielding, on rearranging the terms:

$$X = \cos(A - C) S(\varphi_1 + \varphi_3) S(\varphi_2 + \varphi_3) + \sin(A + D) S(\varphi_1 + \varphi_3) S(\varphi_2 - \varphi_3)$$

In this way we obtain for L_1:

$$L_1 = \iiint_{-\pi}^{\pi} d\varphi_1\, d\varphi_2\, d\varphi_3 \cos\alpha(\varphi_1) \cos\alpha(\varphi_2) \operatorname{tgh} \tfrac{1}{2}\beta A(\varphi_3) \cdot$$
$$\cdot \left[\sin\left\{\lambda'(\varphi_2) - \lambda'(\varphi_1) + \frac{N+1}{2}(\varphi_1 + \varphi_2)\right\} S(\varphi_1 + \varphi_2) + \right.$$
$$\left. \cos\left\{-\lambda'(\varphi_1) - \lambda'(\varphi_2) + \frac{N+1}{2}(\varphi_1 - \varphi_2)\right\} S(\varphi_1 - \varphi_2)\right] \cdot$$
$$\cdot \left[\cos\left\{-\lambda'(\varphi_1) - \lambda'(\varphi_2) - 2\lambda(\varphi_3) + \frac{N+1}{2}(\psi_1 - \varphi_2)\right\} S(\varphi_2 + \varphi_3) \cdot \right.$$
$$S(\varphi_2 + \varphi_3) + \sin\left\{-\lambda'(\varphi_1) + \lambda'(\varphi_2) - 2\lambda(\varphi_3) + \right.$$
$$\left. \left. + \frac{N+1}{2}(\varphi_1 + \varphi_3)\right\}(S\varphi_1 + \varphi_3)\, (S\varphi_2 - \varphi_3)\right]$$

Between both pairs of brackets the first terms change sign under the inversion, $\varphi_1 \to -\varphi_1$, $\varphi_2 \to -\varphi_2$, $\varphi_3 \to -\varphi_3$, the other terms are even. This reduces L_1 to:

$$L_1 = \int\int\limits_{-\pi}^{\pi}\int \mathrm{d}\varphi_1\, \mathrm{d}\varphi_2\, \mathrm{d}\varphi_3 \cos\alpha(\varphi_1) \cos\alpha(\varphi_2)\, \mathrm{tgh}\, \tfrac{1}{2}\beta\Lambda(\varphi_3) \cdot$$

$$\cdot \Big[\sin\Big\{\lambda'(\varphi_2) - \lambda'(\varphi_1) + \frac{N+1}{2}(\varphi_1+\varphi_2)\Big\} \sin\Big\{-\lambda'(\varphi_1) + \lambda'(\varphi_2)$$

$$- 2\lambda(\varphi_3) + \frac{N+1}{2}(\varphi_1+\varphi_2)\Big\} S(\varphi_1+\varphi_2)\, S(\varphi_1+\varphi_3)\, S(\varphi_2-\varphi_3)$$

$$+ \cos\Big\{-\lambda'(\varphi_1) - \lambda'(\varphi_2) + \frac{N+1}{2}(\varphi_1-\varphi_2)\Big\}\cos\Big\{-\lambda'(\varphi_1) - \lambda'(\varphi_2)$$

$$-2\lambda(\varphi_3) + \frac{N+1}{2}(\varphi_1-\varphi_2)\Big\} S(\varphi_1-\varphi_2)\, S(\varphi_1+\varphi_3)\, S(\varphi_2+\varphi_3)\Big\}$$

Now, performing a last substitution $\varphi_2 \to -\varphi_2$ in the last term of this integral, we arrive at:

$$L_1 = \int\int\limits_{-\pi}^{\pi}\int \mathrm{d}\varphi_1\, \mathrm{d}\varphi_2\, \mathrm{d}\varphi_3 \cos\alpha(\varphi_1) \cos\alpha(\varphi_2)\, \mathrm{tgh}\, \tfrac{1}{2}\beta\Lambda(\varphi_3)$$

$$S(\varphi_1+\varphi_2)\, S(\varphi_1+\varphi_3)\, S(\varphi_2-\varphi_3)$$

The function L_2 can be simplified in an analogous way, resulting in the following expression for $\langle M^z(t)\rangle$:

$$\langle M^z(t)\rangle = -\frac{1}{2\pi^3 N}\int\int\limits_{-\pi}^{\pi}\int \mathrm{d}\varphi_1\, \mathrm{d}\varphi_2\, \mathrm{d}\varphi_3 \,[\cos\alpha(\varphi_1)\cos\alpha(\varphi_2)\cos 2\lambda(\varphi_3) +$$

$$+ \sin\alpha(\varphi_1)\sin\alpha(\varphi_2)\cos 2(\lambda'(\varphi_1) - \lambda'(\varphi_2) + \lambda'(\varphi_3))]\cdot$$

$$\cdot\mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi_3)\, S(\varphi_1+\varphi_2)\, S(\varphi_1+\varphi_3)\, S(\varphi_2-\varphi_3)$$

Introducing new variables

$$\frac{\varphi_1+\varphi_2}{2} = \Psi_1,\quad \frac{\varphi_1+\varphi_3}{2} = \Psi_2,\quad \varphi_3 = \Psi_3,$$

and defining:

$$f(\Psi_1, \Psi_2) = \int\limits_{-\pi}^{\pi} [\cos t\Lambda'(2\Psi_2 - \Psi_3)\cos t\Lambda'(2\Psi_1 - 2\Psi_2 + \Psi_3)\cos 2\lambda(\Psi_3)$$

$$+ \sin t\Lambda'(2\Psi_2 - \Psi_3)\sin t\Lambda'(2\Psi_1 - 2\Psi_2 + \Psi_3).$$

$$\cos 2\{\lambda'(2\Psi_2 - \Psi_3) - \Lambda'(2\Psi_1 - 2\Psi_2 + \Psi_3) + \lambda(\varphi_3)\}]\cdot\mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda(\Psi_3)\,\mathrm{d}\Psi_3 \quad (30)$$

we can write

$$\langle M^z(t)\rangle = -\frac{1}{8\pi^3}\int_{-\pi}^{\pi}\int f(\Psi_1, \Psi_2)\,\frac{1}{N}\,\frac{\sin N\Psi_1}{\sin \Psi_1}\cdot\frac{\sin N\Psi_2}{\sin \Psi_2}\cdot$$
$$\cdot\frac{\sin N(\Psi_1-\Psi_2)}{\sin(\Psi_1-\Psi_2)}\,\mathrm{d}\Psi_1\,\mathrm{d}\Psi_2$$

As one may easily check, the function

$$\frac{1}{N}\,\frac{\sin N\Psi_1}{\sin \Psi_1}\cdot\frac{\sin N\Psi_2}{\sin \Psi_2}\cdot\frac{\sin N(\Psi_1-\Psi_2)}{\sin(\Psi_1-\Psi_2)}$$

behaves like a series of δ-functions in the $\Psi_1\Psi_2$ plane as N goes to infinity, the peaks lying in the points $(n\pi, m\pi)$, with n and m integers. Since a few peaks are lying on the integration boundaries, we shift the integration area a little in the right upward direction (see figure 7), which is allowed since the

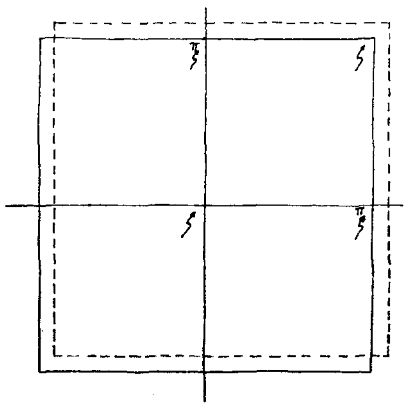

Fig. 7

integrand is a periodic function, in order to get only contributions from the points $(0, 0)$, $(\pi, 0)$, $(0, \pi)$ (π, π), so obtaining

$$\langle M^z(t)\rangle = -\frac{c}{8\pi^3}\,[f(0,0) + f(0,\pi) + f(\pi,0) + f(\pi,\pi)] \tag{31}$$

where c is the normalization constant of the δ-function. Substituting (30) into (31), one finds:

$$\langle M^z(t)\rangle = -\frac{c}{2\pi^3}\int_{-\pi}^{\pi}[\cos 2\lambda(\varphi) - \sin^2 t\Lambda'(\varphi)\{\cos 2\lambda(\varphi) -$$
$$-\cos(2\lambda(\varphi) - 4\lambda'(\varphi))\}]\,\mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi)\,\mathrm{d}\varphi$$

Since, at $t = 0$, this must be equal to $\langle M^z(h)\rangle_\beta$, which is given by formula

(8), we find for the normalization constant: $c = \pi^2/2$, so:

$$\langle M^z(t)\rangle = -\frac{1}{2\pi}\int_0^{\pi} [\cos 2\lambda(\varphi) - \sin^2 t\Lambda'(\varphi)\,\{\cos 2\lambda(\varphi) - \\ - \cos(2\lambda(\varphi) - 4\lambda'(\varphi))\}]\,\mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi)\,d\varphi \tag{32}$$

Another way to determine c would be to put $h_1 = h_2 = h$, since then we should also have $\langle M^z(t)\rangle = \langle M^z(h)\rangle_\beta$; it gives the same value for c.

So we have found the exact evolution in time of a macroscopic observable of a many-body system in a non-equilibrium situation. We can split $\langle M^z(t)\rangle$ in a constant and a timedependent part:

$$\langle M^z(t)\rangle = -\frac{1}{4\pi}\int_0^{\pi} [\cos 2\lambda(\varphi) + \cos(2\lambda(\varphi) - 4\lambda'(\varphi))]\,\mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi)\,d\varphi \\ - \frac{1}{4\pi}\int_0^{\pi} \cos 2t\Lambda'(\varphi)\{\cos 2\lambda(\varphi) - \cos(2\lambda(\varphi) - 4\lambda'(\varphi))\}\,\mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi)\,d\varphi \tag{33}$$

where the time-dependent part is seen to go to zero, by means of the theorem of Riemann-Lebesque, as $t \to \infty$, so:

$$\lim_{t\to\infty} M^z(t) = -\frac{1}{4\pi}\int_0^{\pi} \{\cos 2\lambda(\varphi) + \cos(2\lambda(\varphi) - 4\lambda'(\varphi))\}\,\mathrm{tgh}\,\tfrac{1}{2}\beta\Lambda(\varphi)\,d\varphi$$

This is obviously not equal to $\langle M^z(h_2)\rangle_\beta$ (compare eq. 8), but that could hardly be expected, since the system is isolated.

Unfortunately we have not been able to evaluate the integral of the time-dependent part of $\langle M^z(t)\rangle$, but it is clear that there is no exponential decay. By developing in powers of t one finds that for small values of t the time-dependent part is proportional to t^2, and, by using the method of stationary phase, that for large times it is proportional to $1/\sqrt{t}$. In the next section some numerical results will be considered, to investigate whether there are intermediate time scales for which the decay is exponential.

E. *Comparison of the Kubo approximation to the exact solution, some numerical results and comparison with some other methods of solving the Kubo approximation.* The relaxation of more general spin systems has been considered before[12) 4)]. One usually considers a crystal composed of particles of spin $\frac{1}{2}$, where the spin system is isolated from the lattice and the Hamiltonian is supposed to consist of a Zeeman term, exchange and dipole-dipole interaction. A constant magnetic field H is applied along the z axis, plus a field h which is small compared to H and the system is supposed to be in equilibrium at time $t < 0$. At time $t = 0$ the small field h is suddenly switched off and one studies the temporal development of the magnetization in the in the z direction $\langle M^z(t)\rangle$. Since h is small compared to H, or, if we had taken $H = 0$, small compared to the exchange energy, one usually restricts oneself to the response of the magnetization which is linear in h, i.e. one studies:

$$\langle M^z(t)\rangle - \langle M^z(H)\rangle_\beta = \Phi_{zz}(t)\, h \tag{34}$$

where $\langle M^z(t)\rangle$ is the average magnetization at time t, $\langle M^z(H)\rangle_\beta$ is the static magnetization in presence of only the field H, $\beta = 1/kT$ and $\Phi_{zz}(t)$ is the $z - z$ component of the relaxation tensor. Using first order perturbation theory Kubo and Tomita[3]) derived a general formula for $\Phi_{zz}(t)$, given by, the expression:

$$\Phi_{zz}(t) = \begin{cases} (\chi_0)_{ij} & t < 0 \\ \int_0^\beta \mathrm{d}\lambda\, \mathrm{Tr}\, \rho_0 M^z M^z(t + i\hbar\lambda) - \beta\langle M^z\rangle_\beta^2, & t > 0 \end{cases} \tag{35}$$

where χ_{zz} is the $z - z$ component of the static susceptibility tensor, ρ_0 the equilibrium density matrix at temperature $T(\beta = 1/kT)$ and external field H and M^z is the Heisenberg operator for the magnetic moment in the z direction. One usually considers the case where the temperature is so high that one can expand expression (35) in powers of β, and retaining only the first term one obtains:

$$\Phi_{zz}(t) = \beta\, \frac{\mathrm{Tr}\, M^z M^z(t)}{\mathrm{Tr}\, 1} = \beta\, \langle\!\langle M^z M^z(t)\rangle\!\rangle, \tag{36}$$

or

$$\langle M^z(t)\rangle_{\mathrm{Kubo}} = h\beta\, \langle\!\langle M^z M^z(t)\rangle\!\rangle + \langle M^z(H)\rangle_\beta.$$

Obviously, for the case of the linear chain we are studying the expression $\langle\!\langle M^z M^z(t)\rangle\!\rangle$ is nothing but the function $R(0, t)$ of section C. So for the chain we have an exact solution of Kubo's high-temperature approximation of the $z - z$ component of the relaxation tensor. On the other hand we have shown how to calculate the exact time development of the magnetization in the former section. We now want to compare the exact solution to the Kubo approximation. Since we are looking at cases with a high temperature we can expand expression (33) in powers of β and retain only the first term

$$\langle M^z(t)\rangle_{\mathrm{exact}} = -\frac{\beta}{4\pi}\int_0^\pi \cos(2\lambda(\varphi) - 2\lambda'(\varphi)) \cos 2\lambda'(\varphi)\, \Lambda(\varphi)\, \mathrm{d}\varphi$$

$$+ \frac{\beta}{4\pi}\int_0^\pi \cos 2t\Lambda'(\varphi) \sin(2\lambda(\varphi) - 2\lambda'(\varphi)) \sin 2\lambda'(\varphi)\, \Lambda(\varphi)\, \mathrm{d}\varphi \tag{37}$$

where

$$2\lambda(\varphi) = \operatorname{arctg} \frac{\gamma \sin \varphi}{\cos \varphi - H - h}, \; 2\lambda'(\varphi) = \operatorname{arctg} \frac{\gamma \sin \varphi}{\cos \varphi - H}$$

$$\Lambda(\varphi) = \sqrt{(\cos \varphi - H - h)^2 + \gamma^2 \sin^2\varphi}, \; \Lambda'(\varphi) = \sqrt{(\cos \varphi - H)^2 + \gamma^2 \sin^2 \varphi}.$$

This exact relaxation of the magnetization at high temperatures clearly is an analytic function of h, so in order to compare it with the Kubo formula we only have to develop (37) in powers of h and again retain only the first term. We then obtain the linear part of the exact time development at the magnetization:

$$\langle M^z(t)\rangle_{\text{exact, lin.}} = \langle M^z(t)\rangle_{\text{exact}, h=0} + h\left(\frac{\partial \langle M^z(t)\rangle_{\text{exact}}}{\partial h}\right)_{h=0}$$

$$= \frac{h}{4\pi}\int_0^\pi \{1 - 2\sin^2 2\lambda'(\varphi)\sin^2 \Lambda'(\varphi)\, t\}\, \mathrm{d}\varphi - \frac{\beta}{4\pi}\int_0^\pi \cos 2\lambda'(\varphi)\Lambda'(\varphi)\, \mathrm{d}\varphi \tag{38}$$

On the other hand by inserting (26) and (8) (after replacing tgh $\frac{1}{2}\beta\Lambda(\varphi)$ by $\frac{1}{2}\beta\Lambda(\varphi)$) into the Kubo formula (36) we get:

$$\langle M^z(t)\rangle_{\text{Kubo}} = \frac{h}{4\pi}\int_0^\pi \{1 - 2\sin^2 2\lambda'(\varphi)\sin^2\Lambda'(\varphi)\, t\}\, \mathrm{d}\varphi - \frac{\beta}{4\pi}\int_0^\pi \cos 2\lambda'(\varphi)\, \lambda'(\varphi)\, \mathrm{d}\varphi \tag{39}$$

Formulae (38) and (39) give us the result that $\langle M^z(t)\rangle_{\text{exact, lin.}} = \langle M^z(t)\rangle_{\text{Kubo}}$, for all times.

Since the exact solution contains a constant part, it is natural that the approximation or $R(0, t)$ also contains a constant part. It is due to the fact that when the external field is made smaller, the spins are not as much forced to align, which in turn, if the system would tend to thermodynamical equilibrium for $t \to \infty$, would correspond to a higher temperature, so:

$$\lim_{t\to\infty} \langle M^z(t)\rangle \neq \langle M^z(H)\rangle_\beta.$$

This means that we must have $\lim_{t\to\infty} R(0, t) \neq 0$ as is indeed the case.

As a peculiar feature, which is a freak of the model, we mention the fact that for $h \gg 1$ and $H \ll 1$ the exact solution and the Kubo approximation are equal to a very high degree, for in these cases we have (writing $H + h = h_1$, $H = h_2$):

$$h_1 - h_2 \simeq h_1$$

$$\Lambda(\varphi) \simeq h_1$$

$$2\lambda(\varphi) \simeq \pi$$

Inserting this into formula (39) we obtain:

$$\langle M^z(t)\rangle_{\text{Kubo}} = \frac{\beta h_1}{4\pi}\int_0^\pi \{1 - \sin^2 2\lambda'(\varphi)\sin^2 \Lambda'(\varphi)\, t\}\, d\varphi +$$

$$+ \langle M^z(h_2)\rangle_\beta \simeq \frac{\beta(h_1 - h_2)}{4\pi}\int_0^\pi \{1 - \sin^2 2\lambda'(\varphi)\sin^2 \Lambda'(\varphi)\, t\}\, d\varphi + 0(h_2),$$

and in formula (33):

$$\langle M^z(t)\rangle_{\text{exact}} = -\frac{1}{2\pi}\int_0^\pi [\cos 2\lambda(\varphi) - 2\sin^2 t\Lambda'(\varphi)\{\cos 2\lambda,(\varphi) -$$

$$- \cos(2\lambda(\varphi) + 4\lambda'(\varphi))\}]\ \text{tgh}\ \tfrac{1}{2}\beta\Lambda(\varphi)\, d\varphi$$

$$\simeq -\frac{1}{2\pi}\int_0^\pi [-1 - 2\sin^2 t\Lambda'(\varphi)\{-1 + \cos 4\lambda'(\varphi)\}]\ \text{tgh}\ \tfrac{1}{2}\beta\Lambda(\varphi)\, d\varphi$$

$$\simeq \frac{\beta(h_1 - h_2)}{4\pi}\int_0^\pi \{1 - \sin^2 2\lambda'(\varphi)\sin^2 \Lambda'(\varphi)\, t\}\, d\varphi + 0(h_2).$$

So one sees that under these circumstances

$$\langle M^z(t)\rangle_{\text{exact}} \simeq \langle M^z(t)_{\text{Kubo}}.$$

For several cases the integral expressions for

$$[\langle M^z(t)\rangle_{\text{exact}} - \langle M^z(h_2)\rangle_\beta] \quad \text{and} \quad [\langle M^z(t)\rangle_{\text{Kubo}} - \langle M^z(h_2)\rangle_\beta]$$

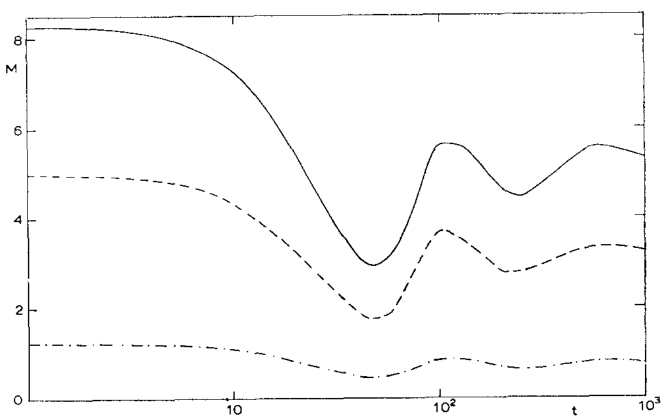

Fig. 8. $[\langle M^z(t)\rangle - \langle M^z(h_2)\rangle_\beta]^{10^{-2}}_{\text{exact}} \cdot = [\langle M^z(t)\rangle - \langle M^z(h_2)\rangle]^{10^{-2}}_{\text{Kubo}} \cdot$ for $h_1 = 10$, $h_2 = 0$, $\beta = 0.033$ (solid line), $\beta = 0.020$ (dashed line) and $\beta = 0.005$ (dash, point, dash); $\gamma = 0.25$.

have been calculated numerically by Drs. E. H. de Groot in order to get an idea how these functions behave. In fig. 8 we have plotted

$$[\langle M^z(t)\rangle_{\text{Kubo}} - \langle M^z(h_2)\rangle_\beta]$$

for the cases $\beta = 0.053, 0.020$ and 0.005 with $h_1 = 10$, $h_2 = 0$ and $\beta = 0.25$. We saw that under these circumstances

$$[\langle M^z(t)\rangle_{\text{Kubo}} - \langle M^2(h_2)\rangle_\beta] = [\langle M^2 t)\rangle_{\text{exact}} - \langle M^z(h_2)\rangle_\beta].$$

It is seen that the magnetization behaves somewhat like a damped oscillator, whose amplitude becomes smaller as the temperature is increased.

When h_1 and h_2 are both much larger than 1, $\langle M^z(t)\rangle$ is almost independent of time, since then we have: $\sin 2\lambda(\varphi) \simeq \sin 2\lambda'(\varphi) \simeq 0$ and $\cos 2\lambda(\varphi) \simeq \simeq \cos 2\lambda'(\varphi) \simeq -1$. Upon inserting this into (33) and (39) the time dependent parts of the integrands are seen to vanish.

An interesting case arises when both h_1 and h_2 are not too large, so that the time dependence does not vanish, and $h_1 - h_2$ is small compared to h_2, while $\beta \ll 1$, since under these conditions the Kubo approximation is supposed to be a good one for more general spin systems. For the X–Y model we can compare the exact solution to the Kubo approximation. We have plotted the following cases:

fig. 9*a*: $h_1 = 1$; $h_2 = 0.9$; $\beta = 0.033$; $\gamma = 0.75$

fig. 9*b*: the same with $\gamma = 0.25$

fig. 10*a*: $h_1 = 1$; $h_2 = 0.9$; $\beta = 0.005$; $\gamma = 0.75$

fig. 10*b*: the same with $\gamma = 0.25$

In figures 9*c* and 10*c* we have plotted $\{[\langle M^z(t)\rangle - \langle M^z(h_2)\rangle_\beta - \langle M^z(\infty)\rangle]\}$ on a logarithmic scale versus t for $h_1 = 1$, $h_2 = 0.9$; $\beta = 0.033$ and 0.005;

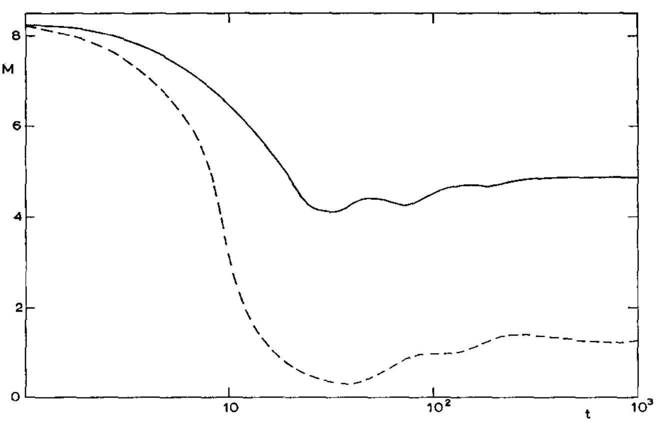

Fig. 9*a*. $[\langle M^z(t)\rangle - \langle M^z(h_2)\rangle_\beta]^{10^{-4}}_{\text{exact}}$ · and $[\langle M^z(t)\rangle - \langle M^z(h_2)\rangle_\beta]^{10^{-4}}_{\text{Kubo}}$ ·, resp. solid and dashed, for $h_1 = 1.0$; $h_2 = 0.9$; $\gamma = 0.75$ and $\beta = 0.033$.

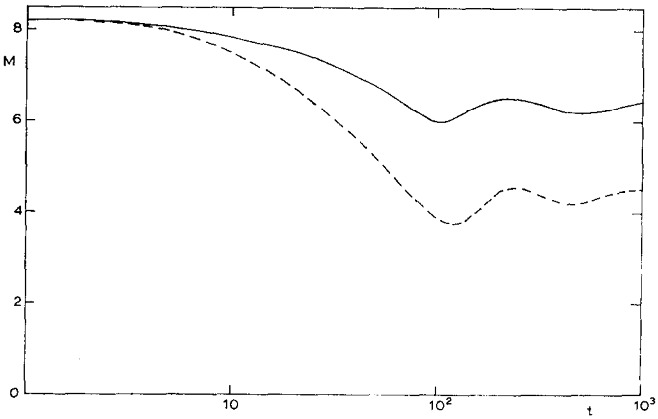

Fig. 9*b*. The same as in fig. 9*a* but $\gamma = 0.25$.

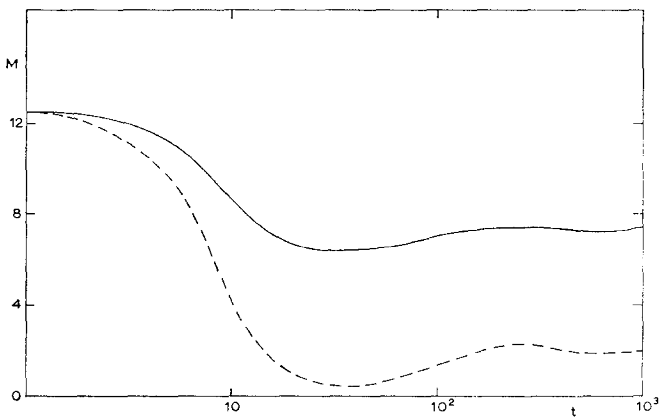

Fig. 10*a*. $[\langle M^z(t) - \langle M^z(h_2)\rangle_\beta]^{10^{-5}}_{\mathbf{exact}}\cdot$ and $[\langle M^z(t)\rangle - \langle M^z(h_2)\rangle_\beta]^{10^{-5}}_{\mathbf{Kubo}}\cdot$ for $h_1 = 1.0$; $h_2 = 0.9$, $\beta = 0.005$ resp. solid and dashed line $\gamma = 0.75$.

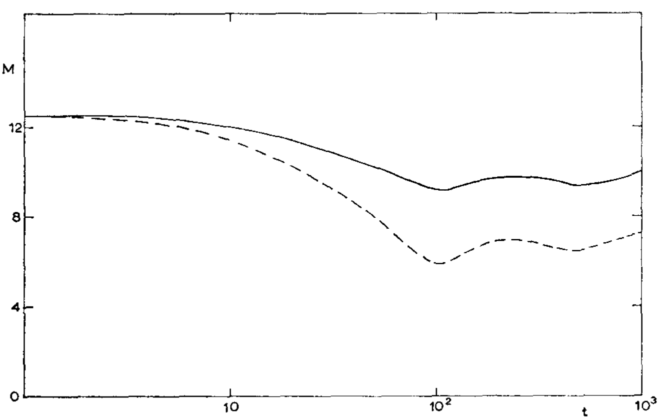

Fig. 10*b*. The same as in fig. 10*a*, but $\gamma = 0.25$.

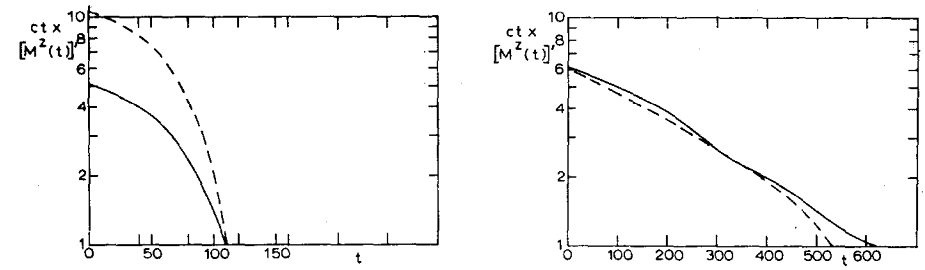

Fig. 9*c*. $[\langle M^z(t)\rangle - \langle M^z(\infty)\rangle_\beta]$ on a logarithmic scale versus t for $h_1 = 1.0$; $h_2 = 0.9$; $\beta = 0.033$; the solid line represents the exact solution, the dashed line is the Kubo solution. Left: $\gamma = 0.75$; right; $\gamma = 0.25$.

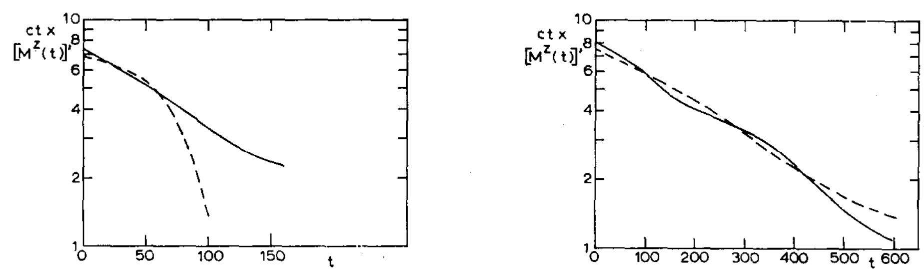

Fig. 10*c*. $[\langle M^z(t)\rangle - \langle M^z(\infty)_\beta\rangle]$ on a logarithmic scale versus t for $h_1 = 1.0$; $h_2 = 0.9$; $\beta = 0.005$; the solid line represents the exact solution, the dashed line is the Kubo solution. Left: $\gamma = 0.75$; right: $\gamma = 0.25$.

$\gamma = 0.75$ and 0.25, in order to see by the straightness of the curve in how far the decay is exponential.

One can observe that the Kubo approximation converges rather slowly. In all cases it is seen that the magnetization first makes a ,,main drop" after which there are oscillations which die out gradually. For large times the Kubo approximation appears to be rather bad, which probably corresponds to the fact that the Kubo approximation relies on first order perturbation theory. It improves fastly when γ becomes smaller, which is understandable since γ characterizes the strength of the non-secular part of the Hamiltonian. For $\gamma = 0.25$ one observes that a part of the "main drop" can be considered to be exponential, but the following oscillations are too large to consider the whole process as an exponential decay. The same is seen in curves for smaller $h_1 - h_2$ and γ. This provides a good example of the danger of using the weak coupling limit, as developed by Van Hove[9]), in order to obtain an exponential decay for more general spin systems as was done by Terwiel and Mazur[4]). The X–Y model can serve as an example that their treatment of spin-spin relaxation probably cannot be extended to spin systems with an anisotropic exchange interaction, since their basic assumption together with the weak coupling limit yields an incorrect result for the case of the

X–Y model. The possibility that the use of the weak coupling limit may obscure the fact that after some time the exponential decay is submerged in the non-exponential part has been pointed out already by Zwanzig[10]).

We can easily apply the method of Terwiel and Mazur to the X–Y model and we will shortly reproduce their argument. The Hamiltonian is split into a secular part H_1 and a non-secular part H_2 (of which the strength is characterized by the parameter γ) which respectively commute and do not commute with the operator M^z:

$$H_1 = \sum_{j=1}^{N} [S_j^x S_{j+1}^x + S_j^y S_{j+1}^y - hS_j^z]$$

$$H_2 = \gamma \sum_{j=1}^{N} [S_j^x S_{j+1}^x - S_j^y S_{j+1}^y]$$

We will study the function $\langle\!\langle M^z M^z(t) \rangle\!\rangle = R(0, t)$ which appears in the Kubo equation (36). In section D it was shown that $R(0, t)$ reaches an equilibrium value $R(0, \infty)$ as t goes to infinity. Following Terwiel and Mazur we define:

$$\beta \Omega(t) = \Phi_{zz}(t) - \Phi_{zz}(\infty) = \beta \langle\!\langle \mu\mu(t) \rangle\!\rangle$$

where

$$\mu = M^z - i[\beta^{-1}\Phi_{zz}(\infty)]^{\frac{1}{2}}.$$

(In our notation we would have $\Omega(t) = R(0, t) - R(0, \infty)$). Without making any further assumption they derive an exact integral equation for $\Omega(t)$ by a technique introduced by Zwanzig[10])

$$\frac{\partial \Omega(t)}{\partial t} = -\gamma^2 \int_0^t \mathrm{d}\tau\, G(\tau, \gamma)\, \Omega(t - \tau) \tag{40}$$

where

$$G(\tau, \gamma) = \frac{\langle\!\langle \mu L' \{\exp iL_0 + iL(1 - P_\mu)\gamma L'\tau\} L'\mu \rangle\!\rangle}{\langle\!\langle \mu^2 \rangle\!\rangle}$$

L is the quantummechanical Liouville operator which is split into two parts:

$$L = L_0 + \gamma L'$$

where

$$L_0 = \frac{i}{\hbar} [H_1, \cdot]$$

$$L' = \frac{i}{\hbar} [H_2, \cdot]$$

and P_μ is a projection operator defined by

$$P_\mu \mu(t) = \mu \frac{\langle\!\langle \mu\mu(t) \rangle\!\rangle}{\langle\!\langle \mu^2 \rangle\!\rangle}.$$

Introducing the Laplace transforms of $\Omega(t)$ and $G(t, \gamma)$:

$$\hat{\Omega}(p) = \int_0^\infty \mathrm{d}\tau\, \mathrm{e}^{-p\tau}\, \Omega(\tau)$$

and

$$\hat{G}(p, \gamma) = \int_0^\infty \mathrm{d}\tau\, \mathrm{e}^{-p\tau}\, G(\tau, \gamma)$$

equation (40) can be written as

$$\hat{\Omega}(p) = \frac{\Omega(0)}{p + \gamma^2 \hat{G}(p, \gamma)}\,. \tag{41}$$

They then deal with equation (41) in the so-called weak coupling limit, i.e. they take the limit $\gamma \to 0$, $t \to \infty$, while keeping $\gamma^2 t$ finite. Equation (41) then takes the form:

$$\lim_{\gamma \to 0} \gamma^2 \hat{\Omega}(\gamma^2 p) = \frac{\Omega(0)}{p + \lim\limits_{\gamma \to 0} \hat{G}(\gamma^2 p, \gamma)} \tag{42}$$

Their basic assumption now is

$$\lim_{\gamma \to 0} \hat{G}(\gamma^2 p, \gamma) = \lim_{\gamma \to 0} \hat{G}(\gamma^2 p, 0) \tag{43}$$

so that (42) reduces to

$$\lim \gamma^2 \hat{\Omega}(\gamma^2 p) = \frac{\Omega(0)}{p + \int_0^\infty \mathrm{d}\tau\, G(\tau, 0)} \tag{44}$$

yielding a simple exponential decay for $\Omega(t)$, with a relaxation time τ_r, defined by

$$\tau_r^{-1} = \gamma^2 \int_0^\infty \mathrm{d}\tau\, G(\tau, 0).$$

For the case of the X–Y model the validity of equation (44) can be checked since we can give explicit expressions for the quantities occurring in (44) and assuming that

$$\int_0^\infty \mathrm{d}\tau\, G(\tau, 0) = a$$

is finite. From (26) one immediately finds that $\Omega(t)$ is given by

$$\Omega(t) = \frac{1}{4\pi} \int_0^\pi \sin^2 2\lambda(\varphi) \cos \{2\Lambda(\varphi)\, t\}\, \mathrm{d}\varphi$$

so we have

$$\Omega(0) = \frac{1}{4\pi} \int_0^\pi \sin^2 2\lambda(\varphi)\, \mathrm{d}\varphi \tag{45}$$

and for the Laplace transform:

$$\hat{\Omega}(p) = \frac{1}{4\pi} \int_0^\pi \sin^2 2\lambda(\varphi) \left\{ \int_0^\infty e^{-pt} \cos 2\Lambda(\varphi)\, t \,\mathrm{d}t \right\} \mathrm{d}\varphi$$

which reduces to:

$$\hat{\Omega}(p) = \frac{p}{4\pi} \int_0^\pi \frac{\sin^2 2\lambda(\varphi)}{p^2 + 4\Lambda^2(\varphi)} \,\mathrm{d}\varphi \tag{46}$$

The integrals (45) and (46) can in principle be evaluated by using the substitution $\cos\varphi = x$ and the so-called "third Eulerian substitution" $\sqrt{1 - x^2} = t(x + 1)$ whereupon the integrands become rational functions of t. It turns out, however, that the denominators are of such a high degree in t that they are quite intractable. If we confine ourselves to the case that the constant magnetic field is zero the integrals (45) and (46) are easily evaluated yielding:

$$\Omega(0) = \frac{1}{4\pi} \int_0^\pi \sin^2 2\lambda(\varphi) \,\mathrm{d}\varphi = \frac{\gamma}{4(1 + \gamma)}$$

and

$$\hat{\Omega}(p) = \frac{p\gamma^2}{4\pi} \int_0^\pi \frac{\sin^2 \varphi}{[p^2 + 4\{\cos^2 \varphi + \gamma^2 \sin^2 \varphi\}][\cos^2 \varphi + \gamma^2 \sin^2 \varphi]} \,\mathrm{d}\varphi$$

$$= \frac{p\gamma}{2^3} \frac{1}{\sqrt{p^2 + 4\gamma^2}\,\{\gamma \sqrt{p^2 + 4} + \sqrt{p^2 + 4\gamma^2}\}}.$$

So the lefthand side of (44) is

$$\lim_{\gamma \to 0} \frac{p\gamma^3}{2^3} \frac{1}{\sqrt{p^2\gamma^2 + 4}\,\{\sqrt{p^2\gamma^4 + 4} + \sqrt{p^2\gamma^2 + 4}\}} \tag{47}$$

and the righthand side

$$\frac{\gamma}{4(1 + \gamma)} \cdot \frac{1}{p + a} \tag{48}$$

It is easily seen that (47) tends to zero when $\gamma \to 0$, whereas the right side is unequal to zero, nor does (47) take the shape of (48) for very small values of γ. So after we have made assumption (43), the weak coupling limit does not give us the correct result, as we could have expected, since the asymptotic time behaviour of $\langle M^z(t) \rangle$ is governed by a time dependence $t^{-\frac{1}{2}}$.

This makes it probable that the use of the weak coupling limit together with assumption (43) is not correct for spin systems with dipole-dipeol interaction and anisotropic exchange interaction since it is not correct for the X–Y model which is a special case of the foregoing class of systems for vanishingly small dipole-dipole interaction.

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