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

II

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Synopsis

The chain of spins $\frac{1}{2}$ with anisotropic nearest neighbour interaction, known as the X–Y model, which was introduced by Lieb, Schultz and Mattis[1]) and studied in ref. 2*) in the presence of a constant field along the z axis, is now studied with a small oscillating field superimposed on the constant field.

Since the autocorrelation function of the magnetization is known from I, the susceptibility, as given by the Kubo formalism, can now easily be calculated. The implicit assumption of Kubo and Tomita[3]) that the aftereffects of the adiabatic switching on of the oscillating field vanish, can now be rigorously justified for this simple case by giving an exact procedure for solving the time-dependent Schrödinger equation in successive orders of the amplitude of the oscillating field.

The imaginary part of the susceptibility is different from zero in a certain frequency range with the effect that energy will be absorbed by the chain if the frequency of the oscillating field lies within this range. If one assumes for the sake of simplicity that the chain is thermally completely isolated and that it always is in thermal equilibrium, the temperature will obviously increase in time since energy is being absorbed. An exact equation for the temperature as a function of time is derived in terms of the parameters characterizing the system in the limit of high temperatures and the temperature is seen to increase exponentially in time.

Introduction. The chain of spins which was studied in I is again placed in a constant field directed along the z axis, but now a small oscillating field superimposed on this constant field is switched on at $t = 0$. The system is supposed to be in thermal equilibrium at times $t < 0$.

By assuming the oscillating field to be switched on adiabatically at $t = -\infty$, Kubo and Tomita[3]) derived the response of a magnetic system up to first order in the amplitude of the oscillating field by making a formal expansion of the density matrix. The susceptibility turns out to be directly related to the autocorrelation function of the magnetization in equilibrium. In the high temperature limit it is nothing but the fourier transform of this quantity.

Since the time-dependent autocorrelation function of the magnetization has been explicitly calculated in I, it now is an easy matter to calculate the

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*) From now on to be referred to as I, any of its equations will be identified by the prefix 1.

susceptibility χ of the X–Y model in the Kubo-formulism. This is done in section A. The imaginary part of the susceptibility turns out to be different from zero for a certain frequency range, indicating that the chain absorbs energy from the oscillating field when its frequency lies within this range.

In section B the oscillating field $h_1 \cos \omega t$ is suddenly switched on at $t = 0$, assuming the system to be in thermal equilibrium in a constant field h_0 at times $t < 0$. The time-dependent Schrödinger equation governing the system can be solved exactly in powers of h_1. Retaining only the first power in h_1 and, to simplify the calculations, also only the first power in β $(\beta = 1/kT)$, the time-dependent magnetization is calculated directly from the Schrödinger equation, yielding exactly the same result as found in section A plus a transient term, thereby justifying the adiabatic switching on procedure of Kubo and Tomita, since the effects of the switching on appear to die out.

It turns out that it is essential that the Schrödinger equation is solved with a time-dependent field which is smeared out over all frequencies. After this has been done the thermodynamic limit should be taken and it is only then, that one can take the limit of a monochromatic oscillating field. The necessity of following this procedure is due to the fact that the finite chain has a discrete energy spectrum, and the physical and mathematical backgrounds of the approach are indicated. They are probably valid for all systems with discrete energy spectra.

Assuming the system to be thermally completely isolated the temperature will gradually rise when the frequency of the oscillating field lies within the required range, since energy is being absorbed. In the high temperature limit an exact equation is derived for the temperature and it is seen to rise exponentially in time. The line of this derivation makes it acceptable that this also holds for more general spin systems.

A. *Calculation of the susceptibility from the relaxation function.* The chain is now placed in a constant magnetic field h_0, which is directed along the z axis, with a field $h_1 \cos \omega t$ superimposed, so the Hamiltonian now reads

$$H = \sum_{j=1}^{N} [(1 + \gamma) S_j^x S_{j+1}^x + (1 - \gamma) S_j^y S_{j+1}^y - (h_0 + h_1 \cos \omega t) S_j^z]. \quad (2.1)$$

In the general treatment of Kubo and Tomita a formal development is made in powers of h_1. Retaining only the first term in h_1 they obtain the following expression for the magnetization:

$$\overline{M^z(t)} = \langle M^z(h_0) \rangle_\beta + h_1 \{ \chi'(\omega) \cos \omega t + \chi''(\omega) \sin \omega t \},$$

where the susceptibility is defined by:

$$\chi(\omega) = \chi'(\omega) - i\chi''(\omega) = -\int_0^\infty \frac{\mathrm{d}\Phi(t)}{\mathrm{d}t} \exp(-i\omega t)\, \mathrm{d}t, \quad (2.2)$$

$\Phi(t)$ being the relaxation function defined in (1.35); in our case it is known exactly. In the high temperature expansion it reduces to:

$$\Phi(t) = \beta \langle\!\langle M^z M^z(t) \rangle\!\rangle$$

which is given by (1.26):

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

and thus:

$$\chi(\omega) = \frac{\beta\gamma^2}{2\pi} \int_0^\pi \frac{\sin^2 \varphi}{\Lambda(\varphi)} \times$$

$$\times \left[\int_0^\infty \frac{\exp[i\{2\Lambda(\varphi) - \omega\}\, t] - \exp[-i\{2\Lambda(\varphi) + \omega\}\, t]\, \mathrm{d}t}{2i} \right] \mathrm{d}\varphi.$$

In our case it would not be necessary to take the high temperature limit, since the relaxation function is known for all temperatures, but we do so in order to simplify the calculations.

If we use the well known relation

$$\frac{1}{2\pi} \int_0^\infty \mathrm{d}t \exp(-ixt) = \frac{1}{2}\left\{\delta(x) + P\left(\frac{1}{i\pi x}\right)\right\}$$

where the symbol P indicates that the principal value has to be taken, we arrive at:

$$\chi(\omega) = -\frac{i\gamma^2\beta}{4} \int_0^\infty \frac{\sin^2 \varphi}{\Lambda(\varphi)} \left[\delta\{2\Lambda(\varphi) - \omega\} - \delta\{2\Lambda(\delta) + \omega\} - \right.$$

$$\left. - P\frac{1}{i\pi\{2\Lambda(\varphi) - \omega\}} - P\frac{1}{i\pi\{2\Lambda(\varphi) + \omega\}} \right] \mathrm{d}\varphi.$$

By choosing $\omega > 0$, the second delta-function vanishes since $\Lambda(\varphi) \geqslant 0$. We obtain for χ' and χ''

$$\chi'(\omega) = \frac{\beta\gamma^2}{\pi} P \int_0^\pi \frac{\sin^2 \varphi}{4\Lambda^2(\varphi) - \omega^2}\, \mathrm{d}\varphi \qquad (2.3)$$

and

$$\chi''(\omega) = \frac{\beta\gamma^2}{2\omega} \int_0^\pi \sin^2 \varphi\, \delta(2\Lambda(\varphi) - \omega)\, \mathrm{d}\varphi. \qquad (2.4)$$

Obviously there will only be absorption if $2\Lambda_{\min} \leqslant \omega \leqslant 2\Lambda_{\max}$. The

physical and mathematical background of this particular feature will become clear when the Schrödinger equation is solved.

One verifies of course directly that $\chi'(\omega)$ and $\chi''(\omega)$ are related to each other by the Kramers-Kronig relations.

B. *Direct calculation of the magnetization from the Schrödinger equation.* We now want to check the susceptibility we have found in this way by solving the Schrödinger equation directly and not switching on the oscillating field adiabatically. We will not yet specify the time-dependence of the magnetic field, but simply write $h = h(t)$. The transformation of the Hamiltonian to fermion operators, which was performed in I, can again be accomplished since it does not depend on $h(t)$, obtaining:

$$H = \tfrac{1}{2} \sum_{j=1}^{N} \{(c_j^* c_{j+1} + \gamma c_j^* c_{j+1}^*) + \text{h.c.}\} - h(t) \sum_{j=1}^{N} c_j^* c_j + \frac{Nh(t)}{2}. \quad (2.5)$$

In principle it would of course still be possible to diagonalize the Hamiltonian in terms of fermion operators, as was done in I, but now this would lead us nowhere since the transformation coefficients depend on time through the magnetic field as can be seen from (1.1), (1.2) and (1.4), and it is not obvious how the equations of motion can be solved. For our purposes the Schrödinger equation becomes most tractable by simply performing a canonical fourier transformation:

$$
\begin{aligned}
c_j^* &= \frac{1}{\sqrt{N}} \sum_{\nu=-N/2}^{N/2} \exp(ij\varphi_\nu)\, a_\nu^*, \\
c_j &= \frac{1}{\sqrt{N}} \sum_{\nu=-N/2}^{N/2} \exp-(ij\varphi_\nu)\, a_\nu,
\end{aligned}
\qquad (2.6)
$$

with $\varphi_\nu = \nu(2\pi/N)$.

The a_ν's are again fermion operators. The Hamiltonian now assumes the form:

$$H = \sum_\nu (\cos\varphi_\nu - h(t))\, a_\nu^* a_\nu - \frac{i\gamma}{2} \sum_\nu \sin\varphi_\nu (a_\nu^* a_{-\nu}^* + a_\nu a_{-\nu}) + \frac{Nh(t)}{2}.$$

Later on we will need to diagonalize this Hamiltonian, starting from this form, for a constant field h_0.

This can be effected by means of a Bogoliubov-transformation as was already pointed out by Pikin and Tsukernik[4]), the transformation being:

$$
\begin{aligned}
a_\nu &= u_\nu \eta_\nu + v_\nu^* \eta_{-\nu}^*, \\
a_{-\nu} &= -u_\nu \eta_{-\nu} + v_\nu^* \eta_\nu^*,
\end{aligned}
\qquad (2.7)
$$

obtaining again (1.5):

$$H = \sum_\nu \Lambda_\nu \eta_\nu^* \eta_\nu - \tfrac{1}{2} \sum_\nu \Lambda_\nu$$

with

$$\Lambda_\nu = \sqrt{(\cos \varphi_\nu - h)^2 + \gamma^2 \sin^2 \varphi_\nu}$$

and

$$u_\nu = \frac{\gamma \sin \varphi_\nu}{[2\Lambda_\nu(R_\nu + \Lambda_\nu)]^{\frac{1}{2}}},$$

$$v_\nu = i\left[\frac{R_\nu + \Lambda_\nu}{2\Lambda_\nu}\right]^{\frac{1}{2}},$$

$$R_\nu = h - \cos \varphi_\nu.$$

The free energy of such a system of non-interacting fermions is:

$$F = -T \sum_\nu \{\ln 2 + \ln \cosh \tfrac{1}{2}\beta\Lambda_\nu\},$$

yielding a magnetization

$$\langle M^z(h) \rangle = -\frac{\partial F}{\partial h} = \frac{1}{2} \sum_\nu \frac{\partial \Lambda_\nu}{\partial h} \, \mathrm{tgh} \, \tfrac{1}{2}\beta\Lambda_\nu \qquad (2.8)$$

which in the limit $N \to \infty$ is of course nothing but (1.8).

It is obvious that the phase space of the system is the direct product of $N/2$ four-dimensional spaces, which are respectively spanned by the basis vectors:

$$\{|0\rangle, a_\nu^* |0\rangle, a_{-\nu}^* |0\rangle, a_\nu^* a_{-\nu}^* |0\rangle\}, \qquad \nu > 0. \qquad (2.9)$$

The Hamiltonian will cause no transitions between these spaces, whatever the time-dependence of the field $h(t)$, a fact that is very useful.

Since we will be working in the Heisenberg-picture the operators a_ν, denoted by the same symbol as in the Schrödinger-picture, will depend on time, just as the operator for the magnetization per spin in the z direction:

$$M^z(t) = \frac{1}{N} \sum_\nu (a_\nu^* a_\nu - \tfrac{1}{2}). \qquad (2.10)$$

Introducing the abbrevations

$$\begin{aligned} \alpha_\nu(t) &= 2\{\cos \varphi_\nu - h(t)\}, \\ 2\gamma \sin \varphi_\nu &= -\delta_\nu, \end{aligned} \qquad (2.11)$$

we have for the Hamiltonian:

$$H(t) = \frac{1}{2} \sum_\nu \left\{ \alpha_\nu(t) \, a_\nu^* a_\nu + \frac{i}{4} \, \delta_\nu(a_\nu^* a_{-\nu}^* + a_\nu a_{-\nu}) \right\} + \tfrac{1}{2}Nh(t). \qquad (2.12)$$

For an arbitrary operator O we have in the Heisenberg-picture the equation of motion:

$$\frac{\mathrm{d}O}{\mathrm{d}t} = i[H, O] + \frac{\partial O}{\partial t}. \qquad (2.13)$$

The operators a_ν depend on time only through the Hamiltonian; for these operators one easily derives the following equation of motion from (12) and (13):

$$\dot{a}_\nu^* = \frac{i}{2}\,\alpha_\nu(t)\,a_\nu^* + \tfrac{1}{2}\delta_\nu a_{-\nu},$$

$$\dot{a}_\nu = -\frac{i}{2}\,\alpha_\nu(t)\,a_\nu + \tfrac{1}{2}\delta_\nu a_{-\nu}^*,$$

$$\qquad\qquad\qquad\qquad\qquad\qquad\qquad \nu > 0 \qquad (2.14)$$

$$\dot{a}_{-\nu}^* = \frac{i}{2}\,\alpha_\nu(t)\,a_{-\nu}^* - \tfrac{1}{2}\delta_\nu a_\nu,$$

$$\dot{a}_{-\nu} = -\frac{i}{2}\,\alpha_\nu(t)\,a_{-\nu} - \tfrac{1}{2}\delta_\nu a_\nu^*.$$

It now is clear that the Schrödinger equation of the total system splits up into $N/2$ systems of four coupled differential equations. This is why the fourier transformation was performed in the Hamiltonian.

However, we are only interested in the magnetization, and therefore define the following hermitian operators:

$$M_\nu = a_\nu^* a_\nu + a_{-\nu}^* a_{-\nu} - 1,$$
$$B_\nu = a_\nu^* a_{-\nu}^* - a_\nu a_{-\nu}, \qquad \nu > 0 \qquad (2.15)$$
$$C_\nu = i(a_\nu^* a_{-\nu}^* + a_\nu a_{-\nu}).$$

Obviously we have

$$M^z(t) = \sum_{\nu=0}^{N/2} M_\nu.$$

Using (14) we obtain the following equations for M, B and C (where now the index ν is omitted until we have to perform the summation (16)):

$$\dot{M} = \delta B,$$
$$\dot{B} = \alpha(t)\,C - \delta M, \qquad (2.17)$$
$$\dot{C} = -\alpha(t)\,B.$$

From now on we no longer consider M, B and C as operators, but as the expectation values thereof in an equilibrium ensemble, described for all times by the density matrix

$$\exp[-\beta\{\sum_{j=1}^{N} (1+\gamma)\,S_j^x S_{j+1}^x + (1-\gamma)\,S_j^y S_{j+1}^y - h_0 S_j^z\}].$$

For $h(t)$ we choose $h(t) = h_0 + h_1 f(t)$, with $f(t) = 0$ for $t < 0$. This means that we choose the chain to be in thermal equilibrium in a constant field h_0 for $t < 0$ and at $t = 0$ switch on a superimposed field $h_1 f(t)$. Writing

$$h' = 2h_1$$

and

$$\alpha_0 = 2(\cos\varphi - h_1),$$

eqs (17) become:

$$\dot{M} = \delta B,$$
$$\dot{B} = \{\alpha_0 - h'f(t)\} C - \delta M, \qquad (2.18)$$
$$\dot{C} = -\{\alpha_0 - h'f(t)\} B.$$

For $t > 0$ we develop M, B and C in powers of h'. One easily checks by means of the Bogoliubov-transformation (7) that the expectation value of B in an equilibrium ensemble is zero: $\langle B \rangle_{\text{eq}} = 0$, which was to be expected, since M and C should be constant in that case. So B has no zeroth order and we have:

$$M = M_0 + h'M_1 + h'^2 M_2 + \dots,$$
$$B = \qquad h'B_1 + h'^2 B_2 + \dots, \qquad (2.19)$$
$$C = C_0 + h'C_1 + h'^2 C_2 + \dots.$$

Substitution in (18) and taking the different orders together yields:

$$0^{\text{th}} \text{ order} \begin{cases} \dot{M}_0 = 0 \\ \alpha_0 C_0 = \delta M_0 \\ \dot{C}_0 = 0 \end{cases}$$

$$2^{\text{st}} \text{ order} \begin{cases} \dot{M}_1 = \delta B_1 \\ \dot{B}_1 = -f(t) C_0 + \alpha_0 C_1 - \delta M_1 \\ \dot{C}_1 = -\alpha_0 B_1 \end{cases}$$

$$2^{\text{nd}} \text{ order} \begin{cases} \dot{M}_2 = \delta B_2 \\ \dot{B}_2 = -f(t) C_1 + \alpha_0 C_2 - \delta M_2 \qquad (2.20) \\ \dot{C}_2 = -\alpha_0 B_2 + f(t) B_1 \end{cases}$$

$$\vdots$$

$$n^{\text{th}} \text{ order} \begin{cases} \dot{M}_n = \delta B_n \\ \dot{B}_n = -f(t) C_{n-1} + \alpha_0 C_n - \delta M_n \\ \dot{C}_n = -\alpha_0 B_n + f(t) B_{n-1}. \end{cases}$$

These equations can obviously be solved systematically. The zeroth order solution of course is $C_0 = (\delta/\alpha_0) M_0$. The first order equations can be written as:

$$\ddot{B}_1 = -(\alpha_0^2 + \delta^2) B_1 - \dot{f}(t) C_0,$$
$$\dot{M}_1 = \delta B_1, \qquad (2.21)$$
$$\dot{C}_1 = -\alpha_0 B_1.$$

The equation for B_1 is nothing but a harmonic oscillator with a driving

force and without damping. Using the abbreviations for α_0 and δ we obtain:

$$\ddot{B}_1 = -4\Lambda_\nu^2 B_1 - \dot{f}(t)\, C_0.$$

If the small field is taken to be harmonic, i.e. $f(t) = \cos \omega t$, the only solution for B_1 is:

$$B_1 = -\frac{\omega C_0}{\omega^2 - 4\Lambda_\nu^2} \sin \omega t$$

giving

$$M_1 = \frac{\delta C_0}{\omega^2 - 4\Lambda_\nu^2} \cos \omega t.$$

So if ω is outside the interval $[2\Lambda_{\min}, 2\Lambda_{\max}]$ all M_1's vary as $\cos \omega t$, which means that the factor $\cos \omega t$ can be taken outside the summation sign in (16): the time-dependent part of the magnetization is completely in phase with the oscillating field. Inside the interval $[2\Lambda_{\min}, 2\Lambda_{\max}]$ however, the amplitude of $A_{1,\nu}$ blows up to infinity when $\omega = 2\Lambda_\nu$, indicating an infinite energy absorption from the field by this particular mode: here $\chi''(\omega)$ consists of a series of $N/2$ delta peaks. This is clearly not what we found in section A, where $\chi''(\omega)$ turned out to be a smooth function of ω.

But in section A we had already taken the thermodynamic limit; if this had not been done, then $\langle\!\langle M^z M^z(t)\rangle\!\rangle$ would have been a periodic function of t and the defining integral (2) for $\chi(\omega)$ would not have existed. Since it is not clear from the article of Kubo and Tomita[3] how this difficulty should be avoided, we will now show that it is possible to assign to every delta peak a certain weight. This can be done by giving the perturbing field only a finite extension in time, so that it is smeared out over all frequencies and every "oscillator" can absorb only a finite amount of energy. After the equations (21) have been solved, one must first take the thermodynamic limit and only then one can take the limit of a monochromatically oscillating field.

For $f(t)$ we take:

$$f_\varepsilon(t) = \begin{cases} e^{-\varepsilon t} \cos \omega t & \varepsilon > 0, t > 0 \\ 0 & t < 0, \end{cases}$$

so that

$$\lim_{\varepsilon \to 0} f_\varepsilon(t) = \cos \omega t.$$

The inhomogeneous second order differential equation for B_1 now becomes:

$$\ddot{B}_1 = -4\Lambda_\nu^2 B_1 + C_0(\varepsilon \cos \omega t + \omega \sin \omega t)\, e^{-\varepsilon t}.$$

The most general solution of this equation is:

$$B_1(t) = \frac{C_0\, e^{-\varepsilon t}}{p^2 + 4\varepsilon^2\omega^2} \{\omega(p - 2\varepsilon^2) \sin \omega t + \varepsilon(p + 2\omega^2) \cos \omega t\} +$$
$$+\, a_1 \sin 2\Lambda t + a_2 \cos 2\Lambda t.$$

where $p = 4\Lambda^2 + \varepsilon^2 - \omega^2$ and a_1 and a_2 are arbitrary constants. As boundary conditions we take $B_1(0) = 0$ and $\dot{B}_1(0) = 0$. This choice is not very important, since it only influences the transient terms as will be shown later on. These boundary conditions yield:

$$a_1 = 0,$$

$$a_2 = -\frac{C_0\omega^2}{2\Lambda p},$$

where the limit $\varepsilon \to 0$ has already been taken, since here it is of no importance. Integrating for M_1 one obtains:

$$M_1 = \frac{\delta C_0\, e^{-\varepsilon t}}{p^2 + 4\varepsilon^2\omega^2} \{2\varepsilon\omega \sin \omega t + p \cos \omega t\} + \frac{\delta C_0\omega^2}{4p\Lambda^2} \cos 2\Lambda t. \qquad (2.22)$$

In the exponent we can already put $\varepsilon = 0$, this is immaterial for the limiting procedure. Inserting (22) into (19) we obtain for the magnetization to first order in h_1:

$$\overline{M^z(t)} = \langle M^z(h_0)\rangle_\beta + h_1[\chi_s'(\omega) \cos \omega t + \chi_s''(\omega) \sin \omega t + F(t)],$$

where

$$\chi_s' = \sum_{\nu=0}^{N/2} \frac{\delta_\nu^2 p_\nu M_{0,\nu}}{\alpha_{0,\nu}(p_\nu^2 + 4\varepsilon^2\omega^2)},$$

$$\chi_s'' = \sum_{\nu=0}^{N/2} \frac{\delta_\nu^2 2\varepsilon\omega M_{0,\nu}}{\alpha_{0,\nu}(p_\nu^2 + 4\varepsilon^2\omega^2)}, \qquad (2.23)$$

$$F_s(t) = \omega^2 \sum_{\nu=0}^{N/2} \frac{\delta_\nu \cos 2\Lambda_\nu t}{4p_\nu\Lambda_\nu^2}.$$

The subscript s indicates the fact that there quantities are calculated directly from the Schrödinger equation.

From expression (8) one immediately sees that $M_{0,\nu}$ is the contribution of the subspace (9) to the magnetization due to the field h_0 and thus equal to:

$$M_{0,\nu} = \frac{(\cos \varphi_\nu - h_0)}{\Lambda_\nu}\, \mathrm{tgh}\, \tfrac{1}{2}\beta\Lambda_\nu.$$

For high temperatures this reduces to

$$M_{0,\nu} = \frac{\beta}{2}(\cos \varphi_\nu - h_0) = \frac{\beta\alpha_{0,\nu}}{4}.$$

Introducing this into eqs (23) ($F(t)$ will be dealt with separately), and also the other abbreviations at the same time going over to the thermodynamic

limit, the sums being replaced by integrals, we obtain:

$$\chi_s'(\omega) = \frac{\beta\gamma^2}{\pi} \int_0^\pi \frac{\sin^2\varphi(4\Lambda^2(\varphi) + \varepsilon^2 - \omega^2)}{(4\Lambda^2(\varphi) + \varepsilon^2 - \omega^2)^2 + 4\varepsilon^2\omega^2}\, d\varphi$$

and

$$\chi_s''(\omega) = \frac{\beta\gamma^2}{\pi} \int_0^\pi \frac{\sin^2\varphi \cdot 2\varepsilon\omega}{(4\Lambda^2(\varphi) + \varepsilon^2 - \omega^2)^2 + 4\varepsilon^2\omega^2}\, d\varphi.$$

We now are ready to take the limit $\varepsilon \to 0$. One easily checks that:

$$\chi_s' = \frac{\beta\gamma^2}{\pi} \lim_{\varepsilon \to 0} \int_0^\pi \frac{\sin^2\varphi}{4\Lambda^2(\varphi) - \omega^2 + \varepsilon^2(1 + 4\omega^2)}\, d\varphi =$$

$$= \frac{\beta\gamma^2}{\pi}\, P \int_0^\pi \frac{\sin^2\varphi}{4\Lambda^2(\varphi) - \omega^2}\, d\varphi = \chi'(\omega),$$

in accordance with (3).

For $\chi_s''(\omega)$ we have, neglecting the term ε^4 in the denominator:

$$\chi_s'' = 2\beta\gamma^2 \int_0^\pi \frac{\omega \sin^2\varphi}{2(4\Lambda^2(\varphi) + \omega^2)} \times$$

$$\times \left[\frac{1}{\pi} \lim_{\varepsilon \to 0} \frac{\varepsilon}{\dfrac{(4\Lambda^2(\varphi) - \omega^2)^2}{2(4\Lambda^2(\varphi) + \omega^2)} + \varepsilon^2} \right] d\varphi =$$

$$= 2\beta\gamma^2 \int_0^\pi \frac{\omega \sin^2\varphi}{2(4\Lambda^2(\varphi) + \omega^2)}\, \delta \left\{ \frac{4\Lambda^2(\varphi) - \omega^2}{[2(4\Lambda^2(\varphi) + \omega^2)]^{\frac{1}{2}}} \right\} d\varphi.$$

Using the relation

$$\delta\{f(x)\} = \sum_i \frac{\delta(x - x_i)}{|f'(x_i)|}$$

where the x_i are the zeropoints of the function $f(x)$, we obtain:

$$\chi_s''(\omega) = \frac{\beta\gamma^2}{2\omega} \int_0^\pi \sin^2\varphi\, \delta(2\Lambda(\varphi) - \omega)\, d\varphi = \chi''(\omega), \qquad (2.24)$$

in accordance with (4).

The function $F_s(t)$ is a transient term. After taking the thermodynamic

limit it can be written in the form:

$$F_s(t) = \int_0^\pi f(\varphi) \cos\{g(\varphi) \, t\} \, \mathrm{d}\varphi$$

where $f(\varphi)$ and $g(\varphi)$ are continuous functions of bounded variation, so the conditions under which the theorem of Riemann-Lebesgue is valid, are fulfilled:

$$\lim_{t \to \infty} F(t) = 0.$$

The fact that $F(t)$ is transient means that we recover the formula of Kubo and Tomita, their adiabatic switching on of the oscillating field giving only rise to transient terms as could be expected.

Since $F(t)$ contains ω^2 in the numerator as well as in the denominator, it will be largely independent of ω.

So by taking the limiting procedures in the right order we have found complete agreement with the susceptibility which was calculated from the relaxation function in section A. The fact that $\chi''(\omega) \neq 0$ only in the interval $[2\Lambda_{\min}, 2\Lambda_{\max}]$ is explained by the fact that the Hamiltonian can be transformed into terms corresponding with $N/2$ noninteracting systems with characteristic frequencies $2\Lambda(\varphi_\nu)$ at which they can absorb energy and that the operator for the magnetization is quadratic in the operators a_ν. In the thermodynamic limit these frequencies become dense in the interval $[2\Lambda_{\min}, 2\Lambda_{\max}]$.

Since $\sin^2 \varphi$ can, for a given value of $2\Lambda(\varphi)$, take on one, two or three values, depending on the values of h_0 and γ, we will determine the lineshape of $\chi''(\omega)$ only for the two cases where $\sin^2 \varphi$ is determined uniquely by $2\Lambda(\varphi)$, since the system is not very realistic anyway.

a. $h = 0$

$$\chi''(\omega) = \begin{cases} \dfrac{\beta\gamma^2}{8(1 - \gamma^2)} \dfrac{\omega_{\max}^2 - \omega^2}{\omega} & \omega_{\min} < \omega < \omega_{\max} \\ 0 & \text{other } \omega\text{'s.} \end{cases}$$

It is a convex, monotonously decreasing function of ω.

b. $\gamma = 1$.

This is again the Ising chain in a transverse field, of which the susceptibility has never been calculated. One easily finds:

$$\chi''(\omega) = \begin{cases} \dfrac{\beta}{8\omega} \left\{ 3h_0^2 - 1 + \dfrac{\omega^2}{4} \right\} & \omega_{\min} < \omega < \omega_{\max} \\ 0 & \text{other } \omega\text{'s.} \end{cases}$$

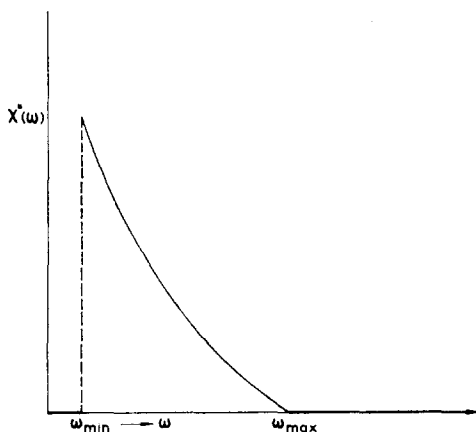If one assumes the spin system to be in contact with a heatbath, e.g. by

Fig. 1

means of spin-lattice interaction, and that the spin system reaches a stationary state which can be described by a new temperature β', in which all non-linear effects are absorbed, one can systematically solve the sequence of equations (20) by substituting the $(n-1)$th order solutions in the n-th order equations.

C. *The increase in temperature due to energy absorption*. When calculating the response of the magnetization to an external oscillating field, it is for small h_1 enough to look only at the linear response. The temperature can be taken to be constant in this approximation, since the energy absorption is a second order effect, being proportional to h_1^2. The influence on the temperature seems therefore never to have been calculated. Assuming the spin chain to be in thermal equilibrium at every moment, we can easily derive an expression for the temperature as a function of time.

The first law of thermodynamics for a spin system is

$$dQ = dU - h\, dM.$$

If the spin system is in contact with a heat bath which has a constant temperature T_b and the temperature of the spin system is T_s, one could set

$$\frac{dQ}{dt} = c(T_b - T_s)$$

for the heat flow. For the sake of simplicity, however, we will suppose the spin system to be thermally completely isolated, so $dQ = 0$ and writing the first law in differential form we obtain:

$$\frac{dU}{dt} = h\,\frac{dM}{dt}.$$

Substituting

$$h(t) = h_0 + h_1 \cos \omega t$$

and

$$\overline{M(t)} = M_0 + h_1(\chi' \cos \omega t + \chi'' \sin \omega t)$$

and integrating over one cycle one finds:

$$\oint \mathrm{d}U = h_1^2 \pi \chi''(\omega). \qquad (2.25)$$

Per unit of time the increase of internal energy in:

$$\Delta U = \tfrac{1}{2} h_1^2 \omega \chi''(\omega)$$

an expression already derived by Du Pré[5]).

For the chain the total energy per spin is:

$$E(\beta, h_0) = \frac{1}{N} \sum_{j=1}^{N} \langle \eta_j^* \eta_j \rangle = \frac{1}{2\pi} \int_0^{\pi} \{1 - \mathrm{tgh}\, \tfrac{1}{2}\beta \Lambda(\varphi)\} \, \mathrm{d}\varphi, \qquad (2.26)$$

so the total internal energy is:

$$U(\beta, h_0) = E(\beta, h_0) + h_0 M(\beta, h_0),$$

which equals, using expression (2.26) and (1.8):

$$U(\beta, h_0) = \frac{1}{2\pi} \int_0^{\pi} \{1 - \cos^2 \lambda(\tfrac{1}{2}\varphi)\, \mathrm{tgh}\, \beta \Lambda(\varphi)\} \, \mathrm{d}\varphi.$$

If after a fraction of time Δt, β has increased by an amount $\Delta \beta$, we can write:

$$U(\beta, h_0) + \tfrac{1}{2} h_1^2 \omega \chi''(\omega)\, \Delta t = -\frac{\Delta \beta}{2\pi} \int_0^{\pi} \Lambda(\varphi) \cos^2 \lambda(\varphi) \, \mathrm{d}\varphi.$$

For high temperature this becomes:

$$h_1^2 \omega \chi''(\omega)\, \Delta t = -\frac{\Delta \beta}{2\pi} \int_0^{\pi} \Lambda(\varphi) \cos^2 \lambda(\varphi) \, \mathrm{d}\varphi. \qquad (2.27)$$

Writing

$$\tfrac{1}{2} \int_0^{\pi} \sin^2 \varphi \, \delta(2\Lambda(\varphi) - \omega) \, \mathrm{d}\varphi = I_1 \qquad (\geqslant 0)$$

and

$$\frac{1}{2\pi} \int_0^{\pi} \Lambda(\varphi) \cos^2 \lambda(\varphi) \, \mathrm{d}\varphi = I_2 \qquad (> 0)$$

we have:

$$\chi''(\omega) = \frac{\beta\gamma^2}{\omega} I_1.$$

and (2.27) becomes:

$$\frac{d \ln \beta}{dt} = -h^2\gamma^2 \frac{I_1}{I_2}.$$

Choosing Boltzmann's constant equal to unity, this yields for the temperature:

$$T(t) = \alpha \exp(at)$$

where α is an integration constant and

$$a = \pi h_1^2 \gamma^2 \frac{\int_0^\pi \sin^2 \varphi \; \delta(2\Lambda(\varphi) - \omega) \, d\varphi}{\int_0^\pi \Lambda(\varphi) \cos^2 \lambda(\varphi) \, d\varphi}.$$

In view of the way in which this exponential increase of the temperature was derived, it will probably also hold for more general spin systems.

In realistic situations however, the spin system will never be isolated, i.e. $c \neq 0$, and the system will reach an equilibrium temperature. The fact that for an ideally isolated system the temperature goes to infinity is caused by the fact that we are dealing with a system of fermions: only a finite amount of energy per spin can be absorbed. When all the excitations are present, the temperature is infinite by definition.

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