Studies in Applied Mathematics, Vol. LI, No. 2, June 1972.

Dynamics of a Local Perturbation in the X-Y Model II—Excitations*

By D. B. Abraham, E. Barouch, G. Gallavotti, and A. Martin-Löf

Excitations of a single spin embedded in the XY chain are studied. We find that the magnetization does not approach equilibrium, even if the external magnetic field approaches a non-zero limit, and that oscillatory excitation resonates with the edge of the one-particle spectrum band.

1. Introduction

In a previous paper we considered the magnetization of a single spin embedded in the XY chain after the external magnetic field is switched off. We have shown that this spin thermalizes [1]. This problem was further studied by Emch and Radin [2] from a C^*-algebra point of view.

In this paper we continue our investigation by considering the reverse question. If at time $t = 0$, we turn on a magnetic field which approaches a limit as $t \to \infty$, does the magnetization of this spin also thermalize and approach a limit? The answer here turns out to be *no:* we find that the magnetization does *not* approach equilibrium, no matter how slowly the external field reaches its limit.

We shall also study the effect of an oscillatory field on the isolated spin. Because of technical difficulties we study this by perturbation theory, and find a resonance of the driving field with the external points of the one particle spectrum.

We have limited ourselves to the isotropic chain. In I, we showed that the anisotropic chain can be studied along the same lines as the isotropic chain, and does not reveal more information to the questions asked. In the case of local oscillatory excitations, we conjecture that the magnetization of a spin in the anisotropic chain with a constant field in the z direction will resonate with one of the global frequencies found earlier [3] for the tanslationally invariant system.

* Partially supported by NSF Grant GP–29463.

2. Formulation

Let the Hamiltonian of the chain be given by (I2.1) with $\gamma = 0$ and

$$h(t) = \begin{cases} 0 & t \leq 0 \\ h(t) & t > 0 \end{cases} \tag{2.1}$$

where $h(t)$ is an explicit time dependence of the external magnetic field, to be discussed later.

The magnetization of the nth site, for $t >$ o is given by

$$\langle 1 + \sigma_n^z(t) \rangle = Z^{-1} \operatorname{Tr}\left[e^{-\beta H_0} \frac{2}{M} \sum_{qq'} e^{in(q'-q)} a_q^\dagger(t) a_{q'}(t) \right] \tag{2.2}$$

where z is the partition function of the lattice, and the operators a_q are defined in (13.3).

To determine the evolution of the operators a_q, we need to solve the equation

$$i \frac{da_q(t)}{dt} = [a_q(t), H(t)] \tag{2.3}$$

where $H(t)$ is given explicitly in terms of the operators a_q by

$$H(t) = \sum_q \cos q a_q^\dagger a_q + 2h(t) \frac{1}{M} \sum_{q,q'} a_q^\dagger a_{q'} \, e^{-i(q'-q)m} \tag{2.4}$$

where m is the site of the impurity subjected to the external magnetic field.

In general, the simplification of the $\gamma = 0$ case is in the lack of necessity to perform a Bogoliubov transformation. In the present case, this allows us to express $a_q(t)$ as a linear combination of the operators a_q, but not $a_q^\dagger$, with time dependent coefficients to be determined.

Explicitly we thus have

$$a_q(t) = \sum_{q'} A_{qq'}(t) a_{q'}. \tag{2.5}$$

Substitution of (2.5) in (2.3), and equating the coefficients of each a_q gives the set of coupled differential equations

$$i\dot{A}_{pp'}(t) = \cos p' A_{pp'}(t) + \frac{2}{M} h(t) \, e^{-ip'm} \sum_k A_{kp}(t) \, e^{ikm} \tag{2.6}$$

with boundary conditions $A_{pp'}(0) = \delta_{p,p'}$. Define

$$X_p(t) = \sum_k A_{kp}(t) \, e^{-im(p-k)}. \tag{2.7}$$

Then, treating the last term in (2.6) as an inhomogeneous term, we have a formal solution of (2.6) as

$$A_{pp'}(t) = e^{-it\cos p'} \left(\delta_{pp'} - \frac{2i}{M} e^{i(p-p')m} \times \int_0^t dt' \, e^{it'\cos p'} h(t') X_p(t') \right) \tag{2.8}$$

In order for us to obtain $A_{pp'}(t)$, we need an equation for $X_p(t)$. This is achieved by performing the sum over p' in (2.8), namely

$$X_p(t) = e^{-it\cos p} - 2i\int_0^t \left(\frac{1}{M}\sum_p e^{i(t'-t)\cos p}\right) h(t')X_p(t')\,dt' \tag{2.9}$$

In the thermodynamic limit, we may replace the sum in (2.9) by an integral, which is the integral representation of the Bessel function of zero-order, so (2.9) may be written as

$$X(p,t) = e^{-it\cos p} - 2i\int_0^t J_0(t-t')h(t')X(p,t')\,dt' \tag{2.10}$$

Direct substitution of $A_{pp'}(t)$, determined from (2.8), in (2.2) using (2.5) yield

$$\langle 1+\sigma_n^z(t)\rangle = Z^{-1}\,\mathrm{Tr}\left\{\exp\left[-\beta\sum_q \cos_q a_q^\dagger a_q\right] \times \frac{2}{M}\sum_{kk'} e^{in(k-k')}\sum_{ss'} A_{sk}^*(t)A_{s'k'}(t)a_s^\dagger a_{s'}\right\} \tag{2.11}$$

Since

$$Z^{-1}\,\mathrm{Tr}\left\{\exp\left[-\beta\sum_q \cos q\, a_q^\dagger a_q\right] a_s^\dagger a_{s'}\right\} = (1+e^{\beta\cos s'})^{-1}\delta_{ss'}, \tag{2.12}$$

we may rewrite (2.11) as

$$\langle 1+\sigma_n^z(t)\rangle = \frac{2}{M}\sum_{s'}(1+e^{\beta\cos s'})^{-1}\sum_{kk'} A_{sk}^* A_{sk'}\,e^{in(k-k')} \tag{2.13}$$

For the special case $m = n$, (2.13) becomes quite simple, namely

$$\langle 1+\sigma_n^z(t)\rangle = \frac{2}{M}\sum_k (1+e^{\beta\cos k})^{-1}|X_k(t)|^2 \tag{2.14}$$

In other words, the problem of evaluating the expected value of the magnetized spin is reduced to the integral equation (2.9).

For $m \neq n$ we need to solve (2.9) and combine its solution with (2.13), and (2.8) to obtain

$$\langle 1+\sigma_n^z(t)\rangle = \frac{2}{M}\sum_k (1+e^{\beta\cos k})^{-1}\{1+S_1(t)+S_2(t)\} \tag{2.15a}$$

where $S_1(t)$ and $S_2(t)$ are given by

$$S_1(t) = 4\,\mathrm{Re}\sum_q \frac{i}{M}\exp\{i[q-k)(n-m)+t(\cos q-\cos k)]\} \times \int_0^t dt'\,e^{-it'\cos q}h(t')X_q(t') \tag{2.15b}$$

$$S_2(t) = \left|\sum_q \frac{2i}{M}\exp\{i[(q-k)(n-m)+t\cos q]\} \times \int_0^t dt'\,e^{-it'\cos q}h(t')X_q(t')\right|^2 \tag{2.15c}$$

These are desired results.

So far the analysis is independent of $h(t)$. Since we cannot give a general solution of (2.10), we wish to specify explicit time dependence of $h(t)$.

3. Step function magnetic field

In order to study the question of approach to equilibrium, it is sufficient to require that $\lim_{t\to\infty} h(t) \neq 0$ exists, so we choose

$$h(t) = \begin{cases} 0 & t \leq 0 \\ h & t > 0 \end{cases} \tag{3.1}$$

Equation (2.10) then becomes

$$X(p, t) = e^{-it\cos p} - 2ih \int_0^t J_0(t - t')X(p, t')\, dt'. \tag{3.2}$$

Taking Laplace transform with respect to t we obtain

$$\tilde{X}(p, \tau) = \frac{1}{\tau + i\cos p} - 2ih(\tau^2 + 1)^{-1/2}\tilde{X}(p, \tau). \tag{3.3a}$$

Namely

$$\tilde{X}(p, \tau) = (\tau + i\cos p)^{-1}[1 + 2ih(\tau^2 + 1)^{-1/2}]^{-1} \tag{3.3b}$$

and

$$X(p, t) = \frac{1}{2\pi i}\int_{\gamma - i\infty}^{\gamma + i\infty} d\tau\, e^{\tau t}(\tau + i\cos p)^{-1}[1 + 2ih(\tau^2 + 1)^{-1/2}]^{-1}. \tag{3.4}$$

So in the thermodynamic limit we have from (3.4) and (2.14)

$$\langle 1 + \sigma_m^z(t)\rangle = \frac{1}{\pi}\int_{-\pi}^{\pi} dk(1 + e^{\beta\cos k})^{-1}|X(k, t)|^2. \tag{3.5}$$

In order to study the approach to equilibrium of (3.5) (we take here $m = n = 0$ for convenience), we need the equilibrium magnetization. This can be obtained by setting $t = 0$ in (I 3.24) and (I 3.26) so

$$\sigma_z(\text{Eq.}) = \frac{2h}{\pi i}\int_c d\lambda(\lambda^2 - 1)^{-1}[1 - 2h(\lambda^2 - 1)^{-1/2}]^{-1}[1 + e^{\beta\lambda}]^{-1}. \tag{3.6}$$

An asymptotic study of (3.5) shows that the magnetization does not approach the equilibrium result (3.6). Furthermore, among the order 1 terms we find an oscillatory term with frequency $(1 + 4h^2)^{1/2}$. This is the isolated frequency discussed by Lebowitz [4], which determines the nonequilibrium final state.

For the step function field (3.1) one can use an alternative method, restricted to this case. Since $H_0 + h\sigma_n^z$ was diagonolized in I we can write (2.2) as

$$\begin{aligned}\langle 1 + \sigma_n^z(t)\rangle = Z^{-1}\,\mathrm{Tr}\Big\{&e^{-\beta H_0}\frac{2}{M}\sum_{qq'} e^{in(q'-q)}\exp[it(\Sigma_j\lambda_j\alpha_j^\dagger\alpha_j)] \\ &\times(\Sigma_j U_{jq}\alpha_j^\dagger)(\Sigma_{j'}U_{j'q'}^*\alpha_{j'})\exp[-it\Sigma_j\lambda_j\alpha_j^\dagger\alpha_j]\Big\}\end{aligned} \tag{3.7}$$

where λ_j, U_{jq} are discussed in section 3 of I. Performing the evolution transformation we find

$$\langle 1 + \sigma_n^z(t)\rangle = Z^{-1}\,\mathrm{Tr}\left\{e^{-\beta H_0}\frac{2}{M}\sum_{qq'}\sum_{jj'} e^{i[n(q'-q)+t(\lambda_j-\lambda_{j'})]}U_{jq}U^*_{j'q'}\alpha_j^\dagger\alpha_{j'}\right\} \tag{3.8}$$

Expressing $\alpha_j^\dagger$, α_j, in terms of the operators a_q using (I3.9) and performing the trace operation, we finally find

$$\langle 1 + \sigma_n^z(t)\rangle = \frac{2}{H}\sum_{qq'}\sum_{jj'}\sum_{k}\{e^{i[n(q'-q)+t(\lambda_j-\lambda_{j'})]}(1 + e^{\beta\cos k})^{-1}U^*_{jk}U_{j'k}U_{jq}U^*_{j'q'}\} \tag{3.9}$$

Equation (3.9) is the desired answer, and with sufficient labor it can be shown to be the same as (3.5). The advantage of this method is that we *have* already all the expressions in it from paper I. However, this method is applicable to fields which are constants over a period of time, namely rather limited.

4. Approach to the final state

We already know [3] that when a global perturbation is turned on, the magnetization does not approach equilibrium no matter how slowly the final field is reached. To illustrate that this is the case for the present problem we choose

$$h(t) = \begin{cases} 0 & t \le 0 \\ h(1 - e^{-t}) & t > 0 \end{cases} \tag{4.1}$$

The field (4.1) has the same values of (3.1) at 0 and ∞.

The Laplace transform of (2.10) yield the difference equation

$$\tilde{X}(p,\tau) = (\tau + i\cos p)^{-1} - 2ih(\tau^2 + 1)^{-1/2}[\tilde{X}(p,\tau) - \tilde{X}(p,\tau + 1)]. \tag{4.2}$$

This is a first order difference equation, with boundary condition $\tilde{X}(p,\infty) = 0$, and its solution is readily obtained as

$$\tilde{X}(p,\tau) = \sum_{r=0}^{\infty}[(\tau + r)^2 + 1]^{1/2}(2ih)^r(i\cos p + \tau + r)^{-1} \times \left\{\prod_{s=0}^{r}[2ih + [(\tau + s)^2 + 1]^{1/2}]\right\}^{-1} \tag{4.3}$$

The first term in (4.3) is exactly (3.3), and the next term gives a contribution, exponentially small in t, to the magnetization. This could also be obtained by direct iteration of (2.10) with the first order term taken as (3.4).

5. Oscillatory fields

In general it is harder to deal with periodic fields $h(t)$ than with monotonic fields (3.1) or (4.1).

To illustrate this consider the square wave

$$h(t) = h(t + \tau),$$

$$h(t) = \begin{cases} h & 0 \le t \le t_1 \\ 0 & t_1 \le t \le \tau \end{cases} \tag{5.1}$$

The evolution operator is thus given by (in the $N + 1$ period)

$$[e^{i(\tau - t_1)H_0}\, e^{it_1(H_0 + h\sigma_0^z)}]^N B(N\tau - t)$$

where $B(t)$ is a simple exponential operator. As to computing the asymptotic behavior of the magnetization we need to solve the eigenvector problem

$$e^{i(\tau - t_1)H_0}\, e^{it_1(H_0 + h\sigma_0^z)}\, \vec{V} = \mu \vec{V}. \tag{5.2}$$

The fact that (5.2) is harder than our previous eigenvector problem raises the guess that it contains some resonance phenomenae, typical to any oscillatory external fields, which is richer in structure.

Since the long-time oscillatory behavior of the thermodynamic averages depends on very few extremal frequencies of the energy spectrum [3], we expect that a resonance phenomenae will occur at $\omega = 2$, where ω is the frequency of the driving external field. To illustrate this point consider

$$h(t) = \begin{cases} 0 & t \le 0 \\ h \cos \omega t & t > 0 \end{cases} \tag{5.3}$$

Equation (2.10) then becomes

$$X(p, t) = e^{-it\cos p} - 2ih \int_0^t J_0(t - t') \cos \omega t' X(p, t')\, dt' \tag{5.4}$$

Let $X(p, t) = Y(p, t) + iZ(p, t)$ with Y and Z real, so (5.4) can be rewritten as

$$Y(p, t) = \cos(t \cos p) + 2h \int_0^t J_0(t - t') \cos \omega t' Z(p, t')\, dt' \tag{5.5a}$$

$$Z(p, t) = -\sin(t \cos p) - 2h \int_0^t J_0(t - t') \cos \omega t' Y(p, t')\, dt' \tag{5.5b}$$

and (2.14) becomes

$$1 + \langle \sigma^z(t) \rangle = \frac{1}{\pi} \int_0^\pi (1 + e^{\beta \cos p})^{-1} [Y^2(p, t) + Z^2(p, t)]\, dp. \tag{5.6}$$

Since we are unable to solve (5.5) exactly, we assume h to be small, and compute $\langle \sigma(t) \rangle$ to first order in h. Neglecting terms of order h^2 we obtain

$$\begin{aligned} m(t) \simeq \frac{8h}{\pi} \int_0^\pi & (1 + e^{\beta \cos p})^{-1}\, dp \\ & \times \left\{ \sin(t \cos p) \int_0^t J_0(t - t') \cos \omega t' \cos(t' \cos p)\, dt' \right. \\ & \left. - \cos(t \cos p) \int_0^t J_0(t - t') \cos \omega t' \sin(t' \cos p)\, dt' \right\} \end{aligned} \tag{5.7}$$

Assuming for convenience that β is small we obtain

$$\begin{aligned} m(t) &\simeq \frac{8h\beta}{\pi} \int_0^\pi dp \cos p \int_0^t J_0(t - t') \cos \omega t' \sin[(t - t') \cos p]\, dt' \\ &= \frac{8h\beta}{\pi} \int_0^t J_0(t - t') J_1(t - t') \cos \omega t'\, dt'. \end{aligned} \tag{5.8}$$

Integrating (5.8) by parts we find

$$m(t) \simeq \frac{4h\beta}{\pi}(J_0^2(t) - \cos \omega t) - \frac{4h\beta}{\pi}\omega \int_0^t J_0^2(\tau) \sin[\omega(t - \tau)]\, d\tau. \qquad (5.9)$$

It is clear that $m(t)$ is not analytic at $\omega = 2$. To see that, we analyze the integral in (5.9). Let

$$I_1(\omega) = \int_0^\infty J_0^2(\tau) \cos \omega\tau\, d\tau \qquad (5.10a)$$

$$I_2(\omega) = \int_0^\infty J_0^2(\tau) \sin \omega\tau\, d\tau. \qquad (5.10b)$$

The integrals $I_1(\omega)$ and $I_2(\omega)$ can be carried out exactly (GR 6.672) [5], and after some manipulations we obtain

$$I_1(\omega) = \pi\left[K\left(\frac{\omega}{2}\right) + K\left(\sqrt{1 - \frac{\omega^2}{4}}\right)\right] \quad \text{for } \omega < 2 \qquad (5.11a)$$

$$I_1(\omega) = 0 \quad \text{for } \omega > 2 \qquad (5.11b)$$

$$I_2(\omega) = \pi K\left(\frac{\omega}{2}\right) \quad \text{for } \omega < 2 \qquad (5.11c)$$

$$I_2(\omega) = \frac{2\pi}{\omega} K\left(\frac{2}{\omega}\right) \quad \text{for } \omega > 2 \qquad (5.11d)$$

where $K(\theta)$ is the complete elliptical integral of the first kind.

These results exhibit a resonance phenomena at $\omega = 2$. These amplitudes are clearly non-analytic, and the perturbation scheme breaks down for $\omega = 2$. Furthermore, the next order correction diverges with time as $\log t$.

So, using (5.11) in (5.9) we find for $\omega \neq 2$

$$m(t) \simeq \frac{4h\beta}{\pi}\left\{J_0^2(t) \cos \omega t - \omega \sin \omega t\left[I_1(\omega) - \int_t^\infty J_0^2(\tau) \cos \omega t'\, d\tau\right]\right.$$

$$\left. + \omega \cos \omega t\left[I_2(\omega) - \int_t^\infty J_0^2(\tau) \sin \omega\tau\, d\tau\right]\right\} \qquad (5.12)$$

In the remaining integrals we may replace J_0 by its asymptotic form, and study the resulting *si* and *ci* functions for large t by integration by parts. So, for $\omega \neq 2$ we finally obtain to first order in βh.

$$m(t) \simeq \frac{4h\beta}{\pi}\{[-\cos \omega t - \omega I_1(\omega) \sin \omega t + \omega I_2(\omega) \cos \omega t] + O(t^{-1})\}$$

In other words, we find that if we drive the system with a frequency ω, different from the resonance frequency, the magnetization would oscillate with the same ω, with a phase lag that depends explicitly on ω, as expected.

Acknowledgement

The authors wish to thank Professors J. Lebowitz, B. M. McCoy and H. Cheng for many interesting discussions.

E. B. would like to thank Professor S. Orszag for his interest in this work, and Professors, C. N. Yang and T. T. Wu for stimulating discussions.

References

1. D. Abraham, E. Barouch, G. Gallavotti and A. Martin-Löf, *Studies of Applied Math.* **50**, 121 (1971). This paper is referred to as I.
2. G. G. Emch and C. Radin, *JMP* **12**, 2043 (1971).
3. E. Barouch, B. McCoy and M. Dresden, *Physical Review*, **A2**, 1075 (1970).
4. J. Lebowitz, Lecture given at the I.U.P.A.P. meeting, Chicago, 1971.
5. I. S. Gradshtein and I. M. Ryzhik, *Table of Integrals Series and Products*, Academy Press, **40**, 1965, page 751.

Cambridge University
Massachusetts Institute of Technology
Universita Di Roma
The Royal Institute of Technology, Stockholm

(Received December 22, 1971)