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Thermalization of a magnetic impurity in the isotropic XY model

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We carry out an exact study of the relaxation of a single magnetic impurity embedded in a linear quantum chain

Recently the time dependent properties of the XY model have been extensively investigated. For instance, it has been shown that if a uniform, time dependent, magnetic field is applied in the z direction *to all spins* of a systeminitially at equilibrium, then the average magnetization in the z–direction approaches a limit which is *not* its equilibrium value, no matter how slowly the field varies[1–4].

In this note we obtain *rigorously* the magnetization at any site when a field wich is applied to a single spin is removed. In the thermodynamic limit we find that the magnetization of any it interior spin approaches its new equilibrium value with time t as t^{-1}. Tjon, [5], has examined the behavior of a *boundary spin* in the weak coupling approximation; approach to equilibrium again obtains, but as t^{-3}.

Consider the Hamiltonian function

$$\mathcal{H} = \mathcal{H}_0 + h(t)\,\sigma_m^z \tag{1}$$

where

$$\mathcal{H}_0 = J\sum_{n=1}^{M}(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y) \tag{2}$$

the σ^α are Pauli matrices, J is the coupling constant, and $\sigma_{M+1}^\alpha = \sigma_1^\alpha$ and

$$h(t) = h \text{ for } t \le 0, \qquad h(t) = 0 \text{ for } t > 0 \tag{3}$$

We assume that for $t \le 0$ the system is in thermal equilibrium at temperature β^{-1}, and that at $t = 0$ the magnetic field h is switched off.

The magnetization of the n–th spin is defined as

$$\langle\sigma_n^z(t)\rangle = \frac{\mathrm{Tr}\left(e^{-\beta\mathcal{H}}e^{i\mathcal{H}_0 t}\sigma_n^z e^{-i\mathcal{H}_0 t}\right)}{\mathrm{Tr}\,e^{-\beta\mathcal{H}}} \tag{4}$$

and it thermalizes if

$$\lim_{t\to\infty}\langle\sigma_n^z(t)\rangle = 0 \tag{5}$$

Since $\mathcal{H}_0$ can be written in terms of fermion operators $a_s^\dagger, a_s$ as

$$\mathcal{H}_0 = 4J\sum_q \cos q\, a_s^\dagger a_s \tag{6}$$

with $a_q^\dagger = M^{-\frac{1}{2}}\sum_1^M e^{iqm}(\sigma_m^x + i\sigma_m^y)\prod_1^{m-1} e^{i\frac{\pi}{2}(\sigma_n^z+1)}$ we have, to within an irrelevant constant,

$$\mathcal{H} = 4J\sum_q \cos q\, a_s^\dagger a_s + \frac{2h}{M}\sum_{q,q'} e^{i(q-q')m} a_q^\dagger a_{q'} \tag{7}$$

Since H is quadratic in $a_q, a_{q'}$ it can be written as

$$\mathcal{H} = \mathit{const} + \sum_j \lambda_j \alpha_j^\dagger \alpha_j \tag{8}$$

where the α_j are new Fermi operators given by

$$\alpha_j = \sum_q U_{jq} a_q \tag{9}$$

There are two kinds of eigenvalue λ_j:
(i) $\lambda_j \neq 4J\cos q$ for all q. Then

$$U_{jq} = e^{imq}\,N(\lambda_j)\,(\lambda_j - 4J\cos q) \tag{10}$$

where $N(\lambda_j)$ is the normalization factor and λ_j are the zeros of

$$F(\lambda) = 1 - \frac{2h}{M}\sum_q \frac{1}{\lambda - 4J\cos q} \tag{11}$$

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(ii) $\lambda_j = 4J\cos q_0$ for some $0 < q_0 < \pi$; then

$$U_{jq} = \frac{1}{\sqrt{2}}\left(e^{imq_0}\delta_{q,q_0} - e^{-imq_o}\delta_{q,-q_0}\right) \tag{12}$$

Combining these results we obtain the final result in the thermodynamic limit:

$$\langle\sigma_n^z(t)\rangle = \frac{2h}{i\pi}\oint_C d\lambda \frac{1}{1+e^{\beta\lambda}} \frac{dq}{1-\frac{h}{\pi}\int_0^{2\pi}} \frac{1}{\lambda - 4J\cos q}$$
$$\int_0^{2\pi} \frac{dqdq'}{(2\pi)^2} \frac{e^{i\left((m-n)(q-q')+4J(\cos q-\cos q')\,t\right)}}{(\lambda-4J\cos q)(\lambda-4J\cos q')} \tag{13}$$

where the contour C is an ellipse which contains the zeros of $F(\lambda)$ but not those $1+e^{\beta}\lambda$.

By the Riemann–Lebsegue lemma, therma;ization in the sense of (5) occurs. An asymptotic study of $\langle\sigma_n^z(t)\rangle$ from (13) gives a leading term proportiona;l to t^{-1}, which is a rather slow approach to equilibrium. An interesting feature of (13) is its analytic properties for fixed t arounf $h = 0$.

The anisotropic case as well as details of the present case will be published elsewhere.

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[1] E. Barouch, B. McCoy, and M. Dresden, Physical Review A **2**, 1075 (1970).
[2] E. Lieb, T. Schultz, and D. Mattis, Annals of Physics **16**, 407 (1961).
[3] H. Narnhofer, Annals of Physics **0**, ??? (1971).
[4] C. Radin, Preprint **0**, ??? (1971).
[5] J. Tjion, Preprint **0**, ??? (1971).

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