Thermalization of a Magnetic Impurity in the Isotropic XY Model

D. B. Abraham* and E. Barouch*†

Department of Mathematics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

and

G. Gallavotti and A. Martin-Löf The Rockefeller University, New York, New York 10021 (Received 18 September 1970)

We carry out an exact study of the relaxation of a single magnetic impurity embedded in a linear quantum chain. We obtain a rigorous result for the expectation value of any spin in the chain, and find that it relaxes to its equilibrium value as t^{-1} .

Recently, the time-dependent properties¹ of the XY model² 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 the spins of a system initially 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.^{1,3} In this note, we obtain <u>rigorously</u> the magnetization at any site when a field which is applied to a single spin is removed. In the thermodynamic limit, we find that the magnetization of any <u>interior</u> spin approaches its new equilibrium value with time t as t^{-1} . Tjon⁴ 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

$$\mathcal{K} = \mathcal{K} + h(t)\sigma_{m,z} \tag{1}$$

where

$$\mathcal{K}_{0} = J \sum_{n=1}^{M} (\sigma_{n,x} \sigma_{n+1,x} + \sigma_{n,y} \sigma_{n+1,y})$$
(2)

and

$$h(t) = h, \quad t \leq 0,$$

= 0, $t > 0.$ (3)

The σ_{α} are Pauli spin matrices, J is the coupling constant, and $\sigma_{\mu+1,\alpha} = \sigma_{1,\alpha}$.

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 nth spin is defined as

$$\langle \sigma_{n,z}(t) \rangle = \operatorname{Tr}[\exp(-\beta \mathcal{H}) \exp(i\mathcal{H}_0 t) \sigma_{n,z} \exp(-i\mathcal{H}_0 t)] / \operatorname{Tr} \exp(-\beta \mathcal{H})$$
(4)

and it thermalizes if

$$\lim_{t \to \infty} \langle \sigma_{n,z}(t) \rangle = 0.$$
⁽⁵⁾

Since H_0 can be written in terms of fermion operators a_a^{\dagger} , a_a as

$$\mathcal{H}_{0} = 4J \sum_{q} \cos q a_{q}^{\dagger} a_{q} \tag{6}$$

with

$$a_{q}^{\dagger} = M^{-1/2} \sum_{1}^{M} e^{iqm} (\sigma_{m,x} + i\sigma_{m,y}) \prod_{1}^{m-1} \exp[i\pi(\sigma_{n,z} + 1)/2],$$

we have, to within an irrelevant constant,

$$\mathcal{K} = 4J\sum_{q} \cos q a_{q}^{\dagger} a_{q} + \frac{2h}{M} \sum_{qq'} e^{i(q'-q)m} a_{q}^{\dagger} a_{q'}.$$
(7)

Since *H* is quadratic in a_q , a_q^{\dagger} , it can be written as

$$\mathcal{K} = \text{const} + \sum_{q} \lambda_{j} \alpha_{j}^{\dagger} \alpha_{j}, \tag{8}$$

1449

where the α_i are new Fermi operators given by

$$\alpha_{j} = \sum_{q} U_{jq} a_{q}.$$
(9)
There are two kinds of eigenvalue λ_{j} :
(i) $\lambda_{i} \neq 4J \cos q$ for all q. Then

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

where $N(\lambda_i)$ is the normalization factor and λ_i are the zeros of

$$F(\lambda) = 1 - (2h/M) \sum_{q} (\lambda - 4J \cos q)^{-1}.$$
 (11)

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

$$U_{ig} = 2^{-1/2} (e^{ima_0} \delta_{ag_0} - e^{-ima_0} \delta_{a_0, -g_0}).$$
(12)

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

$$\langle \sigma_{n,z}(t) \rangle = \frac{2h}{\pi i} \oint_{C} d\lambda \left\{ (1 + e^{\beta \lambda})^{-1} \left[1 - \frac{h}{\pi} \int_{0}^{2\pi} (\lambda - 4J \cos q)^{-1} dq \right]^{-1} \\ \times (2\pi)^{-2} \int_{0}^{2\pi} \int dq \, dq' \exp i \left[(m - n)(q - q') + 4J (\cos q - \cos q')t \right] \left[(\lambda - 4J \cos q)(\lambda - 4J \cos q') \right]^{-1} \right\},$$
(13)

where the contour C is an ellipse which contains the zeros of $F(\lambda)$, but not those of $1 + e^{\beta}\lambda$. By the Riemann-Lebesgue lemma, thermalization in the sense of (5) occurs. An asymptotic study of $\langle \sigma_{n,z}(t) \rangle$ from (13) gives a leading term proportional to t^{-1} , which is a rather slow approach to equilibrium. An interesting feature of (13) is its analytic properties for fixed t around h = 0.

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

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