for l = 1, 2 and m = 1, 2. Here $F(\vec{x}, t)$ is a function which varies slowly as compared to $u_{l}^{(i)}(\vec{x} - \vec{X}_{i})$ in the neighborhood of \vec{X}_{i} . Also Q

is again either the identity operator or the grad operator $\vec{\nabla}$. If the vector $\vec{q}_{12}^{(i)}$ is replaced by

*Work supported by the U. S. Army Research Office (Durham).

¹S. L. McCall and E. L. Hahn, Phys. Rev. Letters <u>18</u>, 908 (1967). ²S. L. McCall and E. L. Hahn, Phys. Rev. <u>183</u>, 457

²S. L. McCall and E. L. Hahn, Phys. Rev. <u>183</u>, 457 (1969).

³F. T. Arecchi, V. Degiorgio, and C. G. Someda, Phys. Letters 27A, 588 (1968).

⁴M. D. Crisp, Phys. Rev. Letters <u>22</u>, 820 (1969). ⁵C. L. Tang and B. D. Silverman, *Physics of Quantum Electronics*, edited by P. L. Kelley, B. Lax, and P. E. Tannenwald (McGraw-Hill, New York, 1966), p. 280.

⁶R. P. Feynman, F. L. Vernon, Jr., and R. W. Hellwarth, J. Appl. Phys. 28, 49 (1957).

⁷As an example, let us consider the case where the wave functions $u_1(\underline{x})$, $u_2(\underline{x})$ correspond to a transition with a change of the magnetic quantum number m by one, i.e., $\Delta m = -1$. Then the electric dipole moment, as given by Eq. (2.4), is equal to ${}^8 \hat{\mu} = (P/\sqrt{2})$ ($\underline{\hat{x}} - i \underline{\hat{y}}$) [See E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge U. P., London, 1964), p.91.], where P is a real negative number and $\underline{\hat{x}}$, $\underline{\hat{y}}$ are unit vectors in the x and y directions, respectively. In this case μ_x

its average value $\vec{q} = \omega \quad \vec{\mu}$ in Eqs. (A25), then Eqs. (2.3a) - (2.3c) follow directly from Eqs. (A25) and the definitions (2.2) when the electromagnetic field propagates in the z direction.

 $=P/\sqrt{2}$, $\mu_y = -i P/\sqrt{2}$, and $\mu_+ = \sqrt{2} P$.

⁸The term $-\eta^2 \omega_r^2/c^2 = -4\pi e^2 N/m_e c^2$ in this dispersion relation appears also in the usual formula for the dielectric constant in the electric dipole approximation. See for example, H. A. Kramers, *Quantum Mechanics* (North-Holland, Amsterdam, 1957), p. 487, first line of the relation following Eq. (229).

⁹E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge U. P., London, 1940), p. 491 et seq.

¹⁰F. Bowman, Introduction to Elliptic Functions (English U. P., London, 1953).

¹¹V. M. Belyakov, P. I. Kravtsova, and M. G. Rappoport, *Tables of Elliptic Integrals* (MacMillan, New York, 1965), part I.

¹²L. M. Milne-Thomson, Jacobian Elliptic Function Tables (Dover, New York, 1950).

¹³See for example, A. Messiah, in *Quantum Mechanics* (Wiley, New York, 1962), Vol. II, p. 1020; and L. I. Schiff, *ibid.*, 1968, 3rd ed., p. 521.

¹⁴For a similar argument, see, for example, E. T. Jaynes and F. W. Cummings, Proc. IEEE <u>51</u>, 89 (1963) or W. Louisell, *Radiation and Noise in Quantum Electronics* (McGraw-Hill, New York, 1964), p. 213.

PHYSICAL REVIEW A

VOLUME 2, NUMBER 3

SEPTEMBER 1970

Statistical Mechanics of the XY Model. I

Eytan Barouch*

IBM Watson Laboratory, Columbia University, New York, New York 10025

and

Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11790

and

Barry M. McCoy and Max Dresden[†]

Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11790 (Received 10 February 1970)

The Liouville equation for the XY model is solved exactly, and the magnetization is computed explicitly. Nonergodic behavior of the magnetization is found for a general class of time-dependent magnetic fields.

I. INTRODUCTION

There is extensive literature on the general aspects of nonequilibrium statistical mechanics. There are many different approaches and procedures, and it is not at all trivial to decide what procedures and approximations, if any, are appropriate in given circumstances. The lack of nontrivial examples, in which the Liouville equation can be solved exactly and the time dependence explicitly obtained, has been keenly felt. With such an exactly soluble example, one can compare the effectiveness and legitimacy of the many approximate procedures. This makes the construction and analysis of such systems especially important.

A considerable amount of success has been achieved in the exact discussion of various one-

dimensional spin systems. The general type of system studied is a one-dimensional chain with nearest-neighbor interactions. Most of the studies start from a Hamiltonian of the form

$$H = \sum_{j=1}^{N} \left(\alpha S_{i}^{x} S_{i+1}^{x} + \beta S_{i}^{y} S_{i+1}^{y} + \gamma S_{i}^{z} S_{i+1}^{z} \right) , \qquad (1.1)$$

where the \overline{S}_i are $\frac{1}{2}$ of the Pauli spin matrices, and $\alpha \beta \gamma$ are the coupling constants.

In spite of the idealization involved in representing an actual magnetic substance by the Hamiltonian (1.1), the analysis of such systems is of considerable difficulty.

From a physical viewpoint, these models are all highly contrived. Whatever interest they might possess depends on the information and insight they yield about the general character and structure of many-body theory and statistical mechanics. There is always the hope that methods which yield exact information about idealized systems will be helpful in discussing more realistic ones. There is also the suspicion that the inability to solve simple systems means that one is poorly prepared to discuss more realistic ones.

Various special cases of (1.1) have been analyzed in detail. Some of these cases are: (i) α = β =0, the Ising model, studied by Ising,¹ Onsager,² and many others; (ii) $\alpha = \beta = \gamma$, the Heisenberg model, studied by Bethe³ and Hulthen⁴; (iii) $\alpha = \beta$ $\neq \gamma$, the Heisenberg-Ising model studied by Yang and Yang⁵; (iv) $\alpha \neq \beta$; $\gamma = 0$, the XY model, studied by Lieb. Schultz, and Mattis⁶ (LSM), and others.⁷⁻¹¹

LSM diagonalized the Hamiltonian of the XY model, found its spectrum and eigenstates, and studied its thermodynamic properties. It is the purpose of this paper to study the nonequilibrium properties of this model.

In the time-dependent case, the eigenvalues of (1.1) are not of primary interest. The discussion here is concerned with the manner in which a system responds to external disturbances and the way that appropriate observables behave for infinite times.

To study such questions, it is useful to introduce an explicitly time-dependent term in the Hamiltonian. In general, H has the form

$$H = H_{ss} + h(t) H_{sh}$$
, (1.2)

where $H_{sh} = \sum_{i} S_{i}^{z}$, (1.3)

where H_{ss} is given by (1.1), and h(t) is the timedependent magnetic field. In the case

$$[H_{ss}, H_{sh}] = 0 \quad , \tag{1.4}$$

the density matrix of the system has a trivial time dependence. Physically this means that the spinspin interaction energy and the spin-field interaction energy are separately conserved. Thus, no energy transfer can take place between the two systems. Hence, it is not surprising that the change of an external field, in this case, does not result in an interesting time evolution of the spin system. The simplest system for which (1.4) is not satisfied is

$$H = \sum_{j=1}^{N} \left[(1+\gamma) S_j^x S_{j+1}^x + (1-\gamma) S_j^y S_{j+1}^y - h(t) S_j^z \right] \quad .(1.5)$$

This is the XY model $[\gamma \neq 0$, since $\gamma = 0$ results in (1, 4)].

This system was chosen for our detailed study. In order to obtain an understanding of the time evolution of this system, the time-dependent density matrix has to be computed. Once this is accomplished, it is possible to calculate the time evolution of physical observables such as the magnetization, which is discussed in this paper. The instantaneous correlation functions are of physical interest, but their calculation is quite involved and will be dealt within a separate paper. From the explicit expression for the magnetization the limit $t \rightarrow \infty$ is obtained. The somewhat surprising result of the detailed analysis is that, although this limit exists, it does not approach its equilibrium value. This may well be connected with the observation of Mazur¹² that the magnetization is not an ergodic observable in this model.

The paper is divided into eight sections. Section II contains a recapitulation of the diagonalization procedure of LSM. The main point is that, by means of an appropriate unitary transformation, the Hamiltonian is transformed into $\Sigma_p H_p$, where each H_p acts in an independent subspace. In Sec. III, it is shown that the density matrix has a direct product structure:

$$\rho(t) = \rho_1(t) \otimes \cdots \otimes \rho_p(t) \otimes \cdots \otimes \rho_{N/2}(t) , \qquad (1.6)$$

where each ρ_p is a 4×4 matrix satisfying

$$i\frac{d}{dt}\rho_{p}(t) = [H_{p}(t), \rho_{p}(t)] \quad . \tag{1.7}$$

The initial condition chosen at t=0 is thermal equilibrium of the system at that time, namely,

$$\rho_{p}(0) = e^{-\beta H_{p}(0)}; \quad \beta = (kT)^{-1} \quad . \tag{1.8}$$

The matrix elements of ρ_p are obtained by elementary means from a function V, which satisfies

$$\frac{d^2}{dt^2} V + [\Lambda^2 + \psi(t)] V = 0 \quad . \tag{1.9}$$

Here ψ is an explicitly given functional of h(t), while Λ depends on the parameters of the system and the value of the magnetic field.

In Sec. IV, the solutions of (1.9) are used to compute the magnetization.

Sections V-VII contain the detailed evaluation

and analysis for three examples of external fields. The general results of these sections is that the asymptotic behavior of m(t) is identical for large times, the specific coefficients depend on the details of h(t), and there is no approach to equilibrium, no matter how slow the field varies.

The conclusions are collected in Sec. VIII, and Appendixes A-C give details of the various asymptotic expansions and some solutions of (1.9).

II. FORMULATION

The equilibrium properties of the XY model in one dimension, have been derived many times.⁶⁻¹⁰ We choose to outline the basic steps used by LSM for sake of completeness.

The XY Hamiltonian is

$$H = J \sum_{j=1}^{N} \left\{ (1+\gamma) S_{j}^{x} S_{j+1}^{x} + (1-\gamma) S_{j+1}^{y} - [\mu h(t)/J] S_{j}^{z} \right\} .$$
(2.1)

This Hamiltonian represents a chain of interacting spins, with nearest-neighbor interaction only. The boundary condition is cyclic, namely, $\vec{S}_{N+1} = \vec{S}_1$. S_j^x , S_j^y , S_j^g , are the spin- $\frac{1}{2}$ operators at the *j*th lattice site (they are $\frac{1}{2}$ the Pauli spin matrices), γ is the anistropy measure, μ is the magnetic moment, h(t) is the time-dependent magnetic field, and *J* is the coupling constant. We set J = 1 and $\mu = 1$ for convenience, and write them explicitly only when necessary.

Define new operators b_j , b_j^{\dagger} , which are neither Fermi nor Bose operators, by

$$S_{j}^{z} = \frac{1}{2} (b_{j}^{\dagger} + b_{j}), \quad S_{j}^{y} = (b_{j}^{\dagger} - b_{j})/2i \quad ,$$

$$S_{j}^{z} = b_{j}^{\dagger} b_{j} - \frac{1}{2} \quad .$$
(2.2)

These operators are expressed in terms of Fermi operators c_K , c_K^{\dagger} by

$$b_{j} = \exp\left(-\pi i \sum_{K=1}^{j-1} c_{K}^{\dagger} c_{K}\right) c_{j} ,$$

$$b_{j}^{*} = c_{j}^{*} \exp\left(\pi i \sum_{K=1}^{j-1} c_{K}^{\dagger} c_{K}\right) .$$
(2.3)

Following LSM, we substitute (2.3) in (2.1) and obtain

$$H = \frac{1}{2} \sum_{j=1}^{N} \left[\left(c_{j}^{\dagger} c_{j+1} + \gamma c_{j}^{\dagger} c_{j+1}^{\dagger} + \text{H. c.} \right) - 2h c_{j}^{\dagger} c_{j} \right] + \frac{1}{2} Nh , \qquad (2.4)$$

with the boundary condition¹³ $c_1 \equiv c_{N+1}$.

The diagonalization of (2.1) for h(t) independent of *t* is completed by using two more transformations: (i) Fourier transformation, and (ii) Bogoliubov transformation.

We can still carry out the Fourier transform

for a general h(t). Define

$$c_{j}^{+} = \frac{1}{\sqrt{N}} \sum_{p=-N/2}^{N/2} \exp(ij\phi_{p}) a_{p}^{\dagger} , \qquad (2.5)$$

$$c_{j} = \frac{1}{\sqrt{N}} \sum_{p=-N/2}^{N/2} \exp(-ij\phi_{p})a_{p}$$
,

where
$$\phi_p = 2\pi p/N$$
 . (2.6)

Substituting (2.5) in (2.4), one obtains

$$H = \frac{1}{2} \sum_{p=1}^{N/2} \left\{ \alpha_{p}(t) \left[a_{p}^{\dagger} a_{p} + a_{-p}^{\dagger} a_{-p} \right] + \frac{1}{2} i \delta_{p} \left[a_{p}^{\dagger} a_{-p}^{\dagger} + a_{p} a_{-p} \right] + 2h(t) \right\} , \qquad (2.7)$$

with
$$\alpha_{p}(t) = 2[\cos \phi_{p} - h(t)]$$
, (2.8)

$$\delta_p = -2\gamma \sin \phi_p \quad , \tag{2.9}$$

and a_p and a_p^{\dagger} are again Fermi operators.

The Bogoliubov transformation that would diagonalize (2.7) in terms of new Fermi operators would have no meaning, since the coefficients of this transformation would be explicitly time dependent. However, we can write (2.7) as

$$H = \sum_{p=1}^{N/2} \tilde{H}_{p} \quad , \tag{2.10}$$

where $\tilde{H}_{p} = \frac{1}{2} \{ \alpha_{p}(t) (a_{p}^{\dagger} a_{p} + a_{-p}^{\dagger} a_{-p}) \}$

$$+\frac{1}{2}i\delta_{p}[a_{p}^{\dagger}a_{-p}^{\dagger}+a_{p}a_{-p}]+2h(t)\} \quad . \qquad (2.11)$$

Clearly, we obtain
$$[\tilde{H}_{p}, \tilde{H}_{p}] = 0$$
, (2.12)

which means the space upon which \tilde{H} acts decomposes into noninteracting subspaces, each of four dimensions. No matter what h(t) is, there will be no transitions among those subspaces.

It is convenient to use the following basis for the pth subspace:

$$(|0\rangle; a_{p}^{\dagger}a_{-p}^{\dagger}|0\rangle; a_{p}^{\dagger}|0\rangle; a_{-p}^{\dagger}|0\rangle) \qquad (2.13)$$

This is the Heisenberg picture. The Hamiltonian (2.10) with the basis (2.13) becomes the matrix

$$\overline{H}(t)\sum_{p=1}^{N/2} \left[I \otimes I \otimes \cdots \otimes \overline{H}_p(t) \otimes \cdots \otimes I\right] \quad , \tag{2.14}$$

where we have explicitly

$$\overline{H}_{p}(t) = \begin{bmatrix} h(t) & \frac{1}{2}i\delta_{p} & 0 & 0 \\ -\frac{1}{2}i\delta_{p} & 2\cos\phi_{p} - h(t) & 0 & 0 \\ 0 & 0 & \cos\phi_{p} & 0 \\ 0 & 0 & 0 & \cos\phi_{p} \end{bmatrix},$$

(2.15)

and I is the 4×4 unit matrix.

III. LIOUVILLE EQUATION

In this section, we reduce the Liouville equation for the density matrix of the system (2.7) to a sec1078

ond-order ordinary differential equation.

Let $U_p(t)$ be the time-evolution matrix in the *p*th subspace, namely, $(\hbar = 1)$:

$$i\frac{d}{dt}U_{p}(t) = U_{p}(t)\overline{H}_{p}(t) \quad , \qquad (3.1)$$

with the boundary condition

$$U_{b}(0) = I$$
 . (3.2)

Then, the Hamiltonian of the system $H^{s}(t)$ in the Schrödinger picture is

$$H^{s}(t) = \sum_{p=1}^{N/2} \left[I \otimes I \otimes \cdots \otimes H_{p}^{s}(t) \otimes \cdots \otimes I \right] , \qquad (3.3)$$

where $H_{p}^{s}(t) = U_{p}(t)\overline{H}_{p}(t)U_{p}(t)^{\dagger}$, (3.4)

and $\overline{H}_{p}(t)$ is given by (2.15).

Let $\rho(t)$ be the density matrix of the system. The Liouville equation of the system is

$$i\frac{d}{dt}\rho(t) = [H^{s}(t), \rho(t)] \quad . \tag{3.5}$$

To complete the specification of $\rho(t)$, we need to provide the differential equation (3.5) with an initial condition. For the purposes of this paper, we will consider only systems which at time t = 0 are in thermal equilibrium at temperature T. Since we obtain

$$H^{s}(0) = \overline{H}(0) \quad , \tag{3.6}$$

we have
$$\rho(0) = e^{-\beta H^{S}(0)} = e^{-\beta \overline{H}(0)}$$
, (3.7)

where $\beta = 1/kT$ and k is the Boltzmann constant.

The boundary condition (3.6), by using (3.3), can be written explicitly

$$\rho(0) = \prod_{p=1}^{N/2} (I \otimes I \otimes \cdots \otimes e^{-\beta H_p(0)} \otimes I \cdots \otimes I)$$
$$= e^{-\beta \overline{H}_1(0)} \otimes e^{-\beta \overline{H}_2(0)} \otimes \cdots \otimes e^{-\beta \overline{H}_{N/2}(0)} \quad . \quad (3.8)$$

This particular algebric form, together with (2.12), suggests the solution of (3.1):

$$\rho(t) = \rho_1(t) \otimes \rho_2(t) \otimes \cdots \otimes \rho_{N/2}(t) \quad . \tag{3.9}$$

By substitution of (3.9) and (3.3) in (3.5), one obtains

$$\sum_{p=1}^{N/2} \left[\rho_1(t) \otimes \rho_2(t) \cdots \otimes \left(i \frac{d}{dt} \rho_p(t) - \left[H_p^s(t), \rho_p(t) \right] \right) \otimes \cdots \otimes \rho_{N/2}(t) \right] = 0 \quad . \quad (3.10)$$

From (3.10), we conclude that if for every integer p, $1 \le p \le \frac{1}{2}N$, ρ_p satisfies

$$i\frac{d}{dt}\rho_{p}(t) = [H_{p}^{s}(t), \rho_{p}(t)]$$
, (3.11)

with the initial condition

$$\rho_{p}(0) = e^{-\beta \, \overline{H}_{p}(0)} \quad ; \qquad (3.12a)$$

then (3.9) is the unique solution of (3.5) under the condition (3.6). Furthermore, because of (3.1) and (3.4), the solution of (3.11) is

$$\rho_{p}(t) = U_{p}(t)\rho_{p}(0)U_{p}(t)^{\dagger}, \qquad (3.12b)$$

and $\rho_p(0)$ is given explicitly

$$\rho_{p}(0) = \begin{bmatrix}
k_{11}^{p} & k_{12}^{p} & 0 & 0 \\
k_{21}^{p} & k_{22}^{p} & 0 & 0 \\
0 & 0 & e^{-\beta \cos\phi_{p}} & 0 \\
0 & 0 & 0 & e^{-\beta \cos\phi_{p}}
\end{bmatrix}, \quad (3.13)$$

where (we omit here the index p for convenience)

$$\Lambda[h(0)] \equiv \{\gamma^2 \sin^2 \phi + [h(0) - \cos \phi]^2\}^{1/2} , \quad (3.14)$$

$$q = -\Lambda[h(0)]^{-1}e^{-\beta\cos\phi}\sinh[\beta\Lambda(h(0))] , (3.15)$$

$$= -\frac{1}{2} \delta q \quad , \qquad (3.16)$$

$$P = \frac{\left[\cos\phi + \Lambda(h(0))\right]e^{-\beta\left[\cos\phi + \Lambda(h(0))\right]}}{2\Lambda[h(0)]}$$
$$\left[\cos\phi - \Lambda(h(0))\right]e^{-\beta\left[\cos\phi - \Lambda(0)\right)\right]} \tag{2.17}$$

$$2\Lambda[h(0)] \tag{0.10}$$

$$e_{12} = k_{21}^{*} = -ir \quad , \qquad (3.18)$$

$$k_{11} = h(0) q + P$$
 , (3.19)

$$k_{22} = P + q [2 \cos \phi - h(0)] \quad . \tag{3.20}$$

Because \overline{H}_{p} is in block form it is clear that

$$U_{p}(t) = \begin{bmatrix} U_{11,p}(t) & U_{12,p}(t) & 0 & 0 \\ U_{21,p}(t) & U_{22,p}(t) & 0 & 0 \\ 0 & 0 & e^{-it\cos\phi_{p}} & 0 \\ 0 & 0 & 0 & e^{-it\cos\phi_{p}} \end{bmatrix},$$
(3.21)

where the upper-left block is determined from

$$i\frac{d}{dt}\begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{bmatrix} = \begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{bmatrix} \begin{bmatrix} h(t) & \frac{1}{2}i\delta \\ -\frac{1}{2}i\delta & 2\cos\phi - h(t) \end{bmatrix}.$$
(3.22)

This matrix equation contains two independent systems of coupled differential equations. By straightforward algebra, we obtain

$$i \frac{d^2}{dt^2} U_{11}(t) = 2 \cos\phi \frac{d}{dt} U_{11}(t) + \left(\frac{dh(t)}{dt} - i \frac{1}{4} \delta^2 + i \left[2 \cos\phi - h(t)\right]h(t)\right) U_{11}, \quad (3.23)$$

with boundary conditions

$$U_{11}(0) = 1$$
 and $\frac{d}{dt} U_{11}(0) = -ih(0)$. (3.24)

Let
$$h(t) = b + h_1(t)$$
, (3.25)

while $\lim h_1(t) = 0$, (3.26)

$$U_{11}(t) = V(t)e^{-it \, \cos\phi} \quad . \tag{3.27}$$

Then (3.22) becomes

$$\frac{d^2}{dt^2} V(t) + [\Lambda^2(b) + \psi(t)] V(t) = 0 \quad , \tag{3.28}$$

where $\Lambda(b)$ is given by (3.14),

$$\psi(t) = h_1^2(t) - 2(\cos\phi - b)h_1(t) + i \frac{d}{dt}h_1(t) , \quad (3.29)$$

and from (3.23), V(t) satisfies the initial conditions

$$V(0) = 1, \quad \frac{d}{dt} V(0) = i [\cos \phi - h(0)] \quad . \tag{3.30}$$

From a well-known theorem,¹⁴ we deduce that all solutions of (3, 28) are bounded as $t \rightarrow \infty$ provided the following conditions are fulfilled:

$$\lim_{t \to \infty} \psi(t) = 0 , \quad \int_0^\infty \left| \psi'(t) \right| dt < \infty \quad . \tag{3.31}$$

Let W_1 and W_2 be two independent solutions of (3.26). Because of (3.31), we know that $\lim_{t\to\infty} V \cong \mu_1 e^{i\Lambda(b)t} + \mu_2 e^{-i\Lambda(b)t}$, where μ_1 and μ_2 are constants to be determined. Accordingly we specify W_{ij} , i = 1, 2, by

$$\lim_{t \to \infty} W_1(t) \sim e^{it \Lambda(b)} , \quad \lim_{t \to \infty} W_2(t) \sim e^{-it \Lambda(b)} . \quad (3.32)$$

Using (3.22), (3.28), and (3.32), we have "immediately'

$$V_{11}(t) = A_1 W_1(t) + A_2 W_2(t) , \qquad (3.33)$$

$$V_{21}(t) = B_1 W_1(t) + B_2 W_2(t) \quad , \tag{3.34}$$

with initial conditions

$$V_{21}(0) = 0$$
 and $\frac{d}{dt} V_{21}(0) = -\frac{1}{2}\delta$. (3.35)

The constants A_1 , A_2 , B_1 , B_2 are easily determined from (3.35) to be

$$A_{1} = \frac{(d/dt)W_{2}(0) - i[\cos\phi - h(0)]W_{2}(0)}{W(0)} ,$$

$$A_{2} = \frac{iW_{1}(0)[\cos\phi - h(0)] - (d/dt)]W_{1}(0)}{W(0)} , \quad (3.36)$$

$$B_{1} = -\frac{\frac{1}{2}\delta W_{2}(0)}{W(0)} , \quad B_{2} = \frac{\frac{1}{2}\delta W_{1}(0)}{W(0)} ,$$

where W(t) is the Wronskian of the two independent solutions W_1 , W_2 , namely,

$$W(t) = W_1(t) \frac{d}{dt} W_2(t) - W_2(t) \frac{d}{dt} W_1(t) \quad . \tag{3.37}$$

IV. MAGNETIZATION

We derive a general expression for the z-direction magnetization in terms of the solutions of (3.28), and obtain its asymptotic behavior.

The magnetization operator per spin is defined

$$M = \frac{1}{N} \sum_{j} S_{j}^{z} \quad . \tag{4.1}$$

M can be written in terms of the operators a_p , a_p^{\dagger} , defined in (2.5) and (2.6) as

$$M = \frac{1}{N} \sum_{p=1}^{N/2} M_p , \qquad (4.2)$$

where
$$M_{p} = a_{p}^{\dagger}a_{p} + a_{-p}^{\dagger}a_{-p} - 1$$
 . (4.3)

Clearly, we obtain

$$[M_{p}, M_{p'}] = 0 \quad . \tag{4.4}$$

Since (4.3) and (4.4) are conditions similar to (2.10) and (2.12), we conclude that *M* has the same algebric structure as *H*.

Let $M_z(t)$ be the average magnetization per spin, namely,

$$M_{z}(t) = \frac{1}{N} \frac{\mathrm{Tr}[M\rho]}{\mathrm{Tr}[\rho]} = \frac{1}{N} \sum_{p=1}^{N/2} \frac{\mathrm{Tr}[M_{p}U_{p}\rho_{p}(0)U_{p}^{\dagger}]}{\mathrm{Tr}[\rho_{p}(0)]}$$
(4.5)

Using (2.13), (3.13), (4.3), and (3.21) in (4.5) we obtain explicitly

$$M_{z}(t) = -\frac{1}{N} \sum_{p} (k_{11}^{p} + k_{22}^{b} + 2e^{-\beta \cos \phi_{p}})^{-1} \\ \times [(k_{11}^{p} - k_{22}^{b})(2 | U_{11}^{p} |^{2} - 1) - 4r_{p} \operatorname{Im}(U_{12}^{p} U_{11}^{p*})] . (4.6)$$

One can replace the U_{ij} in (4.6) by the V_{ij} of (3.33) and (3.34). Using the constants (3.36), (4.6) becomes

N/ 9

$$\begin{split} M_{z}(t) &= \frac{1}{N} \sum_{p=1}^{N-1} \frac{\tanh[\frac{1}{2}\beta\Lambda(h(0))]}{\Lambda(h(0))} \left\{ \begin{bmatrix} h(0) - \cos\phi_{p} \end{bmatrix} \\ &\times \left(2 \left| \frac{W_{2}'(0) - i\left[\cos\phi_{p} - h(0)\right]W_{2}(0)}{W(0)} W_{1}(t) \right. \\ &+ \frac{iW_{1}(0)\left[\cos\phi_{p} - h(0)\right] - W_{1}'(0)}{W(0)} W_{2}(t) \right|^{2} - 1 \right) \\ &+ (-2\gamma\sin\phi_{p})^{2} \operatorname{Im} \left[\frac{W_{2}'(0) - i\left[\cos\phi_{p} - h(0)\right]W_{2}(0)}{W(0)} \\ &\times W_{1}(t) + \frac{iW_{1}(0)\left[\cos\phi_{p} - h(0)\right] - W_{1}'(0)}{W(0)} W_{2}(t) \right) \\ &\times \left(-\frac{\frac{1}{2}W_{2}(0)}{W(0)} W_{1}(t) + \frac{\frac{1}{2}W_{1}(0)}{W(0)} W_{2}(t) \right) \right] \right\} \quad . \quad (4.7) \end{split}$$

This is the exact expression for all N for the magnetization in the z directions in terms of the solutions $W_1(t)$ and $W_2(t)$ of (3.28) with conditions (3.32). However, our major interest is in the thermodynamic limit $N \rightarrow \infty$. This limit is easily obtained from (4.7) by using the definition of inte-

gral to replace ϕ_p by ϕ and

$$rac{1}{N}\sum_{p=1}^{N/2}$$
 by $rac{1}{2\pi}\int_0^{\pi}d\phi$.

V. STEP-FUNCTION MAGNETIC FIELD

A step function in the magnetic field provides us

with the easiest example of the above formalism. Let

$$h(t) = a, t \le 0$$

= b, t > 0; (5.1)

then the solution of (3.22) is readily found to be

$$\begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{bmatrix} = e^{-it\cos\phi} \begin{bmatrix} V_{11} & V_{12} \\ -V_{12}^* & V_{11}^* \end{bmatrix}$$
$$= e^{-it\cos\phi} \begin{bmatrix} i\frac{(\cos\phi - b)}{\Lambda(b)} \sin[t\Lambda(b)] + \cos[t\Lambda(b)] & \frac{\delta}{2}\frac{\sin[t\Lambda(b)]}{\Lambda(b)} \\ -\frac{\delta}{2}\frac{\sin[t\Lambda(b)}{\Lambda(b)} & -i\frac{(\cos\phi - b)}{\Lambda(b)}\sin[t\Lambda(b)] + \cos[t\Lambda(b)] \end{bmatrix}.$$
(5.2)

The explicit density matrix for the pth subspace is also obtained by straightforward matrix multiplication as

$$\rho_{p}(t) = \begin{bmatrix} K_{11}^{p}(t) & K_{12}^{p}(t) & 0 & 0 \\ K_{12}^{*}(t) & k_{11}^{p} + k_{22}^{p} - K_{11}^{p}(t) & 0 & 0 \\ & & & & \\ 0 & 0 & e^{-\beta\cos\phi_{p}} & 0 \\ 0 & 0 & 0 & e^{-\beta\cos\phi_{p}} \end{bmatrix} , \qquad (5.3)$$

where

$$K_{11}^{p}(t) = k_{11}^{p} \left[(\cos\phi_{p} - b)^{2} \left(\frac{\sin[t\Lambda(b)]}{\Lambda(b)} \right)^{2} + \cos^{2}[t\Lambda(b)] \right] + r_{p} \delta_{p} (\cos\phi_{p} - b) \left(\frac{\sin[t\Lambda(b)]}{\Lambda(b)} \right)^{2} + k_{22}^{p} \frac{\delta_{p}^{2}}{4} \left(\frac{\sin[t\Lambda(b)]}{\Lambda(b)} \right)^{2} ,$$

$$K_{12}^{p}(t) = (k_{22}^{p} - k_{11}^{p}) \frac{\delta_{p}}{2} \frac{\sin[t\Lambda(b)]}{\Lambda(b)} \left(i \frac{\cos\phi_{p} - b}{\Lambda(b)} \sin[t\Lambda(b)] + \cos[t\Lambda(b)] \right)$$
(5.4)

$$-ir_{p}\left[\cos^{2}[t\Lambda(b)] + i\frac{\cos\phi_{p} - b}{\Lambda(b)}\sin[2t\Lambda(b)] - (\cos\phi_{p} - b)^{2}\left(\frac{\sin[t\Lambda(b)]}{\Lambda(b)}\right)^{2} + \frac{\delta^{2}}{4}\left(\frac{\sin[t\Lambda(b)]}{\Lambda(b)}\right)^{2}\right] , \quad (5.5)$$

and r_p , k_{11}^p , k_{22}^p , $\Lambda(b)$ are the same as before (3.14)-(3.20). By direct substitution of the matrix elements of (5.2) in the general formula for the magnetization (4.7) one obtains

$$m_{z}(t) = \frac{1}{N} \sum_{p} \frac{\tanh[\frac{1}{2}\beta\Lambda(a)]}{\Lambda(a)} \left(\frac{\cos 2\Lambda(b)t}{\Lambda^{2}(a)} \gamma^{2}(a-b) \sin^{2}\phi_{p} - \frac{(\cos\phi_{p}-b)[(\cos\phi_{p}-b)(\cos\phi_{p}-a)+\gamma^{2}\sin^{2}\phi_{p}]}{\Lambda^{2}(b)} \right)$$
(5.6)

We proceed to take the thermodynamic limit $N \rightarrow \infty$. The sum (5.6) becomes an integral. In other words, only the first term in the Poisson summation formula survives, and the others are exponentially small. It is interesting to note that (5.6) does not approach a limit as $t \rightarrow \infty$. This is not the case if the thermodynamic limit is taken first. Explicitly, (5.6) becomes ¹⁵

$$\lim_{N \to \infty} m_z(t) = \frac{1}{2\pi} \int_0^{\pi} d\phi \, \frac{\tanh[\frac{1}{2}\beta\Lambda(a)]}{\Lambda(a)\Lambda^2(b)} \\ \times \left\{ \cos\left[2\Lambda(b)t\right]\gamma^2(a-b)\sin^2\phi - (\cos\phi - b) \right. \\ \left. \times \left[\cos\phi - a\right)(\cos\phi - b) + \gamma^2\sin^2\phi \right] \right\} \cdot (5.7)$$

One would like to check (5.7) for several limiting cases. Since we have

$$\left[\sum_{i} S_{i}^{z}, \sum_{j} (S_{j}^{x} S_{j+1}^{x} + S_{j}^{y} S_{j+1}^{y})\right] = 0 \quad , \tag{5.8}$$

we expect no time dependence of $m_z(t)$ when $\gamma = 0$, and the time-dependent term of (5.7) is proportional to γ^2 . The limit a = b corresponds to a constant field, and should agree with $m_z(0)$ which is the wellknown statistical equilibrium formula, namely,

$$m_{z}(0) = \frac{1}{2\pi} \int_{0}^{\pi} d\phi \, \frac{\tanh[\frac{1}{2}\beta\Lambda(a)]}{\Lambda(a)} \, (a - \cos\phi) \, . \quad (5.9)$$

On the other hand, the infinite-time limit is

$$m_{z}(\infty) = \frac{1}{2\pi} \int_{0}^{\pi} d\phi \frac{\tanh[\frac{1}{2}\beta\Lambda(\alpha)]}{\Lambda(\alpha)}$$
$$\times \frac{(b - \cos\phi)}{\Lambda^{2}(b)} \left[(\cos\phi - a)(\cos\phi - b) + \gamma^{2}\sin^{2}\phi \right] .$$
(5.10)

 $m_z(\infty)$ depends on a, but for a general value of b this does not mean that $m_z(\infty)$ is not in thermal equilibrium, since the temperature of the finite state could depend on how much the magnetic field had changed. However, when b = 0, $m_z(\infty)$ does not vanish. From (5.9), we see that there is no value of T for which the equilibrium magnetization will be different from zero if no external field is applied. Therefore, we conclude that as $t \to \infty$ the system does not approach thermal equilibrium when h(t) is given by (5.1). In Fig. 1 we plot $m_z(\infty)$ as a function of the initial field a. We see that it is a monotonic function of a and as $a \to \infty$ it saturates at a value smaller than $\frac{1}{2}$, where $\frac{1}{2}$ is the saturation value of the initial magnetization.

In Appendix B, we perform a detailed study of the asymptotic behavior of (5.7) for large t. This expansion is valid for t = O(N) for taking the thermodynamic limit and then letting $t \to \infty$.

The result of this expansion is given in terms of three cases, 16 where

$$f_j(t) = m_z(t) - m_z(\infty), \quad j = 1, 2, 3$$
 (5.11)

Case (i): $|\mu b/J| > (1 - \gamma^2)$; $f_1(t)$ is given up to second order by

$$f_{1}(t) \sim -\frac{(a-b)\gamma^{2}\mu}{2\pi J} \left[\left(\frac{2tJ}{\hbar} \right)^{-3/2} \left\{ - \left[\frac{|\mu b - J|}{\mu b - J(1-\gamma^{2})} \right]^{1/2} \right]^{1/2} \right]^{1/2}$$



FIG. 1. Final magnetization versus initial field a for step function case: a - jumps to 0.

$$\times \Gamma\left(\frac{3}{2}\right) E_{1}\left(\left|\frac{\mu b}{J}-1\right|\right) \qquad \cos\left[\frac{2t}{\hbar}\left|b\mu-J\right|-\frac{1}{4}\pi\right] \\ + \left[\frac{\left|\mu b+J\right|}{\mu b+J(1-\gamma^{2})}\right]^{1/2} \Gamma\left(\frac{3}{2}\right) E_{1}\left(\left|\frac{\mu b}{J}+1\right|\right) \\ \times \cos\left[\frac{2t}{\hbar}\left|b\mu+J\right|+\frac{1}{4}\pi\right]\right\} \\ + \left(\frac{2tJ}{\hbar}\right)^{-5/2} \left\{\left[\frac{\left|\mu b-J\right|}{\mu b-J(1-\gamma^{2})}\right]^{1/2} \Gamma\left(\frac{5}{2}\right) \\ \times E_{1}'\left(\left|\frac{b\mu}{J}-1\right|\right) \cos\left(\frac{2t}{\hbar}\left|b\mu-J\right|+\frac{1}{4}\pi\right) \\ - \left[\frac{\left|\mu b+J\right|}{\mu b+J(1-\gamma^{2})}\right]^{1/2} \Gamma\left(\frac{5}{2}\right) E_{1}'\left(\left|\frac{b\mu}{J}+1\right|\right) \\ \times \cos\left(\frac{2t}{\hbar}\left|b\mu+J\right|-\frac{1}{4}\pi\right)\right\} \right]. \qquad (5.12)$$

 $E_1 \mbox{ and } E_1'$ are given by (B25) and (B26), respectively.

Case (ii): $|\mu b/J| < (1 - \gamma^2)$; $f_2(t)$ is given up to second order by

$$f_2(t) \sim \frac{(a-b)\gamma^2 \mu}{2\pi J} \left\{ (t\,\alpha)^{-1/2} \cos\left[\frac{2t}{\hbar}\,\gamma\right] \right\}$$

$$\times \left(J^{2} - \frac{b^{2}\mu^{2}}{1 - \gamma^{2}}\right)^{1/2} + \frac{1}{4}\pi \left[E_{3}\left(\frac{b}{1 - \gamma^{2}}\right)\Gamma(\frac{1}{2})\right] + \left\{\frac{(a - b)\gamma^{2}\mu}{4\pi J}(t\alpha)^{-3/2}\Gamma(\frac{3}{2})E_{3}''\left(\frac{b}{1 - \gamma^{2}}\right) \times \cos\left[\frac{2t}{\hbar}\gamma\left(J^{2} - \frac{b^{2}\mu^{2}}{1 - \gamma^{2}}\right)^{1/2} - \frac{1}{4}\pi\right] + \left[\text{first-order terms of } f_{1}(t)\right]\right\}.$$
 (5.13)

 $\alpha,\,E_3,\,E_3^{\,\prime}$ are given by (B34), (B41), and (B43), respectively.

Case (iii): $|b| = 1 - \gamma^2$; f_3 is given up to second order by

$$f_{3}(t) \sim \frac{(a-b)\gamma^{2}\mu}{2\pi J} \left[\frac{1}{2}\Gamma(\frac{3}{4})(mt)^{-3/4} E_{4}(0) \right] \\ \times \cos\left(\frac{2t}{\hbar} \left| \mu b - J \right| + \frac{3\pi}{8} \right) + \frac{1}{2}\Gamma(\frac{5}{2})(mt)^{-5/4} \\ \times E_{4}' \cos\left(\frac{2t}{\hbar} \left| \mu b - J \right| + \frac{5\pi}{8}\right) \right], \qquad (5.14)$$

where m is given by (B48) and $E_4(0)$ by (B46).

In Fig. 2, we exhibit the numerical analysis of (5.7) together with its appropriate asymptotic formula (5.12). We obtain the interference of two collective frequencies, which are understood from (5.12) to be "Larmor type" and "spin-exchange type." We cannot give an intuitive interpretation of the other collective frequency in (5.13).

VI. EXPONENTIALLY DECAYING MAGNETIC FIELD

Section V raises the suspicion that nonergodic behavior found in the system is due to the special case (5.1). In other words, when initial field ajumps to a final field b at a very fast rate, the system does not approach equilibrium. However, one might hope that a continuous very slow change of the magnetic field would result in an equilibri-



FIG. 2. $m_z(t)$ exact (numerical) and asymptotic for large t. $a=10, b=2, \gamma=\frac{1}{2}, \beta=1.$

um result.

To demonstrate this hope to be wrong we define a new field, which we can control to change as slow as we please:

$$h(t) = \begin{cases} a, & t \le 0\\ b + (a - b)e^{-Kt}, & t \ge 0 \end{cases}$$
(6.1)

where a > b.

The two solutions $W_1(t)$, $W_2(t)$ [Eq. (3.32)] of Eq. (3.28) are obtained in Appendix A to be

$$W_{1} = \exp\left(i\Lambda(b)t + i\frac{a-b}{K}e^{-\kappa t}\right)_{1}F_{1}\left(\frac{i}{K}\left[-\Lambda(b) + b - \cos\phi\right]; 1 - \frac{2i\Lambda(b)}{K}; -\frac{2i(a-b)}{K}e^{-\kappa t}\right), \quad (6.2)$$

$$W_{2} = \exp\left(-i\Lambda(b)t + i\frac{(a-b)}{K}e^{-\kappa t}\right)_{1}F_{1}\left(\frac{i}{K}\left[\Lambda(b) + b - \cos\phi\right]; 1 + \frac{2i\Lambda(b)}{K}; -\frac{2i(a-b)}{K}e^{-\kappa t}\right), \quad (6.3)$$

where ${}_{1}F_{1}(a, c, x)$ is the confluent hypergeometric function¹⁷ (Kummer series), and $\Lambda(b)$ is again given by (3.14).

One obtains the values of the constants (3.36) by direct substitution of (6.2) and (6.3) in (3.36) at t = 0:

$$W_1(0) = {}_1F_1\left(\frac{i}{K} \left[-\Lambda(b) + b - \cos\phi\right];\right.$$
$$1 - \frac{2i\Lambda(b)}{K}; - \frac{2i(a-b)}{K}\right) , \qquad (6.4a)$$

$$W_{2}(0) = {}_{1}F_{1}\left(\frac{i}{K}[\Lambda(b) + b - \cos\phi];\right.$$

$$1 + \frac{2i\Lambda(b)}{K}; - \frac{2i(a-b)}{K}\right) , \qquad (6.4b)$$

$$\frac{d}{dt} W_1(0) = [i\Lambda(b) - i(a - b)]_1 F_1\left(\frac{i}{K}[-\Lambda(b) + b - \cos\phi]; 1 - \frac{2i\Lambda(b)}{K}; -\frac{2i(a - b)}{K}\right)$$
$$- 2(a - b) \frac{-\Lambda(b) + b - \cos\phi}{K - 2i\Lambda(b)}$$
$$\times {}_1F_1\left(1 + \frac{i}{K}[-\Lambda(b) + b - \cos\phi]; 2 - \frac{2i\Lambda(b)}{K}; -\frac{2i(a - b)}{K}\right), \quad (6.4c)$$

$$\frac{d}{dt} W_2(0) = \left[-i\Lambda(b) - i(a-b) \right]_1 F_1\left(\frac{i}{K} \left[\Lambda(b) + b - \cos\phi \right]; 1 + \frac{2i\Lambda(b)}{K}; -\frac{2i(a-b)}{K} \right)$$

$$-2(a-b)\frac{\Lambda(b)+b-\cos\phi}{K+2i\Lambda(b)}$$

$$\times {}_{1}F_{1}\left(1+\frac{i}{K}\left[\Lambda(b)+b-\cos\phi\right];\right.$$

$$2+\frac{2i\Lambda(b)}{K}; -\frac{2i(a-b)}{K}\right), \quad (6.4d)$$

STATISTICAL MECHANICS...

$$W(0) = W_1(0) \frac{d}{dt} W_2(0)$$

- $W_2(0) \frac{d}{dt} W_1(0) = -2i\Lambda(b)$. (6.4e)

To obtain the magnetization for this case, substitute (6.4a)-(6.4e), (6.2), and (6.3) in (4.7), and take the thermodynamic limit.

We obtain

$$m(a, b, K, t) = \frac{1}{2\pi} \int_0^{\pi} d\phi \frac{\tanh[\frac{1}{2}\beta\Lambda(a)]}{\Lambda(a)} \times \left((a - \cos\phi) \times [2|BW_1(t) - AW_2(t)|^2 - 1] + \frac{\gamma^2 \sin^2\phi}{\Lambda(b)} \operatorname{Im} \left\{i[BW_1(t) - AW_2(t)][W_2(0)W_1(t) - W_1(0)W_2(t)]\right\}\right), (6.5)$$

where

$$A = [W'_{1}(0) - i(\cos\phi - a)W_{1}(0)] / - 2i\Lambda(b), \quad (6.6)$$

$$B = [W_2'(0) - i(\cos\phi - a) W_2(0)] / - 2i\Lambda(b) ,$$
(6.7)

$$W'_{1}(0) = i[-(a-b)+b-\cos\phi] W_{1}(0)$$

- i(- \Lambda + b - \cos \phi) W\frac{*}{2}(0), (6.8)
$$W'_{2}(0) = i[-(a-b)+b-\cos\phi] W_{2}(0)$$

$$-i(\Lambda + b - \cos\phi) W_1^*(0)$$
 . (6.9)

We are interested only in the $t \rightarrow \infty$ limit of (6.5) which is

$$m(a, b, K) = \lim_{t \to \infty} m(a, b, K, t) = \frac{1}{2\pi} \int_0^{\pi} d\phi \frac{\tanh[\frac{1}{2}\beta\Lambda(a)]}{\Lambda(a)}$$

$$\times \left((a - \cos \phi)(2|A|^2 + |B|^2 - 1) + \frac{\gamma^2 \sin^2 \phi}{\Lambda(b)} \operatorname{Re}(BW_1 + AW_2) \right) \quad . \quad (6.10)$$

This expression is an explicit function of K, which means that the final magnetization explicitly depends on how fast the field decays. For example, as $K \rightarrow \infty$

$$\lim_{K \to \infty} m(a, b, K) = \frac{1}{2\pi} \int_0^{\pi} d\phi \frac{\tanh[\frac{1}{2}\beta\Lambda(a)]}{\Lambda(a)} \frac{(b - \cos\phi)}{\Lambda^2(b)}$$
$$\times [\cos\phi - a)(\cos\phi - b) + \gamma^2 \sin^2\phi] \cdot (6, 11)$$

This is identical with (5.10) - a result which is expected, since when $K \rightarrow \infty$, (6.1) reduces to (5.1).

The hope stated at the beginning of this section is that as $K^{-1} \rightarrow \infty$, m(a, b, K) will approach the value it would have in thermal equilibrium at some temperature T_1 . To study this limit let $K^{-1} = s$. As $s \rightarrow \infty$ the asymptotic expansion of $W_1[a, b, s, \Lambda(b)]$ is found in Appendix C to be

$$W_{1}(a, b, s, \Lambda(b)) \sim \frac{[2\Lambda(b)(\Lambda(b) - b + \cos\phi)]^{1/2}}{2(a - b) + (\Lambda(b) - b + \cos\phi)}$$

$$\times \exp\left(i\frac{1}{2}\pi - s(\Lambda - b + \cos\phi) + s(\Lambda - b + \cos\phi) + s(\Lambda - b + \cos\phi)\right)$$

$$+ s(\Lambda - b + \cos\phi)\ln[s(\Lambda - b + \cos\phi) + 2s\Lambda - 2s(a - b) - 2s\Lambda\ln(2s\Lambda) + s(\Lambda + b - \cos\phi)]$$

$$\times \ln[2s(a - b) + s(\Lambda - b + \cos\phi)] , \qquad (6.12)$$

$$W_2(a, b, s, \Lambda(b)) \sim W_1(a, b, s, -\Lambda(b))$$
 (6.13)

By substitution of (6.12) and (6.13) in (6.10), and taking the limit $s \to \infty$, one obtains the final magnetization for this case. Clearly, only terms containing $|W_1|^2$ and $|W_2|^2$ will survive. Otherwise we again have the conditions of the Riemann-Lebesque lemma.

Explicitly, the final magnetization is

$$m(a, b) = \frac{1}{2\pi} \int_{0}^{\pi} d\phi \frac{\tanh[\frac{1}{2}\beta\Lambda(a)]}{\Lambda(a)} \left[(\cos\phi - a) + \left(\frac{3(b - \cos\phi)^{2}(a - \cos\phi)}{\Lambda(b)} + \frac{\gamma^{2}\sin^{2}\phi(a - \cos\phi)}{2\Lambda(b)} + \frac{\gamma^{2}\sin^{2}\phi(b - \cos\phi)}{2\Lambda(b)} \right) \\ \times \frac{2[4(a - b)^{2} + \gamma^{2}\sin^{2}\phi]}{4(a - b)^{2} - 4(a - b)(b - \cos\phi) - \gamma^{2}\sin^{2}\phi} + \left\{ 2(a - \cos\phi) - \gamma^{2}\sin^{2}\phi \right\} \\ \times \frac{(b - \cos\phi)[2(a - b) - (b - \cos\phi)]^{2} + 4\Lambda^{2}[2(a - b) - (b - \cos\phi)] + 2\Lambda^{2}(b - \cos\phi)}{4(a - b)^{2} - 4(a - b)(b - \cos\phi) - \gamma^{2}\sin^{2}\phi} \right] .$$
(6.14)

This magnetization shares with the $t \to \infty$ magnetization of the step function case, the unpleasant feature of failing to vanish when b = 0. Hence, we conclude that the $t \to \infty$ system is not in thermal equilibrium. Therefore, the nonergodic behavior of m_z found in Sec. V does not depend on the rate at which h(t) approaches its $t \to \infty$ limit.

VII. GENERAL PROPERTIES OF $m_{r}(t)$ FOR LARGE t

The final question of interest is the generality of the asymptotic approach of (4.7) to its final value, and its relation to the asymptotic behavior of (5.7).

To understand this point we consider the general field:

$$h(t) = a , \quad t \le 0$$

$$h(t) = g(t), \quad 0 \le t \le t$$

$$h(t) = b , \quad t_0 \le t < \infty$$

The evolution matrix for $t \le t_0$ is, in general,

$$\begin{bmatrix} U_{11}(t) & U_{12}(t) \\ U_{21}(t) & U_{11}(t) \end{bmatrix} = e^{-it \cos\phi} \begin{bmatrix} V_{11}(t) & -V_{21}^{*}(t) \\ V_{21}(t) & V_{11}^{*}(t) \end{bmatrix} , (7.2)$$

where V_{11} and V_{21} are given by (3.31) and (3.32), with constants A_1 , A_2 , B_1 , B_2 given by (3.34). A_1 and A_2 are, in general, independent of δ , and B_1 and B_2 are proportional to $\frac{1}{2}\delta$.

The evolution matrix for $t \ge t_0$ is obtained as

$$Ut = \begin{bmatrix} U_{11}(t) & U_{12}(t) \\ U_{21}(t) & U_{22}(t) \end{bmatrix} = e^{-it_0 \cos\phi} \begin{bmatrix} V_{11}(t_0) & -V_{21}^*(t_0) \\ V_{21}(t_0) & V_{11}^*(t_0) \end{bmatrix} \exp \begin{bmatrix} i(t-t_0) \begin{pmatrix} b & \frac{1}{2}i\delta \\ -\frac{1}{2}i\delta & 2\cos\phi - b \end{pmatrix} \end{bmatrix} .$$
(7.3)

Using (3.36), (6.3) becomes

$$U(t) = e^{-it \cos\phi} \begin{bmatrix} V_{11}(t_0) & -\frac{1}{2}\delta \overline{V}_{21}(t_0) \\ \frac{1}{2}\delta \overline{V}_{21}(t_0) & V_{11}^*(t_0) \end{bmatrix} \\ \times \begin{bmatrix} i \frac{\cos\phi - b}{\Lambda(b)} & \sin[(t - t_0)\Lambda(b)] + \cos[(t - t_0)\Lambda(b)] \\ -\frac{1}{2}\delta \frac{\sin[(t - t_0)\Lambda(b)]}{\Lambda(b)} & -i \frac{(\cos\phi - b)}{\Lambda(b)} & \sin[(t - t_0)\Lambda(b)] + \cos[(t - t_0)\Lambda(b)] \end{bmatrix}$$

where $V_{21} \equiv \frac{1}{2} \delta \overline{V}_{21}$ and \overline{V}_{21} is δ independent. The magnetization for this case is obtained by substitution of the appropriate elements (7.4) in formula (4.6).

The asymptotic expansion of $m_{e}(t)$ is very similar to that of Sec. V and Appendix B. There are three cases.

(i) $|\mu b/J| < 1 - \gamma^2$. In this case, $\Lambda(b)$ has an extremal point in the range $0 \le \phi \le \pi$ and the asymptotic expansion may be performed as a stationary phase integral. We find that the leading term of $m_{e}(t) - m_{e}(\infty)$ is given by the leading term of (5.13), where E_3 is replaced by an expression which depends explicitly on $V_{i,k}(t_0)$.

(ii) $|\mu b/J| > 1 - \gamma^2$. In this case, $\Lambda(b)$ is monotonic for $0 \le \phi \le \pi$, and the asymptotic expansion comes from the endpoint contribution near 0 and π . Because of the presence of the factor δ^2 (note that r is proportional to δ) these contributions are similar to those seen in Sec. V, and we find that the leading terms of $m_{\varepsilon}(t) - m_{\varepsilon}(\infty)$ are given by the leading term of (5.12), where E_1 and E_2 are re-

$$i \frac{(\cos \phi - b)}{\Lambda(b)} \sin[(t - t_0)\Lambda(b)] + \cos[(t - t_0)\Lambda(b)]$$
, (7.4)

placed by expressions which depend explicitly on $V_{j,k}(t_0).$

(iii) $|\mu b/J| = 1 - \gamma^2$. In this case, the extremal point of $\Lambda(b)$ occurs at 0 or π depending upon the sign of b. Again, because of the factor δ^2 this expansion is the same as that of Sec. V and we find the leading term of $m_{e}(t) - m_{e}(\infty)$ is given by the leading term of (5.14), where E_4 now depends on $V_{i,i}(t_0)$.

In summary, the form of the t dependence of the asymptotic behavior of $m_{e}(t) - m_{e}(\infty)$ is the same for all fields of the form (7.1). Only the constants depend on the details of the function g(t).

VIII. CONCLUSION AND SUMMARY

Since the considerations of this paper of necessity involve rather detailed and lengthy calculations, it may be worth while to summarize the various results and comment on their physical significance.

(i) Once the time-independent solutions are known, the time-dependent evolution is described by (1.7). The character of the system is described

(7.1)

by the normal modes Λ_p of the time-independent system relevant to the field h(t). Thus, the nonequilibrium description requires an analysis of Eq. (3.28), over and above the solution of the equilibrium problem.

(ii) The explicit result for the time dependence of the magnetization for the step-function case $m_{z}(a, b, t)$ has the feature, that for a finite system (N finite) the limit $t \rightarrow \infty$ does not exist. The nonexistence of this time limit for physically meaningful observables is the generally known fact that the thermodynamic limit must be taken before an "approach to equilibrium" as $t \rightarrow \infty$ can be expected.

(iii) The main result of this study is the realization that the magnetization m(a, b, t) as $t \rightarrow \infty$ does not approach an equilibrium value. This is indicated by the fact that m(a, o, t) does not go to zero at infinite time. The fact that even as $a \rightarrow \infty$, the limiting value of m is less than $\frac{1}{2}$ is also surprising and shows that this model is not in agreement with the obvious physical intuition. The analysis of the exponentially decaying case, where the change from an external field a to b was carried out as slow as desired, results in the same "nonapproach" to equilibrium. This behavior is not a pecularity of the particular external field. It must be expected that this nonapproach is a general feature of the system at hand.

(iv) In connection with this nonapproach to equilibrium, Mazur¹² formulated a necessary and sufficient condition for a variable X to be ergodic in a classical system. This condition can be expressed in terms of the autocorrelation function as

$$R \equiv \lim \frac{1}{T} \int_0^T \langle X(0) X(t) \rangle dt = \langle \overline{X}^2(E) \rangle \quad . \tag{8.1}$$

Here $\langle X \rangle$ is the canonical average of X and $\overline{X}(E)$ is the microcanonical average of X. It is possible to obtain a generally valid inequality for R (i.e., its validity is independent of the ergodic character of the system or the nature of the variable X). This inequality can be expressed as

$$R \ge Q$$
 . (8.2)

The quantity Q can be expressed exclusively of the canonical average. Thus from the relations (8.1) and (8.2) one can see that a system *cannot* be ergodic if

$$Q > \langle X^2(E) \rangle \quad . \tag{8.3}$$

Mazur has found a condition guaranteeing the nonergodic character of a variable. This is a useful condition since both Q and $\langle X^2(E) \rangle$ are cononical averages, and as such can be obtained without explicit knowledge of the time dependence. Using this inequality for X, the magnetization, Mazur showed that it is not ergodic for the XY model. Thus, harmony exists with the results obtained in this paper. The only point of concern, in a direct application of Mazur's result, is the fact that his analysis is classical, while the spin system is as quantum mechanical as it can be. The results obtained here indicate that there is good reason to expect Mazur's ingenious analysis to be valid in the quantum case, but it would be highly desirable to give a formal proof of Mazur's work for general quantum systems.

(v) The detailed formula for the asymptotic time dependence (for the step function and for the general case) indicates interesting and suggestive beat phenomena which are, as noted, dependent on aand b, but not on g(t). It would be interesting if these various frequencies could be understood in an immediate intuitive fashion. It is believed that this is possible because the results are general, but so far this has not been done. It would be even more interesting if these were experimental situations in which these oscillations could be observed. Perhaps spin-echo experiments might show some of these features. In this connection a detailed examination of the oscillatory approach to the final state would be interesting. Furthermore, the case $h(t) = a + b \cos wt$, should be further analyzed.

(vi) It is possibly not too surprising that equilibrium in the conventional sense is not approached in this system. The system considered is quite simple and reminiscent of a system of coupled oscillators, and it is well known that these are peculiar phenomena associated with the approach to the equipartition of energy for such systems. The system is perhaps not complex enough to produce the mixing between the various degrees of freedom necessary for an approach to equilibrium. Even so, it would be interesting to see whether this system possesses any ergodic observables.¹⁸

ACKNOWLEDGMENTS

The authors are pleased to thank Professor C. N. Yang for his continued interest in this study and his incisive comments. One of us (EB) would like to thank Professor M. C. Gutzwiller for his encouragement and interest in this work, and Professor J. Lebowitz for a most interesting discussion.

APPENDIX A

We analyze here Eq. (3.26) for two cases of interest.

A. Exponential Decay

Let

$$h(t) = b + (a - b)e^{-Kt}, \quad t > 0$$

$$= a, \quad t \le 0, \quad K > 0$$
(A1)

and
$$h_1(t) = (a - b)e^{-Kt}$$
. (A2)

Equation (3.26) for t > 0 becomes

$$\frac{d^2}{dt^2} V + \left[\Lambda^2(b) + (a-b)^2 e^{-2Kt} - 2(\cos\phi - b)e^{-Kt} - iKe^{-Kt}\right]V = 0.$$
(A3)

Let $y(z) = z^R e^{ibz/K} y_z(z) = V(t)$, (A4)

where $z = e^{-Kt}$, (A5)

$$R = \pm i\Lambda(b)/K . \tag{A6}$$

Equation (A3) becomes

$$z\frac{d^{2}}{dz^{2}} y_{2}(z) + \left[z\left(\pm \frac{zi(a-b)}{K}\right) + \left(1 \pm \frac{2i\Lambda(b)}{K}\right)\right] \frac{d}{dz} y_{2}(z) + \left[-i\frac{a-b}{K} + \frac{2(a-b)(b-\cos\phi)}{K^{2}} \pm \frac{i(a-b)}{K} + \frac{2(a-b)(b-\cos\phi)}{K^{2}} \pm \frac{i(a-b)}{K} + \frac{2i\Lambda(b)}{K}\right] y_{2}(z) = 0.$$
 (A7)

Change the variable once more, and let

$$x = -[2i(a-b)/K]z.$$
 (A8)

One obtains confuent hypergeometric equation in Kummer's form,¹⁷ and the two solutions $W_1(z)$ and $W_2(z)$ are

$$W_{1}(z) = z^{(i/K)\Lambda} e^{((b-a)/K)z} {}_{1}F_{1}\left(\frac{i}{K} [\Lambda + b - \cos\phi]; + 2i\Lambda/K; - [2i(a-b)/K]z\right),$$
(A9)

$$W_{2}(z) = z^{-(i/K)\Lambda} e^{i[(b-a)/K]z} {}_{1}F_{1}\left(\frac{i}{K} \left[-\Lambda + b - \cos\phi\right]; \\ 1 - 2i\Lambda/K; - [2i(a-b)/K]z\right), \quad (A10)$$

with z given by (A5).

B. Hyperbolic Decay

Let
$$h(t) = a$$
, $t \le 0$
 $= b + \frac{a-b}{t+1}$, $t \ge 0$
 $h_1(t) = (a-b)/(t+1)$. (A12)

Let t+1=s in (3.26) and V(t)=y(s). We obtain

$$s^{2} \frac{d^{2}}{ds^{2}} y + [\Lambda^{2}(b)s^{2} + 2(a - b) (b - \cos\phi)s + (a - b) (a - b - i)]y = 0 \quad .$$
 (A13)

Let $y(s) = s^{K} e^{i\Lambda s} y_{1}(s)$, (A14)

where

$$K = \frac{1}{2} \left\{ 1 + \left[1 - 4(a-b)(a-b-i) \right]^{1/2} \right\} = -i(a-b) .$$
(A15)

Equation (A13) becomes

$$s\frac{d^{2}}{ds^{2}} y_{1}(s) + (2i\Lambda s + 2K)\frac{d}{ds} y_{1}(s) + [2iK\Lambda + 2(a-b)(b-\cos\phi)]y_{1}(s) = 0.$$
(A16)

This equation is similar to (A7) with different constants, and the solutions are again Kummer function with $-2i\Lambda(t+1)$ as a variable.

There are other cases of interest for $h_1(t)$, for instance an attenuated periodic field $h_1(t)$ = $(a-b)e^{-Kt}\cos\omega t$. To treat such cases, one should substitute his $h_1(t)$ in (3.26) and use the general theory of second-order ordinary differential equations.

APPENDIX B

We perform the asymptotic expansion of (5.8). In the integral (5.8), $\cos\phi$ changes monotonically between $[0, \pi]$, so we can always change the variable.

Let
$$y = \cos \phi$$
 and $d\phi = -\frac{dy}{(1-y^2)^{1/2}}$.
Let $f(t) = A \operatorname{Re} \int_{-1}^{1} dy \frac{(1-y^2)^{1/2} \tanh\left[\frac{1}{2}\beta\Lambda(a,y)\right]}{\Lambda(a,y)\Lambda^2(b,y)}$
 $\times e^{2it\Lambda(b,y)}$. (B1)

This is the time-dependent part of the magnetization m_{xy} . Assume $|\gamma| < 1, b > 0$. Let $A \equiv (a - b)\gamma^2 / 2\pi$; then

$$\begin{split} f(t) &= A \\ &\times \operatorname{Re}\left(\int_{-1}^{1} dy \frac{(1-y^2)^{1/2} \tanh\left\{\frac{1}{2}\beta\left[\dot{\gamma}^{\,2}(1-y^2)+(a-y)^2\right]^{1/2}\right\}}{\left[\gamma^{\,2}(1-y^2)+(a-y)^2\right]^{1/2}\left[\gamma^{2}(1-y^2)+(b-y)^2\right]} \\ &\times \exp\left\{2\,it\left[\gamma^{2}(1-y^2)+(b-y)^2\right]^{1/2}\right\}\right) \,. \end{split} \tag{B2} \\ \operatorname{Case} (I) \qquad b > 1-\gamma^2; \\ \operatorname{Case} (II) \qquad b < 1-\gamma^2; \\ \operatorname{Case} (III) \qquad b = 1-\gamma^2 \,. \end{split}$$

Clearly, in these regions, there will be contributions from the end points. The important question is whether $[\gamma^2(1-y^2)+(b-y)^2]^{1/2}$ has an extremum point for $y \in [-1, 1]$, or not.

Our method of evaluating the integral f(t) for large t is somewhat similar to the method used to evaluate asymptotically Bessel functions. We are going to the complex y plane. Doing so, it appears as if we introduce a serious difficulty:

$$p(y) = \frac{\tanh\{\frac{1}{2}\beta \left[\gamma^2(1-y^2) + (a-y)^2\right]^{1/2}\}}{\left[\gamma^2(1-y^2) + (a-y)^2\right]^{1/2}}.$$
 (B3)

(B5)

(B6)

The function p(y) has an infinite number of poles in the complex y plane. By integrating along a properly chosen contour, one might have to include an infinite sum of the residues of these poles. However, we domonstrate that for large t, these poles decay exponentially; therefore, they do not contribute to the asymptotic expansion for large t.

To demonstrate this last assertion we use the partial fraction decomposition of p(y):

$$\frac{2}{\beta}p(y) = \frac{\tanh\left[\frac{1}{2}\beta\Lambda(a,y)\right]}{\frac{1}{2}\beta\Lambda(a,y)}$$
$$= 2\sum_{n=0}^{\infty} \frac{1}{\left[\frac{1}{2}\beta\Lambda(a,y)\right]^2 - \left[\frac{1}{2}\beta\Lambda_n\right]^2}, \qquad (B4)$$

where $\cosh\left[\frac{1}{2}\beta\Lambda_n\right] = 0$

$$\mathbf{or}$$

Substituting these values in p(y), one obtains

$$p(y) = \frac{4}{\beta} \sum_{n=0}^{\infty} \\ \times \left[(1 - \gamma^2) y^2 - 2ay + \gamma^2 + a^2 + \pi^2 (2n+1)^2 / \beta^2 \right]^{-1}.$$
(B7)

 $\Lambda_n = i\pi(2n+1)/\beta \ .$

An important feature of p(y) is that p(y) does not have any pole in the interval [-1, 1]. This is seen immediately from $\gamma^2(1-y^2) + (a-y)^2 \ge 0$ in [-1, 1], and the square root is always real, therefore (B5) has no solution for $-1 \le y \le 1$.

Poles of p(y) are at the points

$$y_{n}^{\pm} = \frac{a^{\pm} \left[a^{2} - (1 - \gamma^{2}) \left(\gamma^{2} + a^{2} + \pi^{2} \left(2n + 1\right)^{2} / \beta^{2}\right)\right]^{1/2}}{1 - \gamma^{2}}.$$
(B8)

Two possibilities for these poles are: (a) y_n is real so these poles, which must obey $|y_n| > 1$, do not contribute anything; (b) y_n is complex. Let $[(1-\gamma^2) y_n^2 - 2 by_n + b^2 + \gamma^2]^{1/2} \equiv \xi + i\psi$, with $\psi \neq 0$. Then $\xi + i\psi$ is complex unless a = b. But the case a = b is trivial, since the integral f(t) is proportional to a - b. By calculation of the residue, for the simple poles y_n of p(y), we obtain contributions to the value of f(t) of the form

 $\operatorname{const} e^{2it(\xi + i\psi)} = \operatorname{const} e^{-2\psi t} e^{2it\xi}$.

This means that possibly *a*-dependent oscillation frequencies of the magnetization decay exponentially, which is very fast compared to decay of the type t^{-a} , where we have $\alpha > 0$. We conclude that for large *t*, the contribution to f(t) from the poles y_n is negligible.

Case (I) $b > 1 - \gamma^2$; assume $b \neq 1$. (The case b = 1 does not introduce any major difficulty. The result for this case would be sum of two descending series. One series vanishes for b = 1.) We further assume $a \neq 1$. Having a = 1, $\tanh\left[\frac{1}{2}\beta\Lambda\right]/\Lambda$ becomes $\frac{1}{2}\beta$ at the endpoints. Define

$$\begin{split} F(t) &= \int_{-1}^{1} dy \\ &\times \frac{(1-y^2)^{1/2} \tanh\left\{\frac{1}{2}\beta\left[\gamma^2(1-y^2)+(a-y)^2\right]^{1/2}\right\}}{\left[\gamma^2(1-y^2)+(a-y)^2\right]^{1/2}\left[\gamma^2(1-y^2)+(b-y)^2\right]} \\ &\times \exp\left\{2\,it\left[\gamma^2(1-y^2)+(b-y)^2\right]^{1/2}\right\}\,, \end{split}$$

namely, $f(t) = A \operatorname{Re} F(t)$. One can change the variables

$$[\gamma^{2}(1-y^{2})+(b-y)^{2}]^{1/2}=x$$
(B10)

 \mathbf{or}

$$y = \frac{b - [b^2 - (1 - \gamma^2) (b^2 + \gamma^2 - x^2)]^{1/2}}{1 - \gamma^2} \equiv B(x), \quad (B11)$$

where

$$B(|b+1|) = -1, \quad B(|b-1|) = 1,$$
 (B12)

and

$$dy = -\frac{x\,dx}{\left[b^2 - (1 - \gamma^2)\,(b^2 + \gamma^2 - x^2)\right]^{1/2}} \quad , \tag{B13}$$

$$F(t) = \int_{|b-1|}^{|b+1|} \frac{dx}{x} e^{2itx} \frac{\left[1 - B^2(x)\right]^{1/2} \tanh\left\{\frac{1}{2}\beta \left[\gamma^2(1 - B^2(x) + (a - B(x))^2\right]\right\}}{\left\{\gamma^2 \left[1 - B^2(x)\right] + \left[a - B(x)\right]^2\right\}^{1/2} \left[b^2 - (1 - \gamma^2) \left(b^2 + \gamma^2 - x^2\right)\right]^{1/2}}$$
(B14)

Let I(t) be the following contour integral in the complex x plane;

$$I(t) = \oint_C \frac{dx}{x} \frac{\left[1 - B^2(x)\right]^{1/2} \tanh\left\{\frac{1}{2}\beta\left[\gamma^2(1 - B^2(x) + (a - B(x))^2\right]^{1/2}\right\}}{\left\{\gamma^2(1 - B^2(x) + [a - B(x)]^2\right\}^{1/2} \left[b^2 - (1 - \gamma^2)(b^2 + \gamma^2 - x^2)^{1/2}\right]}$$
(B15)

where the contour C_1 is shown in Fig. 3. Apart from possible poles of $[\tanh \frac{1}{2}\beta \Lambda(x,a)] / \Lambda(x,a)$,

which were shown to be negligible for large t, the integral I(t) along the contour C_1 vanishes. The

integral along $z_1 z_2$ vanishes as $\text{Im } x \rightarrow \infty$, especially for t going to infinity. So we are left with

$$F(t) = \int_{b-1}^{x_1} - \int_{b+1}^{x_2} \equiv P_1(t) - P_2(t) .$$
 (B16)
Evaluation of $P_1(t)$:

$$P_{1}(t) = \int_{|b-1|}^{|b-1|+i\infty} \left(\frac{dx}{x} \tanh \left\{ \frac{1}{2}\beta \left[\gamma^{2} (1-B^{2}(x)) + (a-B(x))^{2} \right]^{1/2} \right\} \left[(1+B(x)) (1-B(x)) \right]^{1/2} \\ \times \exp(2 itx) \left[\gamma^{2} (1-B^{2}(x)) + (a-B(x))^{2} \right]^{-1/2} \\ \times \left[b^{2} - (1-\gamma^{2}) (b^{2}+\gamma^{2}-x^{2}) \right]^{-1/2} \right).$$
(B17)
Let $|b-1| + i\xi = x$ (B18)

and $id\xi = dx$.

$$P_{1}(t) = i \int_{0}^{\infty} d\xi \left(\left[1 + B(|b - 1|) + i\xi \right] \right]^{1/2} \left(|b - 1| + i\xi \right)^{-1/2}$$

× tanh $\left\{ \frac{1}{2} \beta \left[\gamma^{2} (1 - B^{2}(|b - 1| + i\xi)) + (a - B(|b - 1| + i\xi))^{2} \right]^{1/2} \right\}$

×
$$[\gamma^2(1 - B^2(|b-1|+i\xi)) + (a - B(|b-1|+i\xi))^2]^{-1/2}$$



FIG. 3. Contour C₁.

×
$$[b^{2} - (1 - \gamma^{2}) (b^{2} + \gamma^{2} - (|b - 1| + i\xi)^{2})]^{-1/2}$$

× $[1 - B(|b - 1| + i\xi)]^{-1/2} \exp [2it(|b - 1| + i\xi)]).$
(B19)

Define next the function $E_1(|b-1|+i\xi)$ such that $P_1(t) = ie^{2it|b-1|} \int_0^\infty d\xi \times E_1(|b-1|+i\xi)$

$$\times e^{-2t\xi} \times [1 + B(|b - 1| + i\xi)]^{1/2}, \qquad (B20)$$

where
$$E_1(|b-1|+i\xi) \simeq E_1(|b-1|)$$

+ $E'_1(|b-1|)(i\xi) - E''_1(|b-1|)\xi^2 + \cdots$
(B21)

exists around $\xi = 0$:

$$B(|b-1|+i\xi) \simeq \frac{b}{1-\gamma^2} - \frac{b-(1-\gamma^2)}{1-\gamma^2} \left(1 + \frac{i|b-1|(1-\gamma^2)}{[b-(1-\gamma^2)]^2} \xi\right) = 1 - \frac{i|b-1|}{b-(1-\gamma^2)} \xi , \quad (B22)$$

$$[1 - B(|b - 1| + i\xi)]^{1/2} \simeq e^{i\pi/4} \times \left[\frac{(b - 1)}{b - (1 - \gamma^2)}\right]^{1/2} \xi^{1/2},$$
(B23)

$$\begin{split} P_{1}(t) &\simeq i e^{i \pi/4} \left(\frac{b-1}{b-(1-\gamma^{2})} \right)^{1/2} e^{2it|b-1|} \\ &\times \left(E_{1}(|b-1|) \int_{0}^{\infty} d\xi \, e^{-2tt} \xi^{1/2} \\ &\quad + i E_{1}'(|b-1|) \int_{0}^{\infty} d\xi \times \xi^{3/2} \, e^{-2tt} \\ &\quad - \frac{E_{1}''}{2!} \int_{0}^{\infty} d\xi \times \xi^{5/2} \, e^{-2tt} \right) \\ &= - e^{-i \pi/4} \left(\frac{|b-1|}{b-(1-\gamma^{2})} \right)^{1/2} e^{2it|b-1|} \\ &\quad \times \left(\frac{E_{1}(|b-1|) \Gamma(\frac{3}{2})}{(2t)^{3/2}} + \frac{i E_{1}'(|b-1|) \Gamma(\frac{5}{2})}{(2t)^{5/2}} + \dots \right), \end{split}$$
(B24)

and

$$E_{1}(b-1) = \frac{\sqrt{2} \tanh[\frac{1}{2}\beta |a-1|]}{|a-1| \times |b-1| [b-(1-\gamma^{2})]}, \quad (B25)$$

= 1/(1-1) $\sqrt{2\{1-\tanh^{2}[\frac{1}{2}\beta |a-1|]\}} \{\frac{1}{2}\beta [a-(1-\gamma^{2})]\}$

$$E_{1}'(|b-1|) = \frac{\sqrt{2}\left(1 - \tan\left[\frac{1}{2}\beta|a-1|\right]\right)\left\{\frac{1}{2}\beta|a-1-\gamma^{2}\right\}}{|a-1|^{2}\left[b-(1-\gamma^{2})\right]^{2}} - \frac{\sqrt{2}\tanh\left[\frac{1}{2}\beta|a-1|\right]}{|a-1|^{2}\left[b-(1-\gamma^{2})\right]} \left(\frac{1}{|b-1|^{2}} + \frac{(1-\gamma^{2})}{[b-(1-\gamma^{2})]^{2}}\right)$$

+
$$\frac{1}{|a-1|^2[b-(1-\gamma^2)]} + \frac{1}{4[b-(1-\gamma^2)]}$$
, (B26)

so $P_1(t)$ is calculated asymptotically for large t, up to second order. It can be done, in principle, to any order desired. In order to obtain $P_2(t)$, we see by close inspection, or better by repeating the above method, that replacing a - 1, b - 1, $b - (1 - \gamma^2)$, $-\frac{1}{4}i\pi$, by a + 1, b + 1, $b + 1 - \gamma^2$, $\frac{1}{4}i\pi$, respectively, in $P_1(t)$ gives the correct formula for $P_2(t)$:

$$P_{2}(t) = -e^{i\pi/4} \left(\frac{|b+1|}{|b+(1-\gamma^{2})|} \right)^{1/2} e^{2it|b+1|} \times \left(\frac{E_{2}(|b+1|)\Gamma(\frac{3}{2})}{(2t)^{3/2}} + \frac{iE_{2}'(|b+1|)\Gamma(\frac{5}{2})}{(2t)^{5/2}} + \cdots \right) ,$$
(B27)

where $E_2(|b+1|) = \frac{2 \tanh[\frac{1}{2}\beta | a+1 |]}{|a+1| |b+1|[b+(1-\gamma^2)]}$, (B28)

$$E_{2}'(|b+1|) = \frac{\sqrt{2}[1-\tanh^{2}(\frac{1}{2}\beta|a+1|)]\left\{\frac{1}{2}\beta[a+(1-\gamma^{2})]\right\}}{|a+1|^{2}[b+(1-\gamma^{2})]^{2}} - \frac{\sqrt{2}\tanh[\frac{1}{2}\beta|a+1|]}{|a+1|(b+(1-\gamma^{2}))}\left(\frac{1}{|b+1|^{2}} + \frac{1-\gamma^{2}}{(b+1-\gamma^{2})^{2}} + \frac{1}{|a+1|^{2}(b+1-\gamma^{2})} + \frac{1}{4(b+1-\gamma^{2})}\right).$$
(B29)

Case II: $b < 1 - \gamma^2$; We compute f(t) for this case up to second order. The existence of a stationary phase in the integrand will contribute the first-order term. The second-order term will consist of two parts, the second-order stationary phase, and the endpoint integration, calculated for $b > 1 - \gamma^2$.

Here we cannot go to the complex x plane, since $\Lambda(b, y)$ is not a monotonic function of y.

We find a stationary phase at the point $y = b/(1 - \gamma^2)$, and expand the two parts of the integral around this point. Rewrite f(t):

$$f(t) = A \operatorname{Re} \int_{-1}^{1} dy \, \frac{(1-y^2)^{1/2} \tanh\left[\frac{1}{2}\beta[\gamma^2(1-y^2) + (a-y)^2]^{1/2}\right] \exp\left\{2it[\gamma^2(1-y^2) + (b-y)^2]^{1/2}\right\}}{[\gamma^2(1-y^2) + (a-y)^2]^{1/2}\left[\gamma^2(1-y^2) + (b-y)^2\right]}$$

$$\equiv A \operatorname{Re} \int_{-1}^{1} dy \, E_3(y) \exp\left\{2it[\gamma^2(1-y^2) + (b-y)^2]^{1/2}\right\} , \qquad (B30)$$

$$f(t) \simeq A \operatorname{Re} \int_{-1}^{1} E_{3}(y) \exp\left\{2it\left[\gamma \left(1 - \frac{b^{2}}{1 - \gamma^{2}}\right)^{1/2} + \frac{1 - \gamma^{2}}{2\gamma} \left(1 - \frac{b^{2}}{1 - \gamma^{2}}\right)^{-1/2} \left(y - \frac{b}{1 - \gamma^{2}}\right)^{2}\right]\right\}.$$
(B31)

We estimate this last integral in the complex y place, along the contour C_2 (Fig. 4). We have introduced two more branch cuts, to define the sign of the square root in the exponent. It is necessary to mention that these branch points do not contribute *any factor* to the answer.

To complete the estimate of f(t) for this case, one needs to compute the line integral $P_3(t)$ along AB.

Let
$$E_{3}(y) = E_{3}\left(\frac{b}{1-\gamma^{2}}\right) + E_{3}'\left(\frac{b}{1-\gamma^{2}}\right)\left(y-\frac{b}{1-\gamma^{2}}\right)$$

 $+\frac{1}{2!}E_{3}''\left(\frac{b}{1-\gamma^{2}}\right)\left(y-\frac{b}{1-\gamma^{2}}\right)^{2} + \cdots,$ (B32)

$$P_3(t) \cong A \operatorname{Re} \exp\left[2it\gamma\left(1-\frac{b^2}{1-\gamma^2}\right)^{1/2}\right]$$

$$\times \left[E_{3} \left(\frac{b}{1 - \gamma^{2}} \right) \int_{AB} dy \ e^{+ it \, \alpha \left[y - b / (1 - \gamma^{2}) \right]^{2}} \\ + E_{3}'' \left(\frac{b}{1 - \gamma^{2}} \right) \int_{AB} dy \ e^{it \, \alpha \left[y - b / (1 - \gamma^{2}) \right]^{2}} \left(y - \frac{b}{1 - \gamma^{2}} \right)^{2} \right] ,$$
(B33)

where
$$\alpha = \frac{1 - \gamma^2}{2\gamma} \left(1 - \frac{b^2}{1 - \gamma^2} \right)^{-1/2}$$
. (B34)

Let
$$y - \frac{b}{1 - \gamma^2} = e^{i\pi/4}z$$
, $dy = e^{i\pi/4}dz$, (B35)

$$P_{3}(t) \stackrel{\sim}{=} A \operatorname{Re} \exp\left[2it\gamma\left(1 - \frac{b^{2}}{1 - \gamma^{2}}\right)^{1/2}\right] \\ \times \left[-E_{3}\left(\frac{b}{1 - \gamma^{2}}\right)\int_{-\infty}^{\infty} e^{i\pi/4}dz \ e^{-t\alpha z^{2}} \\ -\frac{1}{2}E_{3}'\left(\frac{b}{1 - \gamma^{2}}\right)\int_{-\infty}^{\infty} e^{i\pi/4}iz^{2}e^{-t\alpha z^{2}}dz\right].$$
(B36)



$$\times \left[\gamma^{2} \left(1 - \frac{b^{2}}{(1 - \gamma^{2})^{2}} \right) + \left(a - \frac{b}{1 - \gamma^{2}} \right)^{2} \right]^{-1/2} \times \left[\gamma^{2} \left(1 - \frac{b^{2}}{(1 - \gamma^{2})^{2}} \right) + \left(a - \frac{b}{1 - \gamma^{2}} \right)^{2} \right]^{-1} \quad . \tag{B41}$$

Because of its complexity, E_3'' [$b/(1-\gamma^2)$] is expressed in terms of the following constants:

$$Y \equiv \frac{b}{1 - \gamma_2} \quad , \tag{B42a}$$

$$S \equiv \left[1 - b^{-2}(1 - \gamma^2)^{-2}\right]^{1/2}, \qquad (B42b)$$

$$B \equiv \gamma \left[1 - b^{-2} (1 - \gamma^2)^{-1} \right]^{1/2}, \qquad (B42c)$$

$$D \equiv \left[b^{-2}(1-\gamma^2)^{-1} - 2ab(1-\gamma^2)^{-1} + a^2 + \gamma^2\right]^{1/2},$$
(B42d)

$$Q \equiv (b-a) , \qquad (B42e)$$

 $E_{3}^{\prime\prime}(Y) = -Y - S^{-1}QD^{-2}B^{-2}[1 - \tanh^{2}(\frac{1}{2}\beta D)]\frac{1}{2}\beta - S^{-1}D^{-1}B^{-2}\tanh(\frac{1}{2}\beta D) - Y^{2}S^{-3/2}D^{-1}B^{-2}\tanh(\frac{1}{2}\beta D)$

(B37)

(B38)

$$-YS^{-1}D^{-2}B^{-2}Q[1-\tanh^{2}(\frac{1}{2}\beta D)]\frac{1}{2}\beta+YS^{-1}D^{-3}B^{-2}Q\tanh(\frac{1}{2}\beta D)$$

$$-SB^{-2}D^{-3}(\frac{1}{2}\beta)^{2}Q^{2}2\tanh(\frac{1}{2}\beta D)[1-\tanh^{2}(\frac{1}{2}\beta D)]+SD^{-2}B^{-2}\frac{1}{2}\beta(1-\gamma^{2})[1-\tanh^{2}(\frac{1}{2}\beta D)]$$

$$+YS^{-1}D^{-3}B^{-2}Q\tanh(\frac{1}{2}\beta D)-2S(\frac{1}{2}\beta)Q^{2}B^{-2}D^{-4}[1-\tanh^{2}(\frac{1}{2}\beta D)]$$

$$+3SD^{-5}B^{-2}Q^{2}\tanh(\frac{1}{2}\beta D)-(1-\gamma^{2})SB^{-2}D^{-3}\tanh(\frac{1}{2}\beta D)$$

$$-SQ^{2}(\frac{1}{2}\beta)B^{-2}D^{-4}[1-\tanh^{2}(\frac{1}{2}\beta D)]-(1-\gamma^{2})SD^{-1}B^{-4}\tanh(\frac{1}{2}\beta D).$$
(B43)

This completes the calculations for this case. Next we perform the asymptotic expansion for the inter-

esting case $b = 1 - \gamma^2$. This point is the boundary between these two regions. Case III: $b = 1 - \gamma^2$. Having the leading term ~ $t^{-1/2}$ in case II, and $t^{-3/2}$ in case I, one would expect $t^{-\alpha}$ as a leading term for this boundary case, with $\frac{1}{2} \le \alpha \le \frac{3}{2}$. We indeed find $\alpha = \frac{3}{4}$. We perform the first-order calculation for large t. The interesting feature here is that the endpoint coincides with the stationary phase point. $\Lambda(b, y)$ will have now the following form: $[by^2 - 2by + b^2 + 1 - b]^{1/2} = \Lambda(b, y)$, and using the notation of cases I and II, one obtains

$$f(t) = A \operatorname{Re} \int_{-1}^{1} dy \, (1 - y^2)^{1/2}$$

we have



FIG. 4. Contour C_2 .

 $\int_{-\infty}^{\infty} dz \, e^{-t \alpha z^2} z^2 = (t \alpha)^{-3/2} \Gamma(\frac{3}{2}) \,,$

Since $\int_{-\infty}^{\infty} dz \ e^{-t \alpha z^2} = (t\alpha)^{-1/2} \Gamma(\frac{1}{2})$,

$$\times \frac{\tanh\left[\frac{1}{2}\beta\left[(1-\gamma^{2})y^{2}-2ya+a^{2}+\gamma^{2}\right]^{1/2}\right]\exp\left\{i2t\left[by^{2}-2by+b^{2}+1-b\right]^{1/2}\right\}}{\left[(1-\gamma^{2})y^{2}-2ay+a^{2}+\gamma^{2}\right]^{1/2}\left[by^{2}-2by+b^{2}+1-b\right]}$$
(B44)

Near y = -1, one obtains same endpoint integral as case I, but we will see that this gives a contribution, higher than second order. So we concentrate on the endpoint y = 1 (Fig. 5):

$$f(t) = A \operatorname{Re} e^{i3\pi/8} \int_0^\infty d\xi \,\xi^{1/2} E_4(e^{i\pi/4} \,\xi) \\ \times \exp\left[2it\left(\gamma^2 + \frac{1-\gamma^2}{2\gamma^2} e^{i\pi/2} \,\xi^2\right)\right], \quad (B45)$$

where

$$E_{4}(e^{i\pi/4}\xi) = (2 + e^{i\pi/4}\xi)^{1/2} \tanh\left[\frac{1}{2}\beta\Lambda(a, e^{i\pi/4}\xi)\right] \times \left[\Lambda(a, e^{i\pi/4}\xi)\left(\gamma^{2} + \frac{1 - \gamma^{2}}{2\gamma^{2}} (e^{i\pi/4}\xi)^{2}\right)\right]^{-1}.$$
(B46)

Using same method as before one obtains

$$\begin{split} f(t) = A \ \mathrm{Re} \ e^{i 3 \pi \ / 8} \ e^{2 i t \gamma^2} [E_4(0) \frac{1}{2} (m t)^{-3/4} \Gamma(\frac{3}{4}) \\ &+ e^{i \pi \ / 4} E_4'(0) \times \frac{1}{2} (m t)^{-5/4} \Gamma(\frac{5}{4})], \end{split} \tag{B47}$$

where $E_4(0)$ and $d/dz [E_4(z)]$ for $z = e^{i\pi/4} \xi = 0$ can be



FIG. 5. Contour C_3 .

easily determined from (B46) and

$$m = (1 - \gamma^2)/\gamma^2 \qquad . \tag{B48}$$

1091

APPENDIX C

We perform the basic steps of the asymptotic expansion of $W_1(0)$ for large s, where s = 1/K:

$$W_{1}(0) = {}_{1}F_{1}[is(-\Lambda + b - \cos\phi);$$

1 - 2is \Lambda; - 2is(a - b)]. (C1)

We use the integral representation¹⁷

$$W_{1}(0) = -\frac{\Gamma(1-2is\Lambda)\Gamma[1-is(-\Lambda+b-\cos\phi)]}{2\pi i\Gamma[1-is(\Lambda+b-\cos\phi)]}$$
$$\times \int_{C} e^{-2is(a-b)t} (-t)^{-[1-is(-\Lambda+b-\cos\phi)]}$$
$$\times (1-t)^{-is(\Lambda+b-\cos\phi)} dt, \qquad (C2)$$

where C is the contour shown in Ref. 17. Since the asymptotic expansion of the Γ function is well known,¹⁷ it is sufficient to study the asymptotic expansion of the integral in (C2). Let

$$\Phi = \int_{C} e^{-2is(a-b)t} (-t)^{-[1-is(-\Lambda+b-\cos\phi)]} \times (1-t)^{-is(\Lambda+b-\cos\phi)} dt .$$
(C3)

Since the major contribution of Φ , for large *s*, is coming from the vicinity of the endpoint t=1 in the lower half of the complex *t* plane, we deform the contour and approximate Φ by a line integral.

Let
$$t = 1 - iy$$
, $dt = -idy$,
 $\Phi \sim e^{-i\pi [1 - is(-\Lambda + b - \cos \phi)]} (-i)$
 $\times e^{i(\pi/2)[-is(\Lambda + b - \cos \phi)]} e^{-2is(a - b)}$
 $\times \int_0^\infty e^{-2s(a - b)y} (1 - iy)^{-1 + is(-\Lambda + b - \cos \phi)}$
 $\times y^{-is(\Lambda + b - \cos \phi)} dy$. (C4)

(C5)

Let $2s(a-b)y = \zeta$.

 Φ becomes

$$\Phi \sim i e^{s\pi(\Lambda - b + \cos\phi) + (\pi/2)s(\Lambda + b - \cos\phi)} e^{-2is(i-b)}$$

$$\times [2s(a-b)]^{is(\Lambda+b-\cos\phi)-1}$$
$$\times \int_0^\infty e^{-\zeta} \left(1 + \frac{\zeta}{i2s(a-b)}\right)^{is(-\Lambda+b-\cos\phi)}$$

$$\times \zeta^{-is(\Lambda+b-\cos\phi)}d\zeta$$

$$\simeq ie^{s\pi(\Lambda - b + \cos\phi) + (\pi/2)s(\Lambda + b - \cos\phi)}$$

$$\simeq e^{-2is(a - b)[\Omega_{\Omega/a}(-b)]is(\Lambda + b - \cos\phi)} - \frac{1}{1}$$

$$\times e^{-is(\Delta+b-\cos\phi)} \frac{1}{2s(a-b)} \times \int_0^\infty \exp\left[-\zeta \left(1 + \frac{\Lambda - b + \cos\phi}{2(a-b)}\right)\right] \zeta^{-is(\Lambda+b-\cos\phi)} d\zeta .$$
(C6)

Finally, we obtain

 $\Phi \simeq ie^{s\pi(\Lambda - b + \cos\phi) + (\pi/2)s(\Lambda + b - \cos\phi)}e^{-2is(a - b)}$

*Present address: Department of Mathematics, M.I.T., Cambridge, Mass. 02139.

[†]Supported in part by U. S. Atomic Energy Commission, under Contract No. AT(30-1)-3668A.

¹E. Ising, Z. Phyzik 31, 253 (1925).

²L. Onsager, Phys. Rev. <u>65</u>, 117 (1944).

³H. Bethe, Z. Phyzik <u>71</u>, 205 (1931).

⁴L. Hulthén, Arkiv. Mat. Astron. Fysik <u>26A</u>, Na11 (1938).

⁵C. N. Yang and C. P. Yang, Phys. Rev. <u>147</u>, 303 (1966); <u>150</u>, 321 (1966); <u>150</u>, 327 (1966); <u>151</u>, 258 (1966).

 $^6{\rm E.}$ Lieb, T. Schultz, and D. Mattis, Ann. Phys. . (N. Y.) <u>16</u>, 407 (1961). This paper will be referred to

as LSM. ⁷Th. Niemeijer, Physica <u>36</u>, 377 (1967); <u>39</u>, 313 (1968).

⁸B. M. McCoy, Phys. Rev. <u>173</u>, 531 (1968).

⁹S. Katsura, Phys. Rev. <u>127</u>, 1507 (1962).

¹⁰E. Barouch and M. Dresden, Phys. Rev. Letters 23, 114 (1969).

¹¹H. A. W. Van Vianen and J. A. Tjon (unpublished). In this work, the authors study the validity of the Kubo-Tomita linear response theory.

¹²P. Mazur, Physica <u>43</u>, 533 (1969).

$$\times \left[2s(a-b)\left(1 + \frac{\Lambda - b + \cos\phi}{2(a-b)}\right) \right]^{is(\Lambda + b - \cos\phi)}$$
$$\times \left[2s(a-b)\left(1 + \frac{\Lambda - b + \cos\phi}{2(a-b)}\right) \right]^{-1}$$
$$\times \Gamma \left[1 - is(\Lambda + b - \cos\phi)\right]. \quad (C7)$$

Combining (C7) with the asymptotic expansions for $\Gamma(1-2is\Lambda)$ and $\Gamma[1-is(-\Lambda+b-\cos\phi)]$, one obtains (6.12).

¹³This boundary condition is called c cyclic by LSM. It is not the same boundary condition that was imposed on (2.1). In the thermodynamic limit the change of boundary condition is not expected to be significant. See LSM for further discussion.

¹⁴R. Bellman, Stability Theory of Differential Equations (McGraw-Hill, New York, 1953), p. 112. We would like to remark that somewhat weaker conditions can be imposed on $h_1(t)$. However, the conditions (3.29) provide us with sufficiently large class of time-dependent forces. The examples that are explicitly solved in Appendix A obey restrictions (3.31).

¹⁵We remark that example (5.7) was derived in an independent way by Niemeijer. However, he did not study the interesting consequences of this formula, and inaccurately stated that in all cases, the long-time behavior of $m_s(t)$ is proportional to $t^{-1/2}$.

¹⁶At this point we perform the following substitutions: $t \rightarrow tJ/\hbar$; $\beta \rightarrow \beta J$; $a \rightarrow a\mu/J$; $b \rightarrow b\mu/J$.

¹⁷Bateman Manuscript Project, Higher Transcendental Functions, edited by A. Erdelyi (McGraw-Hill, New York, 1953).

¹⁸M. L. Girardeau, Phys. Letters <u>30A</u>, 442 (1969).