Z_{KDP} and Z_F for a 4×4 lattice at three different temperatures, $\epsilon/kT = 0.7$, 0.5, and 0.1. The transition temperature is located at $\epsilon/kT_0 = \ln 2 = 0.693$. Figure 6 confirms that the zeros of the F model in a staggered field lie on the unit circle for $T < T_0$. It is also to be noted that our variable z is related to the conventional fugacity variable $\bar{z} = e^{-\beta\bar{v}}$, where $\bar{v} = \sqrt{2}v$ is the magnitude of the applied field, by the relation $z = \bar{z}^{\sqrt{2}}$. Evidently $|z| = 1$ implies $|\bar{z}| = 1$.

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Integrodifferential Equation for Response Theory

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The problem of response theory in statistical mechanics involves the determination of the density matrix ρ from the Liouville equation and the subsequent computation of the response r from this ρ. Projection techniques are applied to avoid the entire complicated problem of the full dynamics of ρ and to select only that part of ρ which is relevant to the response r. The procedure replaces an inhomogeneous equation by a linear homogeneous integrodifferential equation for response theory. This is a very general equation which can be analyzed in different ways to yield a variety of results. It is shown that the Kubo theory of linear response emerges as the lowest-order approximation. The general equation is solved without approximations for a step-function stimulus, and it is discussed in the context of the steady state.

I. INTRODUCTION

Response theory in physics has a very broad scope, and there is very little in physics that cannot be reformulated in its terms. Its concepts, however, are particularly useful in the treatment of problems of the nature of transport analysis. For this, one uses statistical mechanics, and a response theory essentially proceeds in the following three steps: (i) the determination of the density matrix ρ corresponding to the system in question, (ii) the incorporation of the stimulus s applied to the system in this determination, and (iii) the extraction of the required response r from the ρ thus determined.

The determination of ρ involves its time evolution, which is governed by

$$i\frac{\partial\rho(t)}{\partial t} = L(t)\rho(t)\,, \qquad (1)$$

where we write $\hbar = 1$, and L is the Liouville operator defined by

$$LO = [H_T, O] \quad \text{(for any operator } O), \qquad (2)$$

with H_T as the Hamiltonian of the system with the stimulus applied to it. The stimulus thus appears through H_T.

The extraction of the response is easily accomplished through

$$r(t) = \mathrm{Tr}R\rho(t)\,, \qquad (3)$$

where R is the operator (assumed for convenience to be time independent) corresponding to the response r. In Eq. (3) and from here on we do not display the factor $(\mathrm{Tr}\rho)^{-1}$ multiplying expressions like the right-hand side of Eq. (3).

The usual straightforward analysis therefore involves the complicated solution of the full dynamical problem presented by Eq. (1), followed by the computation in Eq. (3). In the following we employ the projection techniques of Zwanzig[1] to bring about a significant formal simplification by selecting from Eq. (1) only that part of ρ which is required in Eq. (3).

Equations (1) and (3) may be united to yield

$$\frac{\partial r(t)}{\partial t}=\chi(t), \tag{4}$$

where

$$\chi(t)=-i\,\mathrm{Tr}RL(t)\rho(t)\,. \tag{4'}$$

Equation (4)—which is, of course, another way of writing the conjunction of Eqs. (1) and (3)—is not a homogeneous equation. We shall now show that, developing the projection techniques in a certain manner, it is possible to replace Eq. (4) by an equation which is homogeneous and linear in r.

II. PROJECTION TECHNIQUES

The Zwanzig equation,[1] in the form modified by Muriel and Dresden[2] for the case when L is dependent on t, yields, when applied to Eq. (1),

$$i\frac{\partial P\rho(t)}{\partial t}=PL(t)P\rho(t)+PLG(t,0)(1-P)\rho(0)$$
$$-iPL(t)\int_0^t ds\,G(t,s)(1-P)L(s)P\rho(s), \tag{5}$$

where

$$G(t,s)=\exp\left[-i\int_s^t dt'\,(1-P)L(t')\right], \tag{5'}$$

and P is the linear time-independent projection operator which may be suitably chosen. For the application of Eq. (5) particularly to response theory, we now define P through

$$PO\equiv A\,\mathrm{Tr}RO\quad(\text{for any operator } O), \tag{6}$$

where we leave the operator A undefined for flexibility. Substituting Eq. (6) in Eq. (5) and using Eq. (2), we have

$$i\frac{\partial r(t)}{\partial t}=r(t)\mathrm{Tr}RL(t)A+\mathrm{Tr}RL(t)G(t,0)\rho(0)-r(0)$$
$$\times\mathrm{Tr}RL(t)G(t,0)A-i\mathrm{Tr}RL(t)$$
$$\times\int_0^t ds\,G(t,s)(1-P)L(s)Ar(s). \tag{7}$$

We rewrite Eq. (7) as

$$\frac{\partial r(t)}{\partial t}=B(t)r(t)+c_1(t)-r(0)c_2(t)$$
$$+\int_0^t ds\,K(t,s)r(s)\,. \tag{8}$$

The notation is obvious from a comparison with Eq. (7). While this equation can be used as it stands, we have as yet made no improvement over Eq. (4). However since P can be controlled through A [see Eq. (6)], we now define it so that

$$c_1(t)=r(0)c_2(t)\,. \tag{9}$$

This definition obviously requires that we normalize matters such that $r(0)\neq 0$. That is, however, easily done. One way of achieving the result of Eq. (9) is by choosing

$$A=\rho(0)\,, \tag{10a}$$

$$r(0)=1\,. \tag{10b}$$

We shall make this choice. Then Eq. (8) reduces to

$$\frac{\partial r(t)}{\partial t}=B(t)r(t)+\int_0^t ds\,K(t,s)r(s), \tag{11a}$$

$$B(t)=-i\,\mathrm{Tr}RL(t)\rho(0), \tag{11b}$$

$$K(t,s)=-\mathrm{Tr}RL(t)G(t,s)(1-P)L(s)\rho(0). \tag{11c}$$

Equation (11a), which can also be written as

$$\frac{\partial r}{\partial t}=Yr\,, \tag{12}$$

is a homogeneous equation in contrast to the inhomogeneous equation (4) that we started with. In addition, the operator Y in Eq. (12) has the important property of linearity, as may be noticed from Eq. (11a).

We have thus shown that a linear homogeneous equation can be obtained by applying suitable manipulations of the projection techniques to the inhomogeneous equation (4).

Equation (12) can be made the starting point of a whole mathematical framework, by making use of its linearity. We do not carry this out here. We shall show a few simple results that follow, in particular cases, from our general equation (12). Before that we must, however, remark about the shortcomings of the equation. While it has the virtues of being linear and homogeneous, it has the disadvantages of being non-Markoffian and of being riddled with projection operators, which are certainly not the simplest objects to manipulate. And while we state that it is linear with respect to the function $r(t)$ mathematically, it is not linear with respect to the response physically. What we mean is that while $r_1(t)+r_2(t)$ will be a solution if $r_1(t)$ and $r_2(t)$ are, $r_1(t)+r_2(t)$ will not correspond to R_1+R_2 if $r_1(t)$ and $r_2(t)$ correspond to R_1 and R_2, respectively. This follows from the fact that R appears in Y through $B(t)$ and $K(t,s)$. However, once we decide in what response we are interested, R is fixed in Y and then one has a linear equation from the point of view of the mathematical solution. The other shortcoming of Eq. (12) is that it is not possible to apply to Eq. (12) techniques analogous to the ones that are applied to the Schrödinger equation [which incidentally looks quite like Eq. (12)] to yield the Heisenberg and the Dirac "pictures," because Y is not linear in the Hamiltonian.

Having discussed what we cannot do with our equation, we shall now proceed to show a few of the things we can accomplish with its help.

III. LINEAR RESPONSE

We shall first derive the linear-response formula of Kubo[3] as the lowest-order approximation of our Eq. (12). In the manner of Kubo, we shall take

$$H_T = H - \lambda f(t) D, \tag{13}$$

where H is the Hamiltonian of the stimulusless system, and λ and $f(t)$ are c numbers denoting the strength parameter and the time dependence of the applied stimulus, respectively. Defining L_H and L_D to mean taking the commutator with H and D, respectively, we obtain

$$L = L_H - \lambda f(t) L_D. \tag{14}$$

From Eq. (11b) and Eq. (14),

$$B(t) = i\lambda f(t) N, \tag{15}$$

where

$$N = \mathrm{Tr} R L_D \rho(0). \tag{15$'$}$$

In obtaining Eqs. (15) and (15′) we have made use of the fact that the stimulusless Hamiltonian H commutes with the equilibrium density matrix $\rho(0)$.

We thus see that $B(t)$ is of order 1 in λ.

From Eq. (11c) and Eq. (14) we have

$$K(t, s) = \lambda f(s)[\mathrm{Tr} R L(t) G(t, s) L_D \rho(0) - N \mathrm{Tr} R L(t) G(t, s) \rho(0)]. \tag{16}$$

We thus see that $K(t, s)$ is at least of order 1 in λ. Expanding $r(t)$ in orders of the strength parameter λ (we do not discuss the question of the validity of such an expansion here), we obtain

$$r(t) = r_0(t) + \lambda r_1(t) + \cdots. \tag{17}$$

Equations (11a) and (17) give

$$\frac{\partial r_0(t)}{\partial t} = 0, \tag{18}$$

$$\lambda \frac{\partial r_1(t)}{\partial t} = B(t) r_0(t) + \int_0^t K_0(t, s) r_0(s) ds. \tag{19a}$$

In Eq. (19a) terms of order λ have been retained. We also have

$$K_0(t, s) = \lambda f(s) \mathrm{Tr} R L_H G_H(t, s) L_D \rho(0), \tag{19b}$$

$$G_H(t, s) = \exp[-i(t-s)(1-P) L_H]. \tag{19c}$$

Equation (19b) is obtained from Eq. (16) after noting that

$$G_H(t, s)\rho(0) = \rho(0). \tag{19d}$$

In Eqs. (18) and (19a), $r_0(t) = r_0$ is the time-independent initial value of the response which would remain thus unchanged as predicted by Eq. (18) in the absence of a stimulus. This r_0 has been taken equal to 1 in our derivation [see Eq. (10b)]. We may therefore rewrite Eq. (19a):

$$\lambda \frac{\partial r_1(t)}{\partial t} = B(t) + \int_0^t K_0(t, s) ds. \tag{19e}$$

The derivations of the Kubo formulas from our general equation is therefore complete if we show that Eq. (19e) is exactly equivalent to the Kubo formula. The latter[3] may be written in our notation as

$$\lambda r_1(t) = \int_0^t \phi(t-s) f(s) ds, \tag{20}$$

where

$$\phi(t-s) = i\lambda \mathrm{Tr} R e^{-i(t-s)L_H} L_D \rho(0). \tag{20$'$}$$

This equivalence will now be established through an interesting series of manipulations with the projection operators. We first note that, for any operator O,

$$L_H G_H O \equiv L_H (e^{-i(t-s)(1-P)L_H}) O = (e^{-i(t-s)L_H(1-P)}) L_H O, \tag{21a}$$

as may be seen by merely expanding G_H as an exponential. Further, since our projection operator P obeys Eq. (6), it is possible to write

$$L_H P O = 0, \tag{21b}$$

and using this result in Eq. (21a)

$$L_H G_H O = e^{-i(t-s)L_H} L_H O = i \frac{\partial}{\partial t} e^{-i(t-s)L_H} O, \tag{21c}$$

provided O is time independent.

Equation (21c) is a very important result, and when applied to Eq. (19b), it yields

$$K_0(t, s) = i\lambda f(s) \frac{\partial}{\partial t} \mathrm{Tr} R e^{-i(t-s)L_H} L_D \rho(0). \tag{22}$$

A careful examination of Eq. (22) reveals the following curious property of Eq. (19e): The $B(t)$ and $K_0(t, s)$ featuring in that equation are related to each other through the existence of a function $\psi(t, s)$ such that

$$\frac{\partial \psi(t, s)}{\partial t} = K_0(t, s), \tag{23a}$$

$$\lim_{s \to t} \psi(t, s) = B(t). \tag{23b}$$

Obviously

$$\psi(t, s) = i\lambda f(s) \mathrm{Tr} R e^{-i(t-s)L_H} L_D \rho(0). \tag{23c}$$

A comparison of Eq. (23c) with Eq. (20′) immediately shows that our $\psi(t, s)$ is related to the Kubo response function $\phi(t-s)$ through

$$\psi(t, s)=\phi(t-s)f(s). \tag{24}$$

It is now a trivial exercise to differentiate Eq. (20) and use Eqs. (23a), (23b) and (24) to establish the complete equivalence of the Kubo formula [Eq. (20)] and the lowest-order approximation [Eq. (19e)] of our general equation (12).

IV. STEP-FUNCTION STIMULUS

Evidently our exact general Equation (12) has more uses than a mere derivation of the linear formula demonstrated in Sec. III. In this section we show that when the applied stimulus is a step function, Eq. (12) can be solved exactly with the help of Laplace transforms. The magnitude of the step function can be arbitrary, and no approximation is invoked.

The total Hamiltonian H_T is again written as in Eq. (13), but now we have

$$f(t)=\Theta(t), \tag{25}$$

where $\Theta(t)$ is the Heaviside step function; λ in Eq. (13) denotes the magnitude of the step function.

For $t>0$, Eq. (15) shows that $B(t)$ is time independent:

$$B(t)=B=i\lambda N. \tag{26}$$

Equation (11c) shows that

$$K(t, s)=K(t-s)$$
$$=-\operatorname{Tr}R(L_H-\lambda L_D)G(t-s)(1-P)(L_H-\lambda L_D)\rho(0), \tag{27}$$

where

$$G(t-s)=\exp[-i(t-s)(1-P)(L_H-\lambda L_D)]. \tag{27′}$$

The kernel of the integral featuring in Eq. (11a) thus is of the "displacement type" for a step function. This and the fact that $B(t)$ becomes time independent, facilitate the solution of the problem since Eq. (11a) may be Laplace transformed into

$$\epsilon\underline{r}(\epsilon)-r(0)=B\underline{r}(\epsilon)+\underline{K}(\epsilon)\underline{r}(\epsilon). \tag{28}$$

The Laplace transforms are denoted by underscored letters and are defined, for instance, through

$$\underline{r}(\epsilon)=\int_0^\infty r(t)e^{-\epsilon t}dt.$$

Equation (28) will be written as [since $r(0)=1$]

$$\underline{r}(\epsilon)=\frac{1}{\epsilon-B+\underline{K}(\epsilon)}. \tag{29}$$

Equation (29) is thus the exact solution of our Eq. (11a) for the case of a step-function stimulus. An inversion of Eq. (29) will yield the response $r(t)$. It should be noticed that $\mathrm{K}(\epsilon)$ in Eq. (29) has quite a simple form because $(t-s)$ figures in $G(t-s)$ only in an exponential.

We have used Laplace transforms in conjunction with projection techniques elsewhere,[4] but there the final expression [analogous to Eq. (29) above] may not only be used through an inversion of the transform, but also directly. This other manner of utilizing the result is, however, not feasible in our present case because here (unlike in the context of Ref. 4) the expression $\lim_{\epsilon\to 0}\underline{r}(\epsilon)$ has no simple physical interpretation.

V. STEADY STATE

Equation (11a) or Eq. (12) describes the time evolution of the response $r(t)$ at every instant of time. However if one is interested only in the state of affairs after a steady state has been reached, the equation takes a simpler form.

For a steady state we put $\partial r(t)/\partial t=0$ and this reduces Eq. (11a) to

$$r(t)=-\int_0^t ds\frac{K(t, s)}{B(t)}r(s) \text{ in the limit as } t\to\infty. \tag{30}$$

Under certain conditions leading to the validity of the interchange of the orders of the integration and the limit, Eq. (30) may be rewritten as

$$r(\infty)=\int_0^\infty ds\, I(s)r(s), \tag{31}$$

where

$$I(s)=\lim_{t\to\infty}[-K(t, s)/B(t)]. \tag{31′}$$

We do not explore any further details here. Equation (31) should yield interesting information through a careful study of the limiting behavior of $K(t, s)$ and $B(t)$. [$B(t)$, for instance, is expected to tend to a constant.] Work along these lines is in progress.

VI. REMARKS

We have thus shown that projections can be made to transform an inhomogeneous equation of response theory into a homogeneous equation with a linear operator. Not only can the latter be used as a starting point for a general mathematical structure, but it can also yield specific results as has been demonstrated in the foregoing sections. The techniques developed here have been applied in the above discussion for response theory, but it should be clear that the form of our Eq. (11a) or (12) is very general and it will be obtained wherever the quantity of interest may be written as $\operatorname{Tr}Jx$ where

x obeys an equation formally written in the Liouville form. It is not necessary that the evolution described by the equation be a time evolution. It may be a formal equation featuring, for example, the variable $1/kT$ instead of t. Similarly, J can have varied forms. In this paper it is R, the operator corresponding to the response. However, an equation in the exact form of Eq. (11a) can be derived,[5] for example, for the reduced density matrix $\mathrm{Tr}\, a_m^\dagger a_m \rho(t)$, with $J = a_m^\dagger a_m$. These other uses of our method will be reported elsewhere.

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Statistical Mechanics of the XY Model. IV. Time-Dependent Spin-Correlation Functions*

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We compute the correlation functions $\langle S_0^x(t) S_R^x(0)\rangle$ and $\langle S_0^y(t) S_R^y(0)\rangle$ at $T=0$ for the one-dimensional XY model in the presence of a magnetic field.

I. INTRODUCTION

Dynamical properties of many-particle systems which are very near thermal equilibrium are often studied in terms of time-dependent correlation functions $\langle A(r_1, t_1) B(r_2, t_2)\rangle$. Here $\langle \cdots \rangle$ denotes a thermal average in the canonical ensemble. Contact with macroscopic measurements is made by means of the Kubo formulas[1] and the approximation of linear response theory.

In view of the importance of these time-dependent correlation functions, it would be quite useful to have some nontrivial interacting systems for which the correlation functions can be exactly computed. Until recently no such exactly soluble problems were known. However, in 1967 Niemeijer[2] succeeded in computing exactly the correlation function at all temperatures,

$$\rho_{zz}(R, t) = \langle S_1^z(t) S_{R+1}^z(0)\rangle = \langle e^{iHt} S_1^z e^{-iHt} S_{R+1}^z\rangle \,, \tag{1.1}$$

for the XY model defined by

$$H = -\sum_{i=1}^{N} \left[(1+\gamma) S_i^x S_{i+1}^x + (1-\gamma) S_i^y S_{i+1}^y + h S_i^z\right] , \tag{1.2}$$

where S_i^v are $\frac{1}{2}$ the Pauli spin matrices. Niemeijer found that $\rho_{zz}(R, t)$ has the same form as a density-density correlation function of noninteracting fermions which have the dispersion relation

$$\epsilon_k = [(\cos k - h)^2 + \gamma^2 \sin^2 k]^{1/2} \,. \tag{1.3}$$

In particular, if $\gamma \neq 0$ and $h \neq 1$, ϵ_k can never vanish for real values of k, and for fixed R, $\rho_{zz}(R, t)$ approaches its $t \to \infty$ limit of M_z^2 as t^{-1}.

The purpose of the present paper is to extend Niemeijer's work to the transverse ground-state correlation function

$$\rho_{vv}(R, t) = \langle e^{iHt} S_1^v e^{-iHt} S_{R+1}^v\rangle \,, \tag{1.4}$$

where $v = X$ or Y. In contrast to ρ_{zz} these correlation functions are *not* expressible as a correlation function of a finite number of field operators of a noninteracting Fermi system. Instead we find that