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The imaginary parts of the expressions (A6) and (A7) have already been given by Montroll.[14] The expansions of (A3), (A6), and (A7) at $s = \gamma - 1 - i\epsilon$, $\gamma + 1 - i\epsilon$, and ∞ are easily obtained with the aid of the expansion formulas (3.1) and (3.4).

From the general theory of the elliptic integrals, we find that we can, in principle, express the integrals which involve $\cos mx \cos ny$, $m, n = 0, 1, 2, \cdots$, in the numerator of (A1) in terms of the complete elliptic integrals and that then the present method is applicable to these integrals. The investigation of this problem is left as a future problem.

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AC Susceptibility of Biased One-Dimensional Stochastic Ising Model*

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The ac susceptibility for the one-dimensional Ising model is obtained for arbitrary coupling strength in the presence of a dc bias field strong enough to align most of the dipoles in one direction. The dipole flip probability is assumed proportional to the Boltzmann factor corresponding to half the energy change resulting from the flip. The general expression for ac susceptibility is analyzed in three limiting cases: weak coupling with strong bias, strong coupling with strong bias, and strong coupling with weak bias. In the latter case, relatively long chains of anti-aligned dipoles exist and give rise to large susceptibility.

The dynamic behavior of the one-dimensional stochastic Ising model has been studied previously by Meijer, Tanaka, and Barry[1] in the limit of weak spin coupling, and by Glauber,[2] who found the ac susceptibility for the case of zero bias field. In the present work the isothermal ac susceptibility is found for arbitrary coupling strength in the presence of a dc bias field sufficiently large to align most dipoles in one direction. The region of applicability for each of these calculations is indicated in Fig. 1. Glauber's results are exact for zero bias. The present results are complementary to his in that they become exact as the bias field becomes strong enough to align all dipoles.

The one-dimensional Ising model is applicable to materials in which significant coupling of neighboring electric or magnetic dipoles exists in only one direction. The present results are potentially useful for such materials with large bias fields applied, but of particular interest is possible application to crystals of noncentric structure in which the structure rather than an externally applied field favors alignment of electric dipoles in one direction. The relation of this model to such a crystal, lithium hydrazinium sulfate, is briefly discussed.

This model assumes electric or magnetic dipoles of moment μ aligned parallel (up; $\sigma = 1$) or antiparallel (down; $\sigma = -1$) to the dc bias field E_0. The Hamiltonian in the presence of E_0 and a time-varying field E_t is

$$H = -J \sum_l \sigma_l \sigma_{l+1} - \mu(E_0 + E_t) \sum_l \sigma_l, \qquad (1)$$

where the nearest-neighbor interaction energy parameter J is positive, tending to align adjacent dipoles.

The polarization resulting from N dipoles in a

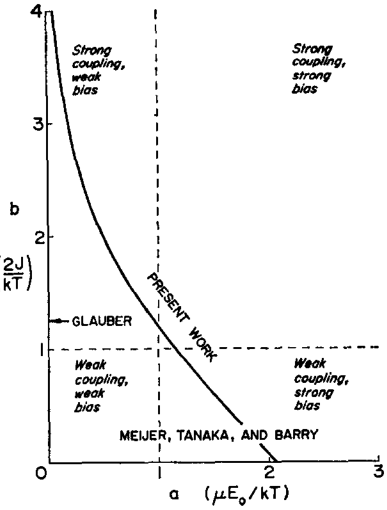

FIG. 1. Regions of applicability for studies of dynamic behavior of one-dimensional stochastic Ising model. Meijer, Tanaka, and Barry (Ref. 1) studied the weak coupling case ($b \ll 1$). Glauber (Ref. 2) found the ac susceptibility for the zero bias case ($a = 0$). In the present work the ac susceptibility given in Eq. (17) should approximate the unknown exact value in the region to the right of the curved line, because in this region the dc limit of Eq. (17) as given in Eq. (18) is within 10% of the exact dc susceptibility (Ref. 3) given in Eq. (19).

volume V is given by

$$P = \frac{\mu}{V}\left[N - 2\sum_m m(N_m + n_m)\right], \qquad (2)$$

where N_m is the equilibrium number of chains each composed of m adjacent down dipoles and n_m is the deviation caused by E_t. The energy required to create a chain is $4J + 2\mu(E_0 + E_t)m$. The large-polarization approximation used herein is that the equilibrium probability of such a chain beginning at any one of the N sites is simply the Boltzmann factor $e^{-\beta(4J+2\mu E_0 m)}$, where $\beta = (kT)^{-1}$. In this approximation the relations

$$N_m = Ne^{-\beta(4J+2\mu E_0 m)}, \qquad (3)$$

$$\sum mN_m = Ne^{-4\beta J}/4\sinh^2(\beta\mu E_0) \qquad (4)$$

are obtained. The equilibrium polarization obtained by combining Eqs. (2) and (4) approaches the exact expression[3]

$$P = \frac{N\mu\sinh(\beta\mu E_0)}{V[\sinh^2(\beta\mu E_0) + e^{-4\beta J}]^{\frac{1}{2}}} \qquad (5)$$

if the large-polarization condition $\sinh(\mu\beta E_0) \gg e^{-2\beta J}$ is fulfilled.

The equilibrium N_m in Eq. (3) can also be obtained by assuming that the flip probability per unit time for a given dipole is a thermally induced basic flip rate ν multiplied by the Boltzmann factor corresponding to half the energy change resulting from the flip. This probability was chosen with electric dipoles in mind. Even if their initial and final states have equal energy, they usually must surmount a large barrier in order to flip. Then a change U in the final state energy will change the barrier height by approximately $\frac{1}{2}U$, giving a flip rate of $\nu e^{-\beta U/2}$. Glauber[2] uses different flip probabilities, $\nu[1 - \frac{1}{2}\tanh(2\beta J)\sigma_l(\sigma_{l-1} + \sigma_{l+1})]$, which were chosen for their simplicity. As he points out, there are infinitely many choices of flip probabilities which will yield the correct equilibrium populations.

In equilibrium, the rates of creation and annihilation of isolated down dipoles must be equal, as indicated below,

$$\left.\frac{dN_1}{dt}\right|_{N_2} = N\nu e^{-\beta(2J+\mu E_0)} - N_1\nu e^{\beta(2J+\mu E_0)} = 0, \quad (6)$$

and a similar relation governs equilibrium between numbers of chains containing $m - 1$ and m down dipoles:

$$\left.\frac{dN_m}{dt}\right|_{N_{m+1}} = 2N_{m-1}\nu e^{-\beta\mu E_0} - 2N_m\nu e^{\beta\mu E_0} = 0. \quad (7)$$

(The 2 occurs because these chains can grow or shrink at either end.) Both flip probabilities in either Eq. (6) or Eq. (7) could be multiplied by the same parameter without upsetting the equilibrium, but the symmetric expressions used seem physically the most reasonable. In Eqs. (6) and (7) the use of N, rather than the more exact value $N - \sum(m + 2)N_m$, and the neglect of the effects of isolated up dipoles, are large-polarization approximations which allow these equations to be satisfied by the approximate N_m of Eq. (3).

Application of a time-dependent field E_t multiplies the transition rates in Eqs. (6) and (7) by the factors of $e^{\pm\beta\mu E_t}$, and these modified transition rates provide differential equations governing the population changes:

$$\begin{aligned}\dot{n}_1 = {} & N\nu e^{-\beta(2J+\mu E_0+\mu E_t)} - (N_1 + n_1)\nu e^{\beta(2J+\mu E_0+\mu E_t)} \\ & + 2(N_2 + n_2)\nu e^{\beta\mu(E_0+E_t)} \\ & - 2(N_1 + n_1)\nu e^{-\beta\mu(E_0+E_t)}, \end{aligned} \qquad (8)$$

$$\begin{aligned}\dot{n}_m = {} & 2(N_{m-1} + n_{m-1})\nu e^{-\beta\mu(E_0+E_t)} \\ & - 2(N_m + n_m)\nu e^{\beta\mu(E_0+E_t)} \\ & + 2(N_{m+1} + n_{m+1})\nu e^{\beta\mu(E_0+E_t)} \\ & - 2(N_m + n_m)\nu e^{-\beta\mu(E_0+E_t)}, \quad m > 1. \end{aligned} \qquad (9)$$

Upon setting $a = \beta\mu E_0$, $b = 2\beta J$, $c = N\beta\mu e^{-4\beta J}$, making the small-field approximation $e^{\pm\beta\mu E_t} = 1 + \beta\mu E_t$, eliminating terms which cancel according to Eqs. (6) and (7), and terms of the form $n_m\beta\mu E_t$, which are of second order in E_t, and using the expression in Eq. (3) for N_m, these equations become

$$\begin{aligned}&\dot{n}_1 + \nu n_1(e^{b+a} + 2e^{-a}) - 2\nu n_2 e^a \\ &\qquad = -2\nu E_t c e^{-2a}(e^{b+a} - 2e^{-a}), \end{aligned} \quad (10)$$

$$\begin{aligned}&\dot{n}_m + 4\nu n_m\cosh a - 2\nu n_{m-1}e^{-a} - 2\nu n_{m+1}e^a \\ &\qquad = -8\nu E_t c e^{-2am}\sinh a, \quad m > 1. \end{aligned} \quad (11)$$

For a small sinusoidal applied field $E_t = E_{t0}e^{i\omega t}$, these equations become

$$(2i\Omega + \tfrac{1}{2}e^{b+a} + e^{-a})S_1 - e^{-a}S_2 = -\tfrac{1}{2}e^{b+a} + e^{-a}, \quad (12)$$

$$(2i\Omega + 2\cosh a)S_m - e^{a}S_{m-1} - e^{-a}S_{m+1} = -2\sinh a, \quad m > 1, \quad (13)$$

where $\Omega = \omega/4\nu$ and $S_m = (n_m/2c)e^{-2am}E_t$. If S_m is assumed to be of the form

$$S_m = S_0G^m - (i\Omega)^{-1}\sinh a, \quad (14)$$

then Eq. (13) is satisfied if G has the values

$$G = e^{a}\{\cosh a + i\Omega \pm [(\cosh a + i\Omega)^2 - 1]^{\frac{1}{2}}\}. \quad (15)$$

The positive sign gives S_m and n_m which increase without limit for large m and Ω, so the negative sign must be chosen for G. The constant S_0 is determined by requiring that Eq. (12) be satisfied by S_1 and S_2 as given in Eq. (14). This value of S_0 inserted into Eq. (14) provides the following simultaneous solution for Eqs. (12) and (13):

$$S_m = -\frac{\sinh a}{i\Omega} - \frac{1 - 2e^{-b} - (i\Omega)^{-1}\sinh a}{(1 - 2e^{-b})G + 2e^{-b}}G^m. \quad (16)$$

The ac susceptibility in the presence of the dc bias field E_0 is $\chi = dP/dE$, which for small E_t reduces to $(P - P_{\text{eq}})/E_t$, and from Eq. (2) $P - P_{\text{eq}} = 2\mu V^{-1} \times \sum_{m=1}^{N} mn_m$. For large N the upper limit can be allowed to become infinite. Then, from Eq. (16), the susceptibility is found to be

$$\begin{aligned}\chi &= -\frac{2\mu}{VE_t}\sum_{m=1}^{\infty} mn_m \\ &= -\frac{4c\mu}{V}\sum_{m=1}^{\infty} mS_m e^{-2am} \\ &= \frac{4N\mu^2\beta e^{-2b}}{V}\bigg(\frac{1}{4i\Omega\sinh a} \\ &\quad + \frac{1 - 2e^{-b} - (i\Omega)^{-1}\sinh a}{[1 + 2e^{-b}(G^{-1} - 1)](e^{a} - e^{-a}G)^2}\bigg). \quad (17)\end{aligned}$$

This expression can be better understood by considering various limiting cases. In the low-frequency limit, $G = (1 - i\Omega/\sinh a - e^{a}\Omega^2/2\sinh^3 a + \cdots)$ to second order in Ω, and substitution of this G gives χ to first order in Ω:

$$\chi \underset{\Omega\to 0}{=} \frac{N\mu^2\beta e^{-2b}\cosh a}{V\sinh^3 a} \times \left(1 - i\Omega\frac{4 + e^{-2a} + 4e^{a-b}\sinh a}{4\sinh^2 a\cosh a} + \cdots\right). \quad (18)$$

The first term is the dc susceptibility in the presence of a bias field $E_0 = a/\beta\mu$. It agrees in the large-polarization limit ($\sinh a \gg e^{-b}$) with the exact value

$$\chi_{\text{exact}}(\Omega = 0) = \frac{N\mu^2\beta e^{-2b}\cosh a}{V(\sinh^2 a + e^{-2b})^{\frac{3}{2}}} \quad (19)$$

obtained by evaluating dP/dE using Eq. (5). The agreement is within 10% in the region to the right of the curved line in Fig. 1. This region within which the large polarization condition $\sinh(\mu E_0/kT) \gg e^{-2J/kT}$ is valid includes three cases, as indicated in Fig. 1. The weak-coupling case has $2J \ll kT$ ($b \ll 1$), so a strong bias field is required for which $\mu E_0 \gg kT$ ($a \gg 1$). In this case there are many chains of down dipoles, but most of the chains are only one dipole long. The strong-coupling, strong-bias case ($b \gg 1$, $a \gg 1$) shows the smallest deviation from maximum polarization. The strong-coupling, weak-bias case ($b \gg 1$, $e^{-b} \ll a \ll 1$) results in relatively few chains of down dipoles having long average chain length since

$$\bar{m} = \sum mN_m / \sum N_m = (e^{a}/2)\sinh a$$

varies from $1 + e^{-a}$ for $a \gg 1$, to $1/2a$ for $a \ll 1$.

To a good approximation, the susceptibility in Eq. (17) can be represented by two components χ_f and χ_s corresponding to fast and slow modes:

$$\chi \simeq \chi_{f0}/(1 + i\omega\tau_f) + \chi_{s0}/(1 + i\omega\tau_s). \quad (20)$$

The fast mode is governed by the frequency dependence of the factor $(1 - 2e^{-b} + 2e^{-b}G^{-1})$ in Eq. (17). The approximation $e^{a}G^{-1} \simeq 2(\cosh a + i\Omega)$ is valid under conditions for which this mode is active. This mode results from the field-induced shift of equilibrium between creation and annihilation of isolated down dipoles ($m = 1$ "chains"). The relaxation times for this mode form a narrow distribution around $\tau_f = (\nu e^{a+b})^{-1}$ for each of the three cases. This is the only mode which exists for the weak-coupling case and is the dominant mode for the $b \gg 1$, $a \gg 1$ case. For both cases, $\chi_{f0} \simeq \chi_0$, where χ_0 is the dc susceptibility given by the first term in Eq. (18). Because $a \gg 1$ for these cases, $\cosh a \simeq \sinh a$, and the large-polarization condition $\sinh a \gg e^{-b}$ requires that $\chi_{f0} \ll N\mu^2\beta/V$.

A comparison can be made with the results of Glauber's[2] study of the zero-bias ($a = 0$) case, which of course does not satisfy the large-polarization condition. His flip probabilities are not exponential in the flip energy, but reduce to those used herein for $b \ll 1$. In this limit he finds $\chi \simeq N\mu^2\beta/V(1 + i\omega/2\nu)$, so his correlation time is $(2\nu)^{-1}$.

For the $b \gg 1$, $a \ll 1$ case, χ_{f0} falls off to $4a^3\chi_0$. The susceptibility for this weak-bias case is dominated by the slow mode, which is caused by the shifts in populations n_m of existing chains of down dipoles. This mode has a narrow range of time constants near $(4\nu a^2)^{-1}$ for this case, and $\chi_{s0} \simeq \chi_0 \simeq N\mu^2\beta e^{-2b}/Va^3$. The large-polarization condition requires that $e^{-2b}/a^2 \ll 1$, but if a is in the lower part of its allowed range $e^{-b} \ll a \ll 1$, it is possible to have $\chi_{s0} \gg N\mu^2\beta/V$. If the coupling were turned off ($b = 0$), the exact expressions in Eqs. (19) and (5) show that χ_{s0} would drop to $N\mu^2\beta/V$, and that the polarization would be near zero rather than near maximum. Accordingly, even in the presence of a dc field which aligns most of the dipoles, the ac susceptibility can show what Wannier[3] has termed "enhanced paramagnetism."

This work was undertaken in order to explain the unusual dielectric properties[4,5] of lithium hydrazinum sulfate, which has generally been considered to be a ferroelectric. The structure[6] contains ordered N–H · · · N–H · · · chains running along the "ferroelectric" c axis. This biased one-dimensional Ising model seems quite applicable to the N–H dipole system if E_0 is the effective field with which the noncentric structure tends to align the N–H dipoles. This model allows for polarization reversal of the N–H dipole system if E_0 can be overcome by an externally applied field smaller than the breakdown field; but it predicts no hysteresis in the dc limit and so is inconsistent with ferroelectric behavior. We have since determined that this crystal is not ferroelectric but that a mechanism other than dipolar reorientation dominates the dielectric behavior, at least below 10 MHz. This mechanism appears to be protonic conduction along the N–H · · · N–H · · · chains, with extrinsic barriers of random height partially blocking the flow. A detailed account of this mechanism will be presented elsewhere. There remains a significant difference between the susceptibilities at 10 MHz and 9.3 GHz. Experimental study of the intervening frequency region could determine whether the effective bias field E_0 and other parameters of this biased Ising model have the correct magnitudes to cause dielectric relaxation in this frequency range.

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Note added in proof: The frequency-wavenumber dependent susceptibility $\chi(q, \omega)$ has been derived for the zero bias case by M. Suzuki and R. Kubo, J. Phys. Soc. Japan **24**, 51 (1968).

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Scaling Behavior of Gravitational Energy

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The transformation property of gravitational energy under scale transformations is presented in the context of a general asymptotically flat space–time. The relevance of scale transformations to the sign of gravitational energy is discussed. Arguments for the positive-definiteness of gravitational energy are presented and criticized.

1. INTRODUCTION

Einstein,[1] in one of his less well-known papers entitled "Demonstration of the Non-Existence of (vacuum) Gravitational Fields with a Non-Vanishing Total Mass Free of Singularities," pointed out a certain scaling property of the energy of asymptotically Schwarzschild space–times. Einstein's model of radiative space–times was oversimplified, and at present the claim made in the title of his paper is widely thought to be wrong. The energy scaling property, however, does have a general validity and, as we show in Sec. 2, can be extended to energy expressions formulated in terms of more recent concepts of asymptotic flatness.