Exact Dynamical Behavior near the Critical Point in the Transverse Ising Model

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In the one-dimensional transverse Ising model, we calculate exactly the time evolution and the admittance of the magnetization and also of the energy near the critical point. The results for the above two quantities are shown to coincide with each other, and are explicitly represented in terms of functions of the inverse static susceptibility. The analyses are made by using the recurrence-relations method developed on the basis of Mori's continued-fraction representation.

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The transverse Ising (TI) model is the simplest solvable quantum model which exhibits a second-order phase transition. Although the equilibrium properties[1] of this system and its dynamical behavior at high temperature[2] are well known, its dynamical behavior near the critical point is less well understood. Recently Vaidya and Tracy[3] studied the time evolution of the XY model with transverse field in various cases, one of which is near the critical point in this model. Müller and Shrock[4] calculated the spin-spin autocorrelation in this model just at critical point; however, from the viewpoint of irreversible processes, to obtain an explicit form of relaxation function of an observable relevant to a phase transition as a function of time has remained an unsolved, and interesting subject.

Experimentally, it is known that there exist quasi-one-dimensional Ising-type substances such as $CsCoCl_3\cdot 2H_2O$.[4,5]

On the other hand, the recurrence-relations (RR)[6] method formulated by Lee has been successfully applied to the analysis of the dynamical behavior of various systems.[7] The formulation is based on the Mori's projection method in the continued-fraction representation.[8]

In this Letter we will apply this method to the TI model near the critical point and calculate exactly the analytic forms of the relaxation function and the admittance both of the magnetization and of the exchange energy. On this basis, we shall also analyze the properties of the dynamical behavior near the second-order phase transition in the TI model.

The Hamiltonian of this model is given by $\mathcal{H}=\mathcal{H}_0+M_x$, where $\mathcal{H}_0=-\tilde{J}\sum_{i=1}^{N}\sigma_i^z\sigma_{i+1}^z$ and $M_x=-H\sum_{j=1}^{N}\sigma_j^x$ are called exchange energy and magnetization, respectively. It is well known that the TI model has a critical point in the ground state ($T=0$) at $H=\tilde{J}/2$.[1]

For small $\epsilon[=(H-H_c)/H_c]$ with $H_c=\tilde{J}/2$, the static susceptibilities of M_x and $\mathcal{H}_0$ take the same form given by $\chi_s=-(\tilde{J}/4\pi)\ln|\epsilon|$.

According to the RR method,[6] the operator $A(t)$ can be expanded in the form $A(t)=\sum_{n=0}^{\infty}a_n(t)f_n$ by an appropriate orthogonal basis. By choosing $f_0=A$, we have the following two recurrence relations: $f_{n+1}=iLf_n+\Delta_n f_{n-1}$ (RR I) and $\Delta_{n+1}a_{n+1}(t)=-\dot{a}_n(t)+\Delta_n a_{n-1}(t)$ (RR II), where $\Delta_n=(f_n,f_n)/(f_{n-1},f_{n-1})$ with the canonical correlation function (A,B),[8] $Lf_n=[\mathcal{H},f_n]$, $\dot{a}_n(t)=(d/dt)a_n(t)$ and $a_{-1}=0$, $f_{-1}=0$. Applying the Laplace transform $\mathcal{L}$ to RR II, one can obtain a continued-fraction representation for $a_0(t)$ of the form

$$a_0(z)=\cfrac{1}{z+\cfrac{\Delta_1}{z+\cfrac{\Delta_2}{z+\cfrac{\Delta_3}{z+\cdots}}}}\,, \tag{1}$$

with $a_0(z)=\mathcal{L}a_0(t)$. By virtue of the inverse Laplace transform $\mathcal{L}^{-1}$, the time evolution of $A(t)$ can be described by a general Langevin equation given by

$$A(t)=a_0(t)A+\int_0^t ds\, a_0(t-s)F(s)\,.$$

In the above, $a_0(t)$ is equal to the relaxation function $\Xi(t)=[A(t),A]/(A,A)$ and $F(t)$ is a generalized random force given by $\sum_{n=1}^{\infty}b_n(t)f_n$ with $b_n(z)=a_n(z)/a_0(z)$.

Now we consider the two cases where f_0 is chosen to be $\mathcal{H}_0$ and M_x, respectively. In the Hamiltonian $\mathcal{H}$, $\mathcal{H}_0$, and M_x are represented in terms of anticommuting Fermi operators with the aid of the Jordan-Wigner transformation. By straightforward calculation, we can obtain $(\mathcal{H}_0^{(n)},\mathcal{H}_0^{(n)})$ and $(M_x^{(n)},M_x^{(n)})$ at $T=0$ to first order in ϵ,

$$(\mathcal{H}_0^{(n)},\mathcal{H}_0^{(n)})=(M_x^{(n)},M_x^{(n)})=\frac{\tilde{J}^{2n+1}}{4\pi}\frac{(2n-2)!!}{(2n+1)!!}\left[1+\frac{2n+1}{2}\epsilon\right],\quad n\geq 1\,, \tag{2}$$

with $M^{(n)}\equiv(iL)^nM$. By inserting Eq. (2) and the static susceptibility into the norm of f_n in RR I and using REDUCE, we calculate numerically Δ_n up to $n=20$ to the first order in $1/\chi_s$ and ϵ. From the result we guess the analytic expression of Δ_n as

$$\Delta_{2n+1}=(1+\epsilon)\tilde{J}^2\frac{2n(2n+1)}{(4n+3)(4n+1)}\left[1+\frac{4n+1}{2n(2n+1)}s\right],\quad n\geq 0, \tag{3a}$$

$$\Delta_{2n}=(1+\epsilon)\tilde{J}^2\frac{2n(2n+1)}{(4n+1)(4n-1)}\left[1-\frac{(4n+1)}{2n(2n+1)}s\right],\quad n\geq 1, \tag{3b}$$

where $s\equiv -1/\ln|\epsilon| = 1/4\pi\chi_s$ and hereafter we note J instead of $(1+\epsilon)^{1/2}\tilde{J}$ for convenience. The continued fraction $\Xi(z)$ constructed by inserting Eqs. (3a) and (3b) into Eq. (1) can be represented by the following quotient of hypergeometric functions, originally found by Gauss[9]:

$$\Xi(z)=\frac{1}{z}\frac{F(s/2,1-s/2;3/2;-J^2/z^2)}{F(s/2,-s/2;1/2;-J^2/z^2)}. \tag{4}$$

The algebraic form of $\Xi(z)$ is written as

$$\Xi(z)=\frac{1}{1-s}\frac{1}{z}\left\{1-\frac{(J^2+z^2)^{1/2}}{J}\frac{[(J^2+z^2)^{1/2}+J]^s-[(J^2+z^2)^{1/2}-J]^s}{[(J^2+z^2)^{1/2}+J]^s+[(J^2+z^2)^{1/2}-J]^s}\right\}. \tag{5}$$

In the above equation, the characteristic dynamical behavior of the system near the critical point is determined by s.

From Eq. (5), one can calculate the admittance, the so-called dynamical susceptibility or response function, by using linear-response theory, i.e., $\chi(\omega)/\chi_s = 1-\lim_{\eta\to 0^+}(i\omega+\eta)\Xi(i\omega+\eta)$. We find that

$$\mathrm{Re}\chi(\omega)=\begin{cases}\dfrac{1}{4\pi s(1-s)}\left\{\dfrac{(J^2-\omega^2)^{1/2}}{J}\dfrac{[(J^2-\omega^2)^{1/2}+J]^{4s}-|\omega|^{4s}}{|\omega|^{4s}+2|\omega|^{2s}[(J^2-\omega^2)^{1/2}+J]^{2s}\cos(s\pi)+[(J^2-\omega^2)^{1/2}+J]^{4s}}-s\right\}, & |\omega|<J,\\[2ex] \dfrac{1}{4\pi s(1-s)}\left\{\dfrac{(\omega^2-J^2)^{1/2}}{J}\tan[s(\pi/2-\theta)]-s\right\}, & |\omega|>J,\end{cases} \tag{6a}$$

$$-\mathrm{Im}\chi(\pm\omega)=\begin{cases}\pm\dfrac{1}{4\pi s(1-s)}\left\{\dfrac{(J^2-\omega^2)^{1/2}}{J}\dfrac{2|\omega|^{2s}[(J^2-\omega^2)^{1/2}+J]^{2s}\sin(s\pi)}{|\omega|^{4s}+2|\omega|^{2s}[(J^2-\omega^2)^{1/2}+J]^{2s}\cos(s\pi)+[(J^2-\omega^2)^{1/2}+J]^{4s}}\right\}, & |\omega|<J,\\[2ex] 0, \quad |\omega|>J,\end{cases} \tag{6b}$$

where $\theta=\tan^{-1}[(\omega^2-J^2)^{1/2}/J]$.

In Fig. 1 we show $-\mathrm{Im}\chi(\omega)$ for two different values of J and various values of s. As is easily seen, the curve approaches the vertical axis near $\omega\simeq 0$ as s goes to zero. For $s\to 0$, which implies the system is just at the critical point, we obtain from Eqs. (6a) and (6b)

$$\lim_{s\to 0}-\mathrm{Im}\chi(\pm\omega)=\begin{cases}\pm\frac{1}{8}(J^2-\omega^2)^{1/2}/J, & |\omega|<J,\\ 0, \quad |\omega|>J,\end{cases} \tag{7a}$$

$$\lim_{s\to 0}\mathrm{Re}\chi(\omega)=\begin{cases}\dfrac{1}{4\pi}\left[\dfrac{(J^2-\omega^2)^{1/2}}{J}\ln\dfrac{(J^2-\omega^2)^{1/2}+J}{|\omega|}-1\right], & |\omega|<J,\\[2ex] \dfrac{1}{4\pi}\left[\dfrac{(J^2-\omega^2)^{1/2}}{J}\left(\dfrac{\pi}{2}-\theta\right)-1\right], & |\omega|>J.\end{cases} \tag{7b}$$

Since the function $-\mathrm{Im}\chi(\omega)$ has a discontinuity at $\omega=0$, by the Kramers-Kronig relations the real part has a singularity at this point, i.e., as $\omega\to 0$, $\mathrm{Re}\chi(\omega)$ tends to $-(4\pi)^{-1}\ln|\omega|$. This agrees with the result obtained by Suzuki.[10] Interchanging the order of taking the limits we have $\lim_{s\to 0}\lim_{\omega\to 0}\mathrm{Re}\chi(\omega)=\chi_s$. For $\omega\to\infty$, we have $\mathrm{Re}\chi(\omega)=O(\omega^{-2})$.

To solve the time-evolution problem, that is, to obtain the relaxation functions of M_x and $\mathcal{H}_0$, we have to apply the inverse Laplace transform $\mathcal{L}^{-1}$ to Eq. (4) or (5). Practically, this is too difficult, and so we shall center our discussion in the following way to avoid this difficulty. First, we write Eq. (4) as the new quotient of the hyper-

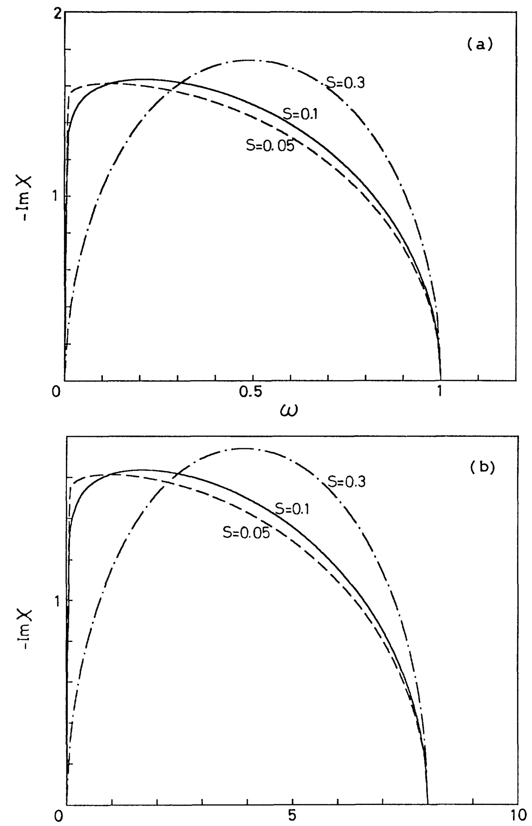

FIG. 1. $-\mathrm{Im}\chi(+\omega)$ vs frequency. (a) and (b) correspond to $J=1$ and 8, respectively.

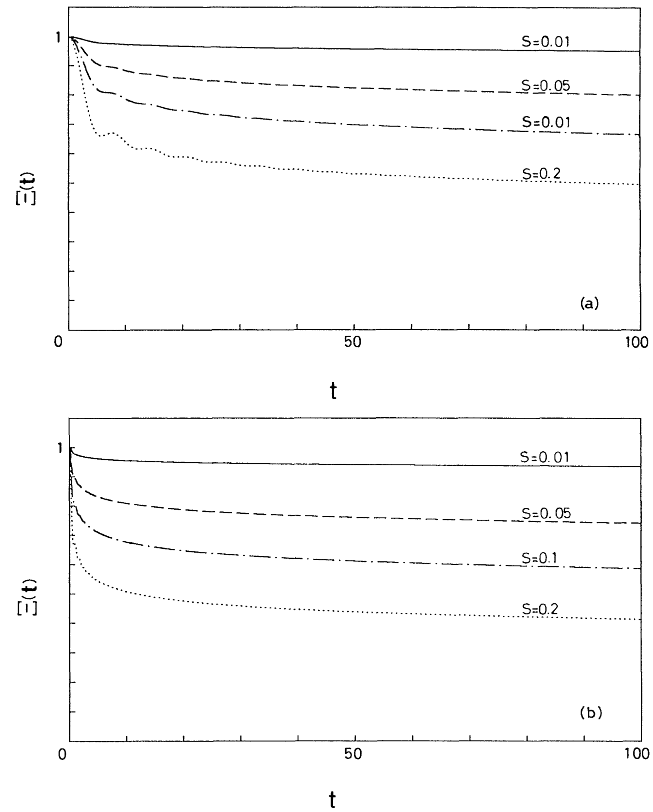

FIG. 2. The relaxation function $\Xi(t)$, the numerical solution of the integral equation (9). (a) and (b) correspond to $J=1$ and 8, respectively.

geometric functions:

$$\Xi(z)=\frac{1}{z}\left[1-\frac{s}{3}\frac{J^2}{z^2}\frac{F(1+s/2,1-s/2;5/2;-J^2/z^2)}{F(s/2,1-s/2;3/2;-J^2/z^2)}\right]^{-1}. \tag{8}$$

In the above, we may set s appearing in the argument of the hypergeometric functions to be 0, because we are only interested in the critical behavior of the system near the critical point $s\simeq 0$. This approximation means that one can simply neglect s in the continued fraction Eq. (1), since $[(4n+1)/2n(2n+1)]s$ in Δ_n with any $n>1$ is small compared with 1. Using the convolution property of $\mathcal{L}^{-1}$, we can construct an integral equation[11] which is called the second Voltera integral equation. It is given by

$$\Xi(t)+s\frac{\pi}{2}\int_0^t du\,\frac{H_1[J(t-u)]}{t-u}\Xi(u)=1\,, \tag{9}$$

where $H_1(t)$ is the Struve's function.[12] We illustrate the t dependence on $\Xi(t)$ for two different values of J and various values of s in Fig. 2.

The asymptotic expansion of the inverse transform $\mathcal{L}^{-1}$ of Eq. (4) or (5) consists of three parts, which are given by the integrals along the branch cuts whose branch points are $z=iJ$, $z=-iJ$, and $z=0$. In general the contribution of branch points $z=iJ$ and $z=-iJ$ is expressed as an infinite series.[13] Then one may expect that the contribution from these branch points decreases faster than the part coming from $z=0$. Therefore, we consider only this part in Eq. (4). It is uniquely represented as $a(s)z^{-1+2s}$ with $\lim_{s\to 0}a(s)=1$. Correspondingly, we find that the long-time tail of the relaxation function is given by

$$\Xi(t)\sim 1/t^{2s}. \tag{10}$$

We can also calculate the random forces together with the response function of the exchange energy. The results will be published elsewhere.

For any realistic Ising-type system, the Hamiltonian can be represented by two parts, the usual TI Hamiltonian and the remaining interaction terms, e.g., non-nearest-neighbor spin-spin coupling. Even though the latter is sufficiently small compared with the former, a critical behavior of the system cannot be characterized by any divergence but only by a sharp maximum. So far, the present study is only at zero temperature ($T=0$). On the other hand, when $\beta J|\epsilon|$ is large, we may write the inverse static susceptibility approximately as

$$s=-1/(1-2\alpha)\ln|\epsilon| , \tag{11}$$

with $\alpha=e^{-\beta J|\epsilon|}$. Further, other temperature-dependent terms appearing in the calculation of Δ_n, Eqs. (3), can be neglected compared with the s-linear terms when $e^{-\beta J|\epsilon|}$ is smaller than $-1/\ln|\omega|$. Therefore we can replace s in Eqs. (4) and (5) by Eq. (11) at low temperature.

If the static susceptibility of a given substance is sufficiently large, i.e., s is small, we expect that the present results can be applied to analyze low-temperature dynamical properties of the substance.

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[11]See, e.g., A. Erdélyi *et al.*, *Tables of Integral Transforms* (McGraw-Hill, New York, 1953), Vol. 1.

[12]The Struve's function is defined by

$$\Gamma(\nu+\tfrac{1}{2})H_\nu(z)=2\pi^{-1/2}\left(\frac{z}{2}\right)^{\nu}\int_0^1(1-t^2)^{\nu-1/2}\sin(zt)\,dt .$$

See, e.g., Vol. 2 of Ref. 9.

[13]See, e.g., R. B. Dingle, *Asymptotic Expansions: Their Derivation and Interpretation* (Academic, London, 1973).