Nonequilibrium properties in the transverse XX chain

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(Received 27 March 2002; published 30 July 2002)

We investigate the nonequilibrium properties of the transverse XX chain. The steady state can be interpreted as the equilibrium state or the ground state of the effective Hamiltonian, which depends on the initial state. We also study the physical properties of the state at various temperatures, in particular, the effects of quantum phase transition.

DOI: 10.1103/PhysRevE.66.016135 PACS number(s): 05.70.Ln, 05.30.−d, 05.60.−k, 82.20.−w

I. INTRODUCTION

During the past few years the thermal conductivity of low-dimensional spin systems has attracted considerable interest [1,2]. There are one-dimensional integrable spin systems whose Hamiltonians have an infinite number of the conserved quantities. Those systems exhibit anomalous heat conduction [3,4], but in real materials, impurities and phonons suppress the anomalous conduction. However, recent experiments showed that such a ballistic transport is realized on a small scale [5]. Sologubenko *et al.* measured the thermal conductivity in Sr_2CuO_3 which can be described by the isotropic Heisenberg chains in equilibrium case, and found that the energy is transmitted by spin excitations (spinon) [6]. This phenomenon is found in many materials including $KCUF_3$ [7], $CuGeO_3$ [8–12], YB_4As_3 [13], and $SrCu_2(BO_3)_2$ [14]. In $CuGeO_3$, the coherent length is estimated at about 100 times the lattice constant above the spin-Peierls transition temperature, i.e., in the regime of the isotropic one-dimensional Heisenberg model. Thus it is very interesting to investigate the nonequilibrium properties in spin systems where the ballistic heat transport is observed. Such nonequilibrium feature may serve to clarify the thermal behaviors of real materials in experiments. In this paper, we consider the transverse XX chain and study the nonequilibrium properties under the transverse field.

The transverse XX chain is regarded as a special case of the XXZ spin chain. Although it is a simple model, it shows the quantum phase transition as a function of the transverse field. This system has the conserved quantities such as the total magnetization of the z component of the spin, so that we expect the ballistic transport. When the exchange interaction is very large in comparison with the energy scale of phonons at low temperatures, this feature will survive on a small scale although the impurities and phonons make the macroscopic heat transport to be normal in real materials. Hence this model may clarify the important effect of the quantum phase transition on the nonequilibrium properties for the materials with large exchange interaction.

This problem was first studied by Antal *et al.*, using the Lagrange multiplier [15]. They devised the effective Hamiltonian composed of the bulk Hamiltonian (transverse XY chain) and the energy current operator that is connected by the Lagrange unknown coefficient. And they investigated the ground state of it. As a result, it was found that the correlations at large distance show oscillations whose amplitudes decay according to the power law. We treat the same problem without resorting to such Lagrange multiplier. Alternatively, we stand on the point of view that the quantum system is in the nonequilibrium steady state in the sense of Ruelle [16] and Jakšić and Pillet [17]. The nonequilibrium steady state is the state asymptotically realized from the initial state that the system is connected to reservoirs of different temperatures. Since the energy is transmitted between the reservoirs at different temperatures, we consider the thermal reservoirs with two different temperatures composed of spin chains. We are interested in the asymptotic behavior. Therefore, we have to treat an infinite system from the beginning. For the purpose, we take the C^*-algebraic approach [18,19].

In order to discuss state with the current, Antal *et al.* added a current term to the original bulk Hamiltonian, to make the effective Hamiltonian [15]. To investigate the corresponding structure, we look for the effective Hamiltonian of the asymptotic state in Sec. III. This is also interesting in the viewpoint of the ensemble argument of the steady state [20]. If the initial temperatures of both the (i.e., right and left) reservoirs are finite, the asymptotic state can be interpreted as the equilibrium state of some effective Hamiltonian at finite temperature $\mathcal{H}_{\mathrm{eff}}^{f}$. It depends on the initial temperatures. On the other hand, if the initial temperature of the left (or right) side is zero, the state can be interpreted as the ground state of some effective Hamiltonian at zero temperature $\mathcal{H}_{\mathrm{eff}}^{0}$. In fact, $\mathcal{H}_{\mathrm{eff}}^{0}$ is formally given as the zero-temperature limit of $\mathcal{H}_{\mathrm{eff}}^{f}$. It is independent of the initial temperature of the right (left) part, and all the asymptotic states with different initial temperatures of the right (left) part are the ground state of $\mathcal{H}_{\mathrm{eff}}^{0}$. They exhibit very different features. The effective Hamiltonian differs from the original one up to the conserved quantities. It is also remarkable that it shows the nonlocal property. That agrees with the general conjecture that the free energy functional of the nonequilibrium steady state is nonlocal. The effective Hamiltonian is different from that of Ref. [15], and consequently, we observe the different physical features.

In Sec. IV, we investigate the transverse field dependence of the energy current. We find that the quantum liquid state enhances the energy current at low temperatures and the transverse field suppresses the enhancement. This phenom-

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enon was observed in $SrCu_2(BO_3)_2$ [14]. On the contrary, in the state at high temperatures, the current becomes smaller as the transverse field increases. The energy current works to localize spin correlations, because it has the thermal origin.

II. THE ASYMPTOTIC STATE

The Hamiltonian we shall consider has the form

$$\mathcal{H}=J\sum_{n=-\infty}^{\infty}(\sigma_n^x\sigma_{n+1}^x+\sigma_n^y\sigma_{n+1}^y)+\Gamma\sum_{n=-\infty}^{\infty}\sigma_n^z, \qquad (1)$$

where σ_n^α $(\alpha=x,y,z)$ is the α component of the Pauli matrix at the site n. $J>0$ is the coupling strength and Γ describes the Zeeman term along the z direction. We denote $\Gamma/2J$ as γ. As the Hamiltonian is invariant under the transformation $\sigma_n^\alpha\to-\sigma_n^\alpha$, $\Gamma\to-\Gamma$, we may consider only the $\gamma>0$ case.

In order to realize the nonequilibrium steady state, the following situations are assumed.

(i) We first divide the whole system into two parts composed of spins, i.e., the left part of negative sites $n<0$ and the right part of positive sites $n\geqslant 1$.

(ii) These parts are initially in equilibrium at the temperatures β_- and β_+, respectively.

(iii) Then the system evolves freely in time, and asymptotically reaches the steady states.

The energy flow operator at the nth site, $\mathcal{J}_E^n$, is easily calculated from the continuity equation of energy;

$$\mathcal{J}_E^n=-2J^2\bigg[\sigma_n^z(\sigma_{n+1}^x\sigma_{n-1}^y-\sigma_{n-1}^x\sigma_{n+1}^y)+\frac{\Gamma}{J}(\sigma_{n+1}^y\sigma_n^x-\sigma_{n+1}^x\sigma_n^y)\bigg]. \qquad (2)$$

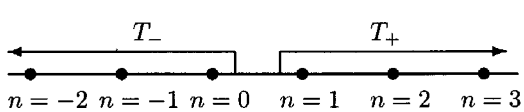
The Hamiltonian (1) and the energy flow (2) are written by the fermion operators using the Jordan-Wigner transformation,

$$\mathcal{H}=-2J\sum_{n=-\infty}^{\infty}[a_{n+1}^\dagger a_n+a_n^\dagger a_{n+1}]+\Gamma\sum_{n=-\infty}^{\infty}(2a_n^\dagger a_n-1),$$

$$\mathcal{J}_E^n=4iJ^2\bigg[-a_{n-1}^\dagger a_{n+1}+a_{n+1}^\dagger a_{n-1}-\frac{\Gamma}{J}(a_{n+1}^\dagger a_n-a_n^\dagger a_{n+1})\bigg], \qquad (3)$$

where a_n and $a_n^\dagger$ are the fermionic annihilation and creation operators of the nth site.

As we are interested in the asymptotic behavior, we treat an infinite system from the beginning. For the purpose, we employ the C^*-algebraic approach [18,19]. In a finite system,



the expectation value of the observable A is determined by the density matrix ρ, as $\mathrm{Tr}\,\rho A$. In C^*-algebraic theory, this is generalized to the positive linear map ψ that is called *state*. The expectation value of A is given by $\psi(A)$. In a finite system, the time evolution in the Heisenberg picture is represented by $A\to U_t^*AU_t$, where $U_t=e^{-iHt}$ is a unitary operator. Instead of this, we have one parameter group of automorphisms α_t, which means the time evolution $A\to\alpha_t(A)$. For the system initially in the state ψ_0, the expectation value of the observable A at the time t is expressed as $\psi_0(\alpha_t(A))$. We consider the asymptotic state in the long-time limit, $\psi_\infty(A)=\lim_{t\to\infty}\psi_0(\alpha_t(A))$.

The initial state has the decoupling form as

$$\psi_0(A_+\otimes A_-)=\psi_+^{\beta_+}(A_+)\otimes\psi_-^{\beta_-}(A_-), \qquad (4)$$

where A_+ and A_- are arbitrary operators of the right part $(n\geqslant 1)$ and the left part $(n\leqslant 0)$ of the chain, respectively. $\psi_+^{\beta_+}$ and $\psi_-^{\beta_-}$ are the states in equilibrium at the inverse temperatures β_+ and β_-. Because of the quadratic form of the equilibrium states $\psi_+^{\beta_+}$ and $\psi_-^{\beta_-}$, the expectation values are enumerated using the Wick product with two-point function. The dynamics corresponding to the Hamiltonian (3) is

$$\alpha_t(a^\dagger(f))=a^\dagger(e^{ith}f), \qquad (5)$$

where we use a notation

$$a^\dagger(f)\equiv\sum_{l=-\infty}^{\infty}f_la_l^\dagger, \quad \sum_{l=-\infty}^{\infty}|f(l)|^2<\infty,$$

and h is the one-particle Hamiltonian with

$$(hf)(n)=-2J(f(n-1)+f(n+1))+2\Gamma f(n).$$

Following the argument of Ho and Araki [21] and Araki [22], we can calculate the asymptotic state ψ_∞: First we derive the exact time evolution at time t (5). Second, take the $t\to\infty$ limit of the expectation value of observables, with the aid of some asymptotic formulas [23,24]. Thus, we have the two-point correlation function

$$\psi_{\infty,\beta_-,\beta_+}(a_l^\dagger a_m)=G(\beta_-,\beta_+,l-m)=G_-(\beta_-,l-m)+G_+(\beta_+,l-m),$$

$$G_-(\beta_-,n)=\frac{1}{2\pi}\int_0^\pi dk\frac{e^{ink}}{1+e^{-4J\beta_-(\cos(k)-\gamma)}}, \qquad (6)$$

$$G_+(\beta_+,n)=\frac{1}{2\pi}\int_{-\pi}^0 dk\frac{e^{ink}}{1+e^{-4J\beta_+(\cos(k)-\gamma)}}.$$

Because the dynamics preserves the quasifree property of the state, ψ_∞ is also given by the Wick product with the two-point function. Note that only the particles with positive momentum $(0\leqslant k\leqslant\pi)$ contribute to the function $G_-(\beta_-,n)$. This implies a situation that quasiparticles with negative momentum in the left part of the chain go to left infinity and do not appear in the correlation function. This feature is also the case in the right part of the chain, as seen in $G_+(\beta_+,n)$.

III. EFFECTIVE HAMILTONIAN

In the view point of the ensemble argument, we look for the effective Hamiltonian: the asymptotic state may be interpreted as an equilibrium state or the ground state of the effective Hamiltonian in the Fermion picture [20]. This also clarifies the difference of our situation from that of Antal *et al.* [15].

It is not always possible to find the effective Hamiltonian for every state, but in our system, we can. Although for an infinite system some automorphism takes the place of the effective Hamiltonian, we can make the argument formally in the Hamiltonian form. The precise meaning of it will be stated in Ref. [25].

First, let us consider the finite temperature case, i.e., where both β_- and β_+ are finite. The two-point function (6) can be interpreted as the Fermi distribution with respect to the Hamiltonian

$$\mathcal{H}_{\rm eff}=\int_{-\pi}^{\pi}\epsilon(k)a_k^\dagger a_k,$$

$$\epsilon(k)=\frac{-8J}{\beta_-+\beta_+}\begin{cases}\beta_-(\cos(k)-\gamma) & k\in[0,\pi],\\ \beta_+(\cos(k)-\gamma) & k\in(-\pi,0),\end{cases}$$

at the inverse temperature $\beta\equiv(\beta_-+\beta_-)/2$. Here $a_k^\dagger$ is the fermion creation operator for a particle with the momentum k. Furthermore, this can be proved to be the uniquely determined effective Hamiltonian. Let us represent the interaction between the sites, in the coordinate representation. In the coordinate representation, $\mathcal{H}_{\rm eff}$ is written in the form

$$\mathcal{H}_{\rm eff}=\mathcal{H}+\sum_{N=0}^{\infty}\mu_N^1 Q_N^1+\mu_N^2 Q_N^2, \tag{7}$$

where, Q_N^1, Q_N^2 are conserved quantities,

$$Q_N^1=\frac{1}{2}\sum_{l=-\infty}^{\infty}(a_{N+l}^* a_l + a_l^* a_{N+l}),$$

$$Q_N^2=\frac{1}{2i}\sum_{l=-\infty}^{\infty}(a_{N+l}^* a_l - a_l^* a_{N+l}).$$

Hence, we can see that the effective Hamiltonian is different from the original one up to conserved quantity, and the difference is determined by $\mu_N(\beta_-,\beta_+)$,

$$\mu_{2l}^2(\beta_-,\beta_+)=-\frac{8J}{\pi}\frac{\beta_- - \beta_+}{\beta_- + \beta_+}\frac{4l}{4l^2-1},\quad l\geqslant 1,$$

$$\mu_{2l+1}^2(\beta_-,\beta_+)=\frac{16J}{\pi}\gamma\frac{\beta_- - \beta_+}{\beta_- + \beta_+}\frac{1}{2l+1},\quad l\geqslant 0,$$

$$\mu_N^1(\beta_-,\beta_+)=0. \tag{8}$$

Next, we consider the case that $\beta_-=\infty$, i.e., the left part is initially at the zero temperature. Since the transverse *XX* model exhibits the phase transition at the zero temperature, this is a physically interesting situation. In the $\beta_-\to\infty$ limit, $\mu_N(\beta_-,\beta_+)$ in Eq. (8) converge to

$$\mu_{2l}^2(\infty,\beta_+)=-\frac{8J}{\pi}\frac{4l}{4l^2-1},\quad l\geqslant 1,$$

$$\mu_{2l+1}^2(\infty,\beta_+)=\frac{16J}{\pi}\gamma\frac{1}{2l+1},\quad l\geqslant 0,$$

$$\mu_N^1(\infty,\beta_+)=0. \tag{9}$$

As is expected, the state $\psi_{\infty,(\infty,\beta_+)}$ is the ground state of the effective Hamiltonian $\mathcal{H}_{\rm eff}^0$ of the form (7), with Eq. (9) [25]. Note that $\mu_N(\infty,\beta_+)$ are β_+ independent. In fact, all the asymptotic states with different β_+ are the ground states of the same effective Hamiltonian, [19,25]. In the following section, these degenerate states will be shown to have very different structures, up to β_+.

Note that Q_N describes to the *N*-sites interaction. So we can interpret the power-law decay of the μ_N as a signal of the nonlocal property of $\mathcal{H}_{\rm eff}$. It is expected in general that, if the free-energy functional exits for the nonequilibrium steady state, it may have the nonlocal property. In fact, Derrida *et al.*, have derived the nonlocal free-energy functional for the nonequilibrium steady state of an exactly solvable model [20]. Our result here agrees with the expectation.

In this way we have obtained the effective Hamiltonian $\mathcal{H}_{\rm eff}$. It is remarkable that our effective Hamiltonian is entirely different from that of Antal *et al.* [15]: They added magnetic current or energy current. The magnetic current case corresponds to the effective Hamiltonian

$$\mathcal{H}-\lambda Q_2^1,$$

and the energy current case corresponds to,

$$\mathcal{H}-\lambda(Q_2^2-\gamma Q_1^2).$$

In the next section, we shall discuss in detail the physical properties of the states.

IV. PHYSICAL PROPERTIES OF THE STEADY STATE

Once the two-point functions are obtained, various quantities are calculated. It is known that the quantum phase transition occurs at the zero temperature at $\gamma=1$. When $\gamma<1$, this system remains in the disordered phase due to the quantum effect. We investigate how this quantum phase transition affects the energy flow and the correlation of spins in a nonequilibrium state. In order to analyze the effect, we consider the $\beta_-\to\infty$ limit, i.e., we take the zero-temperature limit in the left part, and change $1/\beta_+$, the temperature in the right part. As shown in Sec. III, the states with different β_+ can be regarded as the degenerate ground states of the effective Hamiltonian corresponding to $\beta_-=\infty$. We shall calculate the energy current and the two-point correlation function of the spins in the *z* and *x* directions.

The energy current is given by

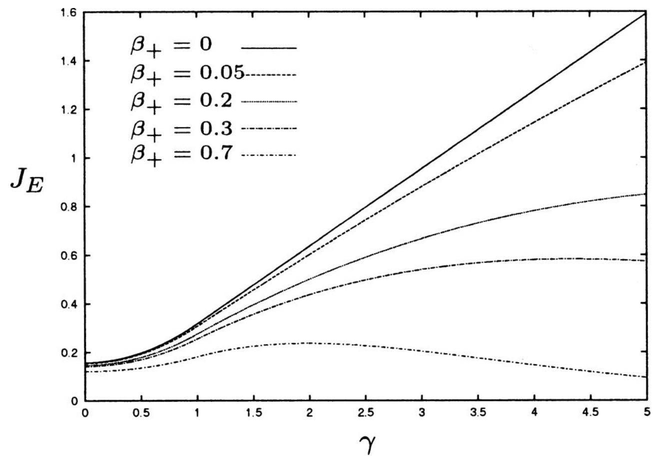


FIG. 1. The transverse field dependence of the energy current for various temperatures: high-temperature regime. The value of the inverse temperature β_+ is attached to the line samples.

$$J_E \equiv \psi_\infty(\mathcal{J}_E^n) = -\frac{4J^2}{\pi}\left[\int_{-\pi}^{0} dk \frac{(\cos k-\gamma)\sin k}{1+e^{-4J\beta_+(\cos(k)-\gamma)}} + \int_0^{\pi} dk \frac{(\cos k-\gamma)\sin k}{1+e^{-4J\beta_-(\cos(k)-\gamma)}}\right]. \quad (10)$$

We see that the quasiparticle with the energy $2J(\cos k-\gamma)$ runs through the chain at the velocity $\sin k$ and that the number of particles is in proportion to $1/(1+e^{-\beta_+(\cos(k)-\gamma)})$ for negative k, and to $1/(1+e^{-\beta_-(\cos(k)-\gamma)})$ for positive k. The positive momenta of particles initially on the right go away to $+\infty$ and only the negative momenta are left. The same applies to particles initially on the left.

Now, we concentrate on the $\beta_- \to \infty$ limit. In this case, the second integral of Eq. (10) is restricted to $0 \leqslant k \leqslant \arccos\gamma$. Thus the energy flow is reduced to

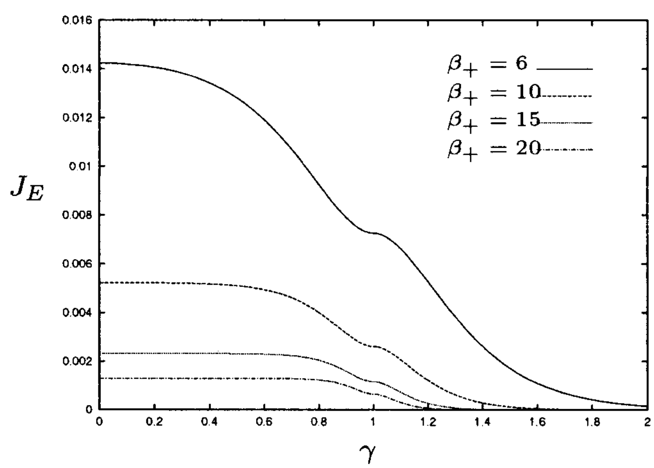


FIG. 2. The transverse field dependence of the energy current for various temperatures: low-temperature regime. The value of the inverse temperature β_+ is attached to the line samples.

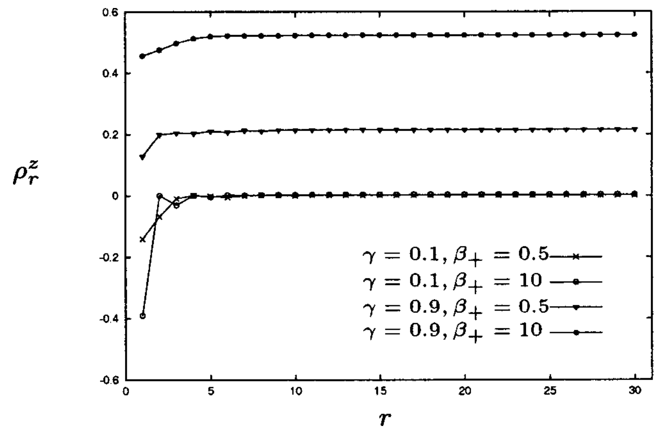


FIG. 3. The correlation function of the z component of spins for various temperatures and transverse fields. The numbers besides the line samples indicate the value of the transverse field γ and the inverse temperature β_+ in order.

$$J_E = -\frac{2J^2}{\pi}\int_{-\pi}^{0} dk \frac{(\sin 2k - 2\gamma\sin k)}{1+e^{-4J\beta_+(\cos(k)-\gamma)}} - 4J^2\begin{cases} \dfrac{(\gamma-1)^2}{2\pi} & 0 \leqslant \gamma < 1, \\ 0 & 1 \leqslant \gamma. \end{cases}$$

There appears a characteristic difference between high- and low-temperatures $1/\beta_+$ (Figs. 1, 2). At high temperature, the transverse field enhances the energy current. At low temperature, it suppresses the current. This phenomenon has been observed in the experiment on $SrCu_2(BO_3)_2$ [14]. At high temperatures, the energy flux behaves as

$$J_E \sim -\frac{4J^2}{\pi}\begin{cases} \dfrac{\gamma^2+1}{2} - \beta_+\left(\dfrac{1}{6}+\dfrac{1}{2}\gamma^2\right) & 0 \leqslant \gamma < 1, \\ \gamma - \beta_+\left(\dfrac{1}{6}+\dfrac{1}{2}\gamma^2\right) & 1 \leqslant \gamma. \end{cases}$$

In the high-temperature limit $\beta_+ \to 0$, this converges to the maximum eigenvalue of the energy flux operator which is called "maximal current" in Ref. [15]. On the other hand, at low temperatures, the opposite γ dependence of the energy flux is observed. That is, J_E decreases as γ increases. For $1 \leqslant \gamma$, it decreases exponentially,

$$J_E \sim -\frac{4J^2}{\pi}\left[e^{4J\beta_+(1-\gamma)}\left(\frac{1}{4J\beta_+}(\gamma-1)+\frac{1}{(4J\beta_+)^2}\right) - e^{-4J\beta_+(1+\gamma)}\left(\frac{1}{4J\beta_+}(\gamma+1)+\frac{1}{(4J\beta_+)^2}\right)\right].$$

Intuitively, in the case of large γ, i.e., $\gamma \gg 1$, spins at the right part flip with the possibility $e^{-\beta\gamma}$. On the other hand, the energy transported per flip is roughly γ. Hence, the energy transported is proportional to $\gamma e^{-\beta\gamma}$. At high temperature, as

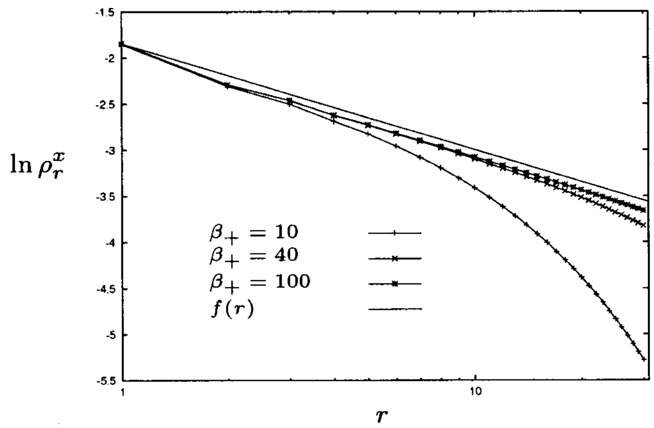


FIG. 4. The correlation function of the x component of spins (in log-log scale) for various temperatures with the transverse field fixed to $\gamma=0.1$. The number besides the line samples indicates the value of the inverse temperature β_+. $f(r)$ is the line with slope of $-\frac{1}{2}$: $\ln \rho_r^x = f(r) = -1.84 - \frac{1}{2}\ln r$.

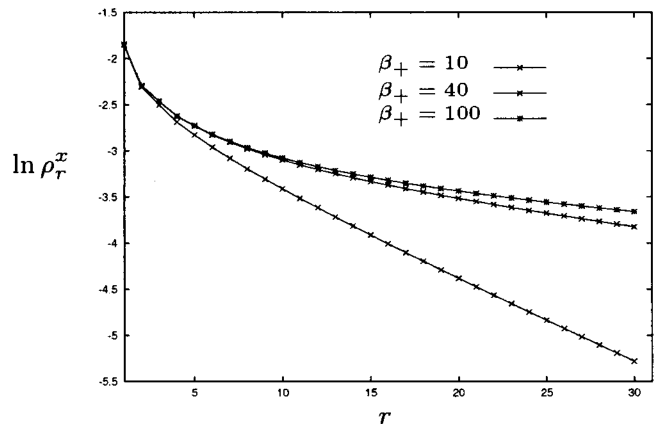


FIG. 5. The correlation function of the x component of spins (in semilog scale) for various temperatures with transverse field fixed to $\gamma=0.1$. The number besides the line samples indicates the value of the inverse temperature β_+.

γ increases, the energy transported increases as γ, while at low temperature it decreases exponentially as calculated above.

We next consider the correlation of the z component of spins,

$$\rho_r^z = \psi_\infty(\sigma_n^z \sigma_{n+r}^z), \quad r>0.$$

As the state ψ_∞ is translation invariant, ρ_r^Z is n independent and is a function of β_-, β_+, γ, and r. The correlation is expressed in terms of the two-point function G,

$$\rho_r^z = [2G(\beta_-,\beta_+,0)-1]^2 - 4|G(\beta_-,\beta_+,r)|^2. \quad (11)$$

To investigate the effects of the phase transition, we present the behavior of the $\beta_- \to \infty$ limit of ρ_r^z, $\lim_{\beta_-\to\infty}\rho_r^z(\beta_-,\beta_+)$. If the right part temperature is also zero, i.e., $\beta_+ = \infty$, the current is absent and the amplitude of oscillation in ρ_r^z is large. In this case, $\gamma=0$ corresponds to the antiferromagnetic phase, while $\gamma \geqslant 1$ to the ferromagnetic phase. When γ increases from 0 to 1, the phase changes from the antiferromagnetic one to the ferromagnetic one. As the temperature increases, the correlation tends to lose the antiferromagnetic structure. At a finite β_+, there is a finite J_E. The current is of thermal origin and disturbs the global correlation between local spins. Hence, the chain shows a more localized structure than the one without current, and loses the antiferromagnetic structure (Fig. 3).

Finally, we consider the correlation function of the x component of spins,

$$\rho_r^x = \psi_\infty(\sigma_n^x \sigma_{n+r}^x).$$

This function is calculated from the determinant of the matrix of the two-point function. In order to see clearly the decay of the correlation at low and high temperatures, we draw the graph in log-log and semilog plot (Figs. 4, 5). In the figure, ρ_r^x is given for various temperatures, with transverse field fixed to $\gamma=0.1$. From Fig. 4, it can be seen that at low temperature (large β_+), the correlation ρ_r^x decreases as $r^{-1/2}$. From Figs. 4 and 5, it can be seen that at high temperature (small β_+), ρ_r^x decreases exponentially for large r, while it decreases as $r^{-1/2}$ for small r.

V. DISCUSSION

We have studied the transverse XX chain and have shown that the nonequilibrium steady state can be interpreted as the equilibrium or the ground state of some effective Hamiltonian in the Fermion picture. The ground state is degenerate and the degenerate states have physically very different properties. The effective Hamiltonian consists of the original one and the conserved quantities. It has been shown that the effective Hamiltonian is nonlocal. The nonlocal form may be due to the fact that the model has an infinitely many conserved quantities. In fact, the sequence of the conserved quantity Q_N that represents N-site interactions implies the existence of the infinitely many conserved quantities. The effective Hamiltonian of strongly interacting systems may have some very different structures.

We have discussed the asymptotic state for local observables; that is, we have fixed some local n that is independent of t, and considered the limit $t\to\infty$. If we instead consider the expectation value of the observable at $n=vt$ for each real v, we can observe the diffusion of the temperature distribution. This interesting consideration was given by Antal *et al.* [26] for zero-temperature system. Modifying the C^*-algebraic argument used in this paper, we can obtain the result that agrees with that of Antal *et al.* [26]. Further argument is possible, which will be stated in Ref. [27].

ACKNOWLEDGMENTS

We thank Professor D. Buchholz, Professor T. Matsui, Dr. T. Miyadera, Dr. K. Saito, and Professor M. Wadati for helpful discussions. We also thank Professor M. Wadati, for instructive advice.

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