Heat transport in quantum spin chains: Relevance of integrability

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We investigate heat transport in various quantum spin chains using the Redfield equation. We find that anomalous heat transport is linked not to the integrability of the Hamiltonian, but to whether it can be mapped to a model of noninteracting fermions. Our results also suggest how seemingly anomalous transport may occur at low temperatures in a much wider class of models.

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I. INTRODUCTION

Heat transport in quantum spin chains, in particular, under which conditions normal (diffusive) transport is observed, is still not understood despite considerable effort.[1–14] For example, it was conjectured that integrability leads to anomalous (ballistic) transport,[8] but it was also argued that integrable but gaped chains have normal conductivity.[10,11] Others have argued that only the spin conductivity is normal in this case, while the thermal conductivity is still anomalous.[12] A consensus as to what the necessary criteria are for normal versus anomalous conductivity is still missing.

Most of this work[3–10] studied infinite and/or periodic chains, and used the Kubo formula[15,16] where finite (zero) Drude weight signals anomalous (normal) transport. For integrable systems, the Kubo formula predicts anomalous heat transport. In fact, full integrability is not even necessary; all that is needed is a finite overlap between the heat current operator and a conserved quantity.[4,14]

The derivation of the Kubo formula for finite systems requires dealing with the currents between the chain's ends and the thermal baths it is connected to. These boundary currents may change the form of the Kubo formula.[17,18] For infinite systems, one may argue that they can be ignored, as they are a boundary effect.[15,16] However, it is obviously not so for finite systems, where coupling to baths should be taken into consideration explicitly.[18] Furthermore, "integrability" of the chain connected to baths may be lost even if the isolated chain is integrable since the terms describing the coupling to the baths lead to a nonvanishing commutator between the heat current operator and the total Hamiltonian. Both of these facts might invalidate the main argument for anomalous transport based on the Kubo formula.

Studies that explicitly consider the effects of the baths on a finite chain, while fewer, also give contradictory results. Using the local-operator Lindblad equation, Prosen *et al.* showed that an integrable gaped ($J_z > J_{xy}$) XXZ chain has normal spin conductivity, while its energy transport is anomalous;[12] whereas, using the same approach, Michel *et al.* claim that, for $J_z > 1.6J_{xy}$, spin chains have normal energy transport.[11]

Such conflicting results exist not only in theoretical studies, but also in experiments. Anomalous heat transport observed experimentally in systems described by integrable models, such as $(Sr,Ca)_{14}Cu_{24}O_{41}$, Sr_2CuO_3 and $CuGeO_3$,[19–21] seems to validate the conjecture linking anomalous transport to integrability, but Ref. 22 finds normal transport in Sr_2CuO_3 at high temperatures.

Even if there was no conflict between results based on the local-operator Lindblad equation, such an approach is likely less reliable than one based on the Redfield equation. For example, only the latter leads to the proper Boltzmann distribution if the baths are not biased. There are, in fact, already several such studies based on the Redfield equation.[23,24] However, these are for spin systems that are either noninteracting (thus, trivially integrable) or are nonintegrable. We call a spin chain "noninteracting" if it can be mapped, for example through a Jordan-Wigner transformation, to a Hamiltonian for noninteracting spinless fermions. Anomalous transport is found for the former and normal transport is found for the latter. Disordered spin systems have also been found to have normal transport.[25] There are no examples of clean, interacting but integrable systems investigated via the Redfield equation.

Here, we systematically investigate many models of finite spin chains coupled to thermal baths using the Redfield equation.[23–27] Our results suggest that integrability is not a sufficient condition for anomalous heat transport. Note that, in this context, we call a model "integrable" if it is so when the system is isolated (i.e., not connected to baths). We find anomalous transport at all temperatures only in models that can be mapped onto homogeneous noninteracting fermionic models. All other models we investigated exhibit normal heat transport, whether they are integrable or not (however, as discussed below, at low temperatures, their heat transport may become anomalous in certain conditions). We therefore conjecture that the existence of a mapping of the spin Hamiltonian to one of noninteracting fermions is the criterion determining anomalous transport, at least for finite-size systems.

The paper is organized as follows. Section II defines the problem and its Redfield equation. In Sec. III, we discuss the numerical methods we use and, in Sec. IV, we define the quantities we use to characterize thermal and spin transport. We then proceed to present our numerical results in Sec. V, and then conclude.

II. THE MODEL AND ITS REDFIELD EQUATION

We consider an N-site chain of spin-$\frac{1}{2}$ described by the Hamiltonian

$$\mathcal{H}_S = \sum_{i=1}^{N-1} \sum_{r=x,y,z} J_r s_i^r s_{i+1}^r - \vec{B} \cdot \sum_{i=1}^{N} \vec{s}_i, \tag{1}$$

while the heat baths are collections of bosonic modes

$$\mathcal{H}_B = \sum_{k,\alpha} \omega_{k,\alpha} b_{k,\alpha}^{\dagger} b_{k,\alpha}, \tag{2}$$

where $\alpha = R/L$ indexes the right- and left-side baths. The system-baths coupling is taken as

$$V = \lambda \sum_{k,\alpha} V_k^{(\alpha)} s_\alpha^y \otimes (b_{k,\alpha}^{\dagger} + b_{k,\alpha}), \tag{3}$$

where $s_L^y = s_1^y$ and $s_R^y = s_N^y$, i.e. , the left (right) thermal bath is only coupled to the first (last) spin of the chain, and can induce its spin flipping. This is because we choose $\vec{B} \cdot \vec{e}_y = 0$ when $|\vec{B}|$ is finite, meaning that spins primarily lie in the $x0z$ plane so that s^y acts as a spin-flip operator. As discussed below, this type of coupling also mimics particle exchange between the system and the baths in systems of bosons or fermions. We use λ to characterize the strength of the system-baths coupling.

The resulting Redfield equation for the density matrix of the system $\rho(t) = \mathrm{Tr}_B \rho_T(t)$, where $\rho_T(t)$ is the full density matrix for system+baths and the trace integrates out the baths while the coupling is treated to second order in perturbation theory, is obtained using standard methods[23,24,26]:

$$\frac{\partial \rho(t)}{\partial t} = -i[\mathcal{H}_S, \rho(t)] - \lambda^2 \sum_{\alpha=L,R} \left(\left[s_\alpha^y, \hat{m}_\alpha \rho(t) \right] + \mathrm{H.c.} \right), \tag{4}$$

where $\hat{m}_\alpha = s_\alpha^y \cdot \Sigma_\alpha$. Here, $(\ldots)$ refers to the element-wise product of two matrices $\langle n|a \cdot b|m\rangle = \langle n|a|m\rangle\langle n|b|m\rangle$. The bath matrices $\Sigma_{L,R}$ are defined in terms of the eigenstates of the system's Hamiltonian $H_S|n\rangle = E_n|n\rangle$ as

$$\begin{aligned}\Sigma_\alpha = \pi \sum_{m,n} |m\rangle\langle n| \Big\{ &\Theta(\Omega_{mn})\, n_\alpha(\Omega_{mn})\, D_\alpha(\Omega_{mn}) \left| V_{k_{mn}}^{(\alpha)} \right|^2 \\ &+ \Theta(\Omega_{nm}) [1 + n_\alpha(\Omega_{nm})]\, D_\alpha(\Omega_{nm}) \left| V_{k_{nm}}^{(\alpha)} \right|^2 \Big\},\end{aligned}$$

where $\Omega_{mn} = E_m - E_n = -\Omega_{nm}$ and k_{mn} is defined by $\omega_{k_{mn},\alpha} = \Omega_{mn}$, i.e., a bath mode resonant with this transition. Furthermore, $\Theta(x)$ is the Heaviside function, $n_\alpha(\Omega) = [e^{\beta_\alpha \Omega} - 1]^{-1}$ is the Bose-Einstein equilibrium distribution for the bosonic modes of energy Ω at the bath temperature $T_\alpha = 1/\beta_\alpha$, and $D_\alpha(\Omega)$ is the bath's density of states. The product $D_\alpha(\Omega_{mn})|V_{k_{mn}}^{(\alpha)}|^2$ is the bath's spectral density function. For simplicity, we take it to be a constant independent of α, m, and n.

For completeness, we note that the local-operator Lindblad equation is a simplified version of Eq. (4), where the bath operators Σ_α are numbers instead of matrices. For example, quite often one uses $\hat{m}_\alpha = s_\alpha^{\pm}\gamma_\pm$,[11,12] where $\gamma_+ \neq \gamma_-$ are constants. This is equivalent to the Redfield equation if and only if the central system consists of a single site, in which case Σ_α becomes a matrix with two off-diagonal numbers, the values of which correspond to $\gamma_\pm$. It can be proven that, for multisite central systems, the Redfield equation predicts the proper thermal equilibrium state as its long-term stationary state, if the baths are kept at the same temperature.[28] This is not true for the local-operator Lindblad equation, except for a single-site central system.[28] This is why we prefer to use the Redfield equation, even though the local-operator Lindblad equation is computationally much more convenient.

III. NUMERICAL METHODS

It is straightforward to use the Runge-Kutta method to integrate the Redfield equation starting from any given initial state.[24,25] The memory cost is proportional to 2^{2N} for an N-spin chain, but it may take a very long time for the integration to converge to the stationary state. This is not surprising since, in principle, the stationary state is reached only as $t \to \infty$.

Another approach[29] is to solve directly for the stationary solution of this Redfield equation (4): $\frac{\partial \rho(t)}{\partial t} = L\rho(t)$, namely,

$$L\rho(\infty) = 0, \tag{5}$$

i.e., to find the eigenstate for the zero eigenvalue of the 2^N-dimensional matrix L. However, in this case, the memory cost is proportional to 4^{2N}, which is much worse than for the Runge-Kutta method.

The method that has better memory efficiency than this eigenvalue problem and also better time efficiency than the Runge-Kutta method is to convert the equation into a linear system and solve it via matrix-free methods such as the Krylov space methods, which require only matrix-vector multiplication but not explicitly the matrix. The eigenvalue problem can be rewritten as a linear system of equations after explicitly using the normalization condition $tr(\rho) = 1$ such that

$$\bar{L}\rho(\infty) = \nu, \tag{6}$$

where $\nu = [1, 0, \ldots]^T$ and $\bar{L}$ is found from L by replacing the first row by $tr(\rho)$. Then we use, for example, the generalized minimal residual method (GMRES),[30] which requires only the matrix-vector multiplication rule. This method has a memory cost of $\sim 2^{2N}$ and time efficiency of a linear system with dimension 2^{2N}.

This is still a direct method, so its efficiency is not comparable with methods such as the Monte Carlo wave-function approach,[11] Hilbert space average method,[31] and the BBGKY-like approach.[32] However, unlike them, this method gives an exact result. This is important until one can understand whether any of the further approximations made in the more efficient methods can, for example, destroy the integrability of the system.

IV. DEFINITIONS OF THE THERMAL CURRENT AND LOCAL TEMPERATURES

We rewrite $\mathcal{H}_S = \sum_{i=1}^{N-1} h_{i,i+1} + \sum_{i=1}^{N} h_i$, where $h_{i,i+1}$ is the exchange between nearest-neighbor spins and h_i is the on-site coupling to the magnetic field. We can then define a local site Hamiltonian

$$h_i^{(S)} = \tfrac{1}{2}h_{i-1,i} + h_i + \tfrac{1}{2}h_{i,i+1} \tag{7}$$

with $h_{0,1} = h_{N,N+1} = 0$, and a local bond Hamiltonian

$$h_i^{(B)} = \tfrac{1}{2}h_i + h_{i,i+1} + \tfrac{1}{2}h_{i+1} \tag{8}$$

such that

$$\mathcal{H}_S = \sum_{i=1}^{N} h_i^{(S)} = \sum_{i=1}^{N-1} h_i^{(B)}. \tag{9}$$

The local bond Hamiltonians can be used to derive the heat current operator from the continuity equation

$$\hat{j}_{i\to i+1} - \hat{j}_{i-1\to i} = \nabla \hat{j} = -\frac{\partial h_i^{(B)}}{\partial t} = -i\big[\mathcal{H}_S, h_i^{(B)}\big]. \quad (10)$$

This results in

$$\hat{j}_{i\to i+1} = i\big[h_i^{(B)}, h_{i+1}^{(B)}\big] \quad (11)$$

for $i = 1,\ldots,N-2$. As expected, in the steady state we find $\langle \hat{j}_{i\to i+1}\rangle = tr[\hat{j}_{i\to i+1}\rho(\infty)] = J$ to be independent of i. Similarly, we define the spin polarization $\langle s_i^z\rangle$ and the spin current for the XXZ model

$$J_s = J_{xy}\left\langle s_i^y s_{i+1}^x - s_i^x s_{i+1}^y\right\rangle. \quad (12)$$

Knowledge of the steady-state heat current J, as such, is not enough to decide whether the transport is normal or not. Consider an analogy with charge transport in a metal connected to two biased leads. In this case, what shows whether the charge transport is anomalous or not is the profile of the electric potential, not the value of the electric current. In anomalous transport (for clean, noninteracting metals) all the voltage drop occurs at the ends of the sample, near the contacts. Away from these contact regions, electrons move ballistically and the electric potential is constant, implying zero intrinsic resistance. For a dirty metal, scattering takes place everywhere inside the sample and the electric potential decreases monotonically in-between the contact regions, i.e., the sample has finite intrinsic resistivity.

In principle, the scaling of the current with the system size, for a fixed effective bias, also reveals the type of transport: For anomalous transport, the current is independent of the sample size once its length exceeds the sum of the two contact regions, while for normal transport, it decreases like inverse length. The problem with this approach is that one needs to keep constant the effective bias, i.e., the difference between the applied bias and that in the contact regions. Furthermore, since we can only study relatively short chains, the results of such scaling may be questionable.

It is therefore desirable to use the equivalent of the electric potential for heat transport and to calculate its profile along the chain in order to determine the type of transport. This, of course, is the "local temperature," which is a difficult quantity to define properly. One consistency condition for any definition is that, if $T_L = T_R = T$, i.e., the system is in thermal equilibrium at T, then all local temperatures should equal T. We define local site temperatures T_i which fulfill this condition in the following way. Since we know all eigenstates of $\mathcal{H}_S$, it is straightforward to calculate its equilibrium density matrix at a given T, $\rho_{eq}(T) = \frac{1}{Z}\sum_n e^{-\beta E_n}|n\rangle\langle n|$, where $Z = \sum_n e^{-\beta E_n}$. Let then $\langle h_i^{(S)}\rangle_{eq}(T) = tr[\rho_{eq}(T)h_i^{(S)}]$. We define T_i to be the solution of the equation

$$\left\langle h_i^{(S)}\right\rangle_{eq}(T_i) = tr\big[\rho(\infty)h_i^{(S)}\big]. \quad (13)$$

In other words, we require that the steady-state value of the energy at that site equals the energy the site would have if the whole system were in equilibrium at T_i. Of course, we can also use other "local" operators such as $h_i^{(B)}$ to calculate a local bond temperature $T_{i+\frac{1}{2}}$. We find that, when these definitions are meaningful, the results are in very good agreement no matter what "local" operator is used.

This type of definition of T_i is meaningful only if a large magnetic field B is applied. For small B, the expectation values $\langle h_i^{(S)}\rangle_{eq}(T)$ are very weakly T dependent, so that tiny numerical errors in the steady-state value can lead to huge variations in T_i. Addition of a large B is needed to obtain $\langle h_i^{(S)}\rangle_{eq}(T)$, which varies fast enough with T for values of interest, so that a meaningful T_i can be extracted. Since we could not find a meaningful definition for T_i when $|\vec{B}| \to 0$, we can not investigate such cases. Note, however, that most integrable models remain integrable under addition of an external field $\vec{B} = B\hat{e}_z$.

V. RESULTS

For reasons detailed above, in most of our calculations we take $B_z = 1$ and the exchange $J \sim 0.1$. The baths' temperatures $T_{L/R} = T(1 \pm \delta/2)$ should not be so large that the steady state is insensitive to the model, or so small that only the ground state is activated. Reasonable choices lie between $\min(J_x, J_y, J_z)$ and NB, which are roughly the smallest and the largest energy scales, respectively, for the N-site spin chain.

In Fig. 1, we show typical results for (a) local temperature profiles $T_i, T_{i+\frac{1}{2}}$ and (b) local spin-polarization profiles $\langle s_i^z\rangle$. We apply a large bias $\delta = (T_L - T_R)/T = 0.4$ for clarity, but we find similar results for smaller δ. For these values, it seems that the "contact regions" include only the end spins. The profile of the central part of the chain is consistent with anomalous transport (flat profile) for the XX chain ($J_x = J_y$, $J_z = 0$) and shows normal transport (roughly linear profile) in all the other cases. XY chains with $J_x \neq J_y$ behave similarly

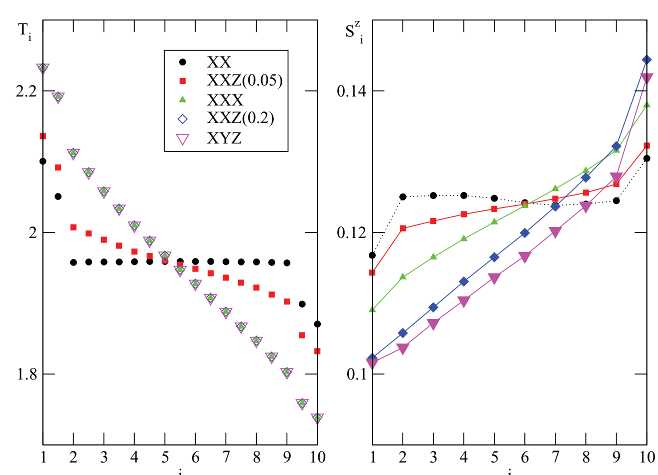

FIG. 1. (Color online) Plot of (a) local temperature profile and (b) local spin-polarization profile for chains with $N = 10$. In all cases, $T_L = 2.4$, $T_R = 1.6$, $\lambda = 0.1$, $J_x = 0.1$, $B_z = 1.0$. Other parameters are $J_y = 0.1$, $J_z = 0.0 (XX)$; $J_y = 0.1$, $J_z = 0.05$ $(XXZ0.05)$; $J_y = J_z = 0.1$ (XXX); $J_y = 0.1$, $J_z = 0.2$ $(XXZ0.2)$ and $J_y = 0.2, J_z = 0.3$ (XYZ). Only the XX chain shows flat T_i and $\langle s_i^z\rangle$ profiles. All other models have essentially linearly varying profiles for both the local temperatures and the local spin polarizations.

with the XX chain (not shown). We find similar results for ferromagnetic couplings. We also find that the ratio between the effective temperature difference $T_2 - T_{N-1}$ and the applied temperature difference $T_L - T_R$ is not a constant for different system sizes N. Therefore, in our numerical calculation, it is not possible to keep the effective temperature difference as a constant by applying the same temperature difference on the ends while changing the system size N. This implies that the dependence of J on N can not be used as an indicator of normal or anomalous transport. At most, it can provide a very rough qualitative picture. We have plotted several of the J versus N curves in Fig. 2. We see that J is independent of N for XX chains while it decreases with increasing N for XYZ and XXX chains.

Another way to examine size dependence is to compare the temperature and spin profiles for all available sizes. We normalize all the profiles for various models with different sizes by harvesting only the data in the central regions and scaling them to vary in [0,1]; for example, instead of (i,T_i), we plot $(\frac{i-2}{N-3},\frac{T_i-T_{N-1}}{T_2-T_{N-1}}), i = 2, 2.5, \ldots, N-1$. In Fig. 3, we plot such normalized profiles. We see that curves for all values of N collapse onto one single straight line and, furthermore, there is no difference between XYZ and XXX chains. Currently, we can only study small systems, but from this limited data, we see no qualitative differences for different sizes.

All these curves correspond to integrable models. The XX model is special because it can be mapped to noninteracting spinless fermions with the Jordan-Wigner transformation.[33] A finite J_z leads to nearest-neighbor interactions between fermions. Eigenmodes for models with $J_z \neq 0$ can be found using Bethe's ansatz, but they can not be mapped to noninteracting fermions.

In order to investigate where this transition between anomalous and normal transport occurs, we plot temperature profiles for systems with small J_z in Fig. 4(a).

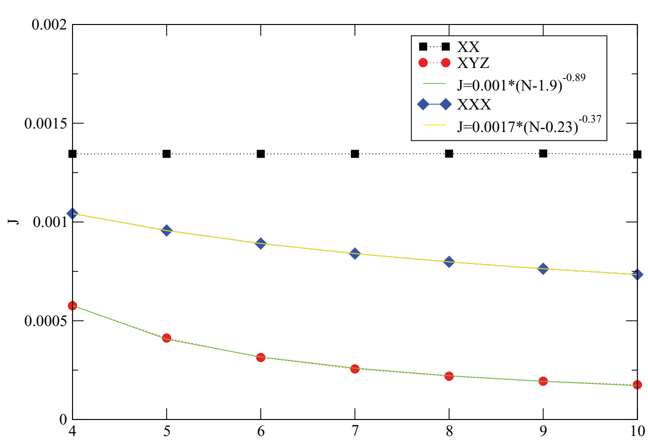

FIG. 2. (Color online) Heat currents J are plotted as a function of the system size for three models: XX, XYZ, and XXX. J is independent of N for XX chains, and it decreases with N for the other two cases. Due to the uncertainty about the effective applied temperature difference for different N, the fitting curves should only be regarded as a guide for eyes. The parameters are the same as in Fig. 1.

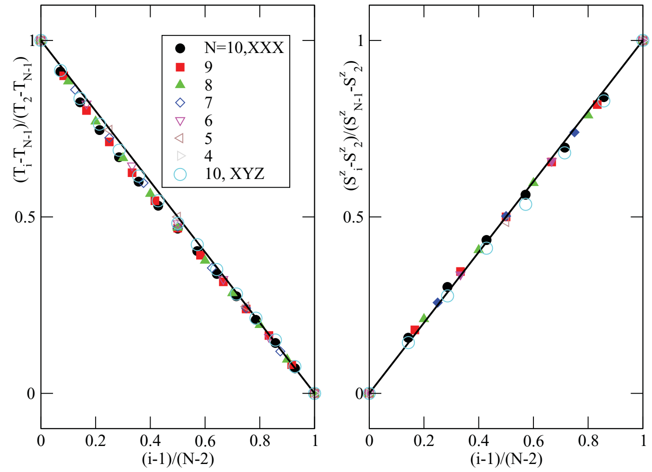

FIG. 3. (Color online) Normalized T_i and $\langle s_i^z \rangle$ profiles are plotted. Curves for different values of N collapse onto a single straight line and we see no difference between XYZ and XXX chains.

We see that, even for very small J_z, the above observation still holds. For $J_z = 0.01$, there is a slight qualitative difference, namely, that the contact regions seem larger than just the end spins, as can be seen from the normalized profiles. We believe that this may be due to limitations of the numerical accuracy. In Fig. 4(b), we investigate what the minimum value of B_z is that we can use with confidence. As we pointed out before, our definition of local temperature and also the idea of a local spin polarization $\langle s_i^z \rangle$ are only meaningful for sufficiently large B_z. We find that roughly we need to take $B_z > 0.3$. This is reasonable since, here, the typical energy due to coupling to the local B_z field $(0.3 \cdot 1/2)$ is comparable with the energy related to exchange $(3 \cdot 0.1/4)$.

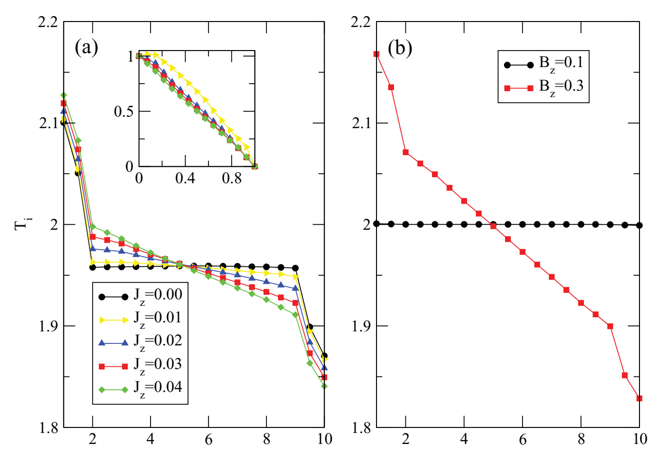

FIG. 4. (Color online) (a) Temperature profiles for small J_z values are shown for $J_x = J_y = 0.1$, $B_z = 1.0$. The effective temperature drop becomes smaller for smaller J_z, but the slope is still finite if $J_z \geqslant 0.02$. The inset plots normalized profiles, and shows no obvious differences for models with $J_z \geqslant 0.02$. The case of $J_z = 0.01$ shows a finite slope, but the normalized profile indicates a slight difference: the contact regions seem to be more extended than in the other cases. (b) Temperature profiles of XXX chains with $J = 0.1$ and small values of B_z. A linear temperature drop is observed for $B_z = 0.3$, but a flat profile for $B_z = 0.1$. Other parameters are as in Fig. 1.

We found this generic behavior for a wide range of parameters. When $\lambda \in [0.03,0.2]$, $T \in [0.3,30.0]$, and $\delta \geqslant 0.01$, the spin chain has normal conductivity when $J_z \in [0.02,0.5]$ and anomalous conductivity when $J_z = 0$ (the conductivity seems to be normal for any $J_z > 0$, but given potential accuracy issues for $0 < J_z < 0.02$ we refrain from making a definite statement for these values). These results lead us to conjecture that it is the presence or absence of interactions, rather than integrability, that determines whether or not the heat transport is normal. We find no difference between thermal transport and spin transport, unlike the results of Prosen *et al.*[12] based on the local-operator Lindblad equation.

The conjecture may be tested further on various other models. One candidate is the Ising model in a transverse field B_x. It maps to noninteracting spinless fermions[34] and if we add a B_z field, it becomes interacting. Another closely related model is a system of spinless fermions on a tight-binding chain, with nearest-neighbor interaction

$$H_S = \epsilon \sum_{l=1}^{N} c_l^\dagger c_l - t \sum_{l=1}^{N-1} (c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l) + V_0 \sum_{l=1}^{N-1} c_{l+1}^\dagger c_{l+1} c_l^\dagger c_l, \tag{14}$$

$$H_B = \sum_{k,\alpha=L,R} \omega_{k,\alpha} b_{k,\alpha}^\dagger b_{k,\alpha}, \tag{15}$$

$$V_{SB} = \lambda \sum_{k,\alpha} (c_\alpha^\dagger b_{k,\alpha} + c_\alpha b_{k,\alpha}^\dagger). \tag{16}$$

The XXZ chains map exactly into this fermionic model after using the Jordan-Wigner transformation. However, the coupling to the baths in this fermionic system is different from that in the spin systems. For a spin system, the Jordan-Wigner transformation maps the σ^y operator into an operator, which is much more complicated than the $c^\dagger$ or c used in this fermionic model. Therefore, although the two models are closely related, they are not identical. Results for this fermionic model can be interpreted as another test of our conjecture or at least a check of whether the observations reported above are influenced by the specific model for the system-bath coupling.

In Fig. 5, we plot local-temperature profiles for Ising spin chains in panel (a) and for fermionic chains in panel (b). The results support our conjecture: interactions lead to normal transport. Similar results for Ising chains in transverse field B_x, with and without B_z terms, have been reported in Ref. 35. However, there the anomalous transport is assigned to integrability. Note that ϵ is set to be much larger than t to mirror the condition $B_z \gg J$. When ϵ is comparable to t, both noninteracting and interacting systems show almost flat temperature profiles.

In summary, the first conclusion we draw from these results is that integrability is not sufficient to guarantee anomalous transport: several integrable models show normal heat transport, in agreement with other studies.[9,11,12,29] The second conclusion is that only models that map onto Hamiltonians of noninteracting fermions exhibit anomalous heat transport.

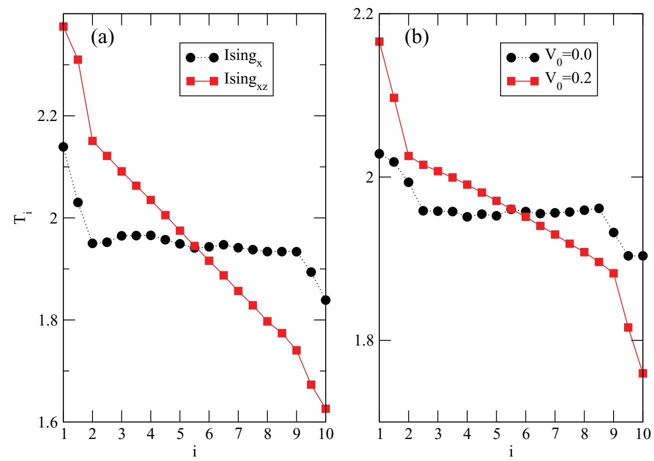

FIG. 5. (Color online) Temperature profiles for (a) Ising spin chains and (b) the V-t fermionic model described in the text. The Ising spin chains have anomalous transport when $B_z = 0$ (Ising$_x$, circles) and normal transport when $B_z = 1.0$ (Ising$_{xz}$, squares). The fermionic chains show a flat temperature profile when $V_0 = 0$ (circles) but a linear temperature drop when $V_0 = 0.2$ (squares). Other parameters are $J_z = 0.1$, $B_x = 1.0$, $\epsilon = 1.0$, $t = 0.1$, $T_L = 2.4$, $T_R = 1.6$, $\mu = -1.0$, $\lambda = 0.1$, $N = 10$.

This is a reasonable sufficient condition since, once inside the sample (past the contact regions), such fermions propagate ballistically. However, we can not, at this stage, demonstrate that this is a necessary condition as well. We therefore can only conjecture that this is the criterion determining whether the heat transport is anomalous. Unless our results are artifacts due to the boundary effects because of the limited system sizes, this conjecture is the only consistent qualitative conclusion that we may draw from all the above results.

In this context, it is important to emphasize again the essential role played by the connection to the baths. In its absence, an isolated integrable model is described by Bethe-ansatz-type wave functions. Diffusion is impossible since the conservation of momentum and energy guarantees that, upon scattering, pairs of fermions either keep or interchange their momenta. For a system connected to baths, however, fermions are continuously exchanged with the baths, and the survival of a Bethe-ansatz-type wave function becomes impossible. In fact, even the total momentum is no longer a good quantum number. We believe that this explains why normal transport in systems mapping to interacting fermions is plausible.

Anomalous transport can also occur in models that map to homogeneous interacting fermions if the bath temperatures are very low. Specifically, consider the XXZ models. Because of the large B_z we use, the ground state of the isolated chain is ferromagnetic with all spins up. The first manifold of low-energy eigenstates has one spin flipped (single-magnon states), followed by states with two spins flipped (two-magnon states), etc. The separation between these manifolds is roughly B_z, although because of the exchange terms each manifold has a fairly considerable spread in energies and usually overlaps partially with other manifolds. At very low temperatures, we find anomalous transport for all models, whether integrable or not, as shown in Fig. 6. This is reasonable since the one magnon

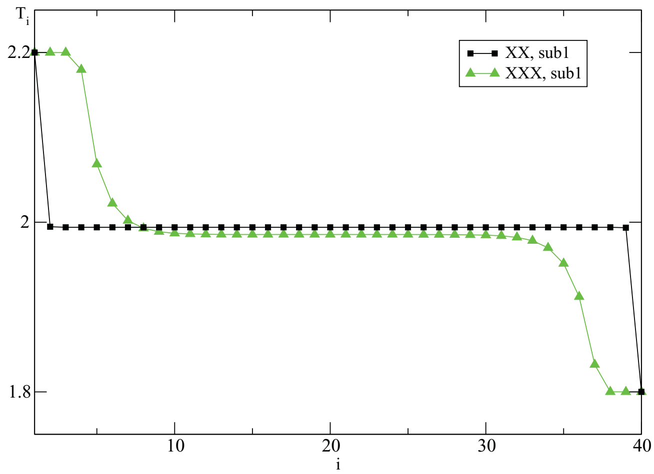

FIG. 6. (Color online) Temperature profiles for XX and XXZ chains are calculated within the single-magnon subspace. Parameters are as in Fig. 1 except here $N = 40$ and $\delta = 0.2$.

(fermion) injected on the chain at such low temperatures has nothing else to interact with, so it must propagate ballistically.

We may repeat this restricted calculation by including the two-magnon, three-magnon, etc., manifolds in the computation. As expected, when these higher-energy manifolds become thermally activated, the transport becomes normal for the models mapping to interacting fermions, in other words, as soon as multiple excitations (fermions) are simultaneously on the chain, and inelastic scattering between them becomes possible. When both $T_L, T_R \ll B_z$, effectively only the single-magnon states participate in the transport and the single-magnon subspace calculation is reasonably accurate. Then, even interacting systems have anomalous transport. These results may explain the heat transport observed experimentally in compounds such as Sr_2CuO_3[22] where, at low temperature, anomalous transport was found, while at high temperature, normal transport was reported. Reference 37 also finds similar behavior, but there the relatively small conductance at high temperature is attributed to phonon-mediated Umklapp scattering of the spinons. Of course, coupling to phonons or other degrees of freedom may well determine the behavior of the system, especially at higher temperatures. Therefore, we note that our study is relevant only for systems where phonon interactions are suppressed, due, for example, to low temperature. While such an assumption may not always hold, we believe that, from a purely theoretical point of view, it is an interesting question to understand the conductance of pure spin systems, as we have tried to do in this paper.

VI. CONCLUSIONS

Based on an extensive study of quantum spin chains using the Redfield equation, we propose a new conjecture for what determines the appearance of anomalous heat transport at all temperatures in finite spin chains. Unlike previous suggestions linking it to the integrability of the Hamiltonian or the existence of energy gaps, we propose that, for clean systems, the criterion is the existence of a mapping of the Hamiltonian onto a model of noninteracting fermions. While the existence of such mapping is certainly a sufficient condition for anomalous transport, we can not prove that it is a necessary condition as well; this conjecture, however, is the only conclusion consistent with all of our results.

We must also point out that we can not rule out the possibility that in the cases where anomalous transport is observed, there is partial overlap of the heat current operator with some conserved quantity. If this were the case, then our findings would be consistent with Ref. 14. Identifying such conserved quantities is a complicated task even in a closed system, and here it is made even more difficult by the coupling to the baths. Because of this coupling, even quantities such as the z-axis magnetization (total number of particles), which are usually conserved for isolated spin chains (fermionic Hamiltonians), are not conserved for the open system. Understanding how to identify the conserved quantities for the open system (if any) is certainly a very interesting question.

Also, our conjecture should be checked for larger systems, where more reliable information on the relation between J and N can be extracted. Such an enterprise is computationally too expensive if direct methods such as those described here are used. The more efficient methods based on the BBGKY-type method[32] might allow us to undertake such a study, but they require a clarification of the effect of the further approximations made there on the integrability of the system. Finally, we point out that, in this paper, we have not taken into consideration the possible coupling to other dissipative degrees of freedom, such as phonon modes,[36] which are also likely a factor in the emergence of normal transport.

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