Thermal transport in a spin-$\frac{1}{2}$ Heisenberg chain coupled to a magnetic or nonmagnetic impurity

A. Metavitsiadis,[1] X. Zotos,[1] O. S. Barišić,[2,3] and P. Prelovšek[3,4]

[1]*Department of Physics, University of Crete and Foundation for Research and Technology-Hellas, P.O. Box 2208, 71003 Heraklion, Greece*

[2]*Institute of Physics, HR-10000 Zagreb, Croatia*

[3]*J. Stefan Institute, SI-1000 Ljubljana, Slovenia*

[4]*Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia*

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We explore the effect of a (non-)magnetic impurity on the thermal transport of the spin-$\frac{1}{2}$ Heisenberg chain model. This unique system allows to probe Kondo-type phenomena in a prototype strongly correlated system. Using numerical diagonalization techniques we study the scaling of the frequency dependent thermal conductivity with system size and host-impurity coupling strength as well as the dependence on temperature. We focus in particular on the analysis of "cutting healing" of weak links or a magnetic impurity by the host chain via Kondo-like screening as the temperature is lowered.

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I. INTRODUCTION

A (non-)magnetic impurity coupled to a spin-$\frac{1}{2}$ Heisenberg chain is a prototype system that exemplifies "Kondo"-type effects in a correlated system. Starting with the proposal of Kane-Fisher,[1] a weak link in a repulsive (attractive) Luttinger liquid was shown to lead to an insulating (transmitting) ground state. The cutting or healing of spin chains by a variety of (non-)magnetic defects has also been established[2–5] as well as the effect of a magnetic impurity on the ground state of the anisotropic easy-plane Heisenberg chain.[6] Generically, a weak link or coupling to a magnetic impurity in a Heisenberg antiferromagnetic chain leads to a ground state corresponding to two open chains. In the exceptional case of two adjacent links or a ferromagnetic (attractive in the Fermionic language) easy axis anisotropy a healing of the defect is conjectured.[6] This screening effect is characterized by a Kondo-like temperature and screening length.[3,4] These phenomena have so far mostly been studied either as they are reflected on ground state properties, e.g., finite size gaps, entanglement or, somewhat indirectly, as a temperature-dependent induced staggered susceptibility.[3]

In this work we use an exceptional physical probe for the study of these effects, namely, the thermal transport in the spin-$\frac{1}{2}$ Heisenberg chain that is truly singular. Although the Heisenberg model describes a strongly correlated system, the thermal conductivity is purely ballistic as the energy current commutes with the Hamiltonian,[7] a result that is related to the integrability of this model.[8] Thus the only scattering present is due to the defect and thus its frequency/temperature/coupling strength dependence can be isolated and clearly analyzed. In this context it was already found that a single potential impurity renders the thermal transport incoherent[9] with the frequency dependence of the thermal conductivity well described by a Lorentzian, at least for a weak impurity. This is in sharp contrast to the case of a noninteracting system where in spite of the impurity the transport remains coherent described within the Landauer formalism by a finite transmission coefficient through the impurity. Thus, a single static impurity materializes the many-body character of scattering states.

Besides its theoretical interest, the effect of (non-)magnetic impurities on the thermal transport of quasi-one-dimensional materials as $SrCuO_2$, Sr_2CuO_3 and the ladder compound $La_5Ca_9Cu_{24}O_{41}$ has recently become possible to explore experimentally.[10]

In this work we use numerical diagonalization techniques—(full) exact diagonalization (ED), the finite-temperature Lanczos method (FTLM)[11] and the microcanonical Lanczos method (MCLM)[12]—to study the thermal transport in the Heisenberg chain model either coupled to a magnetic impurity or perturbed by single and double weak links. These state of the art techniques are crucial in the attempt to look for the subtle low temperature many-body effects associated with Kondo screening.

II. MODEL

We consider the one-dimensional anisotropic spin-$\frac{1}{2}$ Heisenberg model in the presence of a magnetic impurity out of the chain or weak links,

$$H = \sum_{l=0}^{L-1} J_{l,l+1} h_{l,l+1} + J'(s_0^x S^x + s_0^y S^y + \Delta' s_0^z S^z),$$

$$h_{l,l+1} = s_l^x s_{l+1}^x + s_l^y s_{l+1}^y + \Delta s_l^z s_{l+1}^z, \tag{1}$$

where $s^\alpha, \alpha = x,y,z$ are spin-$\frac{1}{2}$ operators, $J_{l,l+1} > 0$ the in-chain magnetic exchange coupling that we take antiferromagnetic, J' the chain-impurity coupling, Δ, Δ' anisotropy parameters and S a spin-S magnetic-impurity operator ($\hbar = 1$). In this work we mostly consider a spin-$\frac{1}{2}$ impurity. We assume periodic boundary conditions, $\mathbf{s}_L = \mathbf{s}_0$, and uniform couplings $J_{l,l+1} = J$, except in the study of weak links (see below). We vary the anisotropy parameters Δ, Δ', with $\Delta = \Delta'$, in order to look for the (healing) cutting of the chain effects mentioned above.

In our study, based on standard linear response theory, the frequency ω dependence of the real part of the thermal conductivity (regular component) is given by

$$\kappa(\omega) = -\frac{\beta}{\omega}\chi''(\omega), \quad \chi(\omega) = \frac{i}{L}\int_0^{+\infty} dt e^{i\omega t}\langle[j^\epsilon(t), j^\epsilon]\rangle, \quad (2)$$

where $\beta = 1/T$, T is the temperature and $k_B = 1$. We determine the energy current from the hydrodynamic $(q \to 0)$ limit of the energy continuity equation $\partial H_q/\partial t \sim q j^\epsilon$ with $H_q = \Sigma_l e^{iql} h_{l,l+1}$ as,

$$j^\epsilon = \sum_{l=0}^{L-1} J_{l-1,l} J_{l,l+1} \mathbf{s}_l \cdot (\mathbf{s}_{l+1} \times \mathbf{s}_{l-1}) + \frac{JJ'}{2}\mathbf{s}_0 \cdot (\mathbf{S} \times \mathbf{s}_{L-1} + \mathbf{s}_1 \times \mathbf{S}), \quad (3)$$

showing for simplicity the case $\Delta = 1$ ($\Delta \neq 1$ is obtained by $s_l^z \to \Delta s_l^z$ in the cross-product terms). When $J' = 0$ and all $J_{l,l+1} = J$ the energy current commutes with the Hamiltonian, the transport is purely ballistic and the thermal conductivity consists of only a $\delta(\omega)$-peak proportional to the thermal Drude weight.

III. HIGH-TEMPERATURE LIMIT

Starting from the high-temperature ($\beta \to 0$) limit we can obtain a first impression on the behavior of the frequency dependence of $\kappa(\omega)$ from the zeroth and second moments, $\mu_n = \int d\omega \omega^n \kappa(\omega)$, which are equal to (for the isotropic point, $\Delta = 1$),

$$\mu_0 = \text{const} \times \frac{6}{T^2}\left(J^2 + \frac{2}{L}\mathcal{B}^2\right), \quad \left(\text{const} = \pi\frac{J^2}{64}\right)$$

$$\mu_2 = \text{const} \times \frac{\mathcal{B}^2}{LT^2}(39J^2 - 12JJ' + 3J'^2 + 36\mathcal{B}^2), \quad (4)$$

where $\mathcal{B}^2 = (J'^2/3)S(S+1)$ is the characteristic impurity spin dependence. One could expect the second moment to reflect the width of $\kappa(\omega)$ and, thus, to be related to the inverse scattering time $1/\tau$. We note that for this impurity problem an assumption of a Gaussian form $\kappa(\omega) = \kappa_{dc}\exp^{-(\omega\tau)^2}$ would imply from the L dependence of $\mu_{0,2}$ that $\kappa_{dc} = \kappa(0)$ would scale as $\sqrt{L}$ and $1/\tau \sim 1/\sqrt{L}$. This is, however, incorrect as is also evident from the disagreement with higher moments, $n > 2$, which behave all as $\mu_n \propto 1/L$. For weak-coupling cases, such as a single impurity weakly coupled to the host chain, we should therefore rather expect a Lorentzian-like frequency dependence with a static $\kappa(0) \propto L$ and a characteristic frequency width $1/\tau \propto 1/L$.

In Fig. 1 we show the frequency dependence of the thermal conductivity, normalized and appropriately scaled with system size. Note that in the high-$T(\beta \to 0)$ limit the relevant (but still nontrivial) quantity is $T^2\kappa(\omega)$, which is implicitly extracted by the normalization. We thus present results of the normalized $\kappa(\omega L)/L$ for a weak, $J' = 0.5J$ and strong, $J' = 2J$ coupling case respectively. The data up to $L = 16$ were obtained by full ED while for $L = 18-22$ the MCLM was used.[12] The δ-peaks at the excitation frequencies are binned in windows $\delta\omega = 0.01$, which also gives the frequency resolution of the spectra. For $J' = 0.5J$ we find a simple Lorentzian form while in the strong coupling case the behavior is nonmonotonic with a maximum at a finite frequency $O(1/L)$. In both cases the proposed L scaling is indeed realized.

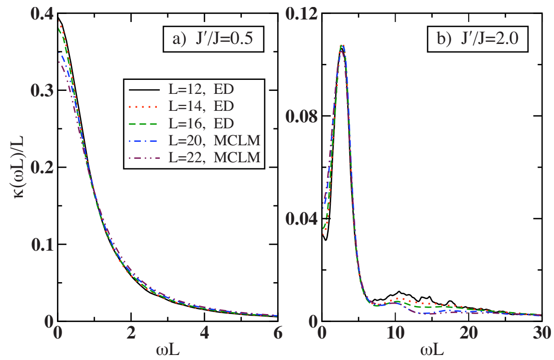

FIG. 1. (Color online) Frequency-dependent thermal conductivity in the high-T limit scaled as $\kappa(\omega L)/L$ for $(\Delta = 1)$: (a) weak coupling $J' = 0.5J$, (b) strong coupling $J' = 2J$ (curves are normalized to unity).

As for the scaling with impurity spin S suggested by the proportionality of the second moment to $\mathcal{B}^2 = (J'^2/3)S(S+1)$ we show in Fig. 2 MCLM results for $\kappa(\omega L)/L$ for a series of S-values and couplings J' so that the effective perturbation strength $\mathcal{B}^2$ retains its value. We find indeed that at both weak as well as strong coupling the scaling is well obeyed, giving a wider applicability to our results. They can be applied to a range of impurity spin values becoming directly relevant in the interpretation of experiments.

Now let us address the generic $L \to \infty$ behavior. We can discuss it by considering the memory function $N(\omega)$ representation defined via the general complex function $\bar{\kappa}(\omega)$,

$$\bar{\kappa}(\omega) = i\beta\frac{\chi_0}{\omega + N(\omega)}, \quad \chi_0 = \chi(\omega \to 0). \quad (5)$$

where the real $\kappa(\omega) = \bar{\kappa}'(\omega)$ and $N''(\omega) \sim 1/\tau$ plays the role of the (frequency dependent) thermal-current relaxation rate. The lowest moments μ_n can be evaluated (in principle) ex-

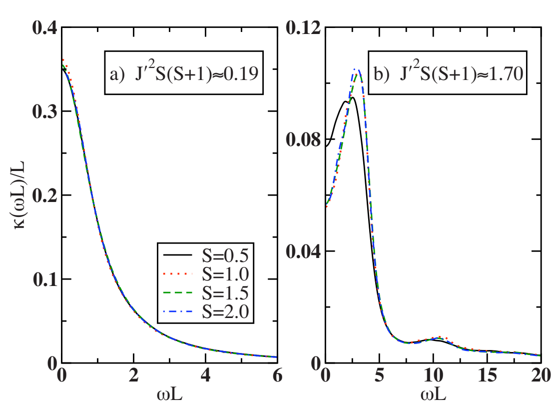

FIG. 2. (Color online) Frequency dependence of the normalized thermal conductivity $\kappa(\omega L)/L$ in the high-T limit for a variety of impurity spin values $S = 1/2, 1, 3/2, 2$ and for: (a) $J'/J = 0.5, 0.3, 0.22, 0.18$ corresponding to the weak coupling $\mathcal{B}^2 = (J'^2/3)S(S+1) \simeq 0.06$, and (b) $J'/J = 1.5, 0.92, 0.67, 0.53$ corresponding to the stronger coupling $\mathcal{B}^2 \simeq 0.57$.

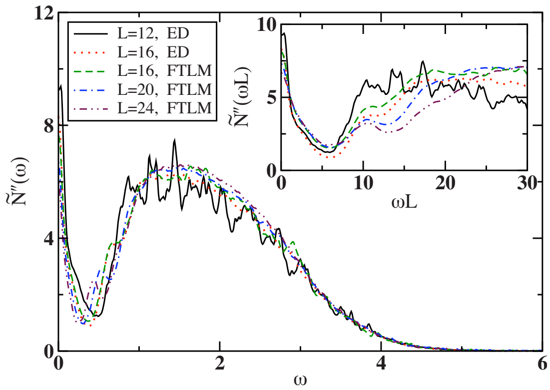

FIG. 3. (Color online) Memory function $\tilde{N}''(\omega)$ for a strong coupling $J'=2J$ and for various lattice sizes $L=12-24$, using both ED and FTLM. Inset: the scaled function $\tilde{N}''(\omega L)$ is shown at low frequencies.

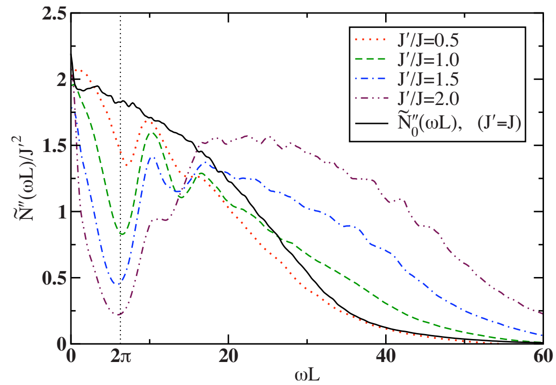

FIG. 4. (Color online) Impurity coupling J' dependence of scaled $\tilde{N}''(L\omega)/J'^2$ and the comparison with the perturbative result. Results are obtained for $\Delta=1$ and $L=16$ via ED.

actly in the high-T limit[13] on a finite size lattice of L sites. Involving only local quantities, at least for $0<n<L/2$, they should behave as $\mu_n=\tilde{\mu}_n/L$ whereby $\tilde{\mu}_n$ is size independent for $n<L/2$. It is plausible that also higher moments, $n>L/2$, behave as $\mu_n\propto 1/L$. If $\tilde{\mu}_n$ for $n>L/2$ would be also size independent, then this would imply the scaling $N(\omega)=\frac{1}{L}\tilde{N}(\omega)$, with a universal (size independent) $\tilde{N}(\omega)$. Consequently

$$\bar{\kappa}(\omega)=\frac{i\beta\chi_0 L}{(\omega L)+\tilde{N}(\omega)},\tag{6}$$

with the real part $\kappa(\omega)$ for $L\to\infty$ and $\omega\to 0$ obeying the Lorentzian scaling relation,

$$\frac{\kappa(\omega L)}{L}=\frac{\beta\chi_0\tilde{N}''(\omega\to 0)}{(\omega L)^2+\tilde{N}''(\omega\to 0)^2},\tag{7}$$

provided that $N''(\omega\to 0)$ is finite. This is, however, clearly not what we observe in Fig. 1, where from the non-Lorentzian shape we must conclude that the memory function also scales as $\tilde{N}(\omega L)$ and thus,

$$\frac{\kappa(\omega L)}{L}=\frac{\beta\chi_0\tilde{N}''(\omega L)}{[\omega L+\tilde{N}'(\omega L)]^2+\tilde{N}''(\omega L)^2}.\tag{8}$$

This is not in contradiction with the moments argument, since the higher moments, $n>L/2$, determine the low frequency behavior. So we can argue that at high frequencies $\tilde{N}(\omega)$ scales as ω while at low frequencies as ωL. This scenario is indeed verified in Fig. 3 at the low/high-frequency regimes, where $N(\omega)$ is extracted from the $\kappa(\omega)$ data. The FTLM method is used for lattice sizes $L\geq 16$ with $M_L=500$ Lanczos steps and smoothed with an additional frequency broadening $\delta\omega=0.03$. On the other hand, we can also explain the observed general $\kappa(\omega L)/L$ scaling with the similarity to a noninteracting system—with an impurity. In the latter case, the characteristic scaling $L\omega$ is signature of "free" oscillations in the system.

To study the crossover from weak to strong coupling regime we show in Fig. 4 the evolution of the relaxation-rate function $\tilde{N}''(\omega L)$ with impurity coupling J' along with a perturbative evaluation $\tilde{N}''_0(\omega L)$ using the eigenstates of the Hamiltonian without the impurity.[14] It is interesting that the memory function shows an increasingly pronounced structure with minima at approximately the same frequencies, multiples of $2\pi/L$ *independently of* J' and which are not present in the perturbative calculation. In particular the characteristic frequency of the minima decreases as the anisotropy parameter Δ decreases and thus it apparently related to the velocity of elementary excitations (spinons) in the system. We can conjecture that this peak structure is due to a resonant mode, created by multiple forward/backward scattering on the impurity, characteristic for the noninteracting system. It is remarkable that this happens even in this high-temperature limit. This effect has already been seen in integrable systems where a perturbation seems to affect the totality of the energy spectrum.[13] Now the picture is clear, $\tilde{N}''(\omega)$ increases as J'^2, scales as ωL at low frequencies and at the same time develops a structure that dominates the behavior of $\kappa(\omega L)$ turning the Lorentzian weak-coupling shape to a nontrivial one at strong coupling.

IV. WEAK LINKS—FINITE *T*

Next we examine the behavior of the thermal conductivity $\kappa(\omega)$ as we lower the temperature, starting with the influence of static weak exchange links.

Kane-Fisher[1] for a Luttinger liquid and Eggert and Affleck[2] (EA) for the isotropic spin-$\frac{1}{2}$ Heisenberg chain, proposed that a weak link leads to an open chain (cutting) in the low energy limit. In contrast, a defect of two adjacent weak links is "healed" leading to a uniform chain at $T=0$.

To analyze this effect we consider a chain with only one weak link, that is one altered bond with coupling e.g., $J_{0,1}=\tilde{J}$ in an otherwise uniform chain ($J'=0$, there is no spin impurity). The characteristic Kane-Fisher temperature is given in the weak coupling limit by $T_{KF}\sim(J-\tilde{J})^2/J$. In Fig. 5(a) we show the corresponding $\kappa(\omega L)/L$ for $\tilde{J}=0.7J$ and a

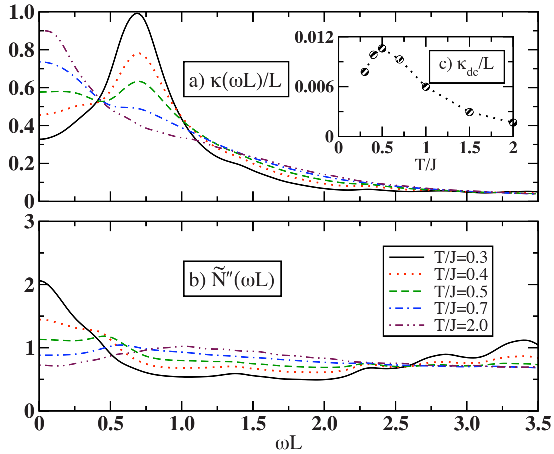

FIG. 5. (Color online) Frequency dependence of: (a) the normalized thermal conductivity $\kappa(\omega L)/L$, (b) the extracted memory function $\tilde{N}''(\omega L)$, for a chain of $L=22$ sites with one weak link $\tilde{J}=0.7J$ and various $T/J=0.3$–2.0. (c) Temperature dependence of $\kappa_{dc}(T)/L$.

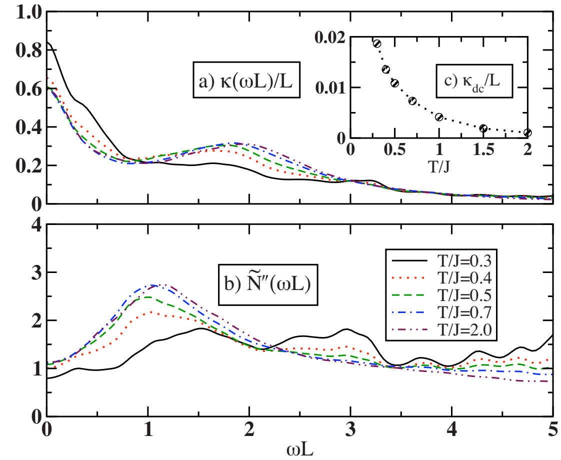

FIG. 6. (Color online) Frequency dependence of: (a) the normalized thermal conductivity $\kappa(\omega L)/L$, (b) the extracted memory function $\tilde{N}''(\omega L)$ for a chain of $L=22$ sites with two adjacent weak links $\tilde{J}=0.7J$ and various $T/J=0.3$–2.0. (c) Temperature dependence of $\kappa_{dc}(T)/L$.

series of temperatures. The data are obtained using the FTLM method for a chain of $L=22$ spins, by $M_L=2000$ Lanczos steps and smoothed by an additional frequency broadening $\delta\omega=0.007$. From Fig. 5(a) we notice that $\kappa(\omega L)/L$ develops a strongly nonmonotonic frequency dependence by lowering the temperature, with a maximum at a finite frequency that suggests a flow to the strong coupling limit similar to the one discussed before by increasing J'. In Fig. 5(b), the extracted $\tilde{N}''(\omega L)$ for various T is presented, with the development of a characteristic structure that explains the nonmonotonic behavior of $\kappa(\omega)$. The increasing value of $\tilde{N}''(0)\sim 1/\tau$ with decreasing temperature indeed corresponds to the effect of "cutting" of the chain.

Nonmonotonic is also the frequency dependence of $\kappa(\omega L)/L$ for the case of two adjacent equal weaker links, $J_{L-1,0}=J_{0,1}=\tilde{J}=0.7J$, as shown in Fig. 6(a). However, in this case we observe in Fig. 6(b) the opposite behavior of $\tilde{N}''(\omega)$. Namely, "healing" of the double defect deduced by the decreasing $\tilde{N}''(0)$ as the temperature is lowered in agreement with theoretical prediction.[2] We should note that both cutting/healing are low-frequency effects at frequencies ωL $O(1)$.

To summarize the observed behavior we show in Fig. 7, the T dependence of the relaxation rate $\tilde{N}''(0)$ for two different couplings $\tilde{J}/J=0.5,0.7$, for one and two weak links, respectively. The presented results confirm the existence of the cutting behavior at low T for a single link, as well as the healing by lowering T for two adjacent and equal links. As expected, both effects appear only at low $T/J<1$ while the dependence of the characteristic T_{KF} on $\tilde{J}/J$ is less pronounced.

V. SPIN COUPLED TO THE CHAIN—FINITE *T*

Finally we can study the effect of lowering the temperature on the scattering by a magnetic impurity. According to EA it leads to cutting the chain at $T=0$ irrespective of the sign of J'. This proposal was extended by Furusaki and Hikihara[6] to the anisotropic spin chain $-1<\Delta\leq 1$ where they furthermore proposed that for $-1<\Delta<0$ (attractive case in the Fermionic language) there is "healing" of the impurity, in analogy to the case of two adjacent weak links.

In the Kondo problem the characteristic temperature in the weak coupling limit is given by $T_K\sim v\,\exp(-c/J')$ with c being a constant, the velocity of spin excitations and J' the Kondo coupling. In the case of a spin-$\frac{1}{2}$ chain it was shown[15] that the exponential dependence is replaced by $T_K\sim\exp(-\pi\sqrt{1/J'-(S'+1/2)^2})$ and a next-nearest neighbor coupling $J_2\simeq 0.2412$ is needed to recover the traditional Kondo case. We should note that in the model studied the impurity spin is attached only at the end of the chain—in contrast to our model—but plausibly the behavior is qualitatively similar. To get a qualitative idea of orders of magnitude for our problem[5] for $J'=0.3J$, $T_K\sim 0.014$, $\xi_K\sim 40$, for $J'=0.6J$, $T_K\sim 0.388$, $\xi_K\sim 4$, and $J'=J$, $\xi_K=0.65$. As in our study we are limited to $T\gtrsim 0.4$ in order to see a "Kondo" crossover we

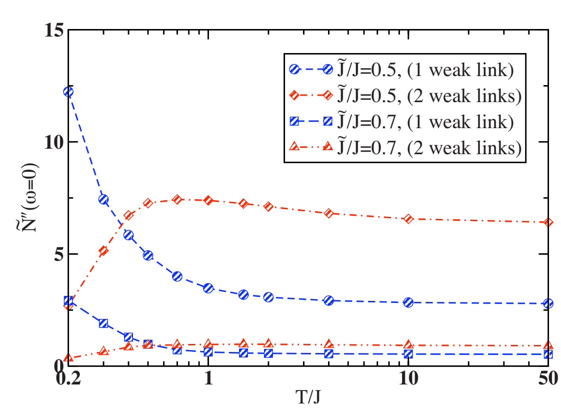

FIG. 7. (Color online) Temperature dependence of $\tilde{N}''(0)$ for $\tilde{J}=0.5,0.7J$ showing cutting/healing behavior for one and two weak links.

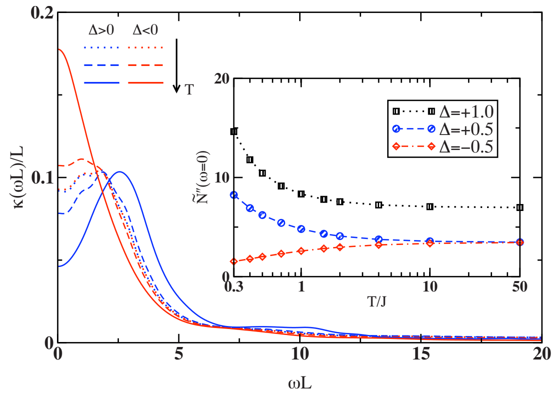

FIG. 8. (Color online) Frequency dependent normalized thermal conductivity $\kappa(\omega L)/L$ for strong coupling $J'=2J$, $\Delta=\pm0.5$, and three $T/J=50,2,0.4$. Inset: T-dependence of $N''(0)$ for $\Delta=\pm0.5$ and $\Delta=+1$.

must consider a coupling $J'\geq 0.5J$ and thus we are in the relatively strong coupling regime, with typical screening length of the order $\xi_K \sim 1$.

In Fig. 8 we show $\kappa(\omega L)/L$ for a chain of $L=22$ sites at strong coupling $J'=2J$ and two representative cases $\Delta=\pm0.5$ as we lower the temperature. Indeed we find at low frequencies the gradual development of the corresponding "cutting/healing" behavior, which we exemplify in the inset by $\tilde{N}''(0)$ as a function of temperature both for $\Delta=\pm0.5$ and the most typical isotropic case $\Delta=+1.0$. It is remarkable that the tendency to increase-decrease the scattering time is already evident from high T, presumably due to the local character of the effect because of the strong J' coupling. We note in passing that the ωL scaling is found not just at high T but rather at all T (not shown).

Next in Fig. 9 we show $\tilde{N}''(0)$ as a function of T for a series of increasing J' couplings. The "cutting" effect for the repulsive case $\Delta=+0.5$ is present for all values of J' with no easily distinguishable "Kondo" temperature. We are always dealing with screening lengths well less than the system size where presumably no subtle many-body effects come into play. On the other hand, in the attractive case $\Delta=-0.5$, we do not observe "healing" for the weakest coupling $J'=+0.5$ where the screening length is expected to be several lattice sites.

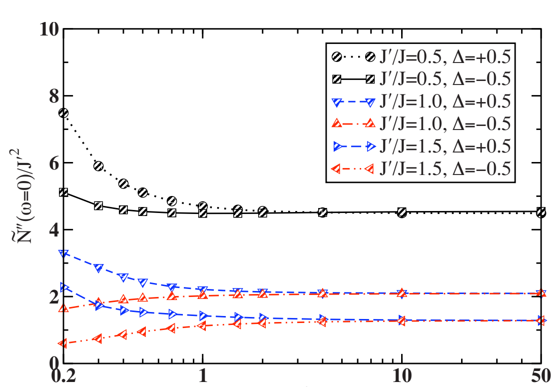

FIG. 9. (Color online) $\tilde{N}''(0)$ vs T for the repulsive (attractive) case $\Delta=+0.5(-0.5)$ for different $J'/J=0.5,1.0,1.5$.

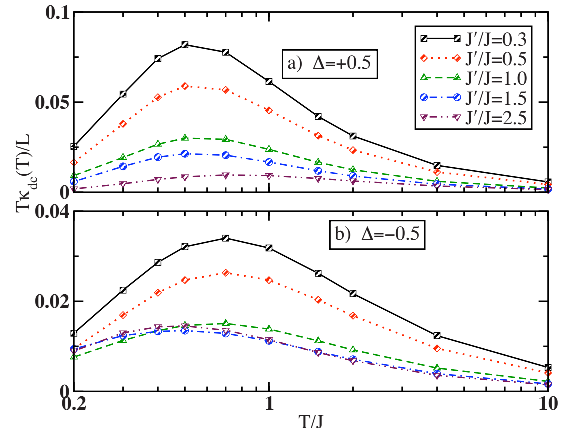

FIG. 10. (Color online) Temperature dependence of κ_{dc}/L for a variety of impurity couplings J' and for: (a) repulsive $\Delta=+0.5$, (b) attractive $\Delta=-0.5$.

Finally, in Fig. 10 we summarize the T-dependence of κ_{dc}/L for a variety of coupling strengths J'/J and $\Delta=\pm0.5$. The experimentally most interesting case $\Delta=+1$ corresponding to isotropic antiferromagnetic as well as ferromagnetic impurity coupling is shown in Fig. 11. For $\Delta>0$ we observe in Figs. 10(a) and 11 a continuous decrease in the κ_{dc} with increasing J'. This can be explained with the formation of a local singlet, at least for $T<J'$ which blocks the current through the impurity region. On the other hand, the $\Delta<0$ case in Fig. 10(b) reveals a saturation of κ_{dc} with J', at least for intermediate large J'. However, for severe perturbations ($J'\gg J$) the impurity cannot be healed by the chain leading inevitably to a further decrease in the κ_{dc}.

VI. CONCLUSIONS

In conclusion, by analyzing the unique behavior of the thermal conductivity of the spin-$\frac{1}{2}$ Heisenberg model several effects of the local static and dynamical impurities have been established:

(a) A single local impurity, either static as the local field[9] and weak link, or dynamical as the spin coupled to the chain

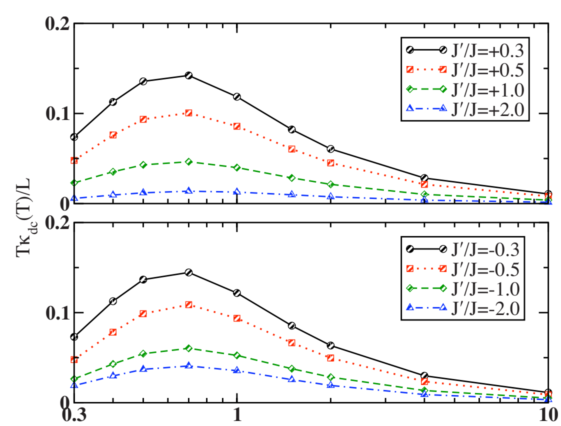

FIG. 11. (Color online) Temperature dependence of κ_{dc}/L for a variety of impurity couplings J', $\Delta=1$ and for: anti-ferromagnetic couplings (top), ferromagnetic couplings (bottom).

turn the dissipationless thermal conductivity into an incoherent one. Numerical results for the dynamical conductivity, best studied at high-T, reveal that a single impurity in a system of L sites shows a universal scaling form $\kappa(\omega L)/L$ at least in the low-ω regime. For weak perturbation, as weakly coupled spins outside the chain, the scaling form is of the simple Lorentzian type. On the contrary large local perturbation can lead to a nontrivial form with the maximum response at $\omega > 0$.

(b) Furthermore, universal oscillations in the dynamical relaxation rate $N''(\omega)$ become visible, from the weak coupling regime already, with the period $\omega \propto 1/L$ being a remnant of the impurity multiple-scattering phenomena in a noninteracting system.

(c) Our results confirm the existence of the Kondo-type effects of impurities on lowering the temperature. In the case of weak links and for the isotropic Heisenberg model cutting and healing effects are observed at lower T for a single weak link and a pair of identical weaker links, respectively, in accordance with theoretical predictions.[1,3] In the case of a spin coupled to the chain the cutting/healing effects at low T depend on the sign of the anisotropy Δ. For ferromagnetic anisotropy ($\Delta < 0$), the chain screens the impurity and the system enters the weak coupling regime as the temperature is decreased. The opposite behavior is obtained for antiferromagnetic anisotropy ($\Delta > 0$), where the system flows to the strong coupling limit at lower temperatures.

(d) Obtained data can be used to model the behavior observed in experiments on materials with spin chains doped with magnetic and nonmagnetic impurities.[10]

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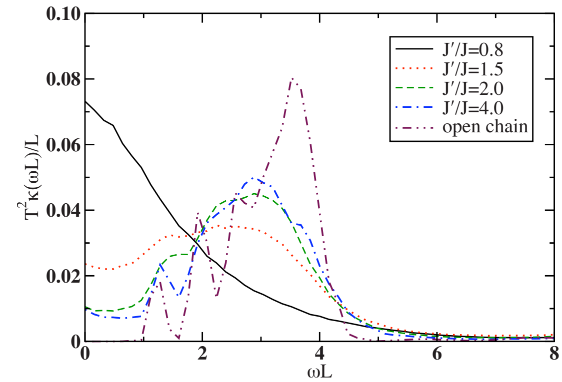

FIG. 12. (Color online) Frequency dependence of the thermal conductivity $\kappa(\omega L)/L$ in the high temperature limit for various values of the coupling $J'/J = 0.8 - 4.0$ and $\Delta = 1.0$.

APPENDIX: OPEN CHAIN

Throughout the article the term "cutting" is used to describe the behavior of the system in the strong coupling limit. In order to justify the term "cutting," we present in Fig. 12 results for the thermal conductivity of a chain of $L = 16$ sites obtained by ED in the high-temperature limit for various couplings J' and the thermal conductivity of a uniform chain with open boundary conditions as well. Figure 12 illustrates the flow of the system from a Drude-like behavior (weak coupling) to a chain with open boundary conditions (strong coupling), which was already proposed for a single nonmagnetic impurity (a local field) from the level statistics analysis.[9] We choose to present the jagged results, i.e., without implementing any smoothing procedure, in order not to wash out the development of the narrow peaks corresponding to the excitations of the open chain. For the strong coupling cases there is some rather significant structure at frequencies $\sim J'$, which correspond to local excitations of the impurity. However, these excitations are irrelevant for the effect of the impurity on the chain which is studied here.

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