Spin conductivity in almost integrable spin chains

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The spin conductivity in the integrable spin-1/2 *XXZ* chain is known to be infinite at finite temperatures T for anisotropies $-1<\Delta<1$. Perturbations, which break integrability, e.g., a next-nearest neighbor coupling J', render the conductivity finite. We construct numerically a nonlocal conserved operator $J_{\parallel}$ which is responsible for the finite spin Drude weight of the integrable model and calculate its decay rate for small J'. This allows us to obtain a lower bound for the spin conductivity $\sigma_s \geqslant c(T)/J'^2$, where $c(T)$ is finite for $J' \to 0$. We discuss the implication of our result for the general question how nonlocal conservation laws affect transport properties.

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I. INTRODUCTION

The behavior of transport properties of integrable systems have attracted considerable interest in the recent past.[1–21] In such models due to the presence of conservation laws, the currents do not decay.[1] As a consequence, the dc conductivity is infinite and characterized by a finite Drude weight D, $\mathrm{Re}\,\sigma(\omega)=\pi D\delta(\omega)+\sigma_{\mathrm{reg}}(\omega)$, where σ_{reg} is the regular part of the conductivity.

In real systems, those conservation laws are violated by perturbations which often can be considered to be small. In these situations, the conductivity becomes finite[1–6] but remains very large as long as the perturbations are small.

A both theoretically[6–15,22] and experimentally[18–20] well studied example is the *XXZ* Heisenberg chain which is equivalent to a model of spinless Fermions with nearest neighbor interactions.

The *XXZ* Heisenberg chain is integrable and therefore an infinite number of constants of motion exist for this model. All eigenstates can be uniquely labeled by a complete set of commuting operators, Q_n with $[Q_n,Q_m]=0$ for all n,m. The first two of these operators are given by the total magnetization $Q_1=\Sigma_k S_k^z$ and the Hamiltonian

$$H_0 = Q_2 = \sum_i h_i, \tag{1}$$

$$h_i = J(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z). \tag{2}$$

All other Q_n can be constructed by a simple recursive formula,[22] $Q_{n+1}=[B,Q_n]$, with the so-called boost operator $B=1/(2i)\Sigma_j j h_j$. All these conservation laws have a property which is important for the following discussion: they are *local* operators in the sense that each Q_n can be written in terms of a local "density" $q_{n,i}$ at site i,

$$Q_n = \sum_i q_{n,i}, \tag{3}$$

where $q_{n,i}$ is local as it contains only spin operators S_j^{α} on maximally n adjacent sites, $i \leqslant j < i+n$.

Besides the Q_n, there exist a huge number of other conservation laws C_i which can in principle be constructed from the exact eigenstates $|j\rangle$, $[H_0,|j\rangle\langle j'|]=0$ for $E_j=E_{j'}$. In general, these operators are highly nonlocal objects in the sense that they cannot be written in the form [Eq. (3)] for finite n.

Only local conservation laws are associated with a continuity equation $\partial_t q_{n,k}+j_{n,k+1}-j_{n,k}=0$, where $j_{n,k}$ is the corresponding current density, and therefore only for local conservation laws a hydrodynamic description can be formulated. A main motivation for the present work is the question to what extent nonlocal conservation laws are relevant in the sense that they lead to experimentally observable consequences in real materials. We therefore study the role of local and nonlocal conservation laws for transport in *XXZ* Heisenberg chains perturbed by weak next-nearest neighbor couplings J'.

For $J'=0$, both the heat conductivity κ and the spin conductivity σ_s (or, equivalently, the electric conductivity in the Fermionic language) are infinite and have a finite Drude weight. However, there is a main conceptual difference between those two cases: the heat current J_E is conserved (and actually given by Q_3 as defined above), while the spin current J_s does not commute with the Hamiltonian. Nevertheless, the presence of a finite Drude weight implies that a certain fraction of the spin current does not decay in time: part of the spin current is "protected" by conservation laws. This has been formalized many years ago by Mazur[23] and later generalized by Suzuki.[24] Suzuki showed that the Drude weight can be expressed in terms of correlators of the current with the conservation laws C_i,

$$D_s = \frac{\beta}{N}\sum_i \frac{\langle J_s C_i\rangle^2}{\langle C_i^2\rangle}, \tag{4}$$

where $\beta=1/T$, N is the number of sites, and the C_i have been chosen such that $\langle C_i C_j\rangle=0$ for $i\neq j$. Note that in Eq. (4), the sum runs over a basis of *all* conservation laws, local and nonlocal, commuting and noncommuting.

Interestingly, it can be shown[1] by simple symmetry arguments that the spin current is orthogonal to all known local conservation laws, $\langle J_s Q_n\rangle=0$ for all n. Therefore, it seems that nonlocal conservation laws are responsible for the infinite conductivity of the integrable model. What will happen to the spin current when the system is weakly perturbed, e.g., by a next-nearest neighbor coupling J' with $J' \ll J$? For local conservation laws, e.g., the heat current Q_3, the answer is known:[6] for small J', Q_3 decays only slowly implying a large dc conductivity proportional to the lifetime of Q_3. Our present goal is to investigate whether the spin conductivity shows a similar behavior.

An example which shows that perturbation theory for local and nonlocal quantities can be drastically different has been discussed in Ref. 25. In this paper, it has been shown that an arbitrarily small interchain coupling can destroy a nonlocal order parameter (e.g., the string order of a spin-1 Haldane chain) in a gapped system. Formally, the perturbations turn out to be proportional to the length of the system. In contrast, local order parameters are always robust against small perturbations for all gapped systems.

In principle, one can try to investigate the transport properties for small J' directly by calculating the spin conductivity from an exact diagonalization of the *XXZ* chain in the presence of finite J'. In such a calculation, Heidrich-Meisner *et al.*[3] were able to show that the spin Drude weight vanishes in the thermodynamic limit, but a reliable determination of the resulting finite spin conductivity is rather difficult even for large J'. Furthermore, finite size effects grow rapidly[3] for small J'.

In the following, we will therefore use a different approach based on a perturbation theory in J'. We construct numerically a nonlocal operator $J_\parallel$ which is conserved for $J'=0$ and responsible for the finite Drude weight of the unperturbed *XXZ* Heisenberg chain. In a second step, we derive a lower bound for the spin conductivity of the perturbed system using results of Ref. 5 and show that the spin conductivity is proportional to $1/J'^2$. Finally, we analyze to what extent $J_\parallel$ is a nonlocal operator and discuss how the result can be interpreted. The Appendix investigates the role of special values of the anisotropies where the Heisenberg model possesses extra symmetries.

II. MODEL

We consider the following Hamiltonian:

$$H = H_0 + H_1, \tag{5}$$

where the *XXZ* Heisenberg chain H_0 has been defined in Eq. (1) and

$$H_1 = J' \sum_k S_k^x S_{k+2}^x + S_k^y S_{k+2}^y + \Delta S_k^z S_{k+2}^z \tag{6}$$

describes the (small) next-nearest neighbor coupling. For this model, the spin current J_s is given by

$$J_s = \frac{i}{2} J \sum_k (S_k^+ S_{k+1}^- - S_k^- S_{k+1}^+) + O(J'), \tag{7}$$

and we have omitted terms linear in J' as they give only subleading contributions to our final result.

For $J'=0$ and $-1<\Delta<1$, the Drude weight defined by

$$\mathrm{Re}\ \sigma_s(\omega) = \pi D \delta(\omega) + \sigma_{\mathrm{reg}}(\omega) \tag{8}$$

is finite[9,10,17] at $T>0$ as discussed above. Equation (4) implies that the finite Drude weight is associated with constants of motion C_i of H_0 with $\langle C_i J_s \rangle \neq 0$, which we need to identify for our further analysis. More precisely, one can split the current operator into two pieces,

$$J_s = J_\parallel + J_\perp, \tag{9}$$

with

$$J_\parallel = \sum_i \frac{\langle J_s C_i \rangle}{\langle C_i^2 \rangle} C_i. \tag{10}$$

$J_\parallel$ can be interpreted as the projection of the the spin current to the space of conserved quantities, i.e., the conserved part of J_s and, indeed, one obtains directly from Eq. (4),

$$D_s = \frac{\beta}{N} \langle J_\parallel^2 \rangle. \tag{11}$$

As described above, the known local conservation laws Q_n do not contribute to J_s, i.e., $\langle J_\parallel Q_n \rangle = 0$. $J_\parallel$ is a very complex nonlocal operator which is difficult to construct and handle analytically. For finite size systems with up to 20 sites, however, one can construct $J_\parallel$ numerically using the exact eigenstates of H_0. As the C_i span the space of energy diagonal operators, we just keep the energy diagonal part of J_s, i.e.,

$$\langle n | J_\parallel | m \rangle = \delta_{E_m E_n} \langle n | J_s | m \rangle. \tag{12}$$

For a finite value of the perturbation J', the Drude weight [Eq. (11)] is absent, as is known from numerical studies[3,16] which were, however, not able to investigate the regime of small J' due to large finite size effects in this limit.

In Ref. 5, we have shown that a lower bound for the leading order contribution to the conductivity σ_s can be obtained in the limit of small J' by evaluating the correlation function $\tilde{\Gamma}$ with respect to H_0,

$$\mathrm{Re}\ \tilde{\Gamma}(\omega) = \frac{1}{N} \int_0^\infty dt e^{i\omega t} \langle [\dot{J}_\parallel(t), \dot{J}_\parallel(0)] \rangle_0. \tag{13}$$

As $[J_\parallel, H_0]=0$, $\tilde{\Gamma}(\omega)$ is proportional to J'^2. The inequality for the spin conductivity reads

$$\sigma_s \geq \frac{\chi^2}{\tilde{\Gamma}(0)}, \tag{14}$$

where $\chi = \beta \langle J_\parallel J_s \rangle / N = D_s$ is the generalized (spin current) susceptibility and $\tilde{\Gamma}(\omega)/\chi$ can be interpreted as a scattering rate of $J_\parallel$, see Ref. 5 for details. Next, we will present our analysis of the correlation function [Eq. (13)].

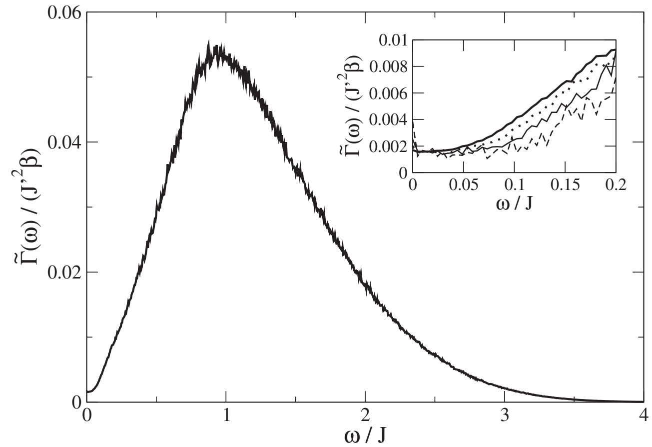

FIG. 1. Leading order contribution to the spin current relaxation rate for $\Delta=0.75$ and system size $L=20$ for $T\rightarrow\infty$. Finite size effects are small and $\tilde{\Gamma}(\omega)$ is finite at $\omega=0$, as can be seen in more detail in the inset (thick line $L=20$, dotted line $L=18$, thin line $L=16$, and dashed line $L=14$).

III. NUMERICAL RESULTS

We investigate $\tilde{\Gamma}(\omega)$ and the generalized susceptibility χ numerically in the $T\rightarrow\infty$ limit via exact diagonalization for system sizes up to $L=20$ and for various anisotropies Δ usingperiodic boundary conditions. In this high temperature limit, the spin-spin correlation length vanishes and therefore finite size effects are smallest. Results for finite $T\gg J$ (not shown) are essentially identical.

The results for an intermediate $\Delta=0.75$ are shown in Fig. 1. $\tilde{\Gamma}(\omega)$ drops rapidly for small frequencies but saturates at a finite value. This saturation value $\lim_{\omega\rightarrow 0}\tilde{\Gamma}(\omega)$ is almost independent of system size (see inset). This indicates that finite size effects are small despite the fact that $J_{\parallel}$ is expected to be a nonlocal operator. We therefore conclude that for small J',

$$\sigma_s \geq \frac{c(T)}{TJ'^2} \tag{15}$$

in the thermodynamic limit. This is the main result of this paper: the spin conductivity of a slightly perturbed *XXZ* Heisenberg chain is very large, despite the fact that the spin current is not protected by any local conservation law. For $\Delta=0.75$, we obtain, for example, $c(T\rightarrow\infty)=0.92J^3$. For any finite temperature, we expect that the same result holds: in the limit of small J', the spin conductivity is proportional to $1/J'^2$.

In Fig. 2, the behavior of the scattering rate $\tilde{\Gamma}/\chi$ as a function of Δ is shown. Interestingly, the scattering rate seems to vanish in the isotropic limit $\Delta\rightarrow 1$, $\tilde{\Gamma}\propto J'^2(1-\Delta)^2$. We have previously[6] observed the same effect for the scattering rate of the heat current, which turns out to be proportional to $1/J'^4$ at the isotropic point. The reason for this unexpected result is that for the isotropic case, one can construct an operator $Q_3'=Q_3+J'\Delta Q_3$ such that the commutator

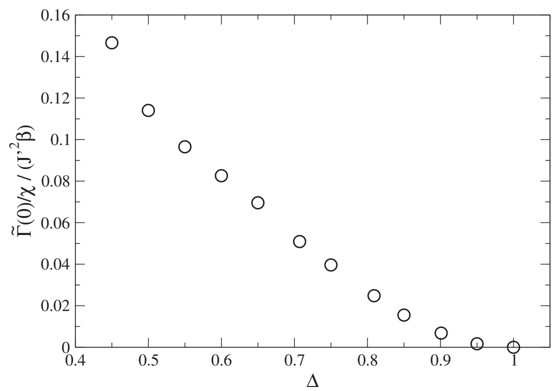

FIG. 2. Scattering rate $\tilde{\Gamma}(0)/\chi$ as a function of the anisotropy parameter Δ for $L=18$, $T=\infty$. For the isotropic system, $\Delta=1$, $\tilde{\Gamma}(0)$ is zero, see text. The errors are comparable to the size of the symbols and are discussed in more detail in the Appendix.

$[Q_3',H_0+H_1]$ is of order J'^2 rather than linear in J'. As a consequence, the decay rate of the heat current at the isotropic point is proportional to J'^4. Very likely, the same mechanism applies to $J_{\parallel}$, too. A subtle and controversial issue[3,10,17] is the value of the Drude weight, $D_s=\chi$, for $\Delta=1$. Both from numerics and from Bethe ansatz, there is evidence pointing either to a finite[3,17] or vanishing[10,17] Drude weight in the thermodynamic limit. If the Drude weight vanishes for $\Delta=1$, our results are only of relevance for $\Delta<1$.

In the Appendix, we discuss a further effect: the Drude weight D_s appears to be a discontinuous function of Δ as for special values of the anisotropies $\Delta=\cos(\pi/\nu)$, $\nu=3,4,5\ldots$, one obtains different values for D_s compared to anisotropies slightly away from these points. For the scattering rate $\tilde{\Gamma}/\chi$, these effects are much smaller and possibly absent in the thermodynamic limit.

IV. NONLOCALITY OF $J_{\parallel}$

As stressed in the Introduction, the spin current J_s is orthogonal to all known local conservation laws Q_n of the *XXZ* Heisenberg chain. This suggests that $J_{\parallel}$, the conserved part of J_s, is a nonlocal operator which cannot be written in the form of Eq. (3). To quantify this statement, we expand the numerically constructed $J_{\parallel}$ in local operators A_{ni} which contain products of spin operators on n adjacent sites,

$$J_{\parallel}=\sum a_{ni}\frac{A_{ni}}{\langle A_{ni}^2\rangle^{1/2}}, \tag{16}$$

where the A_{ni} define a complete orthogonal basis in the space of operators, $\langle A_{ni}A_{mj}\rangle=0$ for $n\neq m$ or $i\neq j$. The A_{ni} are written as sums of products of spin operators, where each product contains spins on n adjacent sites. Here, we use—as above—the $(T=\infty)$ expectation value as the scalar product in the space of operators. In Eq. (16), obviously only translationally invariant Hermitian operators contribute which also conserve S_z. For $n=1$, there is just one such operator,

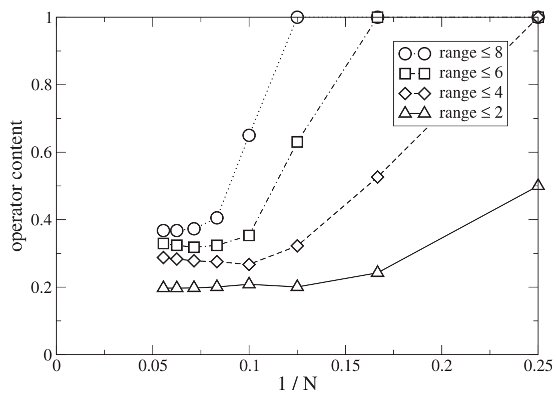

FIG. 3. Relative weight $\Sigma_{m=1}^{n} c_m$, see Eq. (17), of local operators with range up to n ($n=2,4,6,8$) contributing to $J_\parallel$ as a function of inverse system size from $N=4$ to $N=18$.

$A_{11}=\Sigma_i S_i^z$, and for $n=2$, one finds three such terms $A_{21}=\Sigma_i S_i^z S_{i+1}^z$, $A_{22}=\Sigma_i S_i^+ S_{i+1}^- + \text{H.c.}$, and $A_{23}=i\Sigma_i (S_i^+ S_{i+1}^- - \text{H.c.})$. The ten operators of range 3, A_{3i}, contain both products of two spin operators, e.g., $\Sigma_i S_i^z S_{i+2}^z$, and products of three spin operators, e.g., $\Sigma_i S_i^z S_{i+1}^z S_{i+2}^z$.

The ratio,

$$c_n = \frac{\sum_i |a_{ni}|^2}{\sum_{i,m} |a_{mi}|^2}, \qquad (17)$$

shown in Figs. 3 and 4 describes which fraction of the operator $J_\parallel$ can be expressed in terms of operators of range n. For example, if one determines the c_n for H, one obtains $c_2 = J^2/(J^2+J'^2)$ and $c_3=J'^2/(J^2+J'^2)$. By construction, one gets $\Sigma_{n=0}^{N} c_n=1$ for a system with N sites.

What types of behavior can be expected for c_n? First, one has to investigate whether c_n is finite or zero in the thermodynamic limit $N\to\infty$. For example, for the square of a translationally invariant local operator (e.g., H_0^2), one finds that c_n drops proportionally to $1/N$, such that $\lim_{N\to\infty} c_n=0$ for all $n>0$. Even if $\lim_{N\to\infty} c_n$ is finite for each n, one can ask how rapidly $\lim_{N\to\infty} c_n$ drops for $n\to\infty$ and whether $\Sigma_{n=0}^{\infty}\lim_{N\to\infty} c_n$ equals 1 or is smaller.

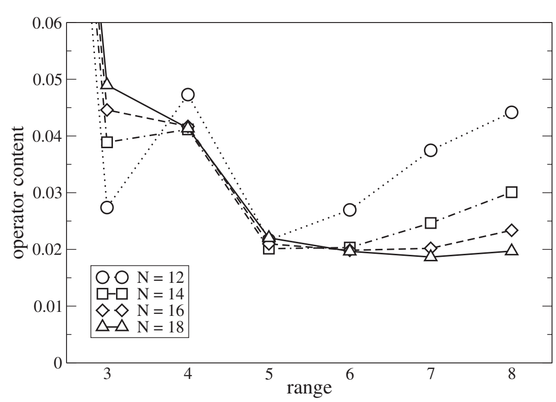

FIG. 4. Relative weight c_n of local operators of range n ($n=3,\ldots 8$) contributing to $J_\parallel$ for different system sizes. Note that in the thermodynamic limit, most of the weight is carried by operators involving more than eight consecutive sites (see Fig. 3).

As shown in Fig. 3, the c_n converge to finite values for $N\to\infty$. For $n=2$, this is a necessary consequence of the fact that the spin current is a range 2 operator and that the Drude weight of the spin current is finite. As the latter is proportional to $\langle J_s J_\parallel\rangle^2$, this implies that $J_\parallel$ has a finite overlap with a range 2 operator in the thermodynamic limit.

A qualitative result of Fig. 3 is, however, that even operators up to range 8 have less than 40% of the total weight of $J_\parallel$ (but $c_8\approx 0.02$ is already very small). As $\Sigma_{n=1}^{\infty} c_n=1$, the c_n have to drop faster than $1/n$ for large n in the thermodynamic limit. Figure 4 shows that the c_n decay extremely slowly with n. In this sense, $J_\parallel$ appears to be a rather nonlocal operator but we cannot decide from our numerics whether $\Sigma_{n=0}^{\infty}\lim_{N\to\infty} c_n=1$ or smaller.

Surprisingly, finite size correction both to χ and Γ remain small (see Appendix), despite the fact that a large fraction of the Drude weight is carried by operators of a range comparable to the system size, see Fig. 3.

V. CONCLUSION

In this paper, we have shown that the spin conductivity of a one-dimensional anisotropic spin chain is strongly enhanced close to the integrable point. It diverges (at least) as $1/J'^2$ for $J'\to 0$. This is the expected behavior for a situation where a local conservation law prohibits the decay of the current at the integrable point. However, as emphasized by Zotos *et al.*,[1] the spin current is orthogonal to all known local conservation laws of the *XXZ* chain.

There are two possible interpretations of this result. First, the conserved part $J_\parallel$ of the spin current could nevertheless be "sufficiently" local to define a slow hydrodynamic mode. Second, the theoretical prejudice that only local conservation laws (i.e., those associated with a continuity equation) lead to slow modes may be wrong. In this respect, the results of sec. IV, where this question is investigated, are ambiguous. On the one hand, we could prove that $J_\parallel$ is a highly nonlocal operator involving products of operators acting on widely separated sites. On the other hand, the relative weight of range-n operators, c_n, is finite in the thermodynamic limit.

In this paper, we have shown that the transport properties of simple one-dimensional problems depend quantitatively and qualitatively on "exotic" and rather complex conserved quantities. For the future, it would be interesting to gain a more analytic understanding of these conservation laws.

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APPENDIX: SPIN CONDUCTIVITY CLOSE TO AND AT $\Delta=\cos(\pi/\nu)$

In this appendix, we discuss the behavior of the spin conductivity for anisotropies $\Delta=\cos(\pi/\nu)$ for integer ν. At these special points, it is known that there are further symmetries which, for example, simplify the Bethe ansatz equations considerably.[26,27] Interestingly, at these special points, thermodynamic quantities show unexpected logarithmic corrections.[27]

In Ref. 7, Naef and Zotos found numerically that the Drude weight at these special points differs for finite systems significantly from the values obtained for slightly different anisotropies. They concluded, however, that these differences vanish in the thermodynamic limit. Heidrich-Meisner *et al.*[3] pointed out that the Drude weight differs substantially for even and odd system sizes for $\Delta \neq \cos(\pi/\nu)$, while such an effect is absent for $\Delta=\cos(\pi/\nu)$. This is shown in the upper panel of Fig. 5. It is therefore very difficult to draw a definite conclusion on the value of D in the thermodynamic limit. The observation that for odd system sizes the Drude weight is a smooth function of Δ suggests[3] that finite size effects are less important in this case.

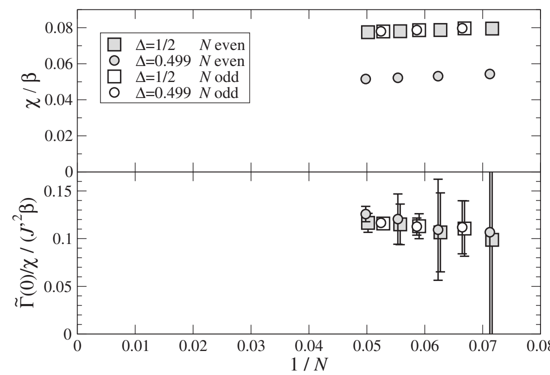

FIG. 5. Drude weight $D=\chi$ (upper panel) and scattering rate $\tilde{\Gamma}(0)/\chi$ (lower panel) for the anisotropy $\Delta=\cos(\pi/3)=1/2$ and a nearby value $\Delta=0.499$ as a function of inverse system size $1/N$ for $N=14,\ldots,20$. The error bars represent the uncertainty inherent in the fitting procedure.

Fortunately, the above described ambiguities seem to be absent for the scattering rate $\tilde{\Gamma}(0)/\chi$, as shown in the lower panel of Fig. 5.

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