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Thermal conductivity of a quantum spin-1/2 antiferromagnetic chain with magnetic impurities

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We present an exact theory that describes how magnetic impurities change the behavior of the thermal conductivity for the integrable Heisenberg antiferromagnetic quantum spin-1/2 chain. Single magnetic impurities and a large concentration of impurities with similar values of the couplings to the host chain (a weak disorder) do not change the linear-in-temperature low-T behavior of the thermal conductivity: Only the slope of that behavior becomes smaller, comparing to the homogeneous case. The strong disorder in the distribution of the impurity-host couplings produces more rapid temperature growth of the thermal conductivity, compared to the linear in T dependence of the homogeneous chain and the chain with a weak disorder. Recent experiments on the thermal conductivity in inhomogeneous quasi-one-dimensional quantum spin systems manifest qualitative agreement with our results.

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71.10–w Theories and models of many-electron systems;
72.10.Di Scattering by phonons, magnons, and other nonlocalized excitations (including Kondo effect);
72.15.Eb Electrical and thermal conduction in crystalline metals and alloys.

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Quasi-one-dimensional quantum spin systems have attracted much attention of researchers in recent years. There are several reasons for that growth of interest. First, during the last decade many real compounds with the properties of quasi-one-dimensional quantum spin chains were synthesized and studied experimentally. On the other hand, namely quantum spin chains provide physicists with the rare opportunity to compare the experimental observations with exact theoretical results, since many exact results have been obtained for one-dimensional quantum spin chains. And, last but not least, one-dimensional spin models are actively used in many modern applications, like in the theory of nano-structures, mesoscopic devices, and, even in the theory of quantum computations.

One of the main models that is frequently considered by physicists, is the Heisenberg spin-1/2 chain with antiferromagnetic interactions, solved exactly by Bethe in 1931 [1]. Since that time many results have been obtained for the model; for recent review see, e.g., Ref. 2. However, in most cases theories were developed for homogeneous spin chains, despite the fact that in nature one more frequently encounters inhomogeneous situations, i.e., real spin chains contain defects, for instance, magnetic impurities. Impurities in quantum systems can drastically change the behavior of the system, especially in low-dimensional cases. For example, it is well known that in the one-dimensional case impurities produce localization of wave functions, changing the behavior from metallic to insulating. This is why the study of models with impurities, especially of systems with strong correlations between particles, is one of the most important and difficult tasks of the modern theoretical physics. The study of the thermal conductivity in systems of weakly coupled quantum spin chains has become popular in recent years, because the thermal conductivity can be a strong experimental instrument to investigate magnetic properties of materials.

In this paper we study theoretically how magnetic impurities can affect the thermal conductivity in quantum spin chains. For our purpose we choose an *integrable* spin chain, because in such chains one can introduce any number of magnetic impurities, and because for that case one can obtain exact results. Earlier studies of integrable spin chains with magnetic impurities manifested a good agreement of theoretical results with experimental data for quasi-one-dimensional inhomogeneous compounds. Therefore, we expect that the calculated thermal conductivity for the integrable model will reveal properties, generic for inhomogeneous quantum spin chains.

We investigate the thermal conductivity of the integrable spin-1/2 antiferromagnetic quantum chain with spin-1/2 magnetic impurities. The Hamiltonian of the system has the form [2,3]: $\mathcal{H} = \mathcal{H}_h + \mathcal{H}_{\rm imp}$, where the host part is $\mathcal{H}_h = \sum_j H_{j,j+1}$, with $H_{j,j+1} = \mathbf{S}_j \mathbf{S}_{j+1}$ (the host exchange constant J is set to unity). The impurity part of the Hamiltonian has the special form, necessary for exact integrability of the model. Suppose the concentration of impurities is such that impurities are not nearest neighbors. Then for the impurity situated between sites m and $m+1$ of the host the integrable Hamiltonian reads

$$\mathcal{H}_{\rm imp} = J_{\rm imp}((H_{m,{\rm imp}} + H_{{\rm imp},m+1}) + \\ + \theta^2 H_{m,m+1} - i\theta\, [H_{m,{\rm imp}}, H_{{\rm imp},m+1}])\,, \qquad (1)$$

where $J_{\rm imp} = 1/(\theta^2+1)$, and $[.,.]$ denotes the commutator. The lattice Hamiltonian Eq. (1) describes the impurity spin coupled to the host with the strength $J_{\rm imp}$, parametrized by the constant θ. One can see that the limit $\theta \to 0$ corresponds to the simple inclusion of an additional site coupled with the bulk interaction to the system. On the other hand, for $\theta \to \infty$ one obtains an impurity spin totally decoupled from the host. The Hamiltonian also contains additional terms which renormalize the coupling between the neighboring sites of the host, and three-spin terms. However, it has been shown [2,3] that in the long-wave limit such a lattice form of the impurity Hamiltonian yields the well-known form of the contact impurity-host interaction, similar to the one of, e.g., the Kondo problem of a magnetic impurity in a metal. The contact impurity coupling in that limit is also determined by the same constant θ. The advantage of the consideration of the integrable Hamiltonian $\mathcal{H}$ is obvious: One can independently incorporate any number of magnetic impurities into the host chain. Each impurity is characterized by its own coupling to the host, i.e., by own θ_j. Finally, we like to note that all considered impurities are *elastic* scatterers, i.e., each excitation only changes its phase when scattering off an impurity, but is not reflected. However, the same property holds for the standard Kondo impurity in a free electron host. Equally important to mention is that we study a *lattice* model, hence all two-particle scattering processes, in particular from one Fermi point to the other (backscattering), are taken into account in the model.

To find the thermodynamic characteristics of our one-dimensional quantum spin Hamiltonian at finite temperature we use the so-called «quantum transfer matrix» approach, see, e.g., [3,4]. Let $R^{\mu_i\mu_{i+1}}_{\alpha_i\beta_i}(u)$ be the standard R-matrix of the Heisenberg spin-1/2 chain [4]. Indices α_i and β_i denote states of the spin at site i, and μ denotes states in the auxiliary space. The «standard» transfer matrices (row-to-row from the viewpoint of statistical 2D problem) $\tau^\beta_\alpha(u)$ have the form of the trace over the auxiliary space of the product of R-matrices

$$\tau^\beta_\alpha(u, \{\theta\}^L_{i=1}) = \sum_\mu \prod_{i=1}^{L} R^{\mu_i\mu_{i+1}}_{\alpha_i\beta_i}(u, \theta_i), \qquad (2)$$

where L is the length of the quantum chain and θ_i are the inhomogeneity parameters, which are shifts of the spectral parameter. The R-matrices satisfy the Yang–Baxter equations, hence the transfer matrices with different spectral parameters commute. Conservation laws of the integrable model can be constructed as derivatives of the logarithm of the transfer matrix as

$$A_n = {\rm const}\cdot\left(\frac{\partial}{\partial u}\right)^n \ln \tau(u)|_{u=0}. \qquad (3)$$

The Hamiltonian of the model corresponds (up to a nonessential constant term) to the $n = 2$ case with const $= 1$. One can introduce R-matrices of different type, related to the initial one by an anticlockwise and clockwise rotation

$$\bar{R}^{\mu\nu}_{\alpha\beta}(u) = R^{\alpha\beta}_{\nu\mu}(u), \\ \tilde{R}^{\mu\nu}_{\alpha\beta}(u) = R^{\beta\alpha}_{\mu\nu}(u)\,. \qquad (4)$$

The transfer matrix $\bar{\tau}(u, \{\theta\}^L_{i=1})$ can be constructed in a way similar to the case of τ. Then we substitute $u = -J/NT$ $(J = 1)$, where N is the Trotter number. We find

$$[\tau(u)\bar{\tau}(u)]^{N/2} = \exp(-\mathcal{H}/T + \mathcal{O}(1/N))\,. \qquad (5)$$

Hence, the partition function of the quantum 1D system is identical to the partition function of an inhomogeneous classical vertex model with alternating rows on a square lattice of size $L \times N$,

$$Z = \lim_{N\to\infty} {\rm Tr}\,[\tau(u)\bar{\tau}(u)]^{N/2}\,. \qquad (6)$$

The interactions on the 2D lattice are four-spin interactions with coupling parameters depending on $(NT)^{-1}$ and interaction parameters θ_j where j is the number of the column to which the considered vertex of the lattice belongs. The corresponding column-to-column transfer matrices are referred to as «quantum transfer matrices»

(where an external magnetic field h is included by means of twisted boundary conditions)

$$\tau_{QTM}(\theta_j, u) = \sum_{\mu} e^{\mu_1 h/T} \prod_{i=1}^{N/2} R^{\mu_{2i-1}\mu_{2i}}_{\alpha_{2i-1}\beta_{2i-1}}(u + i\theta_j) \times$$
$$\times \widetilde{R}^{\mu_{2i}\mu_{2i+1}}_{\alpha_{2i}\beta_{2i}}(u - i\theta_j) . \qquad (7)$$

In general all «quantum transfer matrices» corresponding to the L many columns are different. However, all these operators can be proven to commute pairwise. Therefore, the free energy per lattice site of our system can be calculated from just the largest eigenvalues of the «quantum transfer matrices» (corresponding to only one eigenstate). The partition function of the model is determined by the following nonlinear integral equation for the «energy density» functions a, $\overline{a}$, $A = 1 + a$ and $\overline{A} = 1 + \overline{a}$ in relation to the spectral parameter u:

$$\int [k(u - v) \ln A(v) - k(u - v - \pi i + i\varepsilon) \ln \overline{A}(v)] dv =$$
$$= \ln a(u) + \frac{v_F}{T \cosh u} - \frac{h}{2T} , \qquad (8)$$

with $v_F = \pi / 2$ being the Fermi velocity of low-energy excitations of the chain (spinons) (in what follows we consider the case $h = 0$), with infinitesimally small ε, and the kernel function being defined as

$$k(x) = \frac{1}{2\pi} \int d\omega \frac{e^{(-\pi|\omega| + i2x\omega)}}{\cosh(\pi\omega)} . \qquad (9)$$

The equation for $\overline{a}$ follows from Eq. (8) with the formal changes $h \to -h$, $i \to -i$, $\overline{a} \to a$ and vice versa.

In the linear response theory the Kubo formulas [5] yield the thermal conductivity κ relating the thermal current to the temperature gradient ∇T as $\mathcal{J}_E = \kappa \nabla T$, where

$$\kappa(\omega) = \frac{1}{T} \int_0^{\infty} dt\, e^{-i\omega t} \int_0^{1/T} d\tau \langle \mathcal{J}_E(-t - i\tau) \mathcal{J}_E \rangle_T , \qquad (10)$$

and brackets denote thermal average. It was pointed out [6,7] that for the homogeneous quantum spin chain, i.e., in the limit $\theta_j \to 0$, the operator of the thermal current is equal to the operator of the third conservation current. Following the logic of Refs. 6, 7, we denote the operator of the thermal current, $\hat{J}_E$, for the integrable model of a spin chain with magnetic impurities (i.e., for possible nonzero θ_j) as A_3 (up to a nonessential constant term) with const $= i$ [7]. Then, by construction, the operator of the thermal current for the integrable model with magnetic impurities commutes with the Hamiltonian. It is easy to check that such a definition of the thermal current respects the continuity equation for the considered model; cf. [7]. Hence, one finds

$$\kappa(\omega) = -i \frac{\langle \mathcal{J}_E^2 \rangle_T}{T^2(\omega - i\varepsilon)} |_{\varepsilon \to 0+} . \qquad (11)$$

Therefore the real part of the conductivity can be written as

$$\mathrm{Re}\, \kappa(\omega) = \pi\delta(\omega) \langle \mathcal{J}_E^2 \rangle_T / T^2 . \qquad (12)$$

This means that the thermal conductivity in our integrable model of the antiferromagnetic quantum spin-1/2 chain with magnetic impurities is *infinite* at zero frequency, as for the homogeneous model, without impurities. Naturally, it is the consequence of the exact integrability of the model considered, i.e., of the infinite number of conservation laws. To calculate $\langle \mathcal{J}_E^2 \rangle_T$ for our model we use the trick, proposed in [7]. We define some modified partition function

$$\overline{Z} = \mathrm{Tr} \exp[-(1/T)\mathcal{H} + f \hat{J}_E] . \qquad (13)$$

Using that partition function one can easily find that $\langle \mathcal{J}_E \rangle_T = 0$, and

$$\langle \mathcal{J}_E^2 \rangle_T = \left(\frac{\partial}{\partial f} \right)^2 \ln \overline{Z} |_{f=0} . \qquad (14)$$

The eigenvalue of the modified partition function per site $\Lambda(u)$ is given by

$$\ln \Lambda(u) = \frac{e_0(u)}{T} - \frac{1}{2\pi} \int \frac{\ln[A(v)\overline{A}(v)]\, dv}{\cosh(u - v)} , \qquad (15)$$

where e_0 is the ground-state energy (defined for the system with the partition function Z). The eigenfunction of the modified partition function of the total chain with impurities is

$$\Lambda_{\mathrm{tot}} = \prod_j \Lambda(u = \pi\theta_j / 2) , \qquad (16)$$

where the product is taken over all the sites (for sites without impurities we get $\Lambda(u = 0)$). Equations (8) are easily solved numerically for arbitrary temperatures. For the spin chain with the disordered ensemble of magnetic impurities the random distribution of the values θ_j can be described by a distribution function $P(\theta_j)$.

At low energies the behavior of each impurity depends on the energy scale [2]

$$T_{jK} \propto v_F \exp(-\pi|\theta_j|) , \qquad (17)$$

which plays the same role as the Kondo temperature for a magnetic impurity in a metal. The magnetic impurity behaves asymptotically free for $T >> T_{jK}$, while it is strongly coupled to the spin chain for $T << T_{jK}$. In other words, θ_j measures the shift off the Kondo resonance (higher values of $|\theta_j|$ correspond to lower values on the Kondo scale) of the impurity level with host spin excitations, similar to the standard picture of the Kondo effect in a metallic host. It has been shown [8] that the low-energy thermodynamic characteristics of the considered quantum spin chain with magnetic impurities are determined, in fact, by the distribution of those effective Kondo temperatures. At low temperatures one can replace the functions a, $\bar{a}$, A and $\bar{A}$ by the scaling functions, introduced as

$$a_{\pm}(x) \equiv a[\pm x \pm \ln(\alpha T_{jK}/T)] \tag{18}$$

(α being some constant), etc. [3,7]. For those functions integral equations are transformed in such a way that for that new set of scaling functions the only asymptotic behavior of $A_{\pm}$ and $\bar{A}_{\pm}$ enters. We obtain that each site of the chain contributes to the low-temperature thermal current as

$$\langle \mathcal{J}_{jE}^2 \rangle_T \approx \frac{\pi T_{jK} T^3}{3} + O(T^4), \tag{19}$$

where for sites without impurities one gets $T_{jK} \to v_F$. It means that the contribution from each site to the thermal conductivity is linear in temperature at low T,

$$\mathrm{Re}\,\kappa_j \approx \delta(\omega) \frac{\pi T_{jK} T}{3}. \tag{20}$$

For a single impurity one has $P(T_{jK}) \sim \delta(T_{jK} - T_K)$. Hence, at low temperatures a single magnetic impurity does not change the linear in T dependence of the thermal conductivity of the spin chain.

Consider ensembles of magnetic impurities with a weak disorder (i.e., for ensembles with random distributions of the impurity-host couplings, for which those couplings, and, hence, their effective Kondo temperatures, are similar to each other). Let those Kondo temperatures are close to some T_K. Hence, the total thermal conductivity for integrable spin chains with weakly disordered magnetic impurities can be estimated as

$$\mathrm{Re}\,\kappa_{\mathrm{tot}} = \int dT_{jK} P(T_{jK}) \kappa_j \approx \delta(\omega) \frac{\pi T_K T}{3}. \tag{21}$$

This formula implies that for integrable spin systems with weakly disordered ensembles of magnetic impurities the thermal conductivity is finite. It is proportional to T at low temperatures, but the slope is smaller than the one for the homogeneous integrable chain, because for magnetic impurities, antiferromagnetically coupled to the chain (and we consider here only such impurities) the effective Kondo temperature is smaller than the Fermi velocity of spinons ($v_F = \pi J/2$), i.e., one has $T_K \sim v_F \times \times \exp(-\pi\sqrt{(J - J_{\mathrm{imp}})/J_{\mathrm{imp}}}) < v_F$. Notice that in our model $0 \le J_{\mathrm{imp}} \le J$, and the case without impurities corresponds to $J_{\mathrm{imp}} = J$. Obviously, one should expect a similar behavior for the thermal conductivity of a spin chain with a single antiferromagnetic impurity (or with a small concentration of such impurities).

The situation becomes very different for integrable spin chains with strongly disordered ensembles of magnetic impurities. For those ensembles the distribution function for effective Kondo temperatures is wide. Hence, for a fixed temperature, for a large fraction of the impurities their effective Kondo temperatures are lower than the temperature of the system, and, hence, they remain unscreened. This effect produces the divergency of the magnetic susceptibility and the Sommerfeld coefficient of the specific heat for such chains [2]. It implies that the considered spin chain manifests the Griffiths'-phase-like behavior [9]. Let us consider the realistic distribution of Kondo temperatures for magnetic impurities in the spin chain [2,8,10], which starts from the term

$$P(T_{jK}) \propto G^{-\lambda} (T_{jK})^{\lambda - 1} \tag{22}$$

($\lambda < 1$), valid till some energy scale G for the lowest values of T_{jK}. This distribution was shown to pertain to real disordered quantum spin chains [10,11]. Averaging the thermal conductivity with this distribution, we obtain

$$\mathrm{Re}\,\kappa_{\mathrm{tot}} \sim \delta(\omega) \frac{\pi T^{2+\lambda}}{3(\lambda+1) G^{\lambda}}. \tag{23}$$

Hence, for integrable spin chains with ensembles of strongly disordered magnetic impurities the thermal conductivity is also finite, but it grows with T at low temperatures much faster, than for the homogeneous chain, or for the chain with weakly disordered magnetic impurities.

We can solve nonlinear integral equations analytically also at high temperatures, using the asymptotic form of «energy density» functions a, $\bar{a}$, A and $\bar{A}$, cf. [7]. At high temperatures for our integrable chain with magnetic impurities the thermal conductivity decays with the temperature as

$$\mathrm{Re}\,\kappa(\omega) \sim \delta(\omega) \frac{3}{2T^2}. \tag{24}$$

Obviously, at high temperatures, larger than the coupling constants, the system behaves as a gas of noninteracting spins 1/2, and the result does not depend on the parameters of the impurity-host couplings, as must be the case. Hence, the thermal conductivity of the integrable spin chain with magnetic impurities, as a function of temperature, grows with T at low temperatures, manifests a maximum, and then decays with T, as the homogeneous chain. The main differences, caused by magnetic impurities, are present at low temperatures.

In summary, in the framework of the integrable quantum spin model we have calculated the thermal conductivity for a spin chain with magnetic impurities. Previous theoretical studies of thermodynamic characteristics for the model considered [2,8,10] have shown that the model exhibits generic features of disordered quantum spin systems, e.g., the Griffiths'-phase-like behavior, and the results of those studies well agree with the data of experiments on quasi-one-dimensional antiferromagnetic quantum spin-1/2 systems with magnetic impurities, see, e.g., [11,12]. Our investigation has shown that the presence of magnetic impurities in an integrable quantum chain does not destroy the most exciting property of an integrable spin chain — the infinite thermal conductivity at zero frequency. The δ-function dependence of the thermal conductivity, obtained in this work (as well as for spin chains without impurities), is related to the infinite number of integrals of motion in the integrable model considered, which, in turn, is based on the special choise of the interaction (only elastic scatterings, absence of reflections). In a more realistic situation one should, naturally, take into account the finite value of the width of the frequency dependence of the thermal conductivity, which is present there because of inelastic processes and reflections off impurities. However, we expect that our model reproduces the generic features of the thermal conductivity of a quantum spin chain with impurities.

Our model permits one to include any number of magnetic impurities in the spin chain. Therefore, it permitted us to obtain results for small concentration of impurities, when each impurity behaves as a single one, and for large concentration of impurities. The important conclusion from our study is that the presence of magnetic impurities mostly affects the low-temperature behavior of the zero-frequency thermal conductivity. Single magnetic impurities and a large concentration of impurities with similar values of the couplings to the host chain (a weak disorder) do not change the linear-in-temperature low-T behavior of the thermal conductivity, but the slope of that behavior becomes smaller, compared to the homogeneous case. On the other hand, the strong disorder in the distribution of the impurity-host couplings (when the chain manifests the Griffiths'-phase-like behavior) produces essential changes in the temperature behavior of the low-T thermal conductivity, with the growth with temperature becoming more rapid as compared to the linear temperature dependence of the homogeneous chain and the chain with a weak disorder. We believe that such a behavior of the thermal conductivity for integrable quantum spin chains with impurities has generic features. Similar situation was recently observed in quasi-one-dimensional compounds $Sr_{14-x}Ca_xCu_{24}O_{41}$ [13], $Sr_{1-x}Ca_xCuO_2$ [14], and $Sr_{14}Cu_{24-x}Zn_xO_{41}$ [15], where the introduction of Ca or Zn impurities reduced the slopes of the low-temperature linear-in-T behavior of the magnetic thermal conductivity. It is possible that ions of Zn and Ca, introduced in those compounds, produce local changes in the spin-spin antiferromagnetic coupling between Cu ions. Hence, the situation can be modelled by the magnetic spin-1/2 chain with impurities. Then experiment [15] has revealed that for systems with doped Zn the low-temperature thermal conductivity is linear in temperature, as in the undoped cases. However, the slopes of the linear temperature dependence of the thermal conductivity really became smaller with the doping impurities, which qualitatively agree with our theory. The results of our theory can be also applied, e.g., to quasi-one-dimensional antiferromagnetic systems with magnetic impurities, like $(Sr,Ca,La)_{14}Cu_{24}O_{41}$, $BaCu_2(Si_{1-x}Ge_x)_2O_7$ [12], or organic materials with the properties of inhomogeneous quantum spin chains, see, e.g., [11].

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