

## Heat transport properties of clean spin ladders coupled to phonons: Umklapp scattering and drag

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We study the low-temperature heat transport in clean two-leg spin-ladder compounds coupled to three-dimensional phonons. We argue that the very large heat conductivities observed in such systems can be traced back to the existence of approximate symmetries and corresponding weakly violated conservation laws of the effective (gapful) low-energy model, namely, pseudomomenta. Depending on the ratios of spin gaps and Debye energy and on the temperature, the magnetic contribution to the heat conductivity ( $\kappa_{mag}$ ) can be positive or negative and can exhibit an activated or antiactivated behavior. In most regimes,  $\kappa_{mag}$  is dominated by the spin-phonon drag: the excitations of the two subsystems have almost the same drift velocity, and this allows for an estimate of the ratio  $\kappa_{mag}/\kappa_{ph}$  of the magnetic and phononic contributions to the heat conductivity.

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### I. INTRODUCTION

Recent experiments both on spin-chain<sup>1</sup> and ladder compounds<sup>2</sup> showed a surprisingly large magnetic contribution to the heat conductivity: the heat conductivity in the direction parallel to the ladder (attributed to magnons and phonons) largely exceeds the heat conductivity in directions perpendicular to it (attributed to the phonons alone). The heat conductivity of clean *gapless* spin- $\frac{1}{2}$  chains coupled to phonons shows a simple exponential behavior,<sup>3</sup> associated with a single characteristic energy scale resulting from the high-energy process needed to relax momentum. In contrast, gaps open up in the spectrum of (two-leg) spin ladders, and consequently the heat transport involves a complex interplay between different energy scales, leading to a rich gamut of possible behaviors. In this paper, we present a theoretical framework to describe low-temperature heat transport in such clean *gapped* quasi-one-dimensional systems when they are coupled to phonons.

In the absence of disorder, heat transport in quasi-one-dimensional systems is determined by momentum conservation (or more precisely by “pseudomomentum” conservation<sup>3-5</sup>). In a clean lattice, momentum transfers are quantized and therefore the momentum can only decay via an umklapp process involving a large-momentum high-energy state. This implies that transport in such systems is nonuniversal as it depends on both high- and low-energy features. Therefore, controlled analytic calculations are usually not possible (the situation is, however, simpler for systems with a finite magnetization<sup>3,4</sup>). Nevertheless, we shall show that under certain circumstances, such calculations are possible. Indeed, in many spin systems, the typical spin velocity  $v_s$  is large compared to the sound velocity of the acoustic phonons,  $v_p$ . Therefore, the large-momentum state with the lowest energy (required for an umklapp process) will have most of its momentum carried by phonons. This has two consequences: heat transport is (i) dominated by spin-phonon scattering and is (ii) determined by high-energy features of the phonon system but low-energy properties of

the spin system. The latter observation implies that controlled calculations of transport are in principle possible (up to nonuniversal prefactors describing the electron-phonon coupling), using the fact that high-energy properties of the weakly interacting phonons are often known or can be measured. The necessary low-energy correlators of the gapped spin-system can be obtained from an effective field theory which can be analyzed by semiclassical<sup>6</sup> or form-factor<sup>7</sup> methods for temperatures  $T$  below the gap.

In contrast, in pure systems where phonons are absent (e.g., cold atom realizations) or when  $v_p > v_s$ , no such controlled calculation is possible as little is known about the non-universal high-energy properties of strongly interacting spin systems and one can make only qualitative statements, e.g., that the heat conductivity is exponentially large but finite.<sup>3</sup> Previous numerical studies of pure ladder systems at high  $T$  indicate that the heat conductivity of spin ladders is finite<sup>8,9</sup> but could not reach temperature of the order of the gap and below. On the analytical side, few results are available. The field theoretical treatment of Ref. 10 ignored the role of umklapp processes, thus leading to ballistic transport in a clean and pure system. Rozhkov and Chernyshev<sup>11</sup> included the effect of disorder and phonons in spin chains within a Boltzmann equation approach but did neither consider spin-phonon drag nor addressed the question of umklapp, which becomes essential in a clean system.

In the following, we will first present the general field theoretical framework on which our calculation is based. We discuss the various umklapp processes that induce (pseudo) momentum decay in quanta of size  $G$  or  $G/2$ , where  $G$  is the reciprocal lattice vector. We shall discuss the role of such processes in (weakly) violating the conservation laws of the model, allowing a hydrodynamic description of the system. We then use the memory-matrix formalism to calculate the heat conductivity  $\kappa$  in the various regimes. The memory-matrix approach is generally *not* exact even in the limit of small couplings but it can be shown<sup>12</sup> to give a lower bound to  $\kappa$ , which is saturated in the limit of a large separation of time scales between slow and fast modes, i.e., if a hydrody-

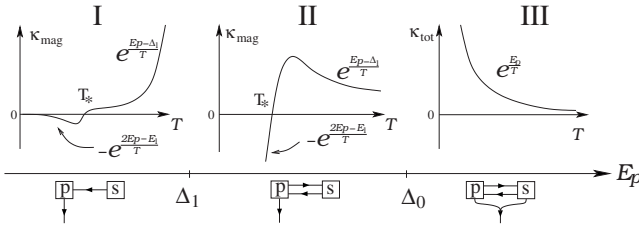


FIG. 1. Schematic plots of  $\kappa(T)$  in three regimes. Depending on the size of  $E_p$  (i.e., the Debye energy) compared to the values of the spin gaps, one obtains qualitatively different behaviors of the heat conductivity (shown for  $T \ll \Delta_1$ ). Note that in regimes, I and II,  $\kappa_{\text{mag}}$  is displayed, while in regime III, the total  $\kappa$  is displayed ( $\kappa_{\text{mag}}$  is not defined in this regime—see text). The dominating momentum transfer processes within the spin and phonon system, and from those modes via umklapp scattering to the lattice, are shown schematically below the horizontal axis.  $T^*$  is of order  $(v_p/v_1)^2 \Delta_1$ .

namic description is possible, as is the case here. Finally, we interpret our results in terms of the spin-phonon drag and the decay rates of various slow modes. The various resulting behaviors of  $\kappa(T)$  are summarized in Fig. 1, where regime I is consistent with the particular data of Ref. 2 for  $T$  below the spin gap but still larger than a lower scale  $T^*$ , where the magnetic heat conductivity displays an activated behavior.

## II. LOW-ENERGY EFFECTIVE THEORY

Our starting point is the following Hamiltonian:

$$H = \sum_{\gamma} H_s(\gamma) + H_p + H_{s,p}, \quad (1)$$

which describes an array of spin ladders (denoted by  $s$ , with  $\gamma$  the ladder index) coupled to acoustic three-dimensional phonons ( $p$ ), via the term  $H_{s,p}$ . For simplicity, we assume  $H_p \approx \sum_{\mathbf{k}, \alpha} v_{\alpha} |\mathbf{k}| a_{\mathbf{k}, \alpha}^{\dagger} a_{\mathbf{k}, \alpha}$ , where the velocities of the various branches of acoustic phonons ( $v_{\alpha}$ ) are approximated by a characteristic velocity  $v_p$ , associated with the Debye energy via  $\Theta_D \sim v_p G/2$ .

A single spin ladder is described by

$$H_s = J_{\parallel} \sum_{j, \ell} \mathbf{S}_{\ell, j} \cdot \mathbf{S}_{\ell, j+1} + J_{\perp} \sum_j \mathbf{S}_{1, j} \cdot \mathbf{S}_{2, j}, \quad (2)$$

where  $\mathbf{S}_{\ell, j}$  is a spin- $\frac{1}{2}$  operator acting on site  $j$  and on leg  $\ell = 1, 2$  of the ladder.

As we are interested in the heat conductivity at low  $T$ , it is useful to consider the effective low-energy theory for  $H_s$  (assuming a small gap,  $\Delta \ll J_{\parallel}$ ) described in terms of four massive Majorana fermions,<sup>13</sup>

$$H_s = H_0^s + \sum_i g_i \int dx \mathcal{O}_i(x),$$

$$H_0^s = \int dx \sum_{a=0}^3 \frac{i v_a}{2} (\xi_L^a \partial_x \xi_L^a - \xi_R^a \partial_x \xi_R^a) + i(-)^{\delta_{a0}} \Delta_a \xi_R^a \xi_L^a. \quad (3)$$

In the above expression, the operators  $\mathcal{O}_i$  are all irrelevant and marginal operators allowed by the symmetry of the

original lattice Hamiltonian [Eq. (2)]. The three Majorana fields  $\xi^a$ ,  $a=1, 2, 3$ , describe the low lying magnon triplet with the velocity  $v_a = v_1$  and (spin) gap  $\Delta_a = \Delta_1$ , while the remaining Majorana field  $\xi^0$  describes a singlet excitation with gap  $\Delta_0$  and velocity  $v_0$ : the single-particle excitations have the dispersion relation  $\epsilon_a(k) = \sqrt{v_a^2 k^2 + \Delta_a^2}$ . While  $\Delta_0/\Delta_1 \sim 3$  for weak  $J_{\perp}$ , this ratio changes for larger  $J_{\perp}/J_{\parallel}$  or when other microscopic interactions are present—so that we shall consider it as a free parameter, yet assuming  $\Delta_0 > \Delta_1$ .

The total heat current, obtained through the continuity equation of the energy density, is

$$J_E \approx v_p^2 P_p + v_0^2 P_0 + v_1^2 P_1, \quad (4)$$

where  $P_p$ ,  $P_0$ , and  $P_1$  are the momentum operators of phonons, singlets, and triplets, respectively, for example,  $P_1 = -\frac{i}{2} \sum_{a=1, \dots, 3, \gamma} \int dx (\xi_{\gamma R}^a \partial_x \xi_{\gamma R}^a + \xi_{\gamma L}^a \partial_x \xi_{\gamma L}^a)$ . In Eq. (4), we neglect further contributions from the interactions which turn out to give only subleading corrections.

The crucial observation on which our following analysis is based is that the effective low-energy theory of our initial Hamiltonian conserves the total momentum,

$$P_T = P_p + P_0 + P_1. \quad (5)$$

A direct consequence is that—within this low-energy description—the heat conductivity is infinite.<sup>14,15</sup> However, the continuous translational invariance of Eq. (3) is not a true symmetry and follows from neglecting umklapp terms whose inclusion leads to a decay of  $P_T$ , which now acquires an exponentially long lifetime at low temperature. This is to be contrasted to all other decaying modes, whose lifetime behaves as power laws of  $T$  and allows for a hydrodynamic description based on the slow modes  $P_a$ ,  $a=p, 0, 1$ . Including these umklapp operators is thus the correct way to obtain a low-energy effective theory suited to the calculation of transport properties.

Three different umklapp terms turn out to be important if we assume that  $v_p < v_0, v_1$ ,<sup>20</sup>

$$H_U^p = \sum_{n \geq 3} g_p^{(n)} \int dx (\partial_x q)^n \cos(Gx), \quad (6)$$

$$H_U^{sp} = g_D^{sp} \int dx (\partial_x q)^2 \mathcal{O}_D(x) \cos(Gx/2) + i \sum_a g_a^{sp} \int dx (\partial_x q)^2 \xi_R^a \xi_L^a \cos(Gx), \quad (7)$$

with  $q(x) \propto \int \frac{1}{\sqrt{v_p |\mathbf{k}|}} e^{ik_x x} (a_{\mathbf{k}}^{\dagger} + a_{-\mathbf{k}}) \frac{d^3 \mathbf{k}}{(2\pi)^3}$  the displacement field for acoustic phonons projected along the ladders ( $a_{\mathbf{k}}^{\dagger}$  is an abbreviation for the sum of contributions from various phonon modes).  $\mathcal{O}_D \equiv \prod_{a=0}^3 \sigma^a$  is the continuum limit of the dimerization operator  $(-)^j (\mathbf{S}_{1, j} + \mathbf{S}_{2, j}) \cdot (\mathbf{S}_{1, j+1} + \mathbf{S}_{2, j+1})$ , where each  $\sigma^a$  ( $a=0, \dots, 3$ ) is the Ising spin operator for the quantum Ising model that is naturally associated with the Majorana  $\xi^a$  theory<sup>13</sup> (in our conventions, Ising model “0” is in its quantum disordered phase, while the three other models are ordered). We checked that linear couplings to phonons in Eq. (7) are subdominant.<sup>21</sup>

On top of the umklapp terms, it is also important to include normal processes

$$H_{N,k}^{sp} = i \sum_a g_a^{N,k} \int dx (\partial_x q)^k \xi_R^a \xi_L^a, \quad (8)$$

which allow momentum exchange between the spin and phonon systems. We do not consider normal operators acting only in the spin sector or only in the phononic sector, as they commute *separately* with the spin and phonon momentum operators and accordingly do not contribute to leading order to the heat conductivity.

### III. HYDRODYNAMIC APPROACH

To obtain a hydrodynamic description, we first identify a basis in the space of slow modes, in our case given by  $P_p$ ,  $P_0$ , and  $P_1$ . Then, we introduce the matrix of static susceptibilities of the slow modes,  $\chi_{ij} = \frac{1}{LT} \langle P_i(0) P_j(0) \rangle$  (equal time correlator) and a matrix of conductivities defined by Kubo formulas for the  $P_i$ 's,  $\sigma_{ij} = \frac{T}{\omega} \int_0^{1/T} d\tau e^{i\omega\tau} \langle T_\tau P_i(\tau) P_j(0) \rangle$ ,  $i, j = p, 0, 1$ . The heat conductivity is then given by

$$\kappa = \frac{1}{T} \sum_{i,j=p,0,1} v_i^2 v_j^2 \sigma_{ij} \equiv \kappa_{ss} + 2\kappa_{sp} + \kappa_{pp}. \quad (9)$$

Note that besides the spin and phonon heat conductivities  $\kappa_{ss}, \kappa_{pp}$ , there is also the drag term  $2\kappa_{ps} = \frac{2}{T} \sum_{b=0,1} v_p^2 v_b^2 \sigma_{bp}$ .

Within the memory-matrix approach,<sup>16,17</sup> the matrix of conductivities  $\hat{\sigma}(\omega)$  is expressed as

$$\hat{\sigma}(\omega, T) = \hat{\chi} \frac{1}{\hat{M}(\omega) - i\omega \hat{\chi}} \hat{\chi}, \quad (10)$$

where  $\hat{M}(\omega)$  is the so-called memory matrix. It can be shown that to leading order in the coupling constants of the umklapp terms  $g^U$  and of the normal spin-phonon term  $g^N$ , the memory matrix is simply given by<sup>3-5</sup>

$$M_{ij} \approx \frac{i}{\omega L} [\langle \dot{P}_i \dot{P}_j \rangle^R(\omega) - \langle \dot{P}_i \dot{P}_j \rangle^R(0)], \quad (11)$$

where  $\langle \cdots \rangle^R$  are the retarded correlation functions evaluated with respect to the unperturbed Hamiltonian as  $\dot{P}_i$  is already *linear* in the perturbations.

To evaluate Eq. (11) to leading order, we need various correlation functions of the decoupled spin-phonon system. As discussed above and checked below, for  $v_p < v_s$  and low  $T$ , one needs the high-energy correlation function in the phonon sector but only the low-energy asymptotics of spin-correlation functions. To obtain the correct low-energy correlators in the spin sector, it is in general necessary to take into account the (unitary) scattering of the thermally excited quasiparticles using generalizations of Sachdev and Young's semiclassical arguments<sup>6</sup>—see the Appendix. For example, the correlator  $\mathcal{G}_D(x, t) = \langle \mathcal{O}_D(x, t) \mathcal{O}_D(0, 0) \rangle$  of the dimerization operator, which is related to the Majorana fields in a highly non linear and nonlocal way, is given by

$$\mathcal{G}_D(x, t) = NK_0 \left( \frac{\Delta_0}{v_0} \sqrt{x^2 - v_0^2 t^2} \right) e^{-(1/2)\Phi(3x/\xi_1, 3t/\tau_1)}, \quad (12)$$

with  $N$  a nonuniversal prefactor,  $\Phi(\bar{x}, \bar{t}) = \bar{x} \operatorname{erf}(\bar{x}/\bar{t}\sqrt{\pi}) + \bar{t} e^{-\bar{x}^2/(\pi\bar{t}^2)}$ ,  $K_0$  the modified Bessel function,  $\tau_1 = \frac{\pi}{2T} e^{\Delta_0/T}$ , and  $\xi_1 = v_1 \sqrt{\frac{\pi}{2\Delta_0 T}} e^{\Delta_0/T}$ . It will, however, turn out that the scattering from other thermally excited quasiparticles described by  $\mathcal{G}_D(x, t)$  is not important as our problem is dominated by the spin-phonon scattering.

A generic umklapp memory-matrix entry at zero frequency can be cast in the form  $q^2 \operatorname{Im} \int dt \int dx e^{iqx} \mathcal{G}_p \mathcal{G}_s$ , with  $q = G/2$  or  $G$  and  $\mathcal{G}_{p(s)}$  the appropriate phonon (spin) correlator. At low  $T < v_p q$ , we evaluate it in the saddle point approximation, by deforming the contour in the complex plane. The saddle point lies at one of the phonon propagator poles,  $v_p t^* = \operatorname{sgn}(q) x^* = -\frac{iv_p}{2T}$ , well within the spin light cone where there are no contributions from the spin-spin scattering. Moreover, the semiclassical approximation for  $\mathcal{G}_D$  is valid at the saddle point.

The memory matrix can be split into four contributions,

$$M = M^N + M^{ph} + M^{G/2} + M^G, \quad (13)$$

corresponding to the relaxation processes described by terms (8), (6), and (7).

Generically, a memory-matrix entry bears an activated form at low temperature and thus can be specified by an activation gap and a prefactor. While the prefactor depends on nonuniversal, high-energy features of the spin system, in the soft phonon limit  $v_p < v_s$ , only *universal* features of the spin system determine the activation gap. This is why we only give the leading, exponential behavior at low  $T$  for the various memory-matrix entries (with the exception of one limiting case, see below). These expressions involve different umklapp gaps,

$$E_p = \frac{v_p G}{2}, \quad E_D = \frac{v_p G}{4} + \frac{\Delta_0}{2} \sqrt{1 - \alpha_0^2},$$

$$E_b = \frac{v_p G}{2} + \Delta_b \sqrt{1 - \alpha_b^2} \quad (14)$$

where  $\alpha_b = \frac{v_p}{v_b} < 1$  and  $b=0, 1$  labeling the spin singlet and triplet excitations. These formulas have a simple interpretation: under the constraints of energy and momentum conservation, they are the lowest energies for processes where the momentum  $q = G$  or  $G/2$  is absorbed by scattering a phonon from  $-q/2 \pm O(\Delta/v_p)$  to  $q/2 \mp O(\Delta/v_p)$  while scattering ( $E_a$ ) or creating ( $E_D$ ) a spin excitation. The simple form of the phonon energy scale appearing in Eq. (14) is a result of our simplified treatment of the phonon sector—high energy features thereof would modify this form but not the fact that it depends on a single scale  $E_p \sim \Theta_D$ .

The leading  $T$  dependence of the various contributions to the memory matrix is summarized as follows. The phonon umklapp [Eq. (6)] gives rise to a single nonvanishing entry,  $M_{pp}^{ph} \sim e^{-E_p/T}$ . Entries due to normal processes are  $M_{pp}^N = x_0 + x_1$ ,  $M_{bb}^N = -M_{pb}^N = x_b$ , and  $x_b \sim e^{-\Delta_b/T}$ . Spin-phonon umklapp processes with momentum transfer  $G$  entries are  $M_{pp}^G = y_0$

$+y_1$  and  $-C_{-1}^b M_{pb}^G = C_b^{-2} M_{bb}^G = y_b$  with  $C_b = \frac{\alpha_b}{\sqrt{1-\alpha_b^2}} \frac{2\Delta_b}{v_b G} \ll 1$  and  $y_b \sim e^{-E_b/T}$ . Finally, the relevant  $G/2$  entries are  $M_{pp}^{G/2} = -C_0^{-1} M_{p0}^{G/2} = C_0^{-2} M_{00}^{G/2} \sim e^{-E_D/T}$ .

With all these elements at hand, using Eqs. (9)–(11) and performing a straightforward matrix inversion yield the heat conductivity, which displays very different behaviors depending on the relative value of the magnetic gaps and Debye energy. In the following, we follow a more physically transparent approach and present in detail the temperature dependence of  $\kappa$  as well as the physical mechanism explaining it, in different parameter regimes.

#### IV. RESULTS AND DISCUSSION

For the interpretation of our results detailed below, it is useful to rewrite the linear-response relation  $\langle P_i \rangle = \sigma_{ij} A_j$ , where  $A_j$  is an external field coupling linearly to  $P_j$ . Using Eq. (4), we can identify it with  $A_j = v_j^2 \frac{\nabla T_j}{T}$ , where  $\nabla T_j$  is a fictitious temperature gradient coupling only to the subsystem  $j$ . Using Eq. (10), one obtains

$$\frac{\partial}{\partial t} \langle P_i \rangle - \chi_i v_i^2 \frac{\nabla T_i}{T} = -(\hat{M} \hat{\chi}^{-1})_{ij} \langle P_j \rangle, \quad (15)$$

where we used  $\chi_{ij} \approx \chi_i \delta_{ij}$ .

This equation has a simple interpretation: it is a rate equation for the momenta and  $\tau^{-1} = \hat{M} \hat{\chi}^{-1}$  can therefore be identified with the matrix of relaxation rates. The matrix of conductivities can be extracted from the equilibrium solution of the rate equation.

We will now discuss our results in the three different regimes depicted in Fig. 1, assuming always  $\Delta_1 < \Delta_0$  and  $v_s > v_p$ . To investigate the relation to experiments, it is useful to define the magnetic contribution to  $\kappa$ ,

$$\kappa_{mag} = \kappa - \kappa_{ph}^0 = \kappa_{ss} + 2\kappa_{ps} + \delta\kappa_{pp}, \quad (16)$$

where  $\kappa_{ph}^0$  is the conductivity of a hypothetical system without magnetic degrees of freedom (estimated in experiments from fits to  $\kappa$  perpendicular to the spin ladders). Note that there is also a negative contribution from the change of the phonon conductivity  $\delta\kappa_{pp} = \kappa_{pp} - \kappa_{ph}^0$  due to scattering from spin excitations.

##### A. Regime I

We first investigate regime I of Fig. 1 where  $E_p, T < \Delta_1$  and the momentum relaxation is dominated by the phonon umklapp ( $E_p < E_1, E_D$ ). As  $\Delta_0 > \Delta_1$ , we can neglect the singlet mode and focus on the  $2 \times 2$  matrix describing the relaxation of phonon and triplet momentum to obtain

$$\kappa_{pp} = v_p^4 \frac{\sigma_{pp}}{T} = \frac{1}{T} \chi_p v_p^4 \tau_p^U \sim e^{E_p/T}, \quad (17)$$

$$\kappa_{ss} = v_1^4 \frac{\sigma_{11}}{T} = \frac{1}{T} \chi_1 v_1^4 \tau_{1 \rightarrow p}^N \sim e^{-\Delta_1/T}, \quad (18)$$

$$\kappa_{ps} = v_1^2 v_p^2 \frac{\sigma_{ps}}{T} = \frac{\chi_1 v_1^2}{\chi_p v_p^2} \kappa_{pp} \sim e^{(E_p - \Delta_1)/T}, \quad (19)$$

where  $\chi_i = \chi_{ii}$  (to leading order,  $\hat{\chi}$  is diagonal) and  $1/\tau_p^U = M_{pp}^{ph}/\chi_p \sim e^{-E_p/T}$  is the phonon umklapp rate. The “pure spin heat conductivity”  $\kappa_{ss}$ —corresponding to the heat being carried by magnons—is determined by the exponentially small number of spin excitations,  $\chi_1 \sim e^{-\Delta_1/T}$ , and the nonexponential rate of momentum transfer,  $1/\tau_{1 \rightarrow p}^N = M_{11}^N/\chi_1$ , from the spin system to the phonon system. Most interesting is the drag term  $\kappa_{ps}$ , which dominates over  $\kappa_{ss}$ . As we can neglect momentum dissipation within the spin system, even a small coupling of the spin and phonon systems by normal processes induces a “perfect drag:” both subsystems have the same drift velocity. Therefore, the ratio of heat currents is given by the ratio of energy densities  $\langle \rho_i^e \rangle = v_i^2 \chi_i$ ,<sup>22</sup> and we find

$$\kappa_{ps} = \kappa_{pp} \langle \rho_i^e \rangle / \langle \rho_p^e \rangle, \quad (20)$$

in complete agreement with our memory-matrix analysis.

In Eq. (17), only the leading behavior of  $\kappa_{pp}$  is shown. To calculate  $\delta\kappa_{pp}$ , one has to consider the leading correction arising from the subdominant mixed spin-phonon umklapp [Eq. (7)] described by the rate  $(\tau_{sp}^U)^{-1} = \sum_{ij} M_{ij}^G/\chi_p$ . We obtain

$$\delta\kappa_{pp} = -\frac{1}{T} \chi_p v_p^4 \left( \frac{\tau_{sp}^U}{\tau_p^U} \right)^2 \sim -e^{(2E_p - E_1)/T}. \quad (21)$$

This term corresponds to “magnetic friction:” the heat current carried by phonons is reduced due to scattering on the dilute gas of magnons.

The competition between the negative  $\delta\kappa_{pp}$  and the positive  $\kappa_{ps}$  leads to a complex cross-over behavior of the magnetic heat conductivity  $\kappa_{mag}$ , see Fig. 1. Below  $T^* = (2E_p - E_1) - (E_p - \Delta_1) \approx \frac{\alpha_1^2}{2} \Delta_1$  (for  $\alpha_1 \ll 1$ ), the negative  $\delta\kappa_{pp}$  dominates. For  $\Delta_1 > T > T^*$ , the behavior is fixed by the pre-exponential factors; in this regime, we find

$$\frac{\kappa_{ps}}{|\delta\kappa_{pp}|} = \frac{\mathcal{N}}{\alpha_1} \left( \frac{v_p G}{\Delta_1} \right)^4 \left( \frac{T}{\Delta_1} \right)^{-9/2} \left( \frac{\bar{g}_{ph}^U}{\bar{g}_{sp-ph}^U} \right)^2, \quad (22)$$

where the  $\bar{g}^U$ 's are the dimensionless microscopic couplings and  $\mathcal{N}$  is a numerical constant. Interestingly, the crossover scale  $T^*$  corresponds to the temperature where the saddle point location crosses the thermal wavelength of the magnons.

Under the hypothesis that for  $T > T^*$  magnetic friction is dominated by the enhancement of conductivity due to the addition of heat carriers, namely, the magnons, we can relate the ratio of the magnetic versus phononic contributions to the heat conductivity, which is of experimental relevance, to purely thermodynamical quantities,

$$\frac{\kappa_{mag}}{\kappa_{ph}^0} \approx \frac{v_1^2 \chi_{11}}{v_p^2 \chi_{pp}}. \quad (23)$$

##### B. Regime II

Next, we consider regime II of Fig. 1, where  $\Delta_1 < E_p < \Delta_0$ . In this regime, formulas (17), (19), and (21) for  $\kappa_{pp}$ ,



$\kappa_{ps}$ , and  $\delta\kappa_{pp}$  remain unchanged; however, in contrast to regime I, both  $\kappa_{ps}$  and  $\delta\kappa_{pp}$  are exponentially large. Furthermore, the momentum transfer rate  $1/\tau_{p\rightarrow 1}$  from the phonon system to the spin system is now larger than the phonon umklapp rate  $1/\tau_p^U$ , and therefore the two subsystems equilibrate before losing momentum via phonon umklapps, yielding

$$\kappa_{ss} = \frac{1}{T} \chi_1 v_1^4 \frac{\tau_{1\rightarrow p}^N}{\tau_{p\rightarrow 1}^N} \tau_p^U \sim e^{(E_p - 2\Delta_1)/T}. \quad (24)$$

$\kappa_{ss}$  is always smaller than  $\kappa_{pp}$ , and generically  $\kappa_{ss} \ll \kappa_{ps}$ . In this regime, the same remark as in regime I, regarding the relative size of the magnetic versus phononic heat conductivity, applies: if the magnetic friction is subdominant, the ratio only depends on thermodynamical quantities.

### C. Regime III

In regime III,  $E_p > \Delta_0$ , a new scattering channel [Eq. (7)] dominates where (pseudo)momentum in quanta of  $G/2$  is transferred to the lattice in a complex process involving singlet, triplet, and phonon modes. The associated umklapp gap  $E_D < E_p$  therefore replaces  $E_p$  in formulas (17), (19), and (24). The leading term is the phonon contribution

$$\kappa_{pp} = \frac{1}{T} v_p^4 \chi_p \tau_D^U \sim e^{E_D/T}, \quad (25)$$

with  $1/\tau_D^U = \sum_{ij} M_{ij}^{G/2} / \chi_p$  the rate of total momentum relaxation. As the phonon contribution is strongly reduced by the presence of the magnetic system, the naive procedure of disentangling the magnon contribution  $\kappa_{mag}$  by subtracting the phonon background [Eq. (16)] is not useful in this regime.

### D. Comparison to experiments

The experimental data presented in Ref. 2 on cuprate ladders clearly display an activated behavior for  $\kappa_{mag}$ , the activation energy being close to the gap value (which is of the order of 400 K). Measurements have been carried on for temperature ranging from a few tens of Kelvins up to 300 K. Due to the operative way to determine the magnetic heat conductivity, namely, by subtracting a ‘‘pure phonon’’ contribution obtained by a low-temperature fit, these data are reliable only for not too low temperatures, i.e.,  $T \gtrsim 50$  K.

Our theory does *not* directly apply to these systems as the low-temperature properties are dominated by disorder. Nevertheless, it is possible to obtain a qualitative understanding of what happens in a situation where the phonon sector is disordered. Then, due to the scattering from defects (in combination with normal phonon-phonon processes<sup>18</sup>), the phonon heat current  $J_e^{ph}$  has no longer an exponentially large lifetime. It is possible to mimic this situation by taking the limit  $E_p \rightarrow 0$  in our equations. This indicates that these compounds are located deep into regime I, and the corresponding activation energy for  $T > T_*$  is then close to the spin gap. Unfortunately, the temperature  $T_* \sim 4$  K turns out to be much lower than the minimal temperature above which the spin contribution to the heat conductivity can be determined reliably in the experiment. Therefore, the characteristic sign

change shown in the first panel of Fig. 1 is not observable in these samples.

## V. CONCLUSION

Our results emphasize the richness of transport phenomena, the actual low  $T$  heat conductivity depending in a subtle way on the different scales present in the system. In particular, we find that in a clean system, the magnetic contribution to the conductivity does not display the trivial activated behavior with activation energy equal to the spin gap. An exception is the limit  $E_p \rightarrow 0$ , which mimics a situation where momentum predominantly relaxes via disorder in the phonon system, as might be the case in the cuprate systems of Ref. 2. We hope that there will be in the future more measures on spin-ladder materials allowing to probe the different regimes discovered by our study.

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## APPENDIX: LONG DISTANCE SPIN CORRELATORS

In this appendix, we present the calculation for the low-temperature dimerization operator correlator,  $\mathcal{G}_D(x, t) = \langle \mathcal{O}_D(x, t) \mathcal{O}_D(0, 0) \rangle$ , which relies on the semiclassical approach developed in Ref. 6. We first recall the results obtained by Sachdev and Young for a single Ising model, and we then apply these ideas to our system, which consists of four weakly coupled Ising models.

### 1. Single Ising model

The central idea of this approach is to exploit the fact that at low enough temperatures in a gapped system,  $T \ll \Delta$ , typical configurations of the system correspond to a very dilute gas of quasiparticles, with mean quasiparticle separation of the order of  $e^{\Delta/T}$ , much larger than their thermal de Broglie wavelength  $\lambda_{th} = \frac{v}{\sqrt{\Delta T}}$ . As shown in Ref. 6, a classical treatment of these quasiparticles is legitimate. Only the scattering rates of two particles (diluteness allows to consider only two-body collisions) has to be calculated from quantum mechanics. In one dimension, particles with a quadratic dispersion are perfectly reflected for any repulsive potential in the limit of small momentum. Therefore, the two-body scattering matrix tends to its so-called superuniversal form,  $S = -1$ , irrespective of the form the two-body potential. Remarkably, these ingredients are sufficient to allow for a closed form evaluation of the Ising operator correlator, both in the ordered and disordered phase, with the result

$$G_{ord} = \langle \sigma(x, t) \sigma(0, 0) \rangle = N^2 e^{-\Phi(x/\zeta, t/\tau)},$$

$$\Phi(\bar{x}, \bar{t}) = \bar{x} \operatorname{erf}\left(\frac{\bar{x}}{\bar{t} \sqrt{\pi}}\right) + \bar{t} e^{-\bar{x}^2/(\pi \bar{t}^2)}, \quad (A1)$$

with  $N = \langle \sigma \rangle$  the local  $T=0$  magnetization,  $\zeta = v \sqrt{\frac{\pi}{2\Delta T}} e^{\Delta/T}$ , and  $\tau = \frac{\pi}{2T} e^{\Delta/T}$ . In the disordered phase, the correlator reads

$$G_{dis} = \langle \sigma(x,t)\sigma(0,0) \rangle = \mathcal{A}K_0 \left( \frac{\Delta}{v} \sqrt{x^2 - v^2 t^2} \right) e^{-\Phi(x/\xi, t/\tau)}. \quad (\text{A2})$$

We are interested in the correlator of the dimerization operator  $\mathcal{O}_D = \prod_{a=0}^3 \sigma^a$ . The crudest approximation consists of neglecting the interaction between the Ising models and leads to a simple product form,  $\mathcal{G}_D = G_{dis}^0 \prod_{a>0} G_{ord}^a$ . Of course, such an approximation is expected to fail to capture the correct long time and space limit since it neglects the scattering between quasiparticles on different Ising models. In reality, the Ising models are coupled—to lowest order, this coupling is given by the spin density–spin density coupling  $\Sigma_{a,b} \int \xi_R^a \xi_R^b \xi_L^a \xi_L^b$ —and the scattering is *relevant* in the sense that it qualitatively affects the form of  $\mathcal{G}_D$  at large  $t, x/v \gg \Delta^{-1}$ . We now proceed to take this interaction into account, in the limit of heavy singlet excitations,  $\Delta_0 > \Delta_1$ . This is *a priori* the relevant physical regime since in actual realizations of the spin ladder, no indication for the existence of the singlet branch, at reasonably low energy, has ever been reported to our knowledge.

## 2. Weakly coupled Ising models

In the semiclassical approximation, field configurations contributing to the path integral representation of the correlation function are classical ones: quasiparticles follow straight lines, each given its corresponding Boltzmann weight. Then, the interaction between two particles is treated quantum mechanically, the  $S$  matrix bearing its superuniversal form ( $k \rightarrow 0$  limit): particles bounce on each other (hard core collisions) with a  $\pi$  phase shift ( $S = -1$ ). We now repeat Sachdev and Young's<sup>6</sup> line of reasoning including the inter-Ising model interaction; this amounts to have the straight lines representing the propagation of thermally excited states to “see” each other, i.e., the quasiparticles belonging to different Ising models to scatter, the  $S$  matrix being again the superuniversal one.

For the Ising models  $a \neq 0$  that are in the ordered phase, quasiparticles are domain walls for the different Ising models that separate domains with different magnetizations. Each domain wall carries an index  $a \neq 0$ . Each time a domain wall  $a \neq 0$  crosses the line joining the points  $(0,0)$  and  $(x,t)$ , the operator  $\prod_{a \neq 0} \sigma^a$  has its  $\pm 1$  eigenvalue flipped. This allows us to conclude that its semiclassical correlator reads

$$\left\langle \prod_{a \neq 0} \sigma^a(x,t) \prod_{a \neq 0} \sigma^a(0,0) \right\rangle = N_1^6 e^{-\Phi(3x/\xi_1, 3t/\tau_1)}. \quad (\text{A3})$$

It is the same as the correlator in a single ordered Ising model, the factor of 3 corresponding to the tripling of the density of excited states [the probability that a given excited state carrying momentum  $p$  crosses the line joining  $(0,0)$  to  $(x,t)$  is  $q' = 3q = 3|x - v_1(p)t|/L$ , with  $L$  the system size and  $v_1(p) = \frac{d\epsilon_1(p)}{dp}$ , where  $\epsilon_1(p) = \sqrt{\Delta_1^2 + v_1^2 p^2}$  is the one-magnon dispersion relation].

However, we are rather interested in the correlator of the dimerization operator which includes both singlet and triplet fields. The singlet Ising model being in its disordered phase,

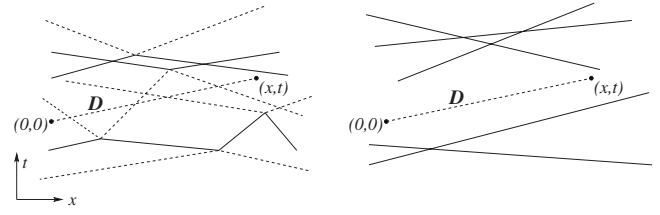


FIG. 2. Typical configurations contributing to  $\mathcal{G}_D$  for different masses. Full lines indicate domain walls of the ordered models  $a \neq 0$ , while dashed lines represent propagation of the quasiparticles of the singlet Ising model. Left: general case. Right: heavy singlet limit.

the spin  $\sigma^0 \equiv \sigma^{0,z}$  has an overlap with the quasiparticle creation operator. Using this remark, the semiclassical calculation can be formulated using the real-space diagrams of Sachdev and Young:<sup>6</sup> full lines represent world lines of domain walls in the ordered models and dashed lines represent the propagation of excitations of the disordered model. There is a line joining  $(x,t)$  to  $(0,0)$  that corresponds to the creation of a 0 particle at point  $(x,t)$  and to its destruction at point  $(0,0)$  (therefore, this line should be dashed on both its extremities), and this line has to be a straight line [the state  $\mathcal{O}_D(x,t)\mathcal{O}_D(0,0)|\Psi\rangle$  has to have a finite overlap with  $|\Psi\rangle$  to contribute to the trace defining the expectation value; therefore, the pattern of world lines with and without the straight line connecting  $(0,0)$  and  $(x,t)$  has to be the same]—in the following, we call this a straight line  $D$ . Additional rules are as follows: each time a dashed line crosses  $D$ , there is a scattering event, particles bounce onto each other, and this contributes an  $S = -1$  factor—note that since we are in one dimension and because the two scattering particles have the same dispersion relation, lines coming out of a scattering event are just continued straight.

To proceed, one has to analyze collisions between dashed and full lines. A simplification occurs in the case of degenerate masses  $\Delta_0 = \Delta_1$ . Then, energy-momentum conservation during the scattering events ensures that lines are also continued straight (particles just exchange their quantum numbers), and it can be shown that the problem maps onto the calculation of Pott's spin correlator in the four-state Pott's model in its disordered phase, a problem which has itself been solved in the low  $T$  regime using the semiclassical approach.<sup>19</sup>

This fine-tuned degenerate limit is, however, not relevant to our situation where masses are generically different. If  $\Delta_0 \neq \Delta_1$ , during a scattering event between a domain wall and a type 0 particle, particles do not just exchange their momenta and lines are deviated after the crossing. In particular, if one considers collisions between domain walls and the line  $D$ , and remembering that the pattern of world lines with and without the line  $D$  should be the same, one concludes that these events just do not give any contribution to the semiclassical correlator—thus, an additional rule is to forbid scattering between plain lines and  $D$  (see Fig. 2, left panel). Note that without  $D$ -full line crossing, the dimerization operator is never flipped by any domain wall.

Given all these rules, one has to sum up contributions over configurations with no crossing between full lines and

*D*. In general, this is a tough problem. A simplification occurs in the case where masses are very different and, for our purpose, when the singlet mass is much greater than the triplet mass. Then, it is possible to neglect all contributions with dashed lines in the thermal background (see Fig. 2, right panel); the error is of the order of  $\exp(-[\Delta_0 - \Delta_1]/T)$ . Enforcing that configurations contributing contain no *D*-full line crossing amounts to the replacement of  $(1 - 2q')^N$  by  $(1 - q')^N$  in Eq. (3) of Ref. 6. Performing the average over *p*, we get

$$\mathcal{G}_D(x, t) = \mathcal{A}K_0 \left( \frac{\Delta_0}{v_0} \sqrt{x^2 - v_0^2 t^2} \right) e^{-(1/2)\Phi(3x/\xi_1, 3t/\tau_1)} \quad (\text{A4})$$

for  $x, t > 0$ .

We will also need to evaluate correlators involving derivatives of just one Ising spin of the kind  $\langle \partial_x \sigma^a \prod_{b \neq a} \sigma^b(x, t) \mathcal{O}_D(0, 0) \rangle$ . Of course, they are not all independent. It suffices for our purpose to compute

$$\mathcal{G}'_D = \left\langle \sigma^0 \partial_x \prod_{a \neq 0} \sigma^a(x, t) \mathcal{O}_D(0, 0) \right\rangle, \quad (\text{A5})$$

which we evaluate using  $\mathcal{G}'_D = \lim_{\epsilon \rightarrow 0} [\langle \prod_{a \neq 0} \sigma^a(x + \epsilon) \sigma^0(x, t) \mathcal{O}_D(0, 0) \rangle - \mathcal{G}_D(x, t)] / \epsilon$ . Contributions to the first term are those with domain walls passing between  $(x + \epsilon, t)$

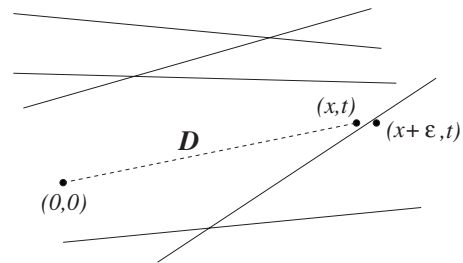


FIG. 3. Typical configuration contributing to  $\mathcal{G}'_D$  in the heavy singlet mass limit.

and  $(x, t)$  but not crossing the line *D* (see Fig. 3).

The probability of having one single domain wall with momentum *p* passing is  $q_\epsilon = \epsilon \Theta(v_1(p)t - x) / L$  (with  $\Theta$  the Heaviside function), and after calculation, we find

$$\mathcal{G}'_D(x, t) = \mathcal{G}_D(x, t) \lambda_1(x, t),$$

$$\lambda_1(x, t) = -\frac{3}{2} \int_{p_0}^{\infty} \frac{dp}{\pi} e^{-\epsilon_1(p)/T}, \quad (\text{A6})$$

where  $p_0$  is the root of the equation  $\frac{\partial \epsilon_1(p)}{\partial p} = x/t$ . We note that  $|\lambda_1(x, t)| < \frac{3}{2} \zeta_1^{-1}$ .

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<sup>20</sup>Additional umklapp terms, acting only in the spin sector, involve much higher energy states in the limit of soft phonons and thus have exponentially suppressed effects.

<sup>21</sup>Scattering events preserving momentum and energy when a single phonon is involved, with momentum transfer of order *G*, force at least one magnon to carry momentum of order *G* and thus involve higher energy states.

<sup>22</sup>This relation follows from  $J_e^i \approx v_i^2 P_i$  and the energy continuity equation for both subsystems. For a derivation in the context of charge transport, see A. Rosch and N. Andrei, J. Low Temp. Phys. **126**, 1195 (2002).