Anomalous spin diffusion in one-dimensional antiferromagnets

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The problem of low-temperature spin dynamics in antiferromagnetic spin chains has so far remained elusive. We reinvestigate it by focusing on isotropic antiferromagnetic chains whose low-energy effective field theory is governed by the quantum nonlinear sigma model. We outline an exact non-perturbative theoretical approach and analyse the low-temperature behaviour in the vicinity of non-magnetized states, obtaining explicit expressions for the spin Drude weight, spin diffusion constant and the NMR relaxation rate. We find several disagreements with previous theoretical predictions obtained by the vacuum form factor and semi-classical approaches. Most prominently in isotropic spin chain we find a crossover from the semi-classical regime to a quantum fully interacting regime at half filling dominated by the strong correlations. In the latter case, we obtain zero spin Drude weight and divergent spin conductivity, yielding superdiffusive spin transport and spin fluctuations belonging to the Kardar-Parisi-Zhang universality class. Moreover, using a numerical approach, we find evidence that the anomalous spin transport can persist at high temperatures even in non-integrable spin chains.

One-dimensional isotropic antiferromagnets reveal several remarkable aspects, which made them a subject of very intense experimental and theoretical investigations in the past. One of the most profound features is a fundamental distinction between spin systems with odd and integer spin. In one dimension, the latter exhibit dynamically generated gapped spectrum while the former are characterised by gapless excitations with fractional statistics [1–3].

In the context of non-equilibrium physics, the main focus has been to explain peculiar properties of the spin relaxation dynamics of the Haldane-gapped spin chain compounds. In spite of various theoretical approaches, ranging from the field-theoretical techniques such as the form-factor expansions [4, 5], to the semi-classical approximations [6–10], the status of the topic still remains controversial to this date, with a number of conflicting statements concerning the spin Drude weight, spin diffusion constant, and the nuclear magnetic resonance (NMR) rate.

In recent years, there has been a rapid theoretical advancement in the domain of non-equilibrium phenomena in exactly solvable interacting systems, largely owing to the formalism of the generalised hydrodynamics [11, 12], see also [13–25], which provides an efficient and universal language to tackle various non-equilibrium problems. Among others, it enables us to obtain closed-form analytic expressions for transport coefficients, such as Drude weights [26–29] (see also [30]) and, more recently, diffusion constants in interacting quantum systems [31–34]. Equipped with this powerful toolbox, we here re-examine a number of perennial issues which lie outside of the scope of methods employed in previous works [4, 35, 36].

In particular, we revisit the problem of spin transport in non-integrable antiferromagnetic spin chains at low temperatures in the half filled sector, focusing on the diffusion constant and the nuclear spin relaxation rate. In the case of gapped anisotropic chains, our results provide the *first* direct confirmation of the semi-classical theory [7]. In *isotropic* $SU(2)$ chains in contrast, our findings markedly differ from the previous predictions and demonstrate that the experimentally relevant regime $h/T \ll 1$, where T is the temperature and h the external magnetic field, is dominated by strong quantum correlations where the full many-body scattering matrix of the underlying effective field theory plays a crucial role. This has several far-reaching physical consequences, most prominently the *divergent* spin (charge) diffusion constant and spin conductivity at any finite temperature, which signals *sub-ballistic*, yet *superdiffusive* spin transport. This anomalous feature, initially observed numerically in an *integrable* isotropic Heisenberg model [37, 38], has been rigorously established in [39]. A recent study of the same model [40] provides a strong numerical evidence that the spin relaxation dynamics falls into the Kardar-Parisi-Zhang (KPZ) universality class, mostly known from the physics of growing interfaces [41–43]. In this work, we offer theoretical arguments which indicate that this type of anomalous spin transport is a distinguished feature of spin/charge transport even in generic one-dimensional *non-integrable* isotropic antiferromagnetic compounds at low temperatures, irrespectively of whether the low-lying theory is gapped or gapless. Moreover, our numerical tDMRG simulations give evidence that the anomalous spin relaxation persists also at higher temperatures.

Spin diffusion constant from integrability. We begin by introducing a new, simpler expression for the spin diffusion constant in integrable models at half filling. Given a spin chain governed a Hamiltonian $\hat{H}$ and conserved total magnetization $\hat{S}^z = \sum_i \hat{s}^z_i$, the linear-response spin diffusion constant $\mathfrak{D}$ is computed as the spatio-temporal integrated spin current autocorrelation function [44, 45],

$$\mathfrak{D}(T,h) = \frac{1}{T\chi_h(T,h)}\int_0^\infty \mathrm{d}t\left(\langle \hat{J}(t)\hat{j}_0(0)\rangle_{T,h} - \mathcal{D}\right), \quad (1)$$

where $\hat{J} = \sum_i \hat{j}_i$ denotes the total current, with $\hat{j}_i$ the spin-current density at site i, $\langle \bullet \rangle_{T,h}$ corresponds to the equilibrium average with respect to the grand-canonical Gibbs ensemble $\hat{\varrho}_{\rm GC}(T,h) \simeq \exp\left(-(\hat{H}-h\hat{S}^z)/T\right)$, while $\chi_h(T,h) = -\partial^2 f(T,h)/\partial h^2$ is the static spin susceptibility, where $f(T,h) = -T\log \mathrm{Tr}(\hat{\varrho}_{\rm GC}(T,h))$. In integrable systems, the spin Drude weight $\mathcal{D}(T,h)$, defined as the large-time limit of the spatially-integrated current-current correlator in Eq. (1), is generically finite and thus has been subtracted in Eq. (1) to ensure that $\mathfrak{D}(T,h)$ is well-defined. At half filling $h=0$ however $\mathcal{D}(T,0)=0$ in the systems considered here, as a consequence of the particle-hole symmetry [27, 46, 47], in agreement with semi-classical results [8].

An explicit expression for the diffusion constant in thermal half-filled states has recently been obtained in [33], using a thermodynamic form-factor expansion and in [34] via kinetic theory. Here we derive a new compact expression for the *exact* spin diffusion constant $\mathfrak{D}$ which is valid in thermal equilibrium *at half filling*,

$$\mathfrak{D} \equiv \mathfrak{D}(T,0) = \frac{\partial^2 \mathcal{D}^{\rm self}(T,\nu)}{\partial \nu^2}\Big|_{\nu=0}, \quad (2)$$

namely as the curvature of the *Drude self-weight* [28] (or zero-frequency noise [48])

$$\mathcal{D}^{\rm self}(T,h) = 2\int_0^\infty \mathrm{d}t \langle \hat{j}_0(t)\hat{j}_0(0)\rangle_{T,h}, \quad (3)$$

with respect to $\nu(T,h) \equiv 4T\langle \hat{S}^z\rangle_{T,h}$. Moreover, formula (2) remains valid for small h, with corrections of the order $\mathcal{O}(h^2)$. The curvature of the spin Drude self-weight at $h=0$ is expressible in terms of equilibrium state functions via the hydrodynamic mode resolution $\partial^2_\nu \mathcal{D}^{\rm self}|_{\nu=0} = \sum_s \int \frac{\mathrm{d}p_s(\theta)}{2\pi} n_s(\theta)(1-n_s(\theta)) \times |v^{\rm eff}_s(\theta)| \partial^2_\nu (m^{\rm dr}_s)^2|_{\nu=0}$, where the integer label s iterates over distinct quasi-particle species [19, 33], and $n_s(\theta)$ correspond to their (thermal) equilibrium Fermi occupation functions, $p_s(\theta)$ their effective (i.e. dressed) momenta as functions of rapidity variable θ, $v^{\rm eff}_s(\theta) = \partial\varepsilon_s(\theta)/\partial p_s(\theta)$ their group velocities and $m^{\rm dr}_s$ their effective magnetization (spin) with respect to a thermal background.

The simple formula (2), can be understood as an improved and optimised analogue of the diffusion lower bound originally proposed in [49] (saturating only in models with a single quasi-particle velocity [50]). It confirms the recent proposal of [34], and is universally valid for any conserved Noether charge in generic integrable systems restricted to half-filled equilibrium states at finite temperature $T>0$. Notice that, in contrast to the conventional Kubo formula, which involves space-integrated current correlations, the correlator in Eq. (13) is evaluated at equal space points. Our result (2) is consistent with the general formula given by Eq. (6.6) in [33] at half filling [51], and can be derived by exploiting a certain identity between thermodynamic functions which we dubbed "*magic formula*". The latter is proven rigorously in the high-temperature limit and confirmed numerically at finite temperatures [47].

Spin transport in spin$-1/2$ chains. To first demonstrate the key concepts, we analyse the integrable XXZ spin-1/2 chain with anisotropy parameter Δ, focusing on the regime $\Delta > 1$ where the quasi-particles (with respect to the ferromagneetic vacuum) are compounds of s bound magnons [47]. In the low-temperature limit and small h, with $h/T \gg 1$ large, the bound-state contributions ($s>1$) are suppressed as $\sim e^{-h(s-1)/T}$, and from Eq. (2) we find (cf. [47])

$$\mathfrak{D}_{\rm XXZ} = \mathfrak{A}\, e^{\mathfrak{m}/T}\left(1 + \mathcal{O}(e^{-h/T}) + \mathcal{O}(e^{-\mathfrak{m}/T})\right), \quad (4)$$

where $\mathfrak{A} = \mathfrak{c}^2/(\mathfrak{n}\,\mathfrak{m})$, $\mathfrak{n}=2$ is the number of low-energy degrees of freedom with the low-momentum dispersion law $\varepsilon_1(k) \approx \mathfrak{m} + (\mathfrak{c}\,k)^2/2\mathfrak{m}$, where $\mathfrak{m}$ denotes the spectral gap, with $\mathfrak{m} = \frac{1}{2}\sinh(\eta) \times \sum_{k\in\mathbb{Z}}(-1)^k/\cosh(k\eta)$, $\eta = \cosh^{-1}\Delta$. The higher-order corrections due to the quasi-particles with finite momenta are of the order $\mathcal{O}(e^{-\mathfrak{m}/T})$ and thus suppressed by the energy gap. These results are aligned with the semi-classical result of ref. [7] and give the first direct confirmation of the semi-classical approximation in anisotropic chains. We are here primarily interested in the physically important, albeit subtle, regime $h/T \ll 1$, where the corrections $\mathcal{O}(e^{-h/T})$ coming from the bound-state contributions, invisible to the semi-classical approach [7], play a pivotal role. While these higher order terms remain sub-leading for anisotropies $\Delta > 1$, they become *divergent* for *isotropic interactions* $\Delta = 1$, as $h \to 0$ at finite T, rendering Eq. (4) invalid. After including these corrections, Eq. (2) gives a spin DC conductivity [47] $\sigma(T,h) = \mathfrak{D}(T,h)\chi_h(T,h) = \kappa(T)|h|^{-1} + \mathcal{O}(h^0)$, with $\kappa(T) \sim T^{-1/2}$, signalling *superdiffusive* spin transport at any finite temperature at half-filling.

Non-integrable isotropic antiferromagnetic chains. We now consider the low-temperature spin dynamics in *generic* antiferromagnetic spin chains with isotropic spin interactions. For definiteness, we focus on the $SU(2)$-symmetric Heisenberg spin-S chains $\hat{H}_S = J\sum_i \hat{\mathbf{s}}_i\cdot\hat{\mathbf{s}}_{i+1}$, with $\hat{\mathbf{s}}\cdot\hat{\mathbf{s}} = S(S+1)$. In the limit of large spin S, one can derive the effective low-energy action, which describes the evolution of the staggered and ferromagnetic fluctuation fields $\hat{\mathbf{s}}_i \approx S(-1)^i\hat{\mathbf{n}} + \hat{\mathbf{m}}$, see [1, 2, 52]. Here magnetization $\hat{\mathbf{m}} = g^{-1}\hat{\mathbf{n}}\times\hat{\mathbf{p}}$ is the generator of the spatial rotations of the unit vector field $\hat{\mathbf{n}} = (\hat{n}^x, \hat{n}^y, \hat{n}^z)$, with the canonically-conjugate

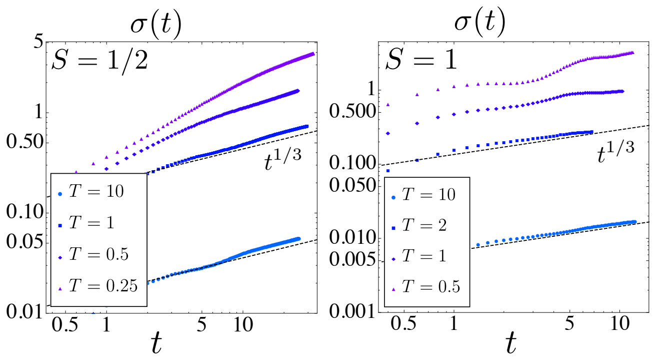

FIG. 1. Log-Log plot of the spin conductivity for the isotropic Heisenberg spin $S=1/2$ (left) and spin $S=1$ (right) chains, as a function of time (in unit of exchange coupling J) at $h=0$, shown for 4 different temperatures (which increase from top to bottom) computed using tDMRG simulations. In both cases we observe time-divergent spin conductivity $\sigma(t)\sim t^{1/3}$.

momentum $\hat{\mathbf{p}}=(1/g)\partial_t\hat{\mathbf{n}}+(\Theta/4\pi)\hat{\mathbf{n}}\times\partial_x\hat{\mathbf{n}}$. This yields a non-abelian quantum field theory described by the Hamiltonian (in dimensionless units $v=2JS\to 1$)

$$\hat{H}^{(\Theta)}_{\Sigma}=\frac{v}{2}\int \mathrm{d}x\left[g\Big(\hat{\mathbf{m}}+\frac{\Theta}{4\pi}\partial_x\hat{\mathbf{n}}\Big)^2+\frac{1}{g}(\partial_x\hat{\mathbf{n}})^2\right], \qquad (5)$$

where $g=2/S$ is the coupling parameter and $\Theta=2\pi S$ is called the topological angle. For $\Theta\in\{0,\pi\}$ the $O(3)$ NLSM model is an *integrable* QFT with a completely factorizable scattering matrix [53, 54]. Specifically, at $\Theta=0$ the model yields the effective low-energy theory for the staggered ($k\approx\pi$) and the ferromagnetic ($k\approx 0$) fluctuations in the Haldane–gapped integer spin chains. The $k\to 0$ component of the spin-lattice magnetization corresponds to the conserved Noether charge $\hat{\mathbf{m}}\simeq\hat{\mathbf{n}}\times\partial_t\hat{\mathbf{n}}$. The elementary excitations are a *massive* triplet of bosons with a relativistic dispersion $e(k)=\sqrt{k^2+\mathfrak{m}^2}$. Here $\mathfrak{m}$ is a dynamically-generated mass $\mathfrak{m}\sim\Lambda\,e^{-\pi S}$, whose magnitude is determined by the underlying spin-S lattice model at momentum scale Λ. While the NLSM has no physical bound states in the spectrum, the scattering is non-diagonal and governed by a non-trivial exchange of spin degrees of freedom. At $\Theta=\pi$, the $O(3)$ NLSM describes the low-energy continuum theory of the half-integer spin chains with *massless* elementary excitations [3, 52].

Low-temperature spin transport. Following the lines from the previous section, taking the $T\to 0$ limit with finite h allows us to disregard the contributions from the internal magnonic excitations labelled by $s>0$. This way, for small T and small h, with $h\gg T$, we arrive (cf. [47]) to the same expression as in Eq. (4), with $\mathfrak{n}=3$, $\mathfrak{c}=1$ and $e(k)\approx\mathfrak{m}+k^2/2\mathfrak{m}$, in agreement with the semi-classical prediction of [6]. Crucially however, the subleading corrections once again blow up when approaching the half filling $h\to 0$ at any finite T and, in exact analogy with the isotropic Heisenberg chain, the resummation over the magnonic degrees of freedom produces a $\sim 1/|h|$ divergence of $\mathfrak{D}_\Sigma$. Consequently, the analogue of Eq. (4) for the $O(3)$ NLSM is only a meaningful approximation *away from half filling* in the regime $T\ll h$. The correct expression for the spin diffusion constant instead follows from Eq. (2),

$$\mathfrak{D}_\Sigma\sim\frac{e^{\mathfrak{m}/T}}{3\mathfrak{m}\,|h|}+\mathcal{O}(h^0). \qquad (6)$$

The divergence $\sim 1/|h|$ signals, once again, infinite spin conductivity and superdiffusive spin transport at half filling at $T>0$. Notice we have made the usual assumption that the 'field-theoretical temperature' of the effective low- energy QFT is, in the leading-order, identifiable with the physical temperature T of the spin chain.

KPZ universality. The peculiar divergence of spin conductivity in the $SU(2)$ chains and $O(3)$ sigma model can be traced to anomalous properties of thermally dressed quasi-particles with large bare spin s (see also [34]). Noticing that the spin diffusion constant (2) is given by an infinite sum $\mathfrak{D}=\sum_s\mathfrak{D}_s$, with $\mathfrak{D}_s$ representing individual quasi-particle contributions to the local spin fluctuations, one can observe that for the isotropic interaction the summand saturates at large s, $\lim_{s\to\infty}\mathfrak{D}_s=\mathfrak{D}_\infty>0$, implying an infinite diffusion constant. Thermal fluctuations of the local spin $\delta\langle\hat{s}^z_x\rangle=\langle\hat{s}^z_x\rangle-\langle\hat{s}^z\rangle_{T,h}$ can on the other hand be linked to fluctuations of 'giant quasi-particles' via [47] $\delta\langle\hat{s}^z\rangle=T\chi_h(T,h)\lim_{s\to\infty}[\delta n_s/(s\,n_s(n_s-1))]$, where δn_s denotes local fluctuations of the Fermi occupation functions. Finite asymptotic value $\mathfrak{D}_\infty$ indicates the presence of a self-interacting term in the dynamics of fluctuations $\delta\langle\hat{s}^z\rangle$, in analogy to the Burger's field: $\partial_t\delta\langle\hat{s}^z_x(t)\rangle=\partial_x[\mathfrak{D}_{\rm reg}\partial_x\delta\langle\hat{s}^z_x(t)\rangle+\lambda(\delta\langle\hat{s}^z_x(t)\rangle)^2+\ldots]$. Here $\mathfrak{D}_{\rm reg}<\infty$ designates the 'regularised' diffusion constant which accounts for the finite contribution of 'light' quasi-particles in a thermal background and $\lambda=\lambda(\mathfrak{D}_\infty)$ is the nonlinearity (self-interaction) coefficient obeying $\lim_{\mathfrak{D}_\infty\to 0}\lambda(\mathfrak{D}_\infty)=0$. This leads to a diverging conductivity in time as $\sigma(t)\sim t^{1/3}$, consistently with the KPZ dynamical exponent $z=3/2$ [34, 55], see Fig. 1. It is thus expected that the spin dynamical structure factor complies with the KPZ universal scaling function $\langle\hat{s}^z_x(t)\hat{s}^z_0(0)\rangle_{T,h=0}\sim f_{\rm KPZ}(x(2\sqrt{2}\lambda t)^{-2/3})$ [55, 56], as corroborated numerically for the spin$-1/2$ Heisenberg chain in a recent work [40].

Comparison with previous results. In the last part of the paper we discuss our theoretical predictions in the broader context and make comparisons with the previous literature.

Semi-classical treatment. In the semi-classical approach to transport, developed in refs. [6, 7] (see also [57–59]), it has been argued that deep below the mass scale the spin transport becomes 'super-universal'; in the regime $T,h\ll\mathfrak{m}$, the mean collision time (i.e. the inverse density) becomes exponentially large ($\sim T^{-1}\,e^{\mathfrak{m}/T}$) and on large spatio-temporal scales (compared to inverse temperature $t\gg T^{-1}$ and the thermal de Broglie wavelength $x\gg\lambda_{\rm T}$). Therefore quasi-particles can be treated classically by retaining only the zero-momentum limit of the full quantum scattering matrix. In the gapped $O(3)$ NLSM ($\Theta = 0$), this allowed a derivation of an expression for the spin diffusion constant [6] $\mathfrak{D}_{\rm cl}(T,h) = e^{\mathfrak{m}/T}/(\mathfrak{m}(1+2\cosh(h/T)))$, yielding a large but *finite* $\mathfrak{D}_{\rm cl} \sim e^{\mathfrak{m}/T}/3\mathfrak{m}$ in the regime $h \ll T \ll \mathfrak{m}$. In the scope of the hydrodynamic theory of spin diffusion employed here, this result is precisely the contribution of massive physical excitations given by the first term ($s = 0$). The semi-classical scattering theory however effectively interchanges the noncommuting $T \to 0$ and $t \to \infty$ limits and consequently completely misses the important coherent contributions of the internal magnonic degrees of freedom (terms with $s > 0$), which become pronounced in the regime $h/T \ll 1$.

Dressed versus bare form factors. Form-factor expansions provide one of the most powerful theoretical framework to deal with integrable QFTs [60–64]. The formalism of thermal form factors is unfortunately a rather technical subject which has not yet been developed to a full extent [65–67]. In this context, it has been advocated, in refs. [4, 5, 36, 68], that a series expansion over multi-particle excitations with respect to the (bare) Fock vacuum rapidly converges, owing to the presence of the spectral gap. It was furthers argued that the ground-state dynamical structure factor experiences a small thermal broadening, which for $T \ll \mathfrak{m}$ matches the diffusive (Lorentzian) peak predicted by the semi-classical approach. However, such a *dilute* gas picture is, strictly speaking, restricted to the zero-temperature sector only, and since equilibrium ensembles possess finite entropy density they ineluctably require a self-consistent renormalization of bare quantities and vacuum form factors even at very low temperatures. Correlation functions should therefore be computed via an expansion of *dressed*, as opposed to bare, form factors of local densities, namely matrix elements of particle-hole type excitations on top of a thermal finite-density background [33, 69–72]. In the case of the longitudinal magnetization component, denoted here by $\hat{s}^z$, the matrix element between a thermal state $|\varrho_{T,h}\rangle$ and an excited state with a single particle-hole excitation of 'type s', with momenta $\Delta k_s = k_s(\theta_s^+) - k_s(\theta_s^-)$, reads

$$\langle \hat{\varrho}_{T,h}|\,\hat{s}^z_x\,|\hat{\varrho}_{T,h};\theta_s^+,\theta_s^-\rangle = e^{ix\Delta k_s} m_s^{\rm dr} + \mathcal{O}(\Delta k_s). \tag{7}$$

The quantity $m_s^{\rm dr}$ is the renormalised (dressed) value of magnetization of a quasi-particle specie s immersed in a finite-density thermal background. The difference from its bare value $m_s^{\rm bare} = s$ turns out to be quite radical in the vicinity of half-filled thermal equilibria, where the effective magnetization exhibits a crossover from paramagnetic $m_s^{\rm dr} \sim s^2\,h$ ($s \ll |h|^{-1}$) to bare $m_s^{\rm dr} \sim s$ ($s \gg |h|^{-1}$) regime. For instance, the vanishing of the spin Drude weight as $h \to 0$, is a direct consequence of the paramagnetic behaviour of the form factors (7), which are key building block of its computation [33].

Furthermore, non-perturbative effects attributed to the quasi-particle dressing also profoundly influence the NMR spin relaxation rate $1/T_1$ [73–75]. Motivated by the preceding studies, see e.g. [4, 74], we specialise to the experimentally relevant regime $h \ll T \ll \mathfrak{m}$, assuming ideal conditions by disregarding possible effects of single-ion anisotropy or inter-chain couplings. The low-temperature dependence of T_1^{-1}, namely the intra-band relaxation rate of the longitudinal component, is expressible as $T_1^{-1} = 2|A^{\rm xz}|^2\sum_s\int {\rm d}p_s(\theta)(1-n_s(\theta))\rho_s(\theta)r_s(\theta)$, where $A^{\rm xz}$ are hyperfine couplings and $r_s(\theta) = (m_s^{\rm dr})^2/(\sqrt{\varepsilon_s''(0)}\sqrt{\varepsilon_s''(0)\theta^2+\omega_{\rm N}})$ with the NMR frequency $\omega_{\rm N} = h$ (in units $\mu_{\rm N} = 1$). In the above computation we have used the thermally-dressed form factor (7). Keeping only the leading contribution in the above sum we find $T_1^{-1} \sim e^{-\mathfrak{m}/T}h^2\log h$, in qualitative agreement with the prediction of refs. [4, 74]. However, taking the $h \to 0$ limit *after* initially performing the summation over the entire quasi-particle spectrum yields

$$\frac{1}{T_1} \sim e^{-(3/2)\mathfrak{m}/T}|h|^{-1/2}. \tag{8}$$

This scaling plays nicely with the experimental study on the $S = 1$ compound [76]. We recall that in the studied regime, the quantum calculation with free spinfull bosons carried out in [74] and the form-factor expansion in [4] yields an incorrect behaviour $T_1^{-1} \sim e^{-\mathfrak{m}/T}\log h$, whereas the semi-classical treatment [6, 7] which predicts $T_1^{-1} \sim T\chi_h|\mathfrak{D}_{\rm cl}h|^{-1/2}$, somewhat surprisingly, matches our result (8) at a qualitative level. In our method however, the activation rate $(3/2)\mathfrak{m}/T$ comes from the contributions of the internal magnonic degrees of freedom.

Numerical results. In Fig. 1 we display the time-dependent spin DC conductivity $\sigma(t) = \frac{1}{T}\int_0^t {\rm d}t'\langle \hat{J}(t')\hat{j}_0(0)\rangle_{T,h=0}$ at half filling for various temperatures, observing the KPZ dynamical exponent $z = 3/2$ dominating the current relaxation process already at intermediate time-scales $t \approx 10J$. While very low temperatures are not accessible, the results at larger temperatures firmly indicate the anticipated $t^{1/3}$ growth of the conductivity, see Fig. 1 as well as [47], which can alternatively be computed from the growth rate of the spin current following a quench from an initial bipartitioned state with a tiny magnetization drop δs^z, that is $\sigma(t) = \lim_{\delta s^z \to 0}\langle\sum_x \hat{j}_x(t)\rangle_{T,\delta s^z}/\delta s^z$ (simpler from the numerical viewpoint). Our simulations employ the finite-temperature time-dependent density matrix renormalization group algorithm [77, 78], using a fixed discarded weight and the maximum bond dimension of 4000 for spin 1/2 and 2000 for spin 1, with system size large compare to the causality light cone at the largest simulation time. Additional numerical results are presented in [47], where it is shown that adding anisotropic interactions restores diffusive transport.

Conclusions. We have outlined a theoretical framework for studying low-temperature spin dynamics in both gapped and gapless one-dimensional isotropic antiferromagnets based on the effective low-energy sigma model field theory. In the gapped spin chains, we find a crossover phenomenon from the semi-classical regime $h/T \gg 1$, to the strongly-correlated regime $h/T \ll 1$, which evaded previous studies. In the limit of half filling $h \to 0$, we have analytically demonstrated the phenomenon of spin superdiffusion and conjectured the onset of the KPZ universality. The spectral gap plays no essential role in this respect. Instead, the anomalous behaviour can be attributed to the formation of isotropically-interacting magnonic waves, accompanied with an anomalous, dynamically generated, self-interaction. Presently, we exclude the conventional interpretation based on mode coupling theory in the phenomenological framework of the classical non-linear fluctuating hydrodynamics [55, 79, 80] due to the vanishing diagonal terms of the Hessian in the current derivative expansion.

Our findings have direct applications in inelastic neutron scattering spectroscopy and quantum transport experiments [76, 81–84] and they open up several interesting venues for further research on the microscopic mechanisms underlying the observed anomalous transport. On the theoretical side, it is puzzling that the phenomenon remains present in the isotropic antiferromagnetic chains even at higher temperatures. While this might be a footprint of the low-lying sigma model physics, it may eventually be related to an emerging classical hydrodynamical description such as e.g. the classical Landau-Lifshitz equation which is also known to exhibits superdiffusive spin transport in equilibrium [85] and far from equilibrium [86]. We leave these exciting questions for future studies.

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Supplemental Material

Anomalous spin transport in one-dimensional antiferromagnets

CONTENTS

I. SPIN DRUDE WEIGHT AND DIFFUSION CONSTANT

We are interested exclusively in the transport of spin (local magnetization) in grand-canonical Gibbs equilibrium states at finite temperature T and external magnetic field h. We specialize to low temperatures and the vicinity of *half filling* $h \sim 0$.

We begin by introducing the relevant linear transport coefficients, namely

- the spin Drude weight,

$$\mathcal{D}(T,h) = \lim_{t\to\infty} \sum_x \langle \hat{j}_x(t) j_0(0)\rangle_{T,h}, \tag{9}$$

- the Drude self-weight,

$$\mathcal{D}^{\rm self}(T,h) = 2\int_0^\infty {\rm d}t \langle \hat{j}_0(t)\hat{j}_0(0)\rangle_{T,h}, \tag{10}$$

- the spin diffusion constant,

$$\mathfrak{D}(T,h) = \frac{1}{T\chi_h(T,h)} \int_0^\infty {\rm d}t \left(\sum_x \langle \hat{j}_x(t)\hat{j}_0(0)\rangle_{T,h} - \mathcal{D}(T,h)\right). \tag{11}$$

In integrable theories, these quantities can be conveniently expressed in terms of the following hydrodynamic mode resolutions

$$\mathcal{D}(T,h) = \sum_s \int d\theta\, \mathcal{D}_s(\theta), \qquad \mathcal{D}^{\rm self}(T,h) = \sum_s \int d\theta\, \mathcal{D}^{\rm self}_s(\theta), \qquad \mathfrak{D}(T,h) = \frac{1}{2}\sum_s \int d\theta\, \mathfrak{D}_s(\theta) + \mathcal{O}(h^2), \tag{12}$$

with kernels

$$\mathcal{D}_s(\theta) = \rho_s(\theta)(1-n_s(\theta))\Big(v^{\rm eff}_s(\theta) m^{\rm dr}_s\Big)^2, \tag{13}$$

$$\mathcal{D}^{\rm self}_s(\theta) = \rho_s(\theta)(1-n_s(\theta))|v^{\rm eff}_s(\theta)|(m^{\rm dr}_s)^2, \tag{14}$$

$$\mathfrak{D}_s(\theta) = \rho_s(\theta)(1-n_s(\theta))|v^{\rm eff}_s(\theta)|\left(\mathcal{W}_s(\theta)\right)^2, \tag{15}$$

which have been derived in refs. [28, 87], [28], and [31, 33], respectively. In the above formulae, integer label s enumerates distinct quasi-particle species in the spectrum with (bare) momenta $k_s = k_s(\theta)$, and $\rho_s(\theta)$ are quasi-particle rapidity distributions in an equilibrium state characterised by (Fermi) occupation functions $n_s(\theta)$. The many-body scattering of quasi-particles is, thanks to integrability, fully encoded in a symmetric two-body scattering kernel

$$K_{s,s'}(\theta,\theta') = \frac{1}{2\pi \mathrm{i}}\partial_\theta \log S_{s,s'}(\theta,\theta'), \tag{16}$$

where $S_{s,s'}(\theta,\theta')$ are the amplitudes of the scattering matrix. The group velocities of propagation are given by the effective dispersion relations

$$v_s^{\mathrm{eff}}(\theta) = \frac{\partial_\theta \varepsilon_s(\theta)}{\partial_\theta p_s(\theta)}, \tag{17}$$

where $\varepsilon_{s'}(\theta)$ and $p_{s'}(\theta)$ are dressed by an interacting of quasi-particles at finite density. Employing a compact vector notation (see a remark on notation in [88]), the dressed energies, momenta and spin are computed as

$$\varepsilon' = (1+Kn)^{-1}e' \tag{18}$$

$$p' = (1+Kn)^{-1}k' \tag{19}$$

$$m^{\mathrm{dr}} = (1+Kn)^{-1}m^{\mathrm{bare}}, \tag{20}$$

respectively, with $e_s(\theta)$, $k_s(\theta)$ and m_s^{bare} being the corresponding single particle (bare) quantities associated to the quasi-particle specie s. The dressed Fredholm operator,

$$(1+K\,n) \equiv \delta_{s,s'}\delta(\theta-\theta') + K_{s,s'}(\theta,\theta')n_{s'}(\theta'), \tag{21}$$

represents a linear integral operator acting on both θ and s variables. Notice that index s usually pertains to the number of constituent quasi-particle within a bound state, typically $m_s^{\mathrm{bare}} = s$. The dressed momentum also specifies the total density of states, $2\pi\rho_s^{\mathrm{tot}} = p_s'$, along with the hole densities, $\bar{\rho}_s = \rho_s^{\mathrm{tot}} - \rho_s$. These are, unlike in non-interacting systems, non-trivial rapidity-dependent functions. Finally, coefficients

$$\mathcal{W}_s = \lim_{s'\to\infty} \frac{K_{s,s'}^{\mathrm{dr}}(\theta,\theta')}{\rho_{s'}^{\mathrm{tot}}(\theta')}, \tag{22}$$

are renormalised dressed (two-body) scattering phase shifts, $K^{\mathrm{dr}} = (1+Kn)^{-1}K$, in the limit of large bare spin/charge. In the above formula, the large-s limit indicates a correspondence between the 'giant quasi-particles' carrying bare spin s and spin fluctuations close to half filling, see sec. V.

Our primary concern here is the low-temperature spin transport in the vicinity of *half filled* Gibbs equilibrium states. We first make a remarkable observation that, in the $h\to 0$ limit, the above exact expression for the spin diffusion constant is nothing but the curvature of the *Drude self-weight*

$$\mathfrak{D}(T,0) = \frac{\partial^2 \mathcal{D}^{\mathrm{self}}(T,\nu)}{\partial \nu^2}\Big|_{\nu=0}, \qquad \nu \equiv 4T\langle S^z\rangle_{T,h}. \tag{23}$$

This result can be also understood as an improved and optimised analogue of the diffusion lower lower bound proposed earlier in refs. [49, 50].

Observe however that the two expressions for the spin diffusion constant, namely Eq. (15) and Eq. (23), do not manifestly coincide. It is easy to see that their equivalence hinges on the following "*magic formula*",

$$\mathcal{W}_s = \frac{1}{2T\chi_h(T,0)}\lim_{h\to 0}\frac{m_s^{\mathrm{dr}}(T,h)}{h} + \mathcal{O}(h^2), \qquad \chi_h(T,h) = -\partial_h^2 f(T,h), \tag{24}$$

where we have introduced $\nu = 4T\chi_h(T,0)h + \mathcal{O}(h^2)$. This statement, which already indirectly appeared in ref. [34] in the XXZ chain at infinite temperature, can be proven analytically in the high-temperature limit. The derivation is presented in sec. VI.

II. NESTED BETHE ANSATZ FOR THE O(3) NONLINEAR SIGMA MODEL

The quantum $O(3)$ nonlinear sigma model (NLSM) is a relativistic QFT for a non-abelian vector field $\hat{\mathbf{n}} = (\hat{n}^x, \hat{n}^y, \hat{n}^z)$ constrained on a unit sphere ($\hat{\mathbf{n}} \cdot \hat{\mathbf{n}} = 1$), described by the Euclidean action

$$\mathcal{A}_0[\hat{\mathbf{n}}] = \frac{1}{2g} \int \mathrm{d}x \, \mathrm{d}t \left((\partial_t \hat{\mathbf{n}})^2 - (\partial_x \hat{\mathbf{n}})^2 \right). \tag{25}$$

The action can be extended by including the topological Θ-term,

$$\mathcal{A}_\Theta[\hat{\mathbf{n}}] = \mathcal{A}_0[\hat{\mathbf{n}}] + \mathrm{i} \frac{\Theta}{4\pi} \int \mathrm{d}x \, \mathrm{d}t \, \hat{\mathbf{n}} \cdot \partial_t \hat{\mathbf{n}} \times \partial_x \hat{\mathbf{n}}. \tag{26}$$

In the following, we are interested in describing the low-energy limit of the $SU(2)$-symmetric antiferromagnetic spin-S chains. The topological angle $\Theta = 2\pi S$ is an integer multiple of π and crucially depends on whether S if an integer or half-integer. While in both cases the low-energy effective field theory is described by an *integrable* relativistic quantum sigma model, only in the former case the elementary spectrum is gapped. The non-trivial topological term $\Theta = \pi$ prevents dynamical mass generation and yields massless excitations.

The quantum sigma model governs the continuum scaling low-energy limit of *non-integrable* spin-S Heisenberg chains

$$\hat{H} = J \sum_i \hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_{i+1}, \tag{27}$$

with antiferromagnetic exchange coupling $J > 0$, normalization $\hat{\mathbf{s}} \cdot \hat{\mathbf{s}} = S(S+1)$, and unit lattice spacing. In the continuum limit, the staggered and ferromagnetic fluctuations are represented by two smooth fields,

$$\hat{\mathbf{s}}_i \approx S(-1)^i \hat{\mathbf{n}} + \hat{\mathbf{m}}, \tag{28}$$

where

$$\hat{\mathbf{m}} = \frac{1}{g} \hat{\mathbf{n}} \times \hat{\mathbf{p}}, \qquad \hat{\mathbf{m}} \cdot \hat{\mathbf{n}} = 0, \tag{29}$$

generates rotations of the field $\hat{\mathbf{n}}$, and

$$\mathbf{p} = \frac{1}{g} \partial_t \mathbf{n} + \frac{\Theta}{4\pi} \mathbf{n} \times \partial_x \mathbf{n}, \tag{30}$$

is the canonically-conjugate momentum. This yields the Hamiltonian

$$\hat{H}_\Sigma = \frac{v}{2} \int \mathrm{d}x \left[g \left(\hat{\mathbf{m}} + \frac{\Theta}{4\pi} \partial_x \hat{\mathbf{n}} \right)^2 + \frac{1}{g} (\partial_x \hat{\mathbf{n}})^2 \right], \tag{31}$$

which matches to the action $\mathcal{A}$ in dimensionless units where the velocity $v = 2JS$ is set to one. The coupling constant g is related to spin S via

$$g = 2/S. \tag{32}$$

A. O(3) NLSM without topological term

The equation of motion is the conservation law for the Lorentz two-current,

$$\partial_\mu \hat{\mathbf{j}}_\mu = 0, \tag{33}$$

with components

$$\hat{\mathbf{j}}_\mu = g^{-1} \hat{\mathbf{n}} \times \partial_\mu \hat{\mathbf{n}}, \qquad \mu = x, t. \tag{34}$$

yielding the conserved Noether charges

$$\hat{\mathbf{m}} = \int \mathrm{d}x\, \hat{\mathbf{j}}_t(x,t). \tag{35}$$

The elementary excitations of the $O(3)$ NLSM form a spin-triplet of massive bosons with relativistic dispersion relation

$$e(k) = \sqrt{k^2 + \mathfrak{m}^2}, \tag{36}$$

where $\mathfrak{m}$ denotes the non-perturbatively generated mass (spectral gap) related to the bare coupling constant g via $\mathfrak{m} \sim J\, e^{-2\pi/g}$. We employ the usual rapidity parametrization in terms of variable θ

$$k(\theta) = \mathfrak{m} \sinh(\theta), \qquad e(\theta) = \mathfrak{m} \cosh(\theta), \tag{37}$$

in the absence of an external applied field.

Exact S-matrix. The creation/annihilation operators for the elementary excitations in the $O(3)$ NLSM constitute the (associative, non-commutative) Faddeev–Zamolodchikov algebra

$$Z_a(\theta_1)Z_b(\theta_2) = \mathcal{S}^{a'b'}_{ab}(\theta_1-\theta_2)Z_{b'}(\theta_2)Z_{a'}(\theta_1), \tag{38}$$
$$Z^\dagger_a(\theta_1)Z^\dagger_b(\theta_2) = \mathcal{S}^{a'b'}_{ab}(\theta_1-\theta_2)Z^\dagger_{b'}(\theta_2)Z^\dagger_{a'}(\theta_1), \tag{39}$$
$$Z_a(\theta_1)Z^\dagger_b(\theta_2) = 2\pi\delta_{ab}\delta(\theta_1-\theta_2) + \mathcal{S}^{b',a}_{b,a'}(\theta_1-\theta_2)Z^\dagger_{b'}(\theta_2)Z_{a'}(\theta_1), \tag{40}$$

where $a,b \in \{x,y,z\}$ are isospin quantum numbers assigned to the $O(3)$ tripet of Bose fields. The Fock space vacuum $|0\rangle$ is a state with the property $Z_a(\theta)\,|0\rangle = 0$. The n-particle scattering states are constructed in the standard manner

$$|\theta_n,\ldots,\theta_2,\theta_1\rangle = Z^\dagger_{a_n}(\theta_n)\cdots Z^\dagger_{a_2}(\theta_2)Z^\dagger_{a_1}(\theta_1)\,|0\rangle\,. \tag{41}$$

The two-body scattering matrix of the $O(3)$ NLSM has the following structure

$$\mathcal{S}^{cd}_{ab}(\theta) = \delta_{ac}\delta_{cd}\,\sigma_1(\theta) + \delta_{ac}\delta_{bd}\,\sigma_2(\theta) + \delta_{ad}\delta_{cd}\,\sigma_3(\theta), \tag{42}$$

where θ designates rapidity difference of the incident particles, and

$$\sigma_1(\theta) = \frac{2\pi\mathrm{i}\theta}{(\theta+\mathrm{i}\pi)(\theta-2\mathrm{i}\pi)}, \quad \sigma_2(\theta) = \frac{\theta(\theta-\mathrm{i}\pi)}{(\theta+\mathrm{i}\pi)(\theta-2\mathrm{i}\pi)}, \quad \sigma_3(\theta) = \frac{2\pi\mathrm{i}(\mathrm{i}\pi-\theta)}{(\theta+\mathrm{i}\pi)(\theta-2\mathrm{i}\pi)}. \tag{43}$$

The non-diagonal multi-particle scattering is completely factorizable and thus fully described by the two-particle (quantum) scattering $\mathcal{S}$-matrix obeying the celebrated Yang–Baxter relation

$$\mathcal{S}^{b_1b_2}_{c_1c_2}(\theta-\theta')\mathcal{S}^{c_1b_3}_{a_1c_3}(\theta)\mathcal{S}^{c_2c_3}_{a_2a_3}(\theta') = \mathcal{S}^{b_2b_3}_{c_2c_3}(\theta')\mathcal{S}^{b_1c_3}_{c_1a_3}(\theta)\mathcal{S}^{c_1c_2}_{a_1a_2}(\theta-\theta'). \tag{44}$$

As a consequence, the model possesses infinitely many local conservation laws.

Thermodynamic Bethe Ansatz

By placing the field theory on space-time worldsheet of a cylinder geometry with circumference L, one imposes a non-trivial quantization condition for n particle rapidities $\{\theta_a\}_{a=1}^n$. The main object of the algebraic diagonalization of the many-body scattering process is the transfer matrix $\mathcal{T}(\lambda;\{\theta_a\})$, acting on a 3^n-dimensional Hilbert space with matrix elements

$$\mathcal{T}^b_a(\lambda;\{\theta_a\})^{j_1\cdots j_n}_{i_1\cdots i_n} = \mathcal{S}^{c_1j_1}_{ai_1}(\lambda-\theta_1)\mathcal{S}^{c_2j_2}_{c_1i_2}(\lambda-\theta_2)\cdots\mathcal{S}^{bj_n}_{c_{n-1}i_n}(\lambda-\theta_n), \tag{45}$$

where λ is a complex spectral parameter. The periodicity constraint for an n-particle wave-function amplitudes $\Psi(\{\theta_a\})$ takes the form of the Bethe equations

$$\left(\mathcal{T}(\theta_j;\{\theta_a\}) + e^{\mathrm{i}p(\theta_j)L}\right)\Psi(\{\theta_a\}) = 0. \tag{46}$$

By virtue of Eq. (44), which implies

$$\mathcal{T}_a^{a''}(\theta)\mathcal{T}_b^{b''}(\theta')\mathcal{S}_{a''b''}^{a'b'}(\theta-\theta') = \mathcal{S}_{ab}^{a''b''}(\theta-\theta')\mathcal{T}_{b''}^{b'}(\theta')\mathcal{T}_{a''}^{a'}(\theta), \tag{47}$$

traces of trances matrices, $\mathcal{T}(\theta) = \sum_a \mathcal{T}_a^a(\theta)$, are in involution for all values of the spectral parameters,

$$[\mathcal{T}(\theta), \mathcal{T}(\theta')] = 0. \tag{48}$$

Presently we deal with a *non-diagonal* scattering theory, referring to non-trivial mixing of internal (spin) degrees of freedom upon elastic quasi-particle collisions. Nonetheless, the scattering can be transformed to a diagonal from at expense of introducing auxiliary magnonic particles, in effect resulting in the so-called nested-type Bethe equations. We shall not reproduce the entire procedure here and instead refer the reader to e.g. [54].

In the case of the $O(3)$ NLSM, the nested Bethe equations have been originally obtained in [89]. In the sector with M_θ physical excitations and M_λ auxilairy rapidities, they take the form

$$e^{\mathrm{i}k(\theta_a)L}\prod_{b=1}^{M_\theta} S(\theta_a,\theta_b)\prod_{c=1}^{M_\lambda} S^{-1}(\theta_a,\lambda_c) = 1, \tag{49}$$

$$\prod_{b=1}^{M_\theta} S^{-1}(\lambda_a,\theta_a)\prod_{c=1}^{M_\lambda} S(\lambda_a,\lambda_c) = -1, \tag{50}$$

where

$$S(\theta) = \frac{\theta - \mathrm{i}\pi/2}{\theta + \mathrm{i}\pi/2}, \tag{51}$$

is the elementary scattering amplitude which depends on the difference of the incident quasi-particles' rapidities θ.

Auxiliary magnons. We wish to stress that the so-called auxiliary rapidities λ_a do not belong to physical (i.e. momentum-carrying) degrees of freedom. Instead, they are the internal quantum numbers assigned to spin degrees of freedom (with respect to the fully polarised reference state). These can be most easily pictured as fictitious particles which propagate in the frozen frame of physical particles which are needed in order to transform the original non-diagonal scattering theory to a diagonal one. The magnonic degrees of freedom play a pivotal role and are crucial, in particular, for understanding and explaining anomalous properties of spin transport. Most importantly, auxiliary rapidities take complex values in general, which signals formation of bound states. According to the fusion properties of the scattering amplitudes, the only allowed complex rapidities λ_a in the large-L limit are those in the form the 'k-string compounds',

$$\lambda_b^{(k)i} = \left\{\lambda_b + \frac{\mathrm{i}\pi}{2}(k+1-2i)\right\}, \tag{52}$$

where $i = 1, 2, \ldots, k$ iterates over the constituent complex λ-rapidities. Therefore, as far as the spin dynamics is concerned, the auxiliary bound states (labelled by a real-valued center λ_b) play a similar role to physical multi-magnon bound states in the integrable Heisenberg spin chains, except that presently these propagate in an inhomogeneous background of physical excitations. To this end, by appropriately shifting the poles of the elementary amplitude S, we introduce the elementary fused amplitudes

$$S_n(\theta) = \frac{\theta - n\,\mathrm{i}\pi/2}{\theta + n\,\mathrm{i}\pi/2}, \tag{53}$$

and the associated scattering phases

$$\Theta_n(\theta) = -\mathrm{i}\log\left(-S_n(\theta)\right) = 2\arctan\left(\frac{2\theta}{n\pi}\right). \tag{54}$$

Bethe–Yang equations. We are interested in the finite-density limit of Eqs. (50), which amounts to take the $L \to \infty$ limit while keeping ratios M_θ/L and M_λ/L finite. Thermodynamic ensembles are understood as macrostates which are characterised by finite densities of physical and auxiliary excitations, denoted by $\rho_0(\theta)$ and $\rho_{s\geq 1}(\theta)$, respectively. Following the standard procedure, namely taking the logarithmic derivative with respect to rapidity θ and converting the discrete summations over rapidities to convolution-type integrals, we arrive at the Bethe–Yang equations of the form (suppressing rapidity dependence for clarity)

$$\rho_0^{\rm tot} = \frac{k'}{2\pi} + \mathcal{K}\star\rho_0 - K_s\star\rho_s, \tag{55}$$

$$\rho_s^{\rm tot} = K_s\star\rho_0 - K_{s,s'}\star\rho_{s'}, \tag{56}$$

with $\rho_{s\geq 0}^{\rm tot}$ denoting the densities of available states for the physical and auxiliary quasi-particles. Here and subsequently we use a compact notation for summations over repeated indices,

$$K_s\star g_s = \sum_{s=1}^{\infty}\int_{-\infty}^{\infty}{\rm d}\theta' K_s(\theta-\theta')g_s(\theta'), \qquad K_{s,s'}\star g_{s'} = \sum_{s'=1}^{\infty}\int_{-\infty}^{\infty}{\rm d}\theta' K_{s,s'}(\theta-\theta')g_{s'}(\theta'). \tag{57}$$

The convolution kernels

$$K_s(\theta) = \kappa_{s-1}(\theta) + \kappa_{s+1}(\theta), \tag{58}$$

$$K_{s,s'}(\theta) = \sum_{\ell=|s-s'|}^{s+s'+2}\kappa_\ell(\theta) + \kappa_{\ell+2}(\theta), \tag{59}$$

with $K_{s\geq 0}\equiv 0$, are given in terms of the differential scattering phases

$$\kappa_s(\theta) = \frac{1}{2\pi{\rm i}}\partial_\theta\Theta_s(\theta) = \frac{2s}{s^2\pi^2+4\theta^2}. \tag{60}$$

Using convention $\hat{f}(k) = \int_{-\infty}^{\infty}{\rm d}\theta e^{-{\rm i}k\theta}f(\theta)$, we have the following Fourier-space representation

$$\hat{\kappa}_s(k) = e^{-(\pi/2)s|k|}. \tag{61}$$

Quasi-local form. The canonical Bethe–Yang integral equations (56) can be further simplified with aid of the fusion identities. The second equation in Eqs. (56) can be presented as a Fredholm-type integral equation

$$(1+K)_{s,s'}\star\rho_s = K_s\star\rho_0 - \bar{\rho}_s. \tag{62}$$

Remarkably, the corresponding resolvent, defined via matrix equation,

$$(1-R)\cdot(1+K) = 1, \tag{63}$$

admits the following compact representation

$$R_{s,s'}\star g_{s'} \equiv I^{A_\infty}_{s,s'}\,\mathfrak{s}\star g_{s'}. \tag{64}$$

Here we have introduced an infinite-dimensional incidence (adjacency) matrix of the A_∞-type Dynkin diagram,

$$I^{A_\infty}_{s,s'} = \delta_{s,s'-1} + \delta_{s,s'+1}, \tag{65}$$

and the $\mathfrak{s}$-kernel, defined as the solution to $\kappa_1 - \mathfrak{s}\star\kappa_2 = \mathfrak{s}$, reading explicitly

$$\mathfrak{s}(\theta) = \frac{1}{2\pi\cosh(\theta)}. \tag{66}$$

It is often convenient to use the its Fourier representation, $\hat{\mathfrak{s}}(k) = (2\cosh(k\pi/2))^{-1}$. Moreover the convolution with the inverse of the Fredholm operator $(1+K)$ has the following important properties

$$\left(1 - I^{A_\infty}\,\mathfrak{s}\right)_{s,s'}\star\kappa_{s'} = \kappa_s - \mathfrak{s}\star(\kappa_{s-1}+\kappa_{s+1}) = \delta_{s,1}\mathfrak{s}, \tag{67}$$

$$\left(1 - I^{A_\infty}\,\mathfrak{s}\right)_{s,s'}\star K_{s'} = K_s - \mathfrak{s}\star(K_{s-1}+K_{s+1}) = \delta_{s,2}\mathfrak{s}, \tag{68}$$

$$\left(1 - I^{A_\infty}\,\mathfrak{s}\right)_{s,s''}\star K_{s'',s'} = I^{A_\infty}_{s,s'}\,\mathfrak{s}, \tag{69}$$

which are straightforward to prove. Inverting Eqs. (62), we find immediately $\rho_s^{\rm tot} = \mathfrak{s}\star I^{A_\infty}_{s,s'}\bar{\rho}_{s'}$ for $s\geq 1$. The remaining equation for the momentum-carrying particle can be simplified with aid of

$$K_s\star\rho_s = K_2\star\mathfrak{s}\star\rho_0 - \mathfrak{s}\star\bar{\rho}_2. \tag{70}$$

This way, we obtain the following quasi-local form of the Bethe–Yang equations

$$\rho_0^{\rm tot} = \frac{k'}{2\pi} + \mathfrak{s}\star\bar{\rho}_2, \tag{71}$$

$$\rho_s^{\rm tot} = \delta_{s,2}\mathfrak{s}\star\rho_0 + \mathfrak{s}\star I^{A_\infty}_{s,s'}\bar{\rho}_{s'}. \tag{72}$$

Notice that the self-coupling term in the canonical equation for $\rho_0^{\rm tot}$ disappears thanks to $\kappa_2 - \mathfrak{s}\star(\kappa_1+\kappa_3) = 0$.

The universal dressing transformation. By identifying the total state densities with the dressed momentum derivatives,

$$2\pi\rho_s^{\rm tot} = p'_s, \qquad s = 0,1,2,\ldots, \tag{73}$$

the Bethe–Yang equation be recast in a more suggestive form

$$p'_0 - \mathfrak{s}\star\bar{n}_2 p'_2 = k'_0, \tag{74}$$

$$p'_s - \mathfrak{s}\star I^{A_\infty}_{s,s'} - \delta_{s,2}\mathfrak{s}\star n_0 p'_0 = 0. \tag{75}$$

Physically speaking, these linear integral equations describe renormalization of particle's bare momenta with respect to an equilibrium macrostate, $k'_s \mapsto p'_s = \mathcal{F}^{\rm dr}_{\{n_s\}}(k'_s)$, where the dressing transformation $\mathcal{F}^{\rm dr}$ is a linear functional which specified by the mode occupation functions

$$n_s(\theta) = \frac{\rho_s(\theta)}{\rho_s^{\rm tot}(\theta)}, \qquad s\geq 0, \tag{76}$$

and $\bar{n}_s(\theta)\equiv 1-n_s(\theta)$ denote the occupations functions of holes.

Thermodynamic Bethe Ansatz. In the formalism of the Thermodynamic Bethe Ansatz (TBA), the equilibrium partition sum is expressed as a functional integral over particle rapidity distributions $\rho_{s\geq 0}(\theta)$. Specifically, the equilibrium free energy density

$$f[\{\rho_s\}] = e[\{\varrho_s\}] - s[\varrho_s], \tag{77}$$

which is a functional of the energy and entropy densities,

$$e = \int_{-\infty}^{\infty} {\rm d}\theta\,(\mathfrak{m}\cosh(\theta) - h)\rho_0(\theta), \qquad s = \sum_{s\geq 0}\int_{-\infty}^{\infty}{\rm d}\theta\left(\rho_s^{\rm tot}\log\rho_s^{\rm tot} - \rho_s\log\rho_s - \bar{\rho}_s\log\bar{\rho}_s\right), \tag{78}$$

respectively, is minimised by demanding the variational derivative to vanish, $\delta f = 0$.

Instead of carrying out an explicit derivation, we can exploit universality of the dressing equation which provides a neat shortcut to derive the TBA equations once the dressing transform for the bare momenta (i.e. the Bethe–Yang equations) is known. The free-energy minimization is essentially nothing but the energy counterpart of the momentum dressing, namely $\varepsilon'_s \mapsto \mathcal{F}^{\rm dr}_{\{n\}}(e'_s)$, reading

$$\varepsilon'_0 - \mathfrak{s}\star\bar{n}_2\varepsilon'_2 = e'_0, \tag{79}$$

$$\varepsilon'_s - \mathfrak{s}\star I^{A_\infty}_{s,s'}\bar{n}_{s'}\varepsilon'_{s'} = 0. \tag{80}$$

By introducing the the TBA Y-functions,

$$Y_s(\theta) = \frac{\bar{\rho}_s(\theta)}{\rho_s(\theta)}, \qquad s\geq 0, \tag{81}$$

and identifying them with the dressed energies ε_s via $\log Y_s = \beta\varepsilon_s$, we readily obtain the quasi-local form of the TBA equations

$$\log Y_0 = \beta\, e - \mathfrak{s}\star\log(1+Y_2), \tag{82}$$

$$\log Y_s = \delta_{s,2}\,\mathfrak{s}\star\log(1+1/Y_0) + \mathfrak{s}\star I_{s,s'}\log(1+Y_{s'}), \tag{83}$$

where we have used

$$\partial_\theta \log(1+Y_s) = \bar{n}_s \varepsilon_s, \qquad \partial_\theta \log(1+1/Y_s) = -n_s \varepsilon_s. \tag{84}$$

With the additional particle-hole transformation on the massive node, the latter that the group-theoretic form

$$\log Y_s = -\delta_{s,0}\beta\, e' + \mathfrak{s} \star I^{D_\infty}_{s,s'} \log(1+Y_b), \qquad s \geq 0, \tag{85}$$

compatible with the so-called Y-system hierarchy associated to the D_∞ Dynkin diagram.

The free energy density is only a functional of energy-carrying Y-function

$$f = -T \int_{-\infty}^{\infty} \mathrm{d}\theta \frac{k'(\theta)}{2\pi} \log(1+1/Y_0(\theta)). \tag{86}$$

B. O(3) NLSM with topological term

Now we consider the addition of the topological Θ-term in the $O(3)$ NLSM action. This now gives a $SU(2)$-symmetric massless relativistic quantum field theory of with completely factorizable non-diagonal scattering [54]. We use subscripts $\pm$ to denote the internal quantum label of the $SU(2)$ doublet, with $+$ designating the 'right movers' ($k > 0$) and $-$ the 'left movers' ($k < 0$). Their bare dispersion relations are

$$e_\pm(\theta) = \pm k(\theta) = \frac{\Lambda}{2} e^{\pm\theta}, \qquad -\infty < \theta < \infty. \tag{87}$$

Here $\Lambda \sim e^{-2\pi/g}$ sets the cut-off scale at which the asymptotically free UV behavior changes into the scale-invariant IR regime. The scattering relations are provided by the following Faddeev–Zamolodchikov algebra [54]

$$R_a(\theta_1)R_b(\theta_2) = \mathcal{S}^{a'b'}_{ab}(\theta_1-\theta_2)R_b(\theta_2)R_{a'}(\theta_1), \tag{88}$$

$$L_a(\theta_1)L_b(\theta_2) = \mathcal{S}^{a'b'}_{ab}(\theta_1-\theta_2)L_b(\theta_2)L_{a'}(\theta_1), \tag{89}$$

$$R_a(\theta_1)L_{\bar{a}}(\theta_2) = \mathcal{U}^{b\bar{b}}_{a\bar{a}}(\theta_1-\theta_2)L_{\bar{b}}(\theta_2)R_b(\theta_1), \tag{90}$$

with scattering amplitudes of the form

$$\mathcal{S}^{a'b'}_{ab}(\theta) = \frac{\mathcal{S}^{(\pi)}(\theta)}{\theta - \mathrm{i}\pi}\left(\theta\delta_{a,a'}\delta_{b,b'} - \mathrm{i}\pi\delta_{a,b'}\delta_{b,a'}\right), \tag{91}$$

$$\mathcal{U}^{b\bar{b}}_{a\bar{a}}(\theta) = \frac{\mathrm{i}\,\mathcal{S}^{(\pi)}(\theta)}{\theta - \mathrm{i}\pi}\left(\theta\delta_{a,b}\delta_{\bar{a},\bar{b}} - \mathrm{i}\pi\delta_{a,\bar{b}}\delta_{\bar{a},b}\right). \tag{92}$$

The scattering phase shift of the model at $\Theta = \pi$, denoted by $\mathcal{S}^{(\pi)}(\theta)$, has the following useful integral representation

$$\log\left(-\mathcal{S}^{(\pi)}(\theta)\right) = \int_0^\infty \mathrm{d}k\, \frac{e^{-\pi k/2}}{2\cosh(\pi k/2)} \frac{\sin(\theta k)}{k}. \tag{93}$$

Note that in the UV regime, $\theta_2 - \theta_1 \to \infty$, the left-right scattering trivializes, and the scattering process becomes indistinguishable from that of the trivial topologically angle $\Theta = 0$.

Bethe, Bethe–Yang and TBA equations. In the periodic box of size L, the quasi-particle rapidities $\{\theta_\alpha\}_{\alpha=1}^N$ are subjected to the Bethe quantization constraints

$$e^{\mathrm{i}p(\theta_\alpha)L} \prod_{\beta=1}^{M_\lambda} \frac{\theta_\alpha - \lambda_\beta + \mathrm{i}\pi/2}{\theta_\alpha - \lambda_\beta - \mathrm{i}\pi/2} \prod_{\gamma=1}^{M_\theta} \mathcal{S}^{(\pi)}(\theta_\alpha - \theta_\gamma) = 1. \tag{94}$$

As usual, here $\{\theta_\alpha\}$ denote a set of physical rapidities which parametrise momenta of the right and left movers, while λ_β pertain to auxiliary magnons which diagonalise the $SU(2)$-invariant scattering.

In the thermodynamic limit $L \to \infty$ (keeping ratios M_θ/L and M_λ/L finite), one arrives at the following equations for the physical and auxiliary quasi-particle densities $\rho_\pm$ and $\rho_{s\geq 1}$,

$$\rho_\pm^{\rm tot} = L\frac{k'_\pm}{2\pi} + \mathcal{K}\star\rho_\pm - K_s\star\rho_s, \tag{95}$$

$$\rho_s^{\rm tot} = K_s\star(\rho_+ + \rho_-) + K_{s,s'}\star\rho_{s'}. \tag{96}$$

Here $k'_\pm(\theta) = (\Lambda/2)e^\theta$ are rapidity derivatives of bare momenta of physical excitations, the convolution kernels K_s are given by (58), and

$$\mathcal{K}(\theta) = \frac{1}{2\pi{\rm i}}\partial_\theta \log \mathcal{S}^{(\pi)}(\theta) = \frac{1}{\pi}(\mathfrak{s}\star K_1)(\theta). \tag{97}$$

The equivalent quasi-local form yields

$$\rho_\pm^{\rm tot} = \frac{L}{2\pi}\frac{\Lambda}{2}e^{\pm\theta} + \mathfrak{s}\star\bar{\rho}_1, \tag{98}$$

$$\rho_s^{\rm tot} = \delta_{s,1}\mathfrak{s}\star(\rho_+ + \rho_-) + \mathfrak{s}\star I^{A_\infty}_{s,s'}\bar{\rho}_{s'}. \tag{99}$$

The TBA equations for the thermodynamic free energy in a finite volume $L = 1/T$ take the form

$$\log Y_\pm = L\frac{\Lambda}{2}e^{\pm\theta} + \mathfrak{s}\star\log(1+Y_1), \tag{100}$$

$$\log Y_s = \delta_{s,1}\mathfrak{s}\star\log(1+Y_+)(1+Y_-) + \mathfrak{s}\star I^{A_\infty}_{s,s'}\log(1+Y_{s'}). \tag{101}$$

III. LOW-TEMPERATURE EXPANSION OF THE SPIN DIFFUSION CONSTANT

A. Heisenberg XXZ chain

We consider the Heisenberg spin-1/2 XXZ chain,

$$\hat{H} = \sum_i \hat{s}^x_i\hat{s}^x_{i+1} + \hat{s}^y_i\hat{s}^y_{i+1} + \Delta\,\hat{s}^z_i\hat{s}^z_{i+1}, \tag{102}$$

in the gapped phase $|\Delta| = \cosh\eta > 1$. The TBA equations for the grand-canonical Gibbs equilibrium are of the form

$$\log Y_s = -T^{-1}\mathfrak{s}^{(\eta)}\delta_{s,1} + \mathfrak{s}\star I^{A_\infty}_{s,s'}\log(1+Y_{s'}), \qquad \lim_{s\to\infty} s^{-1}\log Y_s = (h/T)\,, \tag{103}$$

where

$$\mathfrak{s}(\theta) = \frac{1}{2\pi}\sum_{k\in\mathbb{Z}}\frac{e^{2{\rm i}k\theta}}{\cosh(k\eta)}, \qquad \mathfrak{s}^{(\eta)}(\theta) \equiv \pi\sinh(\eta)\,\mathfrak{s}(\theta), \tag{104}$$

are the usual and the deformed $\mathfrak{s}$-kernels, respectively.

Below we carry out the low-temperature expansion of the TBA quantities, as previously done in e.g. [90, 91]. For the subsequent analysis it is important to work in the regime $h/T \gg 1$. In this case, in the $T\to 0$ limit we have the following behaviour

$$Y_1(\theta) = e^{-\mathfrak{s}^{(\eta)}(\theta)/T}\frac{\sinh(h/T)}{\sinh(h/2T)}\times\big(1+\mathcal{O}(e^{-h/T})\big), \tag{105}$$

$$Y_{s>1}(\theta) = \left(\frac{\sinh^2(s\,h/2T)}{\sinh^2(h/2T)} - 1\right)\times\big(1+\mathcal{O}(e^{-h/T})\big), \tag{106}$$

from where we obtain

$$\rho_1^{\rm tot} = \mathfrak{s}, \qquad \rho_{s>1}^{\rm tot}(\theta) = K_{s+1}\star(\mathfrak{s}\,Y_1), \tag{107}$$

for the state densities and

$$v_1^{\rm eff} = -\sinh{(\eta)}\,\frac{\mathfrak{s}'}{2\mathfrak{s}}, \qquad v_{s>1}^{\rm eff} = -\frac{\sinh{(\eta)}}{2}\frac{K_{s+1}\star(\mathfrak{s}'Y_1)}{K_{s+1}\star(\mathfrak{s}\,Y_1)}, \tag{108}$$

for the dressed velocities, modulo subleading corrections which are of the order $\mathcal{O}(e^{-h/T})$. The low-temperature limit of the Gibbs thermodynamic free energy, $f=-T\int_{-\pi/2}^{\pi/2}{\rm d}\theta\,\mathfrak{s}(\theta)\log(1+Y_1(\theta))$, yields

$$f = -T\int_{-\pi/2}^{\pi/2}{\rm d}\theta\,\mathfrak{s}(\theta)Y_1(\theta)e^{-\mathfrak{s}^{(\eta)}(\theta)/T}\frac{\sinh(h/T)}{\sinh(h/2T)}\times\big(1+\mathcal{O}(e^{-h/T})\big). \tag{109}$$

In the limit $T\to 0$, the latter can evaluated with the saddle point technique. The spectral gap $\mathfrak{m}$ is given by

$$\mathfrak{m} = \mathfrak{s}^{(\eta)}(\pm\pi/2). \tag{110}$$

The dressed dispersion relation for the unbound magnons (1-strings), expanded around $\theta=\pm\pi/2$, reads

$$\varepsilon_1(\theta) = \mathfrak{m} + \frac{(\theta\pm\pi/2)^2}{2}\partial_\theta^2\varepsilon_1(\theta)\Big|_{\theta=\pm\pi/2} + \ldots, \tag{111}$$

with curvature

$$\partial_\theta^2\varepsilon_1(\theta)\Big|_{\theta=\pm\pi/2} = \partial_\theta^2\mathfrak{s}^{(\eta)}(\theta)\Big|_{\theta=\pm\pi/2} = \pi\sinh{(\eta)}\,\mathfrak{s}''(\pi/2). \tag{112}$$

By approximating the dispersion relation in the vicinity of the spectral gap, we find the following low-temperature behavior of the free energy,

$$f(T,h) = -T\mathfrak{s}(\pi/2)e^{-\mathfrak{m}/T}\frac{\sqrt{2\pi\,T}}{\sqrt{\partial_\theta^2\varepsilon_1(\theta)|_{\theta=\pm\pi/2}}}\frac{\sinh(h/T)}{\sinh(h/2T)}\times\big(1+\mathcal{O}(e^{-\mathfrak{m}/T})\big). \tag{113}$$

In a similar manner, we obtain the following low-T limit (with $h/T\gg 1$) of the static spin susceptibility

$$\chi_h(T,h) = -\frac{\partial^2 f(T,h)}{\partial h^2} = \frac{\mathfrak{s}(\pi/2)}{2}\sqrt{\frac{2\pi}{T\partial_\theta^2\varepsilon_1(\theta)|_{\theta=\pm\pi/2}}}e^{-(\mathfrak{m}-h/2)/T}\big(1+\mathcal{O}(e^{-(\mathfrak{m}+h)/T})\big). \tag{114}$$

We proceed by expressing the spin diffusion $\mathfrak{D}(T,h)$ in the vicinity of the half filled state $h\sim 0$ as the curvature of the spin Drude self-weight, employing the exact hydrodynamic mode decomposition

$$\mathfrak{D} = \frac{1}{8(T\chi_h(T,h))^2}\sum_{s\geq 1}\int_{-\pi/2}^{\pi/2}{\rm d}\theta\,\rho_s^{\rm tot}(\theta)n_s(\theta)(1-n_s(\theta))|v_s^{\rm eff}(\theta)|\left(\lim_{h\to 0}\lim_{T\to 0}\frac{m_s^{\rm dr}(T,h)}{h}+\mathcal{O}(h^2)\right)^2. \tag{115}$$

In the limit $T\to 0$ limit, we found the following dressed value of magnetization

$$\lim_{T\to 0}\lim_{h\to 0}\frac{m_1^{\rm dr}(T,h)}{h} = \frac{1}{2}, \qquad \lim_{T\to 0}\lim_{h\to 0}\frac{m_{s>1}^{\rm dr}(T,h)}{h} = \frac{s^2}{3}. \tag{116}$$

Moreover, at low temperatures we have the following properties of the state densities,

$$\rho_1^{\rm tot}(\theta)\sim\mathcal{O}(1), \qquad \rho_{s>1}^{\rm tot}(\theta)\sim\mathcal{O}(\sqrt{T}e^{-\mathfrak{m}/T}), \tag{117}$$

the dressed particle velocities,

$$v_1^{\rm eff}(\theta)\sim\mathcal{O}(1), \qquad v_{s>1}^{\rm eff}(\theta)\sim\mathcal{O}(\sqrt{T}), \tag{118}$$

and the mode occupation functions

$$n_1(\theta)(1-n_1(\theta))\sim e^{-\mathfrak{m}/T}, \qquad n_{s>1}(\theta)(1-n_{s>1}(\theta))\sim e^{-(s-1)h/T}. \tag{119}$$

The above scaling relations imply that the bound-state contributions pertaining to quasi-particles with $s > 1$ get exponentially suppressed as $\sim e^{-s\,h/T}$. The leading contribution thus comes from the unbound magnons ($s = 1$) and reads

$$\mathfrak{D}_{\rm XXZ} = \frac{1}{8(T\chi_h(T,h))^2}\frac{1}{4}\int_{-\pi/2}^{\pi/2} {\rm d}\theta\ \mathfrak{s}(\theta)Y_1(\theta)|v_1^{\rm eff}(\theta)| \times \big(1+\mathcal{O}(e^{-h/T})\big). \tag{120}$$

Contributions of the magnonic bound states with ($s > 1$) are contained in the correction term.

It is important to stress at this point that in the gapped in the XXZ chain, the summation over $s > 1$ converges and for any value of h. This is a corollary of exponential suppression of the dressed velocities $\int d\theta|v_s^{\rm eff}| \sim e^{-s\,\eta}$ for large s. In contrast, in the the isotropic (XXX), where $\int {\rm d}\theta|v_s^{\rm eff}| \sim 1/s$, the sum only converges strictly away from half filling, whereas at $h = 0$ the higher-order contributions due to the spectrum of bound states can no longer be discarded.

Let us further analyse the dominant contribution which comes from $s = 1$. The saddle points of $Y_1(\theta)$ are located at $\theta = \pm\pi/2$ where the velocity vanishes. From the saddle point analysis we deduce

$$\int_{-\pi/2}^{\pi/2} d\theta\ \mathfrak{s}(\theta)|v_1^{\rm eff}(\theta)|e^{-\mathfrak{s}^{(\eta)}(\theta)/T}\frac{\sinh(h/T)}{\sinh(h/2T)} = \frac{\sinh(h/T)}{\sinh(h/2T)}\frac{2T\mathfrak{s}(\pi/2)e^{-\mathfrak{m}/T}}{\partial_\theta^2\varepsilon_1(\theta)\big|_{\theta=\pm\pi/2}}|\partial_\theta v_1^{\rm eff}(\theta)|_{\theta=\pi/2} \times \big(1+\mathcal{O}(e^{-2\mathfrak{m}/T})\big). \tag{121}$$

The spin diffusion constant can therefore be expressed as

$$\mathfrak{D}_{\rm XXZ} = \frac{1}{4}\frac{\sinh(h/T)}{\sinh(h/2T)}\frac{|\partial_\theta v_1^{\rm eff}(\theta)|_{\theta=\pi/2}}{2\pi\mathfrak{s}(\pi/2)}e^{(\mathfrak{m}-h)/T} \times \big(1+\mathcal{O}(e^{-h/T})+\mathcal{O}(e^{-\mathfrak{m}/T})\big). \tag{122}$$

The corrections of the order $\mathcal{O}(T\,e^{-h/T})$ are due to the bound states ($s > 1$), while the corrections of the order $\mathcal{O}(e^{-\mathfrak{m}/T})$ are a consequence of the saddle-point approximation of the rapidity integration in Eqs. (109) and (121). Notice moreover that

$$\partial_k^2\varepsilon_1(k)\Big|_{k=0} = \partial_k v_1^{\rm eff}(k)\Big|_{k=0}, \tag{123}$$

where

$$\frac{\partial_\theta v_1^{\rm eff}}{2\pi\rho_1^{\rm tot}} = \partial_k v^{\rm eff}(k). \tag{124}$$

Finally, in the gapped phase of the XXZ spin-1/2 chain, the leading low-temperature behaviour of the spin diffusion constant, neglecting terms $\mathcal{O}(e^{-h/T})$ and the taking the limit $h \to 0$, we obtain

$$\mathfrak{D}_{\rm XXZ} = \frac{1}{2}\partial_k^2\varepsilon_1(k)\Big|_{k=0}e^{\mathfrak{m}/T}\left(1+\mathcal{O}(e^{-h/T})+\mathcal{O}(e^{-\mathfrak{m}/T})\right), \tag{125}$$

with

$$\partial_k^2\varepsilon_1(k)\Big|_{k=0} = \Big|\frac{\sinh(\eta)\mathfrak{s}''(\theta)}{4\pi\mathfrak{s}(\theta)^2}\Big|_{\theta=\pi/2}. \tag{126}$$

B. $O(3)$ NLSM

Here we analyse the low-temperature limit of the non-topological ($\Theta = 0$) $O(3)$ NLSM given by Eqs. (82). Assuming $h/T \gg 1$ and $T \ll \mathfrak{m}$, and expanding the magnonic Y-functions (see also [4]),

$$Y_{s\geq 1} = \left(\frac{\sinh^2(h(s+1)/2T)}{\sinh^2(h/2T)} - 1\right) \times \big(1+\mathcal{O}(e^{-h/T})\big), \tag{127}$$

we obtain

$$Y_0(\theta)^{-1} = e^{-\,e(\theta)/T}\left(\frac{\sinh(3h/2T)}{\sinh(h/2T)}\right) \times \big(1+\mathcal{O}(e^{-h/T})\big). \tag{128}$$

The dressed magnetization behaves as

$$\lim_{T\to 0}\lim_{h\to 0}\frac{m_0^{\rm dr}(h)}{h}=\frac{4}{3},\qquad \lim_{T\to 0}\lim_{h\to 0}\frac{m_{s\geq 1}^{\rm dr}(h)}{h}=\frac{1}{3}(s+1)^2, \tag{129}$$

implying vanishing spin Drude weight at half filling. The static spin susceptibility,

$$\chi_h(T,h)=-\partial_h^2 f(h)=\sqrt{\frac{2\mathfrak{m}}{T\pi}}e^{-(\mathfrak{m}-h)/T}\times\left(1+\mathcal{O}(e^{-\mathfrak{m}/T})+\mathcal{O}(e^{-h/T})\right), \tag{130}$$

follows from the free-energy density $f(T,h)=-T\int_{-\infty}^{\infty}{\rm d}\theta\,\frac{k'(\theta)}{2\pi}\log(1+1/Y_0(\theta))$.

In precise analogy with the above calculation in the gapped Heisenberg spin chain, by neglecting the contribution of order $\mathcal{O}(e^{-h/T})$, the spin diffusion constants is only given by the physical excitations ($s=0$), reading, taking the limit $h\to 0$ after the limit $T\to 0$,

$$\mathfrak{D}_\Sigma=\frac{1}{3\mathfrak{m}}e^{\mathfrak{m}/T}\left(1+\mathcal{O}(e^{-h/T})+\mathcal{O}(e^{-\mathfrak{m}/T})\right), \tag{131}$$

where we used that curvature of the dispersion relation is now given by

$$\partial_k^2\varepsilon_0(k)\Big|_{k=0}=\Big|\frac{e''(\theta)}{(k'(\theta)^2)}\Big|_{\theta=0}=\frac{1}{\mathfrak{m}}. \tag{132}$$

We wish to stress once again that the corrections $\mathcal{O}(e^{-h/T})$ due to magnonic degrees of freedom ($s>0$) are only negligible provided $h/T\gg 1$. Analogously to the XXX chain, in the half filling limit $h\to 0$ they yield a $\sim 1/h$ type of divergence of $\mathfrak{D}$.

The spin Drude weight is given by

$$\mathcal{D}_\Sigma=\sum_s\int{\rm d}\theta\;\rho(\theta)(1-n(\theta))(v_s^{\rm eff}(\theta)m_s^{\rm dr})^2, \tag{133}$$

and, analogously to the XXX spin 1/2 chain, it goes to zero at small h as $h^2\log h$, due to $m_s^{\rm dr}\sim h$. By including only the contribution from quasiparticles with $s=0$ and, by following the previous reasoning, we obtain

$$T^{-1}\mathcal{D}_\Sigma=\frac{8\mathfrak{m}}{3}\left(h^2+O(h^4)\right)\sqrt{\frac{2T}{\pi}}e^{-\mathfrak{m}/T}\times\left(1+\mathcal{O}(e^{-h/T})+\mathcal{O}(e^{-\mathfrak{m}/T})\right). \tag{134}$$

IV. DIVERGENCE OF SPIN DIFFUSION CONSTANT AT THE ISOTROPIC POINT

We now specialise to the case of isotropic interactions, namely the spin-1/2 XXX chain with $\Delta=1$. We show that the spin diffusion constant $\mathfrak{D}$ diverges when approaching the half filling as h^{-1}. In order to show this is sufficient to analyse the asymptotic behaviour at large s of the summand in (115). We have

$$\mathfrak{D}\simeq\frac{1}{8(T\chi_h(T,h))^2}\sum_{s\geq 1}\int{\rm d}\theta\;\rho_s^{\rm tot}(\theta)n_s(\theta)(1-n_s(\theta))|v_s^{\rm eff}(\theta)|\left(s^2+\mathcal{O}(s)\right)^2. \tag{135}$$

For non-zero h, the sum is convergent since $n_s\sim e^{-sh/T}$. However, the $h\to 0$ limit is rather subtle and eventually results in a divergent $\mathfrak{D}$. This type of anomaly can be attributed to the large-s behaviour of the integrand which reveals that contributions in the limit of infinitely massive strings saturates with increasing the bare spin s. The sum (137) is a clear signature of non-perturbative physics in the vicinity of half filling: the sum over quasi-particle spices s must be evaluated *before* taking the limit $h\to 0$. Using the occupation functions for large s and $h>0$,

$$n_s(\theta)\simeq\left(\frac{\sinh\left(h/(2T)\right)}{\sinh\left(s\,h/(2T)\right)}\right)^2, \tag{136}$$

one can readily extract the type of divergence as $h\sim 0$,

$$\begin{aligned}\mathfrak{D}\simeq&\frac{1}{(T\chi_h(T,0))^2}\sinh^2\left(\frac{h}{2T}\right)\sum_{s\geq 1}s^4e^{-sh/T}\int{\rm d}\theta\,|\varepsilon_s^{\rm dr}(\theta)|\\ &\sim\frac{1}{(T\chi_h(T,0))^2}\sinh^2\left(\frac{h}{2T}\right)\tanh\left(\frac{h}{2T}\right)\sum_{s\geq 1}s^3e^{-sh/T}\sim\frac{1}{(T\chi_h(T,0))^2}\frac{T}{h}.\end{aligned} \tag{137}$$

We have used

$$\int \mathrm{d}\theta\, |\varepsilon_s^{\mathrm{dr}}(\theta)| = \tanh\left(\frac{h}{2T}\right)\frac{1}{s} + \mathcal{O}(s^{-2}). \tag{138}$$

which is valid only at the isotropic point $\Delta = 1$. Since the spin susceptibility at the isotropic point and at $h = 0$ is $\chi_h(T,0) \sim T^{-1/2}$, we immediately have that at $h \sim 0$

$$\mathfrak{D}(T,h)\chi_h(T,h) \sim \frac{\kappa(T)}{|h|} + \mathcal{O}(h^0). \tag{139}$$

with $\kappa(T) \sim T^{-1/2}$ at low T. An analogous result can be found with a similar calculation in the $O(3)$ non-linear sigma model since the structure of the dressing equations for the thermodynamic quantities is quite similar.

V. SPIN FLUCTUATIONS FROM GIANT MAGNONS

Here we explain why fluctuations of the Fermi functions δn_s pertaining to quasi-particle in the limit of infinitely large bare spin s are directly connected to fluctuations of the local magnetization $\delta\langle s^z_x\rangle = \langle s^z_x\rangle - \langle s^z\rangle_{T,h=0}$ with respect to a half-filled thermal state. First, recall that the occupation functions $n_s(\theta)$ are linked to the TBA $Y_s(\theta)$ functions via

$$n_s(\theta) = \frac{1}{1+Y_s(\theta)}. \tag{140}$$

Information about the filling is contained in the large-s asymptotics, namely

$$h/T = \lim_{s\to\infty} \frac{\log Y_s}{s}. \tag{141}$$

Combining the two, we find close to half filling

$$\langle s^z\rangle = T\,\chi_h(T,h)\frac{h}{T} + \mathcal{O}(h^2) = T\,\chi_h(T,h) \lim_{s\to\infty}\frac{\log(Y_s)}{s} + \mathcal{O}(h^2). \tag{142}$$

Considering small fluctuations of local magnetization in the vicinity of a half-filled state, $\delta\langle s^z\rangle = T\,\chi_h\delta(h/T)$, we deduce

$$\delta\langle s^z\rangle = T\,\chi_h(T,h) \lim_{s\to\infty} \delta(\log Y_s/s) = T\,\chi_h(T,h)\delta n_\infty. \tag{143}$$

where

$$\delta n_\infty = \lim_{s\to\infty} \frac{1}{s}\frac{\delta n_s}{n_s(n_s-1)}. \tag{144}$$

pertain to fluctuations of 'giant magnons'. As a specific example of this principle we mention the spin diffusion in the XXZ spin-1/2 chain, which can be understood as the equation of motion

$$\partial_t \delta n_\infty(x,t) = \widetilde{w}_\infty \partial_x^2 \delta n_\infty(x,t). \tag{145}$$

Here the coefficient $\widetilde{w}_\infty$ corresponds to the variance of the fluctuations of the giant magnons and it is precisely the spin diffusion constant at half filling, $\tilde{w}_\infty = \mathfrak{D}$, see Eq. (6.38) in [33].

VI. "THE MAGIC FORMULA"

We begin by the exact hydrodynamic formula for the spin diffusion constant valid in the vicinity of the half-filled thermal state,

$$\mathfrak{D}(T,h) = \frac{1}{2}\sum_s \int \mathrm{d}\theta\, \rho_s(\theta)(1-n_s(\theta))|v_s^{\mathrm{eff}}(\theta)|[\mathcal{W}_s]^2 + \mathcal{O}(h^2) \tag{146}$$

obtained in [33] via the thermodynamic form-factor expansion. Here the rapidity-independent weights $\mathcal{W}_s$ are related to the suitably normalised dressed differential scattering phases,

$$\mathcal{W}_s = \lim_{b\to\infty} \frac{K^{\rm dr}_{bs}(\alpha,\theta)}{\rho^{\rm tot}_b(\alpha)}. \tag{147}$$

We subsequently demonstrate that formula (146) can be rewritten as follows

$$\mathfrak{D}(T,h) = \frac{1}{8(T\chi_h(T,0))^2}\sum_s \int {\rm d}\theta\, \rho_s(\theta)(1-n_s(\theta))|v^{\rm dr}_s(\theta)|\left(\lim_{h\to 0}\frac{m^{\rm dr}_s}{h}\right)^2 + \mathcal{O}(h^2), \tag{148}$$

where the prefactor,

$$\chi_h(T,0) = \frac{\partial\langle s^z\rangle}{\partial h}\Big|_{h=0} = -\partial_h^2 f(T,h)\Big|_{h=0}, \tag{149}$$

is the static spin susceptibility at half filling. The formulae (146) and (148) can be identified provided

$$\mathcal{W}_s(T) = \frac{1}{2T\chi_h(T,0)} \times \left[\lim_{h\to 0}\frac{m^{\rm dr}_s(T,h)}{h}\right], \tag{150}$$

holds true at half filling.

In the next section, we establish the above identity in the limit of infinite temperature where the dressing equations take an algebraic form. We to this for two representative models, (i) the Heisenberg spin-1/2 XXZ chain and (ii) the integrable $SU(3)$-symmetric Lai–Sutherland spin chain. Notice that in the $T\to\infty$ limit the prefactor simplifies,

$$\chi_\mu(T,0) = T\chi_h(T,0), \qquad \lim_{T\to\infty}\chi_\mu(T,\mu=0) = \partial_\mu^2 \log\chi_\square(\mu)\Big|_{\mu=0} = \frac{d^2-1}{12}, \tag{151}$$

where $\chi_\square(h)$ is the fundamental character and d is the dimension of the local Hilbert space. Therefore, writing $\mu\equiv h/T$, the relation which we shall prove below reads

$$\lim_{T\to\infty}\mathcal{W}_s(T) = \frac{6}{d^2-1}\times\left[\lim_{\mu\to 0}\frac{m^{\rm dr}_s(\mu)}{\mu}\right] + \mathcal{O}(\mu^2). \tag{152}$$

A. Proof of the magic formula

1. *Isotropic Heisenberg chain*

The core part of the proof is based on the explicit calculation of the dressed differential scattering phase shifts $K^{\rm dr}_{s,s'}(\theta,\theta')$. We consider the large temperature $T\to\infty$ the dressing transformation becomes a coupled system algebraic equations which can be solved in a closed analytic form.

Identities for the scattering amplitudes. Using the fusion identities amongst the scattering amplitudes, the calculation boils down to computing the dressed momenta of quasi-particle excitations for the entire familyof integrable $SU(2)$ spin chains with higher spin local Hilbert spaces. To this end, let the representation label $s'\in\mathbb{N}$ denote the physical spin $S=s'/2$ degrees of freedom of the spin chain. The bare momenta of physical excitations (i.e. unbound magnons) are then given by

$$k^{(s')}_1(\theta) = -{\rm i}\log S^{-1}_{s'}(\theta), \tag{153}$$

where we have introduced the single-index 'magonon-string' scattering amplitudes

$$S_s(\theta) = \frac{\theta - s\,{\rm i}/2}{\theta + s\,{\rm i}/2}. \tag{154}$$

The inter-particle interactions allow for formation of bound states. These correspond to the so-called s-stings compounds, consisting of s magnons each carrying bare spin s', with bare momenta

$$k^{(s')}_s(\theta) = -{\rm i}\log S^{-1}_{s,s'}(\theta). \tag{155}$$

Here the two-particle scattering amplitudes are obtained by fusion

$$S_{s,s'}(\theta) = S_{|s-s'|}(\theta)S_{s+s'}(\theta) \prod_{\ell=1}^{\min(s,s')-1} S^2_{|s-s'|+2\ell}(\theta), \tag{156}$$

and depend only on the difference of the incident rapidities. Accordingly, we introduce the elementary scattering kernels,

$$K_s(\theta) = \frac{1}{2\pi \mathrm{i}}\partial_\theta \log S_s(\theta). \tag{157}$$

whose Fourier representation, using $\hat{f}(k) = \int_{\mathbb{R}} \mathrm{d}\theta f(\theta) e^{-\mathrm{i}k\theta}$, reads

$$\hat{K}_s(k) = e^{-|k|s/2}. \tag{158}$$

Similarly, the kernels for the two-body differential scattering phases are given by

$$K_{s,s'}(\theta) = \frac{1}{2\pi \mathrm{i}}\partial_\theta \log S_{s,s'}(\theta). \tag{159}$$

It is worthwhile noticing the following two important kernel identities

$$(1+K)_{s,s'} \star K_{s'} = \delta_{s,1}\mathfrak{s}, \qquad (1+K)_{s,s''} \star K_{s'',s'} = I^{A_\infty}_{s,s'}\mathfrak{s}. \tag{160}$$

Moreover, for later purpose it is convenient to define the 'bare momentum tensor',

$$G_{s,s'}(\theta) = \sum_{\ell=1}^{\min(s,s')} K_{|s-s'|-1+2\ell}(\theta), \qquad G_{s,s'}(\theta,\theta') = G_{s',s}(\theta',\theta), \tag{161}$$

given by

$$G_{s,s'}(\theta) = \frac{1}{2\pi}|\partial_\theta k_s^{(s')}(\theta)|. \tag{162}$$

Notice that the two-particle scattering phase decompose as

$$K_{s,s'}(\theta) = G_{s-1,s'}(\theta) + G_{s+1,s'}(\theta) = G_{s,s'-1}(\theta) + G_{s,s'+1}(\theta). \tag{163}$$

Dressed magnetization. In the infinite temperature limit $T \to \infty$ with the $U(1)$ chemical potential $\mu \equiv h/T$, the Fermi occupation function become rapidity independent and only depend on μ. The solution can be compactly expressed in terms of classical $SU(2)$ characters $\chi_s = \chi_s(h)$ (to not be confused with spin susceptibility $\chi_h(T,h)$),

$$n_s^{(0)} = \frac{1}{\chi_s^2(h)}, \qquad \bar{n}_s^{(0)}(h) = 1 - n_s^{(0)}(h). \tag{164}$$

Introducing the variable $z \equiv e^{\mu}$, the characters of irreducible $(s+1)$-dimensional representation read

$$\chi_s(\mu) = \frac{z^{-(s+1)} - z^{s+1}}{z^{-1} - z}. \tag{165}$$

The dressed magnetization can most easily extracted from the log-derivative of the infinite-temperature Y-functions

$$Y_s^{(0)}(\mu) = \chi_s^2(\mu) - 1, \tag{166}$$

as

$$m_s^{\mathrm{dr}}(\mu) = \partial_\mu \log Y_s^{(0)}(\theta;\mu), \tag{167}$$

At half filling, the lattice behave as

$$m_s^{\mathrm{dr}}(\mu) = \frac{1}{3}(s+1)^2\mu + \mathcal{O}(\mu^3). \tag{168}$$

Dressed momenta. By splitting the dressed scattering kernel into two parts,

$$K^{\rm dr}_{s,s'}(\theta) = G^{\rm dr}_{s,s'-1}(\theta) + G^{\rm dr}_{s,s'+1}(\theta), \tag{169}$$

we proceed by calculating the the dressed values of the bare energy tensor $G^{\rm dr}_{s,s'}$. Recall that the latter provides the dressed rapidity derivatives, $\partial_\theta p^{(s')}_s(\theta)$.

In order to analytically solve the dressing transformation we represent it in the quasi-local form. In this respect, it is crucial to determined the position of the source node depending on the spin label s'. This can be inferred by convolving tensor G with the (pseudo)inverse of the Fredholm kernel, that is

$$(1+K)^{-1}_{s,s'\prime} \star G_{s'',s'} = \left(1 - I^{A_\infty}\mathfrak{s}\right)_{s,s''} \star G_{s'',s'} = \delta_{s,s'}\mathfrak{s}. \tag{170}$$

The source term thus resides at the s'-th node. Therefore, to find the dressed momentum tensor $G^{\rm dr}$, one has to solve the following system

$$(1 - I^{A_\infty}\,\bar{n}\,\mathfrak{s})_{s,s''} \star G^{\rm dr}_{s'',s'} = \delta_{s,s'}\mathfrak{s}. \tag{171}$$

By introducing variables $F^{(s')}_s \equiv G^{\rm dr}_{s,s'}$ and transferring to Fourier space, $F^{(s')}_s(\theta;z) \mapsto \hat{F}^{(s')}_s(k;z)$, we arrive at the following three-point inhomogeneous recurrence relation

$$\mathfrak{s}^{-1}\cdot \hat{F}^{(s')}_s - I^{A_\infty}_{s,s''}\bar{n}^{(0)}_{s''}\hat{F}^{(s')}_{s''} = \delta_{s,s'}, \tag{172}$$

where $n^{(0)}_s$ denote the infinite-temperature mode occupation functions and $\mathfrak{s}^{-1}(k) = 2\cosh(k/2)$.

First we find the homogeneous solution to the above recurrence, which is given by

$$\hat{\Phi}^{(s')}_s(k;z|C_-,C_+) = \sum_{\alpha=\pm}\frac{\chi_s(z)}{\chi_1(z)}\left[\frac{e^{\alpha(s+1)k/2}}{\chi_{s-1}(z)} - \frac{e^{\alpha(s+1)k/2}}{\chi_{s+1}(z)}\right]C_\alpha(k;z), \tag{173}$$

for two unknown functions $C_\pm(k;z)$. The particular solution is singled out by imposing appropriate initial and boundary conditions. To satisfy the large-s asymptotics, $\lim_{|\theta|\to\infty} F^{(s')}_s(\theta) = 0$, we put

$$\hat{F}^{(s')}_{s\geq s'} \leftarrow \hat{\Phi}^{(s')}_s(k;z|\mathcal{C},0), \qquad \hat{F}^{(s')}_{s<s'} \leftarrow \hat{\Phi}^{(s')}_s(k;z|\mathcal{A},\mathcal{B}), \tag{174}$$

and write a closed system of equations at the initial node and the two gluing conditions at nodes $s'-1$ and s'. The solution for the fundamental particles is simply given by

$$s' = 1: \qquad \mathcal{C}(k;z) = e^{-k/2}. \tag{175}$$

The general solution for higher representations, namely for $s' \geq 3$, is more unwieldy and reads

$$\mathcal{A}(k;z) = \frac{(1+z^2)\left(e^k(z^{4-2s'}-1) - z^2(z^{2s'-1})\right)}{(e^k-1)(z^{2(s'+1)}-1)\left(z^2(1+e^{2k}) - e^k(1+z^4)\right)}e^{-s'k/2}, \tag{176}$$

$$\mathcal{B}(k;z) = -e^k\mathcal{A}(k;z), \tag{177}$$

$$\mathcal{C}(k;z) = \frac{(1+z^2)\left(z^2(z^{2s'}-1) - z^2(z^{2s'}-1)e^{(s'+2)k} + (z^{4+2s'}-1)(e^{(s'+1)k}-e^k)\right)}{(e^k-1)(z^{2(s'+1)}-1)(z^2(1+e^{2k}) - e^k(1+z^4))}. \tag{178}$$

Since we are interested in $s \gg s'$, only $\mathcal{C}(k;z)$ will be of our interest. The full k-dependent solution $\hat{F}^{(s')}_s(k;z)$ is quite lengthy and we thus suppress it here. Importantly however, since the final solution, after taking the $s\to\infty$ limit contains no rapidity dependence, it suffices to consider only the $k\to 0$ limit. In particular, one can explicitly verify that

$$\lim_{s\to\infty}\frac{\hat{K}^{\rm dr}_{s,s'}(k)}{\eta_{s,s'}} = \delta(k), \qquad \eta_{s,s'} = \frac{2}{3}(s'+1)^2\frac{s+1}{s(s+2)}, \tag{179}$$

implying that in Fourier space the rescaled dressed scattering kernels converge towards a delta function. In the $k\to 0$ limit, we find a simpler expression

$$\lim_{k\to 0}\hat{F}^{(s')}_{s>s'}(k;z) = \frac{(z^{2(s+1)}-1)(z^{2(s+1)}+1)\left(s'(z^2-1)(z^{2(s'+1)}+1) - 2z^2(z^{2s'}-1)\right)}{(z^2-1)(z^{2(s'+1)}-1)(z^{2s}-1)(z^{4+2s}-1)}, \tag{180}$$

and, using the relation

$$K^{\rm dr}_{s,s'}(\theta;z) = G^{\rm dr}_{s,s'-1}(\theta;z) + G^{\rm dr}_{s,s'-1}(\theta;z) = F^{(s'-1)}_{s}(\theta;z) + F^{(s'+1)}_{s}(\theta;z), \tag{181}$$

we obtain

$$\lim_{k\to 0}\hat{K}^{\rm dr}_{s,s'}(k;z) = \frac{2(z^{2(b+1)}-1)(z^{4(s+1)}-1)\left(b(z^2-1)(z^{2(b+1)}+1)-2z^2(z^{2b}-1)\right))}{(z^2-1)(z^{2b}-1)(z^{4+2b}-1)(z^{2s}-1)(z^{4+2s}-1)}. \tag{182}$$

Taking furthermore the limit of half filling, $\mu\to 0$ ($z\to 1$), the above result reduces to

$$\lim_{z\to 1}\lim_{k\to 0}\hat{K}^{\rm dr}_{s,s'}(k;z) = \frac{2}{3}(s'+1)^2\frac{s+1}{s(s+2)}. \tag{183}$$

In particular, $\hat{K}^{\rm dr}_{s,s'}(k=0,z=e^{\mu})$ decays to zero in both the large-s and small-μ limit:

$$\lim_{\mu\to 0}\lim_{k\to 0}\hat{K}^{\rm dr}_{sb}(\mu) = \frac{2}{3}(s'+1)^2\frac{1}{s} + \mathcal{O}(s^{-2}), \tag{184}$$

$$\lim_{s\to \infty}\lim_{k\to 0}\hat{K}^{\rm dr}_{s,s'}(\mu) = \frac{2}{3}(s'+1)^2\mu + \mathcal{O}(\mu^{3}). \tag{185}$$

Likewise, for the total state densities $\rho^{\rm tot}_{s}(\theta) = \frac{1}{2\pi}|\partial_\theta p^{(s'=1)}_{s}(\theta)|$, we find

$$\lim_{\mu\to 0}\lim_{k\to 0}\hat{\rho}^{\rm tot}_{s}(k;\mu) = \frac{1}{s} + \mathcal{O}(s^{-2}), \qquad \lim_{s\to \infty}\lim_{k\to 0}\hat{\rho}^{\rm tot}_{s}(k;\mu) = \mu + \mathcal{O}(\mu^{3}). \tag{186}$$

2. *Integrable SU(N) spin chains*

In this section we repeat computation for a class of model solvable with the nested Bethe Ansatz. We consider integrable the $SU(N)$-symmetric spin chains made of fundamental particles. The quasi-particle spectrum now arranges on vertices of an infinite lattice known as 'the T-strip'. Since the nodes are in one-to-one correspondence with rectangular irreducible unitary representations of $\mathfrak{su}(N)$ Lie algebra we will label them by (a,s), with integers $1\leq a\leq N$ and $s\in\mathbb{N}$. In particular, the row label a runs over different species (flavors) of particles, while the column label s belongs to bound states with s constituent particles. By convention, the momentum-carrying particles belong are assigned to the bottom row $a=1$.

In the *fundamental* $SU(N)$ spin chains, the elementary magnon excitations have momenta $k_{1,s}(\theta) = -{\rm i}\log S_1(\theta)$. All other magnons ($a=2,\ldots,N$) can be though of as auxiliary particles which carry no momenta and energy, that is $p_{a>1,s}=e_{a>1,s}=0$. Each particle species participate in the formation of bound state (Bethe strings). The mechanism is analogous to that of the $SU(2)$ chain. The momenta of s-strings read $k_{a,s}(\theta) = -{\rm i}\,\delta_{a,1}\log S^{-1}_{s}(\theta)$. Therefore, we have $|\partial_\theta k_{a,s}(\theta)/2\pi| = \delta_{a,1}G_{1,s}(\theta) = \delta_{a,1}K_s(\theta)$.

Bethe equations. The Bethe equations for the fundamental $SU(N)$ chain of length L have the nested form

$$e^{{\rm i}\delta_{\ell,1}k(\theta^{(\ell)}_{\alpha})L}\prod^{M_\ell}_{\beta\neq\alpha}S_2(\theta^{(\ell)}_{\alpha},\theta^{(\ell)}_{\beta})\prod^{N-1}_{r=1;r=\ell\pm 1}\prod^{M_r}_{\beta=1}S^{-1}_1(\theta^{(\ell)}_{\alpha},\theta^{(r)}_{\beta}) = 1, \qquad \ell=1,\ldots,N-1, \tag{187}$$

where $\{\theta^{(\ell)}_{\alpha}\}^{M_\ell}_{\alpha=1}$ denote (complex) rapidity variables for different quasi-particle species $\ell=1,2,\ldots N-1$.

Bethe–Yang equations. In the thermodynamic limit, obtained by taking $L\to\infty$ while keeping all filling fractions $M_\ell/L\sim\mathcal{O}(1)$ finite, Bethe equations (187) can be reformulated as the Bethe–Yang equations for analytic rapidity densities $\rho_{a,s}$,

$$\rho_{a,s} + \bar{\rho}_{a,s} = \left|\frac{k'_{a,s}}{2\pi}\right| - K_{(a,s),(a',s')}\rho_{a's'}. \tag{188}$$

This follows from (187) by (i) taking the logarithmic rapidity derivative, (ii) reducing the product of scattering amplitudes by using string configurations, and (iii) passing to continuum description by approximating large sum with convolution-type integrals. Another (equivalent) form of Eqs. (188) is

$$(1+K)_{(a,s),(a',s')}\star\rho_{a',s'} = \left|\frac{k'_{a,s}}{2\pi}\right| - \bar{\rho}_{a,s}. \tag{189}$$

Kernels $K_{(a,s),(a',s')}(\theta)$ encode differential scattering phases associated to the scattering even between (a,s) and (a',s') string excitations with rapidity difference θ, where a is the flavour label and s the number of constituent magnons. As can be seen from the structure of the (nested) Bethe equations, the Fredholm kernel $(1+K)$ is such that only the neighbouring species interact among each other, namely $K_{(a,s),(a',s')}$ is non-zero only if $a'=a\pm 1$.

Higher representations. Next, we consider a family of spin chains whose local Hilbert spaces belong to the one-row tableaux with s' boxes. In analogy to the $N=2$ case, we introduce the bare momentum tensor $G_{(a,s),(a',s')}(\theta)\equiv G^{(a',s')}_{a,s}(\theta)$, which carries all information about the bare momenta $k^{(a',s')}_{a,s}(\theta)\equiv k^{(s')}_{s}$ of elementary magnon excitations in a spin-$s'/2$ chain (including their s-magnon bound states, namely

$$G_{s,s'}(\theta)=\left|\frac{\partial_\theta k^{(s')}_s(\theta)}{2\pi}\right|. \tag{190}$$

Dressed magnetization. The rank of $\mathfrak{su}(N)$ Lie algebra is $N-1$, which is the number of globally conserved Noether charges. This means that the whole Cartan sector is parametrised by $N-1$ distinct chemical potentials. Here we focus only to a single charge, namely the total magnetization $S^z_{\rm tot}=\sum_i S^z_i$, with local density $S^z=\mathrm{diag}(S,S-1,\ldots,-S)$. The conjugate chemical potential will be denoted by μ.

The classical characters of rectangular Young tableau are functions of the Cartan elements

$$G=\mathrm{diag}(x_1,\ldots,x_N)=\exp\left(-\mu S^z\right), \tag{191}$$

and can be compactly expressed with help of the Weyl formula

$$\chi^{(N)}_{a,s}(\mu)=\frac{\mathrm{Det}\left(x_k^{N-j+s+\Theta_{s,j}}\right)_{1\le j,k,\le N}}{\mathrm{Det}\left(x_k^{N-j}\right)_{1\le j,k\le N}}, \tag{192}$$

where $\Theta_{i,j}=1$ if $i\ge j$ and zero otherwise. In fact, all $\chi^{(N)}_{a\ge 2,s}(\mu)$ are uniquely determined by the symmetric functions $\chi^{(N)}_{1,s}(\mu)$ by virtue of the Giambelli–Jacobi–Trudi formula

$$\chi^{(N)}_{a,s}(\mu)=\mathrm{Det}\left(\chi^{(N)}_{1,s+j-k}(\mu)\right)_{1\le j,k,\le a}. \tag{193}$$

The occupation functions of the grand-canonical Gibbs ensembles at infinite-temperature are encoded in the classical Y-functions $Y^{(0)}_{a,s}(\mu)$. The latter are the following non-linear combinations of the $\mathfrak{su}(N)$ characters,

$$Y^{(0)}_{a,s}(\mu)=\frac{\chi_{a,s-1}(\mu)\chi_{a,s+1}(\mu)}{\chi_{a-1,s}(\mu)\chi_{a+1,s}(\mu)},\qquad a\in\{1,2\},\quad s\in\mathbb{N}, \tag{194}$$

with boundary conditions $\chi_{a,s}\equiv 0$ for $a\in\{0,3\}$. For example, to extract the dressed magnetization for $N=3$, we set $G=\mathrm{diag}(e^{-\mu},1,e^{\mu})$ and compute

$$m^{\rm dr}_{a,s}(\mu)=\partial_\mu\log Y^{(0)}_{a,s}(\mu). \tag{195}$$

In the vicinity of a half-filled state, we find

$$m^{\rm dr}_{a,s}(\mu)=\frac{1}{6}(s+1)(s+2)\mu+\mathcal{O}(h^3),\qquad a\in\{1,2\}. \tag{196}$$

Dressed momenta. In the $SU(3)$ case, the dressing equation for the rapidity derivatives of the bare momenta become (written in Fourier space) a coupled system of recurrence relations for functions $\{F_{1,s},F_{2,s}\}_{s\ge 1}$,

$$\hat{\mathfrak{s}}^{-1}\cdot\hat{F}_{1,s}-\bar{n}^{(0)}_{s-1}\hat{F}_{1,s-1}-\bar{n}^{(0)}_{s+1}\hat{F}_{1,s+1}-n^{(0)}_{s-1}\hat{F}_{2,s-1}=\delta_{s,s'}, \tag{197}$$
$$\hat{\mathfrak{s}}^{-1}\cdot\hat{F}_{2,s}-\bar{n}^{(0)}_{s-1}\hat{F}_{2,s-1}-\bar{n}^{(0)}_{s+1}\hat{F}_{2,s+1}-n^{(0)}_{s-1}\hat{F}_{1,s-1}=0. \tag{198}$$

In the half filled case $\mu=0$ we consider here, the infinite-temperature occupation functions read

$$n^{(0)}_{a,s}=\frac{2}{(s+1)(s+2)}. \tag{199}$$

In Eqs. (198) ,the position of the source node, located at $(a,s)=(1,S)$, is prescribed by the one-row tableau associated to local physical degrees of freedom in the spin chain.

By introducing two independent linear combinations

$$\hat{F}^{\pm}_s = \hat{F}_{1,s} \pm \hat{F}_{2,s}, \tag{200}$$

the system of equation (198) reduces to a one-dimensional recurrence,

$$\hat{s}^{-1}\cdot \hat{F}^{\pm}_s - \bar{n}^{(0)}_{s-1}\hat{F}^{\pm}_{s-1} - \bar{n}^{(0)}_{s+1}\hat{F}^{\pm}_{s+1} \mp n^{(0)}_s \hat{F}^{\pm}_s = \delta_{s,1}, \tag{201}$$

which can in turn be solved using a similar strategy as previously in the $N=2$ case. Specifically, for the fundamental representation $S=1$, we find

$$\hat{F}^{\pm}_1(k) = \hat{K}_1(k) \pm \frac{1}{3}\hat{K}_1(k) - \frac{1}{3}\hat{K}_3(k) \mp \frac{1}{6}\hat{K}_4(k), \qquad \hat{C}^{\pm}(k) = 2\hat{K}_1(k), \tag{202}$$

implying

$$\hat{F}_{1,s}(k) = \frac{1}{3s}\Big((s+2)\hat{K}_s(k) - s\,\hat{K}_{s+2}(k)\Big), \tag{203}$$

$$\hat{F}_{2,s}(k) = \frac{1}{3(s+3)}\Big((s+3)\hat{K}_{s+1}(k) - (s+1)\hat{K}_{s+3}(k)\Big). \tag{204}$$

Next, we obtain solutions for generic one-row tableaux with S boxes. These can be found with a similar strategy, except that the source term in Eq. (201) now jumps to the s'-th node. Although it is not difficult to obtain closed-form expressions, e.g. with assistance with symbolic algebra routines, we unfortunately could not display them in a sufficiently economic way. Their general structure, valid for $S\geq 3$, is however of the form

$$\hat{F}^{(s')}_{1,s} = \sum_{k=0}^{s'} c^{(1)}_{s,k}\hat{K}_{s-s'+1+2k}, \qquad \hat{F}^{(s')}_{2,s} = \sum_{k=0}^{s'} c^{(2)}_{s,k}\hat{K}_{s-s'+2+2k}. \tag{205}$$

The $k\to 0$ limits are nonetheless rather simple,

$$\lim_{k\to 0}\hat{F}^{(s')}_{1,s}(k) = \frac{s'(s'+3)(5s+3s'+12)}{30s(s+3)}, \tag{206}$$

$$\lim_{k\to 0}\hat{F}^{(s')}_{2,s}(k) = \frac{s'(s'+3)(5s-3s'+3)}{30s(s+3)}, \tag{207}$$

Moreover, we have the following large-s limits (with $s>s'$)

$$\hat{F}^{(s')}_{a,s}(0) = \frac{1}{6}s'(s'+3)\frac{1}{s} + \mathcal{O}\left(s^{-2}\right), \tag{208}$$

$$\hat{F}^{(s'-1)}_{a,s}(0) + \hat{F}^{(s'+1)}_{a,s}(0) \simeq \frac{1}{3}\left((s')^2+3s'+1\right)\frac{1}{s} + \mathcal{O}\left(s^{-2}\right), \tag{209}$$

which do not depend on label a. To complete the proof of the magic formula, the dressed scattering kernels $K^{\rm dr}_{(a,s),(a',s')}$ are finally expressed in terms of the dressed bare momentum tensor $G^{\rm dr}_{s,s'}$. Specifically,

$$\lim_{s\to\infty}\lim_{k\to 0}\hat{K}^{\rm dr}_{(a,s),(a',s')}(k) = \lim_{s\to\infty}\lim_{k\to 0}\left[\delta_{a,a'}(\hat{G}^{\rm dr}_{s,s'-1}(k) + \hat{G}^{\rm dr}_{s,s'+1}(k)) - I^{A_2}_{a,a'}\hat{G}^{\rm dr}(k)_{s,s'}\right], \tag{210}$$

$$= \frac{1}{6}(s'+1)(s'+2)\frac{1}{s} + \mathcal{O}(s^{-2}). \tag{211}$$

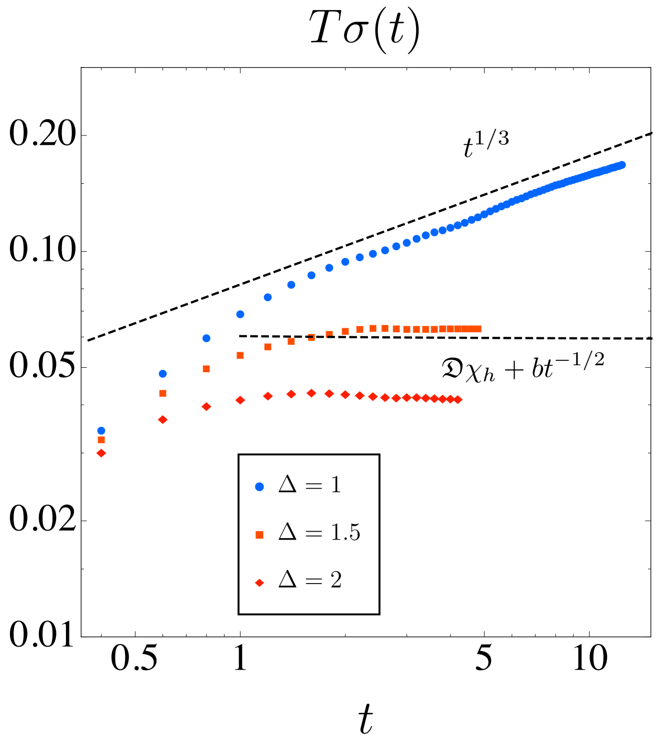

FIG. 2. Log-Log plot of the spin conductivity for the spin $S = 1$ XXZ chain $\hat{H}_\Delta$ at $\Delta = \{1, 1.5, 2\}$ and $T = 10$ and $h = 0$.

VII. ADDITIONAL NUMERICAL DATA

We here report additional numerical data on the time dependent conductivity of the spin current $\hat{j}$

$$\sigma(t) = \frac{1}{T}\int_0^t \mathrm{d}t' \langle \hat{J}(t')\hat{j}_0(0)\rangle_{T,h=0} \qquad \hat{J} = \sum_i \hat{j}_i. \tag{212}$$

We first examine the restoration of normal diffusion upon explicitly breaking the interaction isotropy. We consider the uniaxially anisotropic version of the Haldane spin-1 chain, see Fig. 2, namely

$$\hat{H}_\Delta = \sum_i \hat{s}_i^x \hat{s}_{i+1}^x + \hat{s}_i^y \hat{s}_{i+1}^y + \Delta \hat{s}_i^z \hat{s}_{i+1}^z. \tag{213}$$

The $SU(2)$-symmetric point $\Delta = 1$ displays superdiffusion with $\sigma(t) \sim t^{1/3}$. For $\Delta > 1$ we instead find normal diffusion with $\sigma(t) \sim \mathfrak{D}\chi_h + b/t^{1/2}$ with $\mathfrak{D}$ finite. In this respect, the situations is analogous to that of the $S = 1/2$ XXZ spin chain.

In Fig. 3 we study the growth of the time-dependent conductivity for a one-parametric family of $SU(2)$-invariant spin $S = 1$ Hamiltonians

$$\hat{H}_\vartheta = \sum_i \left(\cos(\vartheta)\hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_{i+1} + \sin(\vartheta)(\hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_{i+1})^2\right), \tag{214}$$

for several different values of ϑ, including the Haldane gapped phase, $\vartheta = 0, \pi/8$, the ferromagnetic phase, $\vartheta = 0.6\pi$, and the dimerised phase, $\vartheta = 3\pi/2$, see for example [92]. While withing the Haldane-gapped phase we find clear evidence of superdiffusion (as expected from the low-lying $O(3)$ non-linear sigma model theory), the results for the other two phases are less conclusive. Finally, in Fig. 4, we display the spin conductivity in the $SU(2)$ spin $S = 1$ chains $\hat{H} = \sum_i \cos(\vartheta)\hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_{i+1} + \sin(\vartheta)(\hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_{i+1})^2$ at $\vartheta = \pi/8$ (inside the Haldane phase) for two different values of temperature, both compatible with the superdiffusion.

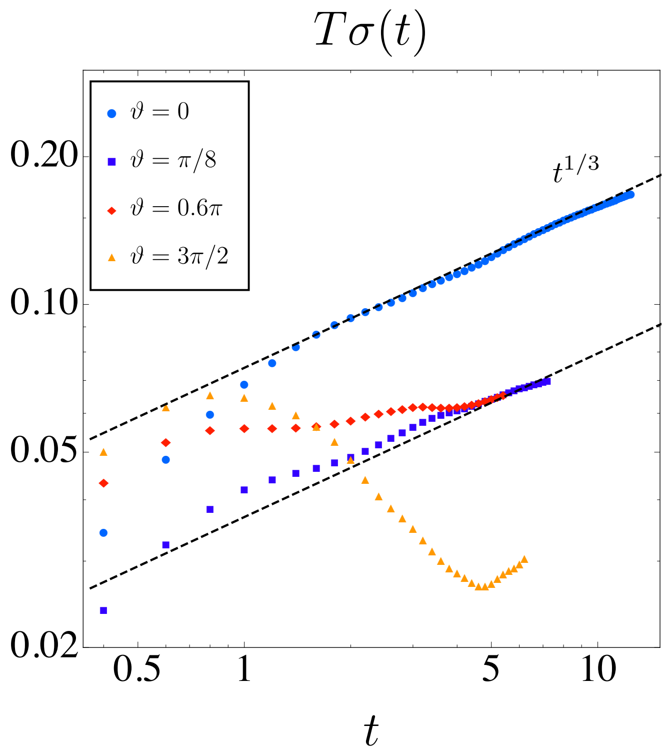

FIG. 3. Log-Log plot of the spin conductivity at $T = 10$ and $h = 0$ for the $SU(2)$ spin $S = 1$ chains $\hat{H}_\vartheta$.

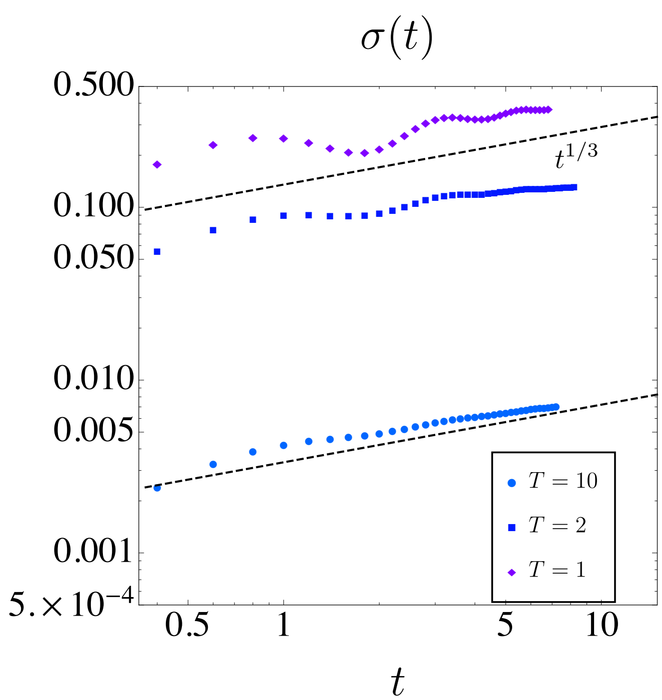

FIG. 4. Log-Log plot of the spin conductivity at $h = 0$ for the $SU(2)$ spin $S = 1$ chain $\hat{H}_{\vartheta=\pi/8}$ for three different values of temperature.