







Local dynamics and thermal activation in the transverse-field Ising chain

Jiahao Yang ¹, Weishi Yuan ², Takashi Imai ², Qimiao Si ^{3,*}, Jianda Wu ^{1,4,†} and Márton Kormos ^{5,6,‡}

¹*Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai 201210, China*

²*Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada L8S 4M1*

³*Department of Physics & Astronomy, Rice University, Houston, Texas 77005, USA*

⁴*School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China*

⁵*Department of Theoretical Physics, Budapest University of Technology and Economics, 1111 Budapest, Hungary*

⁶*MTA-BME Quantum Dynamics and Correlations Research Group (ELKH), BME-MTA Statistical Field*

Theory ‘Lendület’ Research Group, Institute of Physics, Budapest University of Technology and Economics, 1111 Budapest, Hungary



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There has been considerable recent progress in identifying candidate materials for the transverse-field Ising chain (TFIC), a paradigmatic model for quantum criticality. Here, we study the local spin dynamical structure factor of different spin components in the quantum disordered region of the TFIC. We show that the low-frequency local dynamics of the spins in the Ising- and transverse-field directions have strikingly distinctive temperature dependencies. This leads to the thermal-activation gap for the secular term of the nuclear magnetic resonance $1/T_2'$ relaxation rate to be half of that for the $1/T_1$ relaxation rate. Our findings reveal a surprise in the nonzero-temperature dynamics of the venerable TFIC model and uncover a means to evince the material realization of the TFIC universality.

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I. INTRODUCTION

While classical matter freezes at zero temperature, quantum many-body systems often display multiple ground states due to the competition between different couplings. Upon a continuous transformation from one ground state to another, quantum criticality develops. It is anchored by a quantum critical point (QCP) at zero temperature, in contrast to a classical critical point that appears at a thermally induced phase transition. Quantum criticality has emerged as a general organizing principle to understand many of the richest phenomena that have been observed in quantum materials [1,2]. These include the cuprates [3,4], heavy fermion metals [5–7], and iron pnictides [8,9]. One of the prominent features of quantum criticality is that it mixes spatial and temporal fluctuations [10,11]. While this intermixing complicates the description of quantum criticality, it also implies that dynamical properties can be used to characterize the nature of quantum criticality. As another outstanding feature of quantum criticality, approaching the QCP by a nonthermal control parameter (g) and by temperature (T) represent two independent ways to examine its universal behavior. As such, it is instructive to probe quantum criticality by analyzing dynamical properties as a function of temperature, which can be conveniently studied experimentally.

A paradigmatic model for continuous quantum phase transitions is the transverse field Ising model in one spatial

dimension [11–17]. It represents a prototype setting to explore the properties of quantum criticality. Yet, in spite of its venerable status, there is much about it that remains to be understood. Suitable materials to study this model have only been emerging recently [18–22]. They have allowed new experiments that are providing puzzling experimental results, especially on dynamical properties at nonzero temperatures. At the same time, calculating dynamical quantities near a QCP (g_c) are always challenging. That is also the case for the transverse field Ising chain, notwithstanding the considerable efforts [12,13,23]. One of the particularly interesting quantities is the local dynamical structural factor [24–26], which can be measured by the longitudinal relaxation rate $1/T_1$ in the nuclear magnetic resonance (NMR) experiment [27].

In this work, we begin the investigation by focusing on the quantum disordered region of the transverse-field Ising chain (TFIC) ($g > g_c$). The critical behavior of the transverse and longitudinal dynamical structure factors, S^{xx} and S^{zz} , are analytically determined at low frequency. Our result shows that S^{xx} has a thermally activated behavior with one single particle gap, since Pauli matrix σ^x is \mathbb{Z}_2 symmetric in TFIC. In contrast, the thermal-activation energy in S^{zz} is twice as large as that of S^{xx} since σ^z is not \mathbb{Z}_2 invariant [25,26]. This characteristic contrast is very unique and can serve as a telltale sign to ascertain whether candidate materials realize the TFIC universality. Accordingly, we propose an experimental signature for the TFIC realization, viz. that the activation gap for the secular term of $1/T_2$, named $1/T_2'$ (Ref. [28]), will be half of its counterpart for $1/T_1$ in NMR relaxation rate measurements.

The remainder of the paper is organized as follows. Section II introduces the lattice Hamiltonian of TFIC and its field theory description in the scaling limit. Section III

*qmsi@rice.edu

†wujd@sjtu.edu.cn

‡kormosmarton@gmail.com

specifies the expression of the dynamical structure factor. The results of local dynamics at low frequency in transverse and longitudinal directions are obtained in Sec. IV and are discussed in detail in Sec. V. The proposal for using NMR experiments as a means of identifying candidate materials for the TFIC universality is presented in Sec. VI. Finally, Sec. VII contains the conclusion and discussions.

II. MODEL

The Hamiltonian of the transverse field Ising chain is given by [13]

$$H_I = -J \sum_{i=1}^N (\sigma_i^z \sigma_{i+1}^z + g \sigma_i^x), \quad (1)$$

where σ_i^x and σ_i^z are Pauli matrices associated with the spin components $S^\mu = \sigma^\mu/2$ ($\mu = x, y, z$) on site i and g is the coupling with the transverse field. Below we shall refer to the z (Ising) direction as *longitudinal* and to the x direction as *transverse*. At zero temperature, the system undergoes a quantum phase transition when the transverse field is tuned across its QCP $g = g_c = 1$. The Hamiltonian can be conveniently converted to fermionic operators c_i and c_i^\dagger through Jordan-Wigner transformation. After introducing a Bogoliubov rotation, the Hamiltonian takes the canonical form $H_I = \sum_k \epsilon_k (\gamma_k^\dagger \gamma_k - \frac{1}{2})$ with single-particle energy dispersion

$$\epsilon_k = 2J\sqrt{1 + g^2 - 2g \cos k}, \quad (2)$$

where momentum k is dimensionless in all calculations. At zero momentum, the gap, $\Delta = 2J|g - g_c|$, vanishes at g_c .

In the vicinity of the QCP, the low energy effective description of the system is given by an Ising field theory obtained as the scaling limit of the lattice Hamiltonian (cf. Appendix A). In this limit the lattice spacing goes to zero, $a \rightarrow 0$, while $J \rightarrow \infty$ and $g \rightarrow 1$ such that the energy gap and the ‘‘speed of light’’ are kept fixed, $2J(1 - g) = \Delta$, $2Ja/\hbar = c$. The resulting Hamiltonian describes a relativistic field theory of free Majorana fermions with mass $m = \Delta/c^2$

$$\mathcal{H}_I = \int dx \left[\hbar c \frac{i}{2} \left(\psi \frac{\partial \psi}{\partial x} - \bar{\psi} \frac{\partial \bar{\psi}}{\partial x} \right) \pm \Delta \frac{i}{2} (\bar{\psi} \psi - \psi \bar{\psi}) \right], \quad (3)$$

where the sign of the second term is $+$ ($-$) for the paramagnetic (ferromagnetic) phase, corresponding to $g > g_c$ ($g < g_c$) in the lattice model. The field operators are related to the lattice operators as $\bar{\psi}(ja) = \frac{(-)}{\sqrt{2a}} (e^{\mp i\pi/4} c_j + e^{\pm i\pi/4} c_j^\dagger)$. Correspondingly, the single-particle energy Eq. (2) becomes relativistic,

$$\epsilon(p) = \sqrt{\Delta^2 + p^2 c^2} = \Delta \cosh \theta, \quad (4)$$

where $p = \hbar k/a$ and θ is the relativistic rapidity parameter. In the scaling limit, the σ_j^x operator is related to the energy density operator $\epsilon(x)$ through the following relation:

$$\sigma_j^x = -2a \epsilon(x = ja) \equiv -2a i \bar{\psi}(x) \psi(x), \quad (5)$$

where $\epsilon(x) = i\bar{\psi}(x)\psi(x)$ is quadratic in fermion operators. And σ_j^z is related to the magnetization density operator $\sigma(x)$

as ($\hbar = c = 1$) [13]

$$\sigma_j^z = \bar{s}^{-1} J^{-1/8} \sigma(x = ja), \quad (6)$$

where $\bar{s} = 2^{1/12} e^{-1/8} \mathcal{A}^{3/2}$ and $\mathcal{A} = 1.2824271291\dots$ is Glaisher’s constant. The $\sigma(x)$ operator corresponds to the order parameter after taking its expectation value with respect to the vacuum. Note that $\sigma(x)$ is nonlocal in the fermion operators and cannot be simply expressed in terms of the latter.

III. DYNAMIC STRUCTURE FACTOR

In the quantum disordered region of TFIC ($g > g_c$), we compute the local spin dynamical structure factor (DSF) at low frequency $\omega \ll k_B T$, which are relevant to the NMR relaxation rates [28,29]. The DSF with spin component $\alpha = x, y, z$ is given by ($k_B = 1$)

$$\begin{aligned} S^{\alpha\alpha}(\omega, q) &= \frac{-2}{1 - e^{-\omega/T}} \text{Im} \chi^{\alpha\alpha}(\omega, q) \\ &= \sum_l \int_{-\infty}^{\infty} dt e^{i\omega t - iqla} \langle \sigma_{l+1}^\alpha(t) \sigma_l^\alpha(0) \rangle_T, \end{aligned} \quad (7)$$

where $\chi^{\alpha\alpha}(\omega, q)$ is the dynamical spin susceptibility at the transferred energy ω and momentum q . In the field theory, we consider the continuum operators $\epsilon(x)$, $\sigma(x)$ and the summation over lattice sites in Eq. (7) is replaced by an integral over x . The local DSF is $S^{\alpha\alpha}(\omega) = \int \frac{dq}{2\pi} S^{\alpha\alpha}(\omega, q)$. Using field theory language [30], the DSF can be written in Lehmann spectral representation as

$$S^{\alpha\alpha}(\omega, q) = \frac{1}{\mathcal{Z}} \sum_{r,s=0}^{\infty} C_{r,s}^{\alpha\alpha}(\omega, q), \quad (8)$$

where \mathcal{Z} is the partition function and

$$\begin{aligned} C_{r,s}^{\alpha\alpha}(\omega, q) &= \int \frac{d\theta_1 \dots d\theta_r}{(2\pi)^r r!} \int \frac{d\theta'_1 \dots d\theta'_s}{(2\pi)^s s!} e^{-E_r/T} (2\pi)^2 \\ &\times \delta(\omega + E_r - E_s) \delta(q + P_r - P_s) |(\theta_1 \dots \theta_r| \\ &\times \sigma^\alpha(0, 0) | \theta'_1 \dots \theta'_s \rangle|^2, \end{aligned} \quad (9)$$

where the energy and momentum eigenvalues of the multi-particle states $|\theta_1, \dots, \theta_n\rangle$ are $E_n = \Delta \sum_i^n \cosh \theta_i$ and $P_n = \Delta \sum_i^n \sinh \theta_i$. The term $C_{r,s}^{\alpha\alpha}$ carries a factor $e^{-E_r/T} < e^{-r\Delta/T}$; thus the small expansion parameter is $e^{-\Delta/T}$. Its dependence on s is less obvious but thanks to the energy conserving Dirac delta, the energies of the two states with r and s particles are related. For a fixed frequency ω and at low temperature one can truncate the double sum in both r and s . As shown in Appendix B, Eq. (8) is a low-temperature expansion which has term-by-term divergences that can be regularized in a linked cluster expansion [31,32], $S^{\alpha\alpha}(t, x) = \sum_{r=0, s=0}^{\infty} D_{r,s}^{\alpha\alpha}(t, x)$, where the finite terms $D_{r,s}^{\alpha\alpha}$ are certain linear combinations of $C_{r,s}^{\alpha\alpha}$ and terms appearing in the expansion of the partition function.

IV. LOCAL DYNAMICS AT LOW FREQUENCY

Let us first consider the leading critical behavior of $S^{xx}(\omega)$ in the quantum disordered region with $\omega \ll T \ll \Delta$. Since σ_j^x

and $\varepsilon(x)$ are quadratic in the fermionic operators, Eq. (9) has nonzero matrix elements between states that either have an equal number of particles or the particle number difference is 2.

The first term in Eq. (8) is the vacuum contribution $C_{00}^{xx} = |\langle 0|\varepsilon|0\rangle|^2 \delta(\omega)\delta(k)$, i.e., 0 particle–0 particle (0p–0p) contribution. In the field theory this is a divergent contribution and requires renormalization (e.g., by normal ordering) [32]. However, since we are interested in the finite (but small) ω domain, we ignore this term. The terms $D_{0,s}^{xx}$ and $D_{s,0}^{xx}$ contribute to frequencies $\omega \geq s\Delta$ outside of our domain of interest, $0 < \omega \ll \Delta$. Thus the first contributing term is the 1p–1p term,

$$C_{11}^{xx}(\omega, q) = \iint \frac{d\theta}{2\pi} \frac{d\theta'}{2\pi} |F_2^\varepsilon(\theta|\theta')|^2 e^{-\Delta \cosh \theta/T} (2\pi)^2 \times \delta[q + \Delta(\sinh \theta - \sinh \theta')] \times \delta[\omega + \Delta(\cosh \theta - \cosh \theta')], \quad (10)$$

where the 1p–1p form factor $F_2^\varepsilon(\theta|\theta')$ is $F_2^\varepsilon(\theta|\theta') \equiv \langle \theta|\varepsilon(0)|\theta'\rangle = -i\Delta \cosh(\frac{\theta-\theta'}{2})$, as can be obtained from the plane wave expansion of the fields in a straightforward way (cf. Appendix C). Then, after performing two integrals of Eq. (10), the leading contribution to local transverse DSF at $\omega \ll T \ll \Delta$ region is

$$C_{11}^{xx}(\omega) \approx -\frac{\Delta}{\pi} e^{-\Delta/T} \left[\ln\left(\frac{\omega}{4T}\right) - \frac{T}{2\Delta} + \gamma_E \right], \quad (11)$$

where γ_E is Euler's constant. The main features of the result are the $\sim e^{-\Delta/T}$ temperature dependence and the $\sim \ln(\omega/T)$ logarithmic frequency dependence. From Eq. (9) the higher particle number contributions $D_{r,s}^{xx}$ with $\max(r, s) \geq 2$ contain the factor $e^{-E_r/T} \delta(\omega + E_r - E_s)$, so they are exponentially suppressed at low temperature $T \ll \Delta$ for frequencies $\omega \ll \Delta$; in particular, $D_{r,s}^{xx} \sim e^{-\max(r,s)\Delta/T}$. So we find that the leading order contribution to the local transverse DSF $S^{xx}(\omega)$ in the quantum disordered region with $\omega \ll T \ll \Delta$ is given by the 1p–1p term, i.e., Eq. (11).

Because the σ_j^x operator is local and quadratic in terms of the fermion operators, it is promising to calculate the transverse DSF S^{xx} from the discrete spin chain directly without taking the scaling limit. As shown in Appendix E, we further utilize two methods: one is an exact lattice calculation and the other is the truncated form factor expansion. Both of them give the same leading behavior for $S^{xx}(\omega)$ as Eq. (11) obtained by using field theory.

We next turn to the leading critical behavior of S^{zz} in the quantum disordered region with $\omega \ll T \ll \Delta$. Following the same strategy for calculating $S^{xx}(\omega)$ in the scaling limit, we can obtain (cf. Appendix F)

$$S^{zz}(\omega) \approx \frac{\bar{\sigma}^2}{\Delta} \frac{3\sqrt{3}}{2\pi} \left(\frac{T}{\Delta}\right)^2 e^{-2\Delta/T}, \quad (12)$$

where $\bar{\sigma} = \Delta^{1/8} \bar{s}$. This result exhibits a characteristic thermal-activation gap, i.e., 2Δ , which agrees with the scaling limit of the corresponding result found in Refs. [25,26].

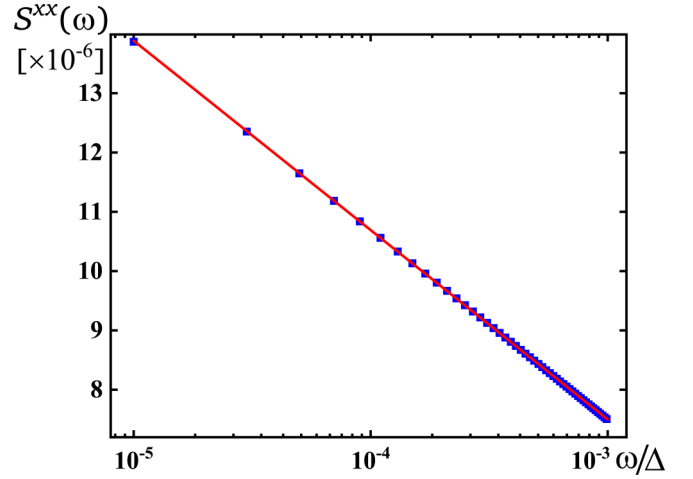


FIG. 1. Local transverse DSF S^{xx} vs frequency (blue dots) at fixed $\Delta = 0.1J$ and $T = 0.01J$. The logarithmic frequency dependence is well fitted by the red solid line.

Figure 1 shows the frequency dependence of $S^{xx}(\omega)$ and its fitting function with parameters $\Delta = 0.1J$ and $T = 0.01J$. The data points are calculated by numerically integrating out q from $S^{xx}(\omega, q)$ (cf. Appendix E) and the fitting function gives the expected logarithmic divergence in ω : $10^6 \times S^{xx}(\omega) = -2.08 - 1.39 \ln(\omega/\Delta)$. This agrees well with the asymptotic result Eq. (11), $10^6 \times S^{xx}(\omega) = -1.99 - 1.38 \ln(\omega/\Delta)$.

We also study the temperature dependence of S^{xx} with $\omega = 10^{-4}J$ and $\Delta = 0.1J$. The data points shown in Fig. 2 are calculated by numerically integrating out q from $S^{xx}(\omega, q)$ (cf. Appendix E) and the corresponding fitting function $S^{xx}(T) = e^{-\Delta/T} [0.24 + 0.03 \ln(T/\Delta)]$ indicates that the thermal behavior of $S^{xx}(T)$ is dominated by the 1p–1p term and the activation gap is Δ . This fitting conforms with the result obtained from the asymptotic expression Eq. (11), $S^{xx}(T) = e^{-\Delta/T} [0.23 + 0.02(T/\Delta) + 0.03 \ln(T/\Delta)]$. In the fitting, the

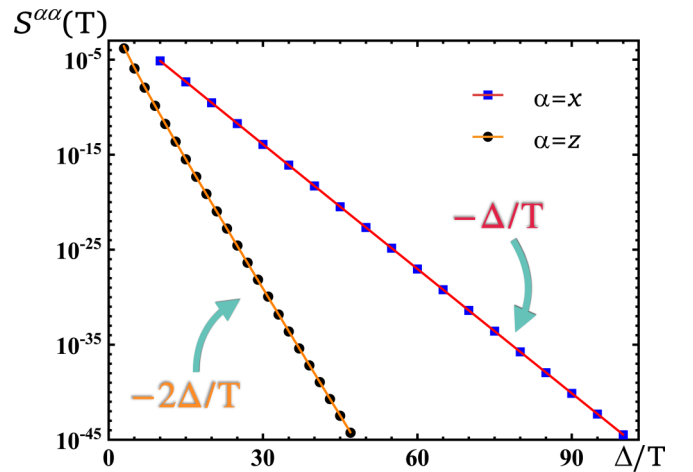


FIG. 2. Contrast of the thermal-activation gaps between S^{xx} (blue dots) and S^{zz} (black dots). The exponential decay behaviors of S^{xx} and S^{zz} are well fitted by red and orange lines, respectively, showing the gap for S^{xx} is half of that for S^{zz} .

T/Δ term is not taken into account since it is negligible compared with other terms in the considered region.

Similarly, we show the temperature dependence of S^{zz} by numerically integrating out q from $S^{zz}(\omega, q)$ with fixed frequency $\omega = 0.1\Delta$ (cf. Appendix F). The fitted line $S^{zz}(T) = 0.87(T/\Delta)^{2.06}e^{-1.99\Delta/T}$, which is consistent with the prediction of Eq. (12), $S^{zz}(T) = 0.83(T/\Delta)^2e^{-2\Delta/T}$. Here $S^{zz}(T)$ exhibits a distinct thermal behavior with the activation gap being 2Δ compared with $S^{xx}(T)$.

V. CONTRASTING THERMAL ACTIVATIONS OF S^{xx} AND S^{zz}

Our key result is the different exponential temperature dependence, $e^{-\Delta/T}$ vs $e^{-2\Delta/T}$, for S^{xx} and S^{zz} , respectively. This is eventually a consequence of the \mathbb{Z}_2 symmetry of the model, i.e., $\sigma^x \rightarrow \sigma^x$ and $\sigma^z \rightarrow -\sigma^z$. For large transverse fields $g \gg 1$, the ground state corresponds to spins pointing in the x direction, so intuitively excitations in the paramagnetic phase can be thought of as spin flips in the transverse direction generated by σ^z . This means that σ^z creates and destroys particles that carry the same quantum numbers as the operator itself, i.e., they are odd under spin reversal in the z direction. As a consequence, the nonzero matrix elements of σ^z in the paramagnetic phase are between states with different particle number parity [33,34]. For σ^x it is the opposite: Its only nonvanishing matrix elements are between states of the same parity because it is quadratic in the fermionic operators.

As for the discussion about Eq. (11), at low frequencies $\omega \ll \Delta$ only those matrix elements can contribute to the Lehmann representation where the energies of the two states are close to each other due to the Dirac-delta expressing energy conservation. This implies that matrix elements between the ground state and the excited states do not contribute. Moreover, independent of which state carries the Boltzmann factor, the contribution of the matrix element will be $\sim e^{-n\Delta/T}$, where n is the larger of the particle numbers in the two states. Together with the parity property of σ^z , this implies that the leading temperature dependence of the longitudinal DSF is $e^{-2\Delta/T}$ coming from 1p-2p contributions, while that of the transverse DSF is $e^{-\Delta/T}$ coming from 1p-1p matrix elements. Therefore, this characteristic contrast of the temperature dependence of S^{xx} and S^{zz} can serve as a universal behavior of TFIC and can also be verified in NMR experiments.

From a symmetry perspective, σ^z can also have a nonzero 1p-1p matrix element if the \mathbb{Z}_2 symmetry of the system is broken. One such case is the quantum E_8 integrable model, which emerges from longitudinal-field perturbed quantum critical TFIC [35]; the additional longitudinal field breaks the \mathbb{Z}_2 symmetry. In the model, the low-temperature DSF S^{zz} exhibits $e^{-m/T}$ (where m is the mass of the lightest E_8 particle) [24]; we stress, however, that it is due to a physical mechanism of broken \mathbb{Z}_2 symmetry that is completely different from what happens in the present work.

VI. NMR RELAXATION RATES

The transverse field applied along the x axis in the TFIC serves as the applied static magnetic field in an NMR setup

[27]. The longitudinal NMR relaxation rate $1/T_1$ of TFIC is given by [28,29]

$$\frac{1}{T_1} \sim |A_y|^2 S^{yy}(\omega_n) + |A_z|^2 S^{zz}(\omega_n). \quad (13)$$

Here, A_j ($j = x, y$, and z) is the scalar hyperfine coupling, which we take as constants for simplicity, and ω_n is the resonant frequency (\sim MHz) of NMR measurements. Therefore, $1/T_1$ probes local spin dynamics through S^{zz} and S^{yy} along the two orientations orthogonal to the transverse-field direction x . In the TFIC, we have $S^{yy}(\omega) = S^{zz}(\omega)\omega^2/[4(gJ)^2]$ [24], so the contribution from S^{yy} can be ignored in an NMR setup (at a very low frequency). As such, we expect $1/T_1 \sim S^{zz}(\omega = \omega_n) \sim e^{-2\Delta/T}$, where the thermal-activation gap is 2Δ [26,27].

To probe $S^{xx}(\omega)$, we consider the transverse NMR relaxation rate $1/T_2$ of TFIC, which is given by [28,29]

$$\frac{1}{T_2} = \frac{1}{T_1'} + \frac{1}{T_2'}, \quad (14a)$$

$$\frac{1}{T_1'} = A \frac{1}{T_1}, \quad (14b)$$

$$\frac{1}{T_2'} = |A_x|^2 S^{xx}(\omega_n). \quad (14c)$$

Here, the nonsecular contribution $1/T_1'$ can be estimated from the result of $1/T_1$ measurement and the prefactor A is calculated based on Bloch-Wangsman-Redfield theory (cf. Appendix I). Then, the secular term $1/T_2'$ can be determined from Eq. (14a) by subtracting $1/T_1'$ from $1/T_2$. Therefore, at relatively low temperature, $1/T_1'$ is exponentially suppressed by the larger gap 2Δ of S^{zz} but $1/T_2' \sim S^{xx}(\omega = \omega_n) \sim e^{-\Delta/T}$ still remains sizable with a thermal-activation gap Δ . Since $1/T_1$ and $1/T_2$ measurements are two independent NMR experiments, we predict that the ratio of extracted thermal-activation gaps for $1/T_1$ and $1/T_2'$ is 2.

VII. CONCLUSION

To conclude, we determined the leading behavior of the local *transverse* DSF in the quantum disordered region of the TFIC at small transfer energy with temperature much smaller than the gap. It is shown that when the transfer energy is much smaller than the temperature the local transverse DSF exhibits a logarithmic singularity. We found that the extracted thermal activation gap from the local *transverse* DSF is half of that for the *longitudinal* one, which can be attributed to the different parities of σ^x and σ^z in the quantum disordered region of the TFIC. This sharp contrast can be directly tested in a proper NMR setup through $1/T_1$ and $1/T_2$ relaxation rate measurements. In addition, it is worth noticing that for unpolarized-spin measurements, our results unveil the underlying physical mechanism for the observed single-particle gap in the thermal activation [36,37], where the transverse DSF is expected to dominate the low-energy behavior.

It is known that a thermodynamic quantity of the TFIC, the Grüneisen ratio—the ratio of magnetic expansion coefficient to specific heat—exhibits a unique quantum critical behavior [23]. Here, our work reveals a sharp contrast of the temperature dependence of the *transverse* and *longitudi-*

nal local DSFs of the TFIC, which represents a unique and surprising dynamical feature for the TFIC. Furthermore, accessing the universality of the TFIC in experiments is a crucial step toward a realization of the exotic quantum phenomena such as the E_8 particles in the quantum E_8 integrable model [21,22,24,38]. Our work implies that combined measurements of the dynamical and thermodynamic quantities provide tell-tale experimental signs for the class of TFIC universality.

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APPENDIX A: DIAGONALIZATION OF THE LATTICE AND FIELD THEORY HAMILTONIANS

After Jordan-Wigner transformation, $\sigma_i^x = 1 - 2c_i^\dagger c_i$ and $\sigma_i^z = -\prod_{j<i} (1 - 2c_j^\dagger c_j)(c_i + c_i^\dagger)$, the TFIC Hamiltonian Eq. (1) becomes

$$H_I = -J \sum_{i=1}^N [(c_i^\dagger c_{i+1} + c_i^\dagger c_{i+1}^\dagger + \text{H.c.}) + g(1 - 2c_i^\dagger c_i)] \quad (\text{A1})$$

in terms of the fermionic operators c_i, c_i^\dagger . After Fourier transformation, $c_j = \frac{1}{\sqrt{N}} \sum_k c_k e^{ikj}$, the Hamiltonian is diagonalized by a Bogoliubov rotation $\gamma_k = u_k c_k - i v_k c_{-k}^\dagger$, where $u_k = \cos(\theta_k/2)$, $v_k = \sin(\theta_k/2)$ with the Bogoliubov angle $\tan(\theta_k) = \frac{\sin k}{g - \cos k}$. After these steps, we arrive at

$$H_I = \sum_k \epsilon_k \left(\gamma_k^\dagger \gamma_k - \frac{1}{2} \right), \quad (\text{A2})$$

with single-particle energy dispersion $\epsilon_k = 2J\sqrt{1 + g^2 - 2g \cos k}$.

The field theory Hamiltonian Eq. (3) can be diagonalized by the plane wave expansion of the Majorana fields which in the paramagnetic phase reads (setting $\hbar = 1$)

$$\psi(x, t) = \sqrt{\frac{mc}{2}} \int \frac{d\theta}{2\pi} e^{-\theta/2} [\alpha a(\theta) e^{ip_\theta x - i\varepsilon_\theta t} + \alpha^* a^\dagger(\theta) e^{-ip_\theta x + i\varepsilon_\theta t}], \quad (\text{A3a})$$

$$\bar{\psi}(x, t) = i \sqrt{\frac{mc}{2}} \int \frac{d\theta}{2\pi} e^{\theta/2} [\alpha a(\theta) e^{ip_\theta x - i\varepsilon_\theta t} - \alpha^* a^\dagger(\theta) e^{-ip_\theta x + i\varepsilon_\theta t}], \quad (\text{A3b})$$

where $\alpha = e^{-i\pi/4}$, and $p_\theta = mc \sinh(\theta)$ and $\varepsilon_\theta = mc^2 \cosh(\theta)$ are the momentum and energy in terms of the rapidity variable θ . The creation/annihilation operators obey the algebra

$$\{a(\theta), a^\dagger(\theta')\} = 2\pi \delta(\theta - \theta') \quad (\text{A4})$$

and diagonalize the Hamiltonian, which becomes

$$\mathcal{H}_I = \int \frac{d\theta}{2\pi} a^\dagger(\theta) a(\theta) mc^2 \cosh \theta. \quad (\text{A5})$$

APPENDIX B: FORM-FACTOR METHOD AND LINKED CLUSTER EXPANSION

Exploiting the local nature of the transverse magnetization in terms of the fermions, the transverse DSF $S^{xx}(\omega, q)$ can be obtained exactly. This is however not true for the longitudinal DSF $S^{zz}(\omega, q)$. Still, in both cases one can give a systematic low-temperature expansion [31,32]. As we are mainly interested in the low-temperature NMR relaxation rates, we first discuss this more general approach, applicable both in the spin chain and in the field theory. We shall use the field theory notations but everything can be translated to the spin chain in a straightforward manner.

Our starting point is the Lehmann spectral representation,

$$\begin{aligned} S^{\alpha\alpha}(\omega, q) &= \sum_l \int_{-\infty}^{\infty} dt e^{i\omega t - iq l} \langle \sigma_{l+1}^\alpha(t) \sigma_l^\alpha(0) \rangle_T \\ &= \frac{1}{\mathcal{Z}} \sum_{n,m} e^{-\beta E_n} (2\pi)^2 \delta(\hbar\omega + E_n - E_m) \\ &\quad \times \delta(q + P_n - P_m) |\langle n | \sigma_l^\alpha(0) | m \rangle|^2. \end{aligned} \quad (\text{B1})$$

Using the multiparticle energy eigenstates¹ $|\theta_1, \dots, \theta_n\rangle$ in the Lehmann representation (B1) leads to

$$S^{\alpha\alpha}(\omega, q) = \frac{1}{\mathcal{Z}} \sum_{r,s=0}^{\infty} C_{r,s}^{\alpha\alpha}(\omega, q), \quad (\text{B2})$$

with $\alpha = x, y, z$ and

$$\begin{aligned} C_{r,s}^{\alpha\alpha}(\omega, q) &= \int \frac{d\theta_1 \dots d\theta_r}{(2\pi)^r r!} \int \frac{d\theta'_1 \dots d\theta'_s}{(2\pi)^s s!} e^{-\beta E_r} \\ &\quad \times (2\pi)^2 \delta(\hbar\omega + E_r - E_s) \delta(q + P_r - P_s) \\ &\quad \times |\langle \theta_1 \dots \theta_r | \sigma^\alpha(0, 0) | \theta'_1 \dots \theta'_s \rangle|^2, \end{aligned} \quad (\text{B3})$$

¹More generally, in interacting field theories the basis of asymptotic scattering states is used.

where the energy and momentum eigenvalues are $E_n = mc^2 \sum_i^n \cosh \theta_i$ and $P_n = mc \sum_i^n \sinh \theta_i$.

This series is a low-temperature expansion in the following sense. The term $C_{r,s}$ (we omit the $\alpha\alpha$ superscript) carries a factor $e^{-\beta E_r} < e^{-r\beta m}$; thus the small expansion parameter is $e^{-\beta m}$. Its dependence on s is less obvious but note that, thanks to the energy conserving Dirac delta, the energies of the two states with r and s particles are related. For a fixed frequency ω and at low temperature one can truncate the double sum in both r and s . The partition function can also be written as $\mathcal{Z} = \sum_{n=0}^{\infty} \mathcal{Z}_n$, where \mathcal{Z}_n has a factor of $e^{-\beta E_n}$.

Now the main problem to be solved is the regularization of the singularities present in the partition function and in the matrix elements (form factors) of the operators in question. In infinite volume all \mathcal{Z}_n are singular due to the fact that they contain a scalar product of two momentum eigenstates. Similarly, $C_{r,s}$ inherits the kinematical poles of the form factors whenever two rapidities in the two sets coincide, i.e., $\theta_i = \theta'_j$ for some i, j . Since the structure factor is a well-defined physical quantity, these singularities must cancel each other. In order to make this manifest we reshuffle the infinite series in a linked cluster expansion [31,32]

$$\chi^{\alpha\alpha}(t, x) = \sum_{r=0, s=0}^{\infty} D_{r,s}^{\alpha\alpha}(t, x), \quad (\text{B4})$$

where the terms

$$D_{0,s} = C_{0,s}, \quad (\text{B5})$$

$$D_{1,s} = C_{1,s} - \mathcal{Z}_1 C_{0,s-1}, \quad (\text{B6})$$

$$D_{2,s} = C_{2,s} - \mathcal{Z}_1 C_{1,s-1} + (\mathcal{Z}_1^2 - \mathcal{Z}_2) C_{0,s-2} + \dots \quad (\text{B7})$$

are supposed to be finite and equivalent relations hold with the indices interchanged. In order to obtain a finite result one needs to regularize the divergencies either in a continuum scheme by adding infinitesimal imaginary parts to the rapidities [31] or by going to a large but finite volume L that satisfies $1 \ll mL \ll e^{m\beta}$, so that the density of thermally excited particles is small [31,32]. The singularities manifest themselves as positive powers of L , while the final result for the $D_{r,s}$ should be $\sim O(L^0)$. All the $D_{1n}(t, x)$ terms are given for any massive relativistic diagonal scattering theory in Ref. [32], while the general expression for $D_{22}(t, x)$ can be found in Ref. [39].

The resulting series still can have diverging terms, signaling that the zero temperature quantity is already singular. This happens around the single particle dispersion relation $\hbar\omega \sim \epsilon(k)$, where the zero temperature DSF is proportional to an on-shell Dirac delta which broadens at nonzero temperatures [31]. In these cases a resummation of infinitely many terms is necessary in order to obtain the finite result. However, if we are interested in the small- ω behavior in the disordered phase of the Ising model, then due to $\hbar\omega \ll mc^2$ we are far from the mass shell. In this case the individual terms are not singular and the truncated series should give a good approximation.

APPENDIX C: DETAILED FIELD THEORY CALCULATION OF LOCAL TRANSVERSE DSF

In this Appendix we provide the details of the calculations leading to Eq. (11). Our starting expression is Eq. (10) from the main text,

$$C_{11}(\omega, q) = \iint \frac{d\theta}{2\pi} \frac{d\theta'}{2\pi} |F_2^\epsilon(\theta|\theta')|^2 e^{-\beta m \cosh \theta} (2\pi)^2 \times \delta[q + m(\sinh \theta - \sinh \theta')] \times \delta[\omega + m(\cosh \theta - \cosh \theta')]. \quad (\text{C1})$$

Both integrals can be performed using the Dirac-delta constraints. The system of equations can be brought to the following form in terms of $x = e^{\theta'}$ and $y = e^{\theta}$:

$$x - y = \tilde{\omega} + \tilde{p} \equiv A, \quad (\text{C2a})$$

$$\frac{1}{x} - \frac{1}{y} = \tilde{\omega} - \tilde{p} \equiv B, \quad (\text{C2b})$$

where $\tilde{\omega} = \omega/m$, $\tilde{q} = q/m$. This leads to the two solutions $\{x_+, y_+\}$ and $\{x_-, y_-\}$

$$x_{\pm} = \frac{AB \pm \sqrt{AB(AB-4)}}{2B}, \quad (\text{C3a})$$

$$y_{\pm} = \frac{-AB \pm \sqrt{AB(AB-4)}}{2B}. \quad (\text{C3b})$$

These roots must be real and positive, so their product must be positive, implying

$$x_+ y_+ = x_- y_- = -x_+ x_- = -\frac{A}{B} = \frac{\tilde{q} + \tilde{w}}{\tilde{q} - \tilde{w}} > 0, \quad (\text{C4})$$

so $\tilde{q}^2 - \tilde{w}^2 > 0$. Their sum is also positive, leading to

$$x_{\pm} + y_{\pm} = \frac{\pm \sqrt{AB(AB-4)}}{B}, \quad (\text{C5})$$

so only the “+” solution is valid for $B = \tilde{\omega} - \tilde{q} > 0$ and only the “-” solution is valid for $B = \tilde{\omega} - \tilde{q} < 0$. Note that, since $AB < 0$, the expression under the square root is always positive so the reality condition is automatically satisfied. Summarizing,

$$e^{\theta_{\pm}} = \frac{q^2 - \omega^2 \pm \sqrt{(q^2 - \omega^2)(q^2 - \omega^2 + 4m^2)}}{2m(\omega - q)}, \quad (\text{C6})$$

$$e^{\theta'_{\pm}} = \frac{-q^2 + \omega^2 \pm \sqrt{(q^2 - \omega^2)(q^2 - \omega^2 + 4m^2)}}{2m(\omega - q)}, \quad (\text{C7})$$

where the “+” roots are valid for $q < -|\omega|$ and the “-” roots are valid for $q > |\omega|$. The Jacobian of the change of variables

$$\{m(\cosh \theta' - \cosh \theta), m(\sinh \theta' - \sinh \theta)\} \rightarrow \{\theta, \theta'\} \quad (\text{C8})$$

is $m^2 \sinh(\theta - \theta')$. Conveniently,

$$\begin{aligned} \cosh(\theta - \theta') &= 1 + (q^2 - \omega^2)/(2m^2), \\ \cosh \theta_{\pm} &= (-\omega \mp q \sqrt{1 + 4m^2/(q^2 - \omega^2)})/(2m). \end{aligned} \quad (\text{C9})$$

Using $|F^{(\varepsilon)}(\theta|\theta')|^2 = m^2[1 + \cosh(\theta - \theta')]/2$ we obtain

$$\begin{aligned} C_{11}(\omega, q) &= e^{-m\beta \cosh \theta_{\pm}} \frac{q^2 - \omega^2 + 4m^2}{2\sqrt{(q^2 - \omega^2)(q^2 - \omega^2 + 4m^2)}} \\ &= \frac{1}{2} e^{\beta\omega/2} \sqrt{1 + \frac{4m^2}{q^2 - \omega^2}} e^{-\frac{\beta}{2}|q| \sqrt{1 + \frac{4m^2}{q^2 - \omega^2}}}, \end{aligned} \quad (\text{C10})$$

$$\begin{aligned} C_{11}(\omega) &\approx \frac{1}{2} e^{\beta\omega/2} \int_{|\omega|}^{\infty} \frac{dq}{\pi} \left(\frac{2m}{q} + \frac{q}{4m} \right) e^{-\frac{\beta m}{2} \left(\frac{q^2}{4m^2} + 2 + \frac{\omega^2}{q^2} \right)} \\ &\approx \frac{1}{2} e^{\beta\omega/2} \int_{\omega}^{p_m} \frac{dq}{\pi} \left(\frac{2m}{q} + \frac{q}{4m} \right) e^{-\frac{\beta m}{2} \left(2 + \frac{\omega^2}{q^2} \right)} + \frac{1}{2} e^{\beta\omega/2} \int_{p_m}^{\infty} \frac{dq}{\pi} \left(\frac{2m}{q} + \frac{q}{4m} \right) e^{-\frac{\beta m}{2} \left(\frac{q^2}{4m^2} + 2 \right)} \\ &= \frac{e^{\beta\omega/2} e^{-m\beta}}{32\pi} \left\{ \frac{2\omega}{m} e^{-\frac{\beta m(m+\omega)}{2m+\omega}} \left(e^{\frac{\beta m}{2}} (2m + \omega) - \omega e^{\frac{\beta m\omega}{4m+2\omega}} \right) + (16m - \beta\omega^2) \left[\Gamma\left(0, \frac{m\beta\omega}{4m+2\omega}\right) - \Gamma\left(0, \frac{m\beta}{2}\right) \right] \right\} \\ &\approx -\frac{m}{\pi} e^{\beta\omega/2} e^{-m\beta} \left[\ln\left(\frac{\beta\omega}{4}\right) - \frac{1}{2m\beta} + \gamma_E \right], \end{aligned} \quad (\text{C12})$$

where the incomplete gamma function $\Gamma(a, z) = \int_z^{\infty} t^{a-1} e^{-t} dt$, Euler's constant $\gamma_E \approx 0.57712$, and $p_m = \sqrt{\omega(2m + \omega)}$ is the extreme point of the exponent.

1. Alternative derivation of the local transverse DSF

Another way to obtain the result in Eq. (11) is to focus on the *local* DSF from the start, defined as

$$S^{\varepsilon}(\omega) = \int dt e^{i\omega t} \langle \varepsilon(0, t) \varepsilon(0, 0) \rangle_T. \quad (\text{C13})$$

This contains a disconnected piece proportional to $\delta(\omega)$. The first nontrivial term in the expansion of the connected part is

$$\begin{aligned} C_{11}(\omega) &= \int \frac{d\theta}{2\pi} \int \frac{d\theta'}{2\pi} |F_2^{\varepsilon}(\theta|\theta')|^2 e^{-\beta m \cosh \theta} 2\pi \delta \\ &\quad \times [\omega + m(\cosh \theta - \cosh \theta')]. \end{aligned} \quad (\text{C14})$$

Let us assume that $\omega > 0$ so the energy conservation condition has two real solutions θ_+ and $\theta_- = -\theta_+$ for all θ , where we denote the positive solution by

$$\theta_+ = \text{arccosh}(\cosh \theta + \omega/m) > 0. \quad (\text{C15})$$

Now $\delta[\omega + m(\cosh \theta - \cosh \theta')] = \frac{1}{m \sinh \theta_+} [\delta(\theta' - \theta_+) + \delta(\theta' + \theta_+)]$, so

$$\begin{aligned} C_{11}(\omega) &= m \int \frac{d\theta}{2\pi} \frac{e^{-\beta m \cosh \theta}}{\sqrt{(\cosh \theta + \omega/m)^2 - 1}} \\ &\quad \times [1 + \cosh \theta (\cosh \theta + \omega/m)], \end{aligned} \quad (\text{C16})$$

where we used the identity $\cosh^2[(\theta - \theta_+)/2] + \cosh^2[(\theta + \theta_+)/2] = 1 + \cosh \theta \cosh \theta_+$. Introducing the shorthand notation $\tilde{\omega} = \omega/m$ and changing the integration variable to $u =$

where we used $\pm q = -|q|$. The local dynamic structure factor is given by

$$C_{11}(\omega) = \int \frac{dq}{2\pi} C_{11}(\omega, q) = 2 \int_{|\omega|}^{\infty} \frac{dq}{2\pi} C_{11}(\omega, q). \quad (\text{C11})$$

Note that, as long as ω is nonzero, the exponential cuts off the diverging prefactor and the integrand remains finite. This is no longer true for $\omega = 0$, which signals a logarithmic singularity. We can extract the leading behavior in the small- ω (and low- T) limit as

$\cosh \theta$,

$$\begin{aligned} C_{11}(\omega) &= \frac{m}{\pi} \int_1^{\infty} du e^{-m\beta u} \\ &\quad \times \frac{u^2 + \tilde{\omega}u + 1}{\sqrt{(u-1)(u+1)(u-1+\tilde{\omega})(u+1+\tilde{\omega})}}. \end{aligned} \quad (\text{C17})$$

The integral is singular for $\omega = 0$. To extract the small- ω behavior, we can approximate the integral by

$$\begin{aligned} C_{11}(\omega) &\approx \frac{m}{\pi} \int_1^{\infty} du e^{-m\beta u} \frac{u^2 + 1}{(u+1)\sqrt{(u-1)(u-1+\tilde{\omega})}} \\ &\approx \frac{m}{\pi} \int_0^{\infty} dv e^{-m\beta(1+v)} \frac{1+v/2}{\sqrt{v(v+\tilde{\omega})}} \\ &= \frac{m}{\pi} e^{-m\beta} \left[e^{\beta\omega/2} K_0\left(\frac{\beta\omega}{2}\right) + \frac{\sqrt{\pi}}{4m\beta} U(1/2, 0, \beta\omega) \right], \end{aligned} \quad (\text{C18})$$

where $K_0(x)$ is the modified Bessel function of the second kind and $U(a, b, z)$ is the confluent hypergeometric function. Expanding the result for small ω we find

$$C_{11}(\omega) \approx \frac{m}{\pi} e^{-m\beta} \left[-\ln\left(\frac{\beta\omega}{4}\right) + \frac{1}{2m\beta} - \gamma_E \right], \quad (\text{C19})$$

which agrees with the result in Eq. (C12).

APPENDIX D: CALCULATIONS OF LOCAL TRANSVERSE DSF IN THE SPIN CHAIN: TRUNCATED FORM FACTOR SERIES METHOD

In this Appendix we present the form factor calculation, analogous to that in Appendix C, in the spin chain. The transverse magnetization on the lattice is given in terms of

the Jordan-Wigner fermions as

$$\sigma_j^x = 1 - 2c_j^\dagger c_j. \quad (\text{D1})$$

The Hamiltonian is quadratic in these fermionic operators and it is diagonalized by going to momentum space and performing the Bogoliubov transformation

$$\begin{aligned} \frac{1}{\sqrt{L}} \sum_{j=1}^L c_j e^{ikj} &= c(k) = \cos(\vartheta_k/2)\alpha(k) \\ &+ i \sin(\vartheta_k/2)\alpha^\dagger(-k), \end{aligned} \quad (\text{D2a})$$

$$\begin{aligned} \frac{1}{\sqrt{L}} \sum_{j=1}^L c_j^\dagger e^{ikj} &= c^\dagger(-k) = i \sin(\vartheta_k/2)\alpha(k) \\ &+ \cos(\vartheta_k/2)\alpha^\dagger(-k), \end{aligned} \quad (\text{D2b})$$

with

$$e^{i\vartheta_k} = \frac{g - e^{ik}}{\sqrt{1 + g^2 - 2g \cos k}} = \frac{2J(g - e^{ik})}{\varepsilon(k)}. \quad (\text{D3})$$

The ground state expectation value of σ_j^x is then easily calculated to be

$$\begin{aligned} \langle \sigma^x \rangle &\equiv \langle 0 | \sigma_j^x | 0 \rangle = 1 - 2 \frac{1}{L} \sum_{n=1}^L \sin^2(\vartheta_k/2) \\ &= \frac{1}{L} \sum_{n=1}^L [1 - 2 \sin^2(\vartheta_k/2)] \\ &= \frac{1}{L} \sum_{n=1}^L \cos(\vartheta_k) \longrightarrow \int_{-\pi}^{\pi} \frac{dk}{2\pi} \cos(\vartheta_k). \end{aligned} \quad (\text{D4})$$

We can also compute the matrix elements

$$\langle 0 | \sigma_j^x | k, k' \rangle \equiv \langle 0 | \sigma_j^x \alpha_k^\dagger \alpha_{k'}^\dagger | 0 \rangle = \frac{2i}{L} e^{-i(k+k')j} \sin\left(\frac{\vartheta_k - \vartheta_{k'}}{2}\right), \quad (\text{D5})$$

$$\begin{aligned} \langle k | \sigma_j^x | k' \rangle &\equiv \langle 0 | \alpha_k \sigma_j^x \alpha_{k'}^\dagger | 0 \rangle \\ &= -\frac{2}{L} e^{i(k-k')j} \cos\left(\frac{\vartheta_k + \vartheta_{k'}}{2}\right) + \delta_{k,k'} \langle \sigma^x \rangle. \end{aligned} \quad (\text{D6})$$

The first contributions to the local DSF in the Lehmann representation are

$$C_{00}(\omega) = 2\pi \delta(\omega) \langle \sigma^x \rangle^2, \quad (\text{D7})$$

$$C_{11}(\omega) = \sum_{n,m} e^{-\beta \varepsilon_n} 2\pi \delta(\omega + \varepsilon_n - \varepsilon_m) \left[\delta(\omega) \langle \sigma^x \rangle^2 \delta_{n,m} + \left(\frac{2}{L}\right)^2 \cos^2\left(\frac{\vartheta_{k_n} - \vartheta_{k_m}}{2}\right) - \delta_{n,m} \frac{4}{L} \cos\left(\frac{\vartheta_{k_n} - \vartheta_{k_m}}{2}\right) \right], \quad (\text{D8})$$

where $\varepsilon_n = \varepsilon(k_n)$ with $k_n = 2\pi n/L$, $n = -L/2 + 1, \dots, L/2$ (Ramond sector). When calculating $D_{11}(\omega)$, the first term in $C_{11}(\omega)$ cancels exactly $\mathcal{Z}_1 C_{00}(\omega)$. The remaining terms containing $\delta_{n,m}$ contribute to the $\omega = 0$ response. Let us focus on the first nontrivial term contributing at finite ω ,

$$\begin{aligned} F(\omega) &\equiv \left(\frac{2}{L}\right)^2 \sum_{n,m} e^{-\beta \varepsilon_n} 2\pi \delta(\omega + \varepsilon_n - \varepsilon_m) \cos^2\left(\frac{\vartheta_{k_n} - \vartheta_{k_m}}{2}\right) \\ &\longrightarrow 4 \int_{-\pi}^{\pi} \frac{dk}{2\pi} \int_{-\pi}^{\pi} \frac{dk'}{2\pi} e^{-\beta \varepsilon(k)} 2\pi \delta(\omega + \varepsilon(k) - \varepsilon(k')) \cos^2\left(\frac{\vartheta(k) - \vartheta(k')}{2}\right). \end{aligned} \quad (\text{D9})$$

The energy Dirac delta can only be satisfied if

$$\varepsilon_{\min} = 2J|1 - g| \leq \varepsilon(k) + \omega \leq 2J(1 + g) = \varepsilon_{\max}, \quad (\text{D10})$$

which implies

$$\cos k_0 \equiv -1 + \frac{1+g}{g} \tilde{\omega} - \frac{\tilde{\omega}^2}{2g} \leq \cos k \leq 1 + \frac{|1-g|}{g} \tilde{\omega} - \frac{\tilde{\omega}^2}{2g}, \quad (\text{D11})$$

where $\tilde{\omega} \equiv \omega/(2J)$. Note that for $\omega < 0$ the first inequality is automatic, while for $0 < \omega < 2\Delta$ the second inequality is automatically satisfied. We focus on the latter case from now on. Then $\cos k'$ is given by

$$\cos k' = \frac{1 + g^2 - [\omega + \varepsilon(k)]^2 / (4J^2)}{2g} = \cos k - \frac{\tilde{\omega}}{g} \sqrt{1 + g^2 - 2g \cos k} - \frac{\tilde{\omega}^2}{2g}, \quad (\text{D12})$$

which has two solutions which we denote by $k'_1 > 0$ and $-k'_1$. Changing variables and performing the integration over k' we obtain

$$F(\omega) = \frac{2}{\pi} \int_{-k_0}^{k_0} dk e^{-\beta \varepsilon(k)} \frac{\varepsilon(k'_1(k))}{4J^2 g \sin(k'_1(k))} \left[\cos^2\left(\frac{\vartheta(k) - \vartheta(k'_1(k))}{2}\right) + \cos^2\left(\frac{\vartheta(k) + \vartheta(k'_1(k))}{2}\right) \right]. \quad (\text{D13})$$

Now we use the identity $\cos^2[(x-y)/2] + \cos^2[(x+y)/2] = 1 + \cos(x)\cos(y)$, the explicit forms of $\varepsilon(k)$ and

$$\cos \vartheta(k) = \frac{g - \cos k}{\sqrt{1 + g^2 - 2g \cos k}}, \quad (\text{D14})$$

together with $\varepsilon(k'_1) = \varepsilon(k) + \omega$ to arrive at

$$F(\omega) = \frac{1}{Jh\pi} \int_{-k_0}^{k_0} dk e^{-\beta\varepsilon(k)} \frac{2\tilde{\varepsilon}(k)[\tilde{\varepsilon}(k) + \tilde{\omega}] - \sin^2 k - \tilde{\omega}/g \cos k[\tilde{\varepsilon}(k) + \tilde{\omega}/2] + \tilde{\omega}^2/2}{\tilde{\varepsilon}(k)\sqrt{1 - [\cos k - \tilde{\omega}/g\tilde{\varepsilon}(k) - \tilde{\omega}^2/(2g)]^2}}, \quad (\text{D15})$$

where $\tilde{\varepsilon}(k) = \varepsilon(k)/(2J)$. We would like to obtain an approximate analytical result in the $\omega \rightarrow 0$ limit. Then we can keep only the $O(\tilde{\omega}^0)$ terms in the numerator. Changing variables to $u = \cos k$,

$$F(\omega) \approx \frac{2}{Jg\pi} \int_{-1+(1+g)/g\tilde{\omega}-\tilde{\omega}^2/(2g)}^1 du e^{-\beta 2J\varepsilon(u)} \frac{2e(u)^2 - (1-u^2)}{\sqrt{1-u^2}e(u)\sqrt{1-[u-\tilde{\omega}e(u)/g-\tilde{\omega}^2/(2g)]^2}} \sim \frac{4}{\pi} \frac{|1-g|}{2Jg} e^{-\beta\Delta} \ln \tilde{\omega} = \frac{1}{\pi} \frac{\Delta}{J^2g} e^{-\beta\Delta} \ln \tilde{\omega}, \quad (\text{D16})$$

with $e(u) = \sqrt{1+g^2-2gu}$. It is not surprising that the same logarithmic divergent behavior appears as in Eq. (E13) and Eq. (11). Comparing to the field theory we have to keep in mind that between ε and σ^x there is a rescaling factor of $-2a = -\hbar c/J$, which leads to a perfect match of the prefactors of $\ln \omega$.

APPENDIX E: TRANSVERSE DSF $S^{xx}(q, \omega)$ IN THE SPIN CHAIN

In this section we discuss the transverse DSF in the spin chain. In this section, we report the calculation of the exact transverse DSF and specify its low temperature and low frequency behavior at the end of the calculation. The

analogous derivation in the scaling limit can be found in Appendix G.

The transverse DSF follows by

$$S^{xx}(\omega, q) = \sum_{l=1}^N \int_{-\infty}^{\infty} dt e^{i\omega t - iqla} [\langle \sigma_l^x(t) \sigma_0^x \rangle_T - \langle \sigma_l^x(t) \rangle_T \langle \sigma_0^x \rangle_T], \quad (\text{E1})$$

where $\hbar\omega$ and $\hbar q$ are transferred energy and momentum, respectively. In the following we set the lattice spacing as $a = 1$ and $\hbar = 1$. Starting from $\sigma_i^x = 1 - 2c_i^\dagger c_i$, going to momentum space, and performing the Bogoliubov rotation, the thermal expectation values can be calculated in a straightforward way using the Hamiltonian Eq. (A2) and Wick's theorem. The resulting expression for $S^{xx}(\omega, q)$ reads

$$\begin{aligned} S^{xx}(\omega, q) &= \frac{4}{N} \sum_k [2\pi\delta(\omega - \epsilon_{k+q/2} + \epsilon_{k-q/2})(u_{k+q/2}^2 u_{k-q/2}^2 - u_{k+q/2} v_{k+q/2} u_{k-q/2} v_{k-q/2})(1 - n_{k+q/2}) n_{k-q/2} \\ &\quad + 2\pi\delta(\omega + \epsilon_{k+q/2} + \epsilon_{k-q/2})(u_{k-q/2}^2 v_{k+q/2}^2 + u_{k+q/2} v_{k+q/2} u_{k-q/2} v_{k-q/2}) n_{k+q/2} n_{k-q/2} \\ &\quad + 2\pi\delta(\omega - \epsilon_{k+q/2} - \epsilon_{k-q/2})(u_{k+q/2}^2 v_{k-q/2}^2 + u_{k+q/2} v_{k+q/2} u_{k-q/2} v_{k-q/2})(1 - n_{k+q/2})(1 - n_{k-q/2}) \\ &\quad + 2\pi\delta(\omega + \epsilon_{k+q/2} - \epsilon_{k-q/2})(v_{k+q/2}^2 v_{k-q/2}^2 - u_{k+q/2} v_{k+q/2} u_{k-q/2} v_{k-q/2}) n_{k+q/2} (1 - n_{k-q/2})] \\ &= \int_{-\pi}^{\pi} dk \{ 2[1 + f(k, q)] \delta(\omega - \epsilon_{k-q/2} + \epsilon_{k+q/2}) (1 - n_{k-q/2}) n_{k+q/2} + [1 - f(k, q)] \\ &\quad \times [\delta(\omega - \epsilon_{k-q/2} - \epsilon_{k+q/2}) (1 - n_{k-q/2}) (1 - n_{k+q/2}) + \delta(\omega + \epsilon_{k-q/2} + \epsilon_{k+q/2}) n_{k-q/2} n_{k+q/2}] \}, \quad (\text{E2}) \end{aligned}$$

with Fermi distribution function $n_k = [e^{\epsilon_k/(k_B T)} + 1]^{-1}$ and

$$f(k, q) = 4J^2 \{ [g - \cos(k - q/2)][g - \cos(k + q/2)] - \sin(k - q/2) \sin(k + q/2) \} / (\epsilon_{k-q/2} \epsilon_{k+q/2}). \quad (\text{E3})$$

Here we have taken advantage of particle and energy conservation during the derivation, for example, $\int_{-\infty}^{\infty} dt e^{i\omega t} \langle e^{iHt} \gamma_{k-q/2}^\dagger \gamma_{k+q/2}^\dagger e^{-iHt} \gamma_{k+q/2} \gamma_{k-q/2} \rangle_T = 2\pi\delta(\omega + \epsilon_{k+q/2} - \epsilon_{k-q/2}) (1 - n_{k-q/2}) n_{k+q/2}$. Focusing on the $\omega > 0$ region, after integration, we obtain

$$S^{xx}(\omega, q) = \sum_{s=\pm} \left[2[1 + f(k_s, q)] \frac{(1 - n_{k_s - q/2}) n_{k_s + q/2}}{|D_{k_s}^-(\omega, q)|} + [1 - f(k_s, q)] \frac{(1 - n_{k_s - q/2})(1 - n_{k_s + q/2})}{|D_{k_s}^+(\omega, q)|} \right], \quad (\text{E4})$$

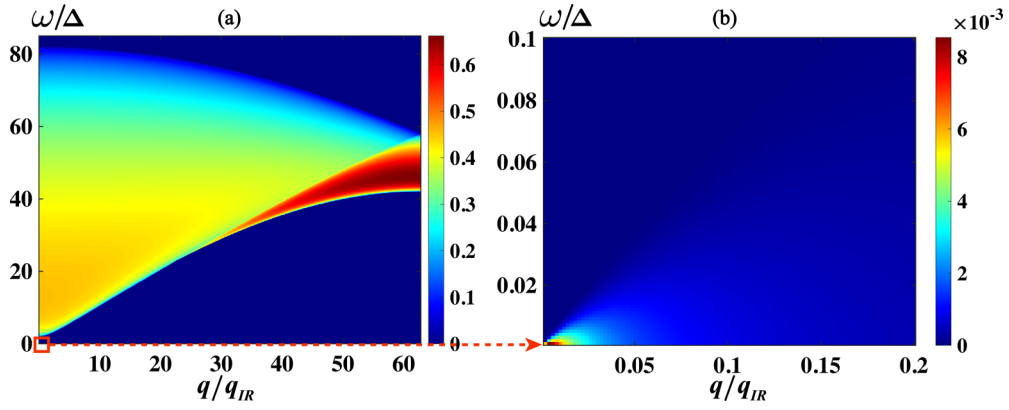


FIG. 3. (a) Transverse DSF $(J/\hbar)S^{xx}(\omega, q)$ for $\omega > 0$ at $\Delta = 0.1J$ and $k_B T = 0.01J$. $q_{IR}/a = \Delta/(\hbar c) = (g-1)/a$ is the infrared wave number scale. The continuum above 2Δ is contributed from the second term of Eq. (E4). (b) The enlarged view of the small rectangular region in (a) exhibits $S^{xx}(\omega, q)$ in the small momentum and low energy region, which comes from the first term in Eq. (E4).

where k_{\pm} are solutions of energy conservation constraint

$$\cos(k_{\pm}) = \frac{\omega^2 \cos(\frac{q}{2})}{16J^2 g \sin^2(\frac{q}{2})} \pm \left(\frac{\omega^2}{16J^2 g \sin^2(\frac{q}{2})} - 1 \right)^{1/2} \left(\frac{\omega^2}{16J^2 g^2 \sin^2(\frac{q}{2})} - 1 \right)^{1/2} \quad (\text{E5})$$

and the Jacobians are

$$|D_{k_s}^{--}(\omega, q)| = \left| 4J^2 g \left(\frac{\sin(k_s + \frac{q}{2})}{\epsilon_{k_s+q/2}} + \frac{\sin(k_s - \frac{q}{2})}{\epsilon_{k_s-q/2}} \right) \right|, \quad s = \pm, \quad (\text{E6})$$

$$|D_{k_s}^{-+}(\omega, q)| = \left| 4J^2 g \left(\frac{\sin(k_s + \frac{q}{2})}{\epsilon_{k_s+q/2}} - \frac{\sin(k_s - \frac{q}{2})}{\epsilon_{k_s-q/2}} \right) \right|, \quad s = \pm. \quad (\text{E7})$$

The transverse DSF, measured in units of \hbar/J , is plotted in Fig. 3 as a function of dimensionless variables using the infrared frequency and wave number scales Δ/\hbar and $\Delta a/(\hbar c)$, respectively. The upper threshold in Fig. 3(a) is given by

$$\omega_{\text{up}}(q) = 2\epsilon_{q/2\pm\pi} = 4J\sqrt{g^2 + 2g \cos(q/2) + 1}, \quad (\text{E8})$$

while the lower thresholds are

$$\omega_{\text{low1}}(q) = 2\epsilon_{q/2} = 4J\sqrt{g^2 - 2g \cos(q/2) + 1}, \quad (\text{E9})$$

$$\omega_{\text{low2}}(q) = \epsilon_0 + \epsilon_q = 2J(\sqrt{g^2 - 2g \cos q + 1} + |g-1|). \quad (\text{E10})$$

In Fig. 3(b), the thresholds are $\omega_{\text{low}'}(q) = \epsilon_{q/2+k}$ and $\omega_{\text{up}'}(q) = \epsilon_{q/2-k}$ with $k = \arccos[\cos(q/2)/g]$.

1. Low temperature behavior of the local transverse DSF

We now focus on the local transverse DSF in the quantum disordered region with gap much larger than the temperature, i.e., $k_B T \ll \Delta$. The leading contribution in Eq. (E4) is of the order $e^{-\Delta/(k_B T)}$ and is given by the first term of Eq. (E4). Then the local transverse DSF follows immediately,

$$\begin{aligned} S^{xx}(\omega) &= \int_{-\pi}^{\pi} \frac{dq}{2\pi} S^{xx}(\omega, q) = \int_{q_c}^{\pi} \frac{dq}{\pi} S^{xx}(\omega, q) \\ &\approx \int_{q_c}^{\pi} \frac{dq}{\pi} \sum_{s=\pm} 2[1 + f(k_s, q)] \frac{(1 - n_{k_s-q/2})n_{k_s+q/2}}{|D_{k_s}^{-+}(\omega, q)|} \end{aligned} \quad (\text{E11})$$

$$\approx \int_{q_c}^{\pi} \frac{dq}{\pi} \left| \frac{\sqrt{1 + g^2 - 2g \cos \frac{q}{2}}}{gJ \sin \frac{q}{2}} \right| e^{-\epsilon_{k_-+q/2}/(k_B T)}, \quad (\text{E12})$$

where $q_c \approx \omega/2J$ is the lower bound obtained from $\omega = \omega_{\text{up}}(q)$ at $\omega \rightarrow 0$ limit. The asymptotic behavior of the integral in the $\omega \ll k_B T \ll \Delta$ regime is determined in Appendix H with the result

$$\begin{aligned} S^{xx}(\omega) &\approx \frac{e^{-\frac{\Delta}{k_B T}}}{\pi} \left\{ -\frac{2\Delta}{J(\Delta + 2J)} \left[\ln\left(\frac{\omega}{4k_B T}\right) + \gamma_E \right] \right. \\ &\quad \left. + \frac{\Delta^2 + 12J^2 + 6\Delta J}{6J^2(\Delta + 2J)^2} k_B T \right\}. \end{aligned} \quad (\text{E13})$$

The asymptotic result Eq. (E13) shows that finite temperature local transverse DSF diverges logarithmically as $\omega \rightarrow 0$. The energy conservation constraints in Eq. (E4) imply only the first term of Eq. (E4) can contribute to such low-energy behavior. Furthermore, the energy conservation leads to a constraint for the phase space. After integration of Eq. (E2), the constraint gives rise to the $1/q$ dependency in the integrand of Eq. (E12) for small q , which is just the case for the lower

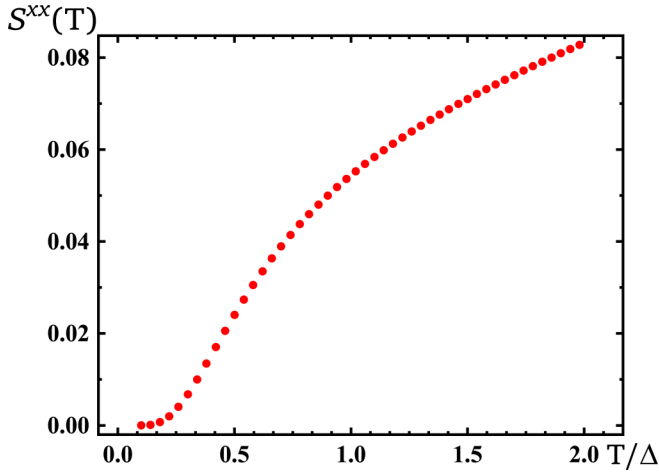


FIG. 4. Local transverse DSF as a function of temperature at fixed $\Delta = 0.1J$ and $\omega = 10^{-4}J$.

bound dependent on the frequency. This finally results in the logarithmic behavior. The temperature dependence shows an exponential decay together with a logarithmic correction in the prefactor. In the scaling limit we obtain

$$S^{xx}(\omega) \approx \frac{\Delta}{\pi J^2} e^{-\frac{\Delta}{k_B T}} \left[-\ln \left(\frac{\omega}{4k_B T} \right) + \frac{k_B T}{2\Delta} - \gamma_E \right]. \quad (\text{E14})$$

Using $J = c/(2a)$ and recalling the rescaling factor $2a$ between the σ^x and the field theory operator ε , we find perfect agreement with the result (11).

In the $k_B T \ll \omega \ll \Delta$ region, we can simply approximate the integral by the steepest descent method and obtain the asymptotic result

$$S^{xx}(\omega) \approx \frac{1}{\pi} e^{-\Delta/(k_B T)} \sqrt{\frac{\pi k_B T}{\omega}} \frac{2\Delta}{J(2J + \Delta)}. \quad (\text{E15})$$

In the high T region it clearly deviates from the exponentially decaying behavior, as shown in Fig. 4.

APPENDIX F: DETAILED FIELD THEORY CALCULATION OF LONGITUDINAL DSF

In this section we turn to the DSF of the order parameter field. This operator is highly nonlocal in terms of the Jordan-Wigner fermions prohibiting an exact calculation based on free fermion techniques. However, one can still use the trun-

cated form factor series approach. This approach has been used in the study of local spin DSF and NMR relaxation rate $1/T_1$ in Refs. [24–26]. The calculations of the form factors of σ^z are far from being trivial, but are known exactly even on the finite spin chain [34]. Here we perform the calculation in the paramagnetic phase in the scaling limit, focusing on the DSF of the continuum spin operator $\sigma(x)$ in Eq. (6). In the disordered phase, the $\sigma(x)$ operator creates and destroys particles, so its only nonzero matrix elements are between states with particle numbers of different parity, that is, the total number of particles in the two states must be odd. The vacuum form factors are given by [33]

$$F_n^\sigma(\theta_1, \dots, \theta_n) = \langle 0 | \sigma | \theta_1, \dots, \theta_n \rangle = \bar{\sigma} \sum_{i < j} \tanh \left(\frac{\theta_i - \theta_j}{2} \right), \quad (\text{F1})$$

with $\bar{\sigma} = \bar{s} m^{1/8}$, where \bar{s} is defined in Eq. (6) and we work with $\hbar = c = 1$ for the following field theory calculation. All other matrix elements can be obtained by the crossing relation. For example,

$$\langle \theta | \sigma | \theta_1, \dots, \theta_n \rangle = \langle 0 | \sigma | \theta + i\pi, \theta_2, \dots, \theta_n \rangle \quad (\text{F2})$$

whenever $\theta \neq \theta_j$, which will be the case in our calculations.

Thus the first contributions to the DSF come from $D_{01}(t, x) = C_{01}(t, x)$ and $D_{10}(t, x) = C_{10}(t, x)$, yielding

$$S_{01}^{zz}(\omega, q) = \bar{\sigma}^2 \int \frac{d\theta}{2\pi} (2\pi)^2 \delta(\omega - m \cosh \theta) \delta(q - m \sinh \theta) \quad (\text{F3})$$

and $S_{10}(\omega, q) = e^{\beta\omega} S_{01}(-\omega, -q)$. Due to the energy conserving Dirac delta, both S_{10} and S_{01} are zero for $\omega < m$. It is clear that all $D_{0,s}$ and $D_{r,0}$ will also give zero contribution, which reflects the fact that the zero temperature result is identically zero.

Energy conservation at small frequencies also leads to a great simplification in higher orders, similar to the case of the transverse magnetization in the previous sections. Because of the Dirac delta and $\omega \approx 0$ the two states in each matrix element must have almost equal energies, so $S_{r,s}(\omega \approx 0, q) \sim e^{-\max(r,s)\beta m}$. This implies that the classification in terms of orders of $e^{-\beta m}$ is simplified, because in every order there is only a finite number of terms. For instance, in the second order one has $S_{12} + S_{21}$, in the third order $S_{23} + S_{32}$, in the fourth $S_{14} + S_{41} + S_{34} + S_{43}$, and so on.

Thus up to the second order one needs only two terms, S_{12} and S_{21} . We use the expression for D_{12} given in Ref. [31] that can be shown to be equivalent to the more general formula in Ref. [32],

$$\begin{aligned} D_{12} = & \frac{1}{2} \int \frac{d\theta}{2\pi} \int_{C_+} \int_{C_-} \frac{d\theta_1}{2\pi} \frac{d\theta_2}{2\pi} |F_3^\sigma(\theta + i\pi, \theta_1, \theta_2)|^2 e^{-\beta m \cosh \theta} \\ & \times 2\pi \delta[q + m(\sinh \theta - \sinh \theta_1 - \sinh \theta_2)] 2\pi \delta[\omega + m(\cosh \theta - \cosh \theta_1 - \cosh \theta_2)] \\ & - \bar{\sigma}^2 \int \frac{d\theta}{2\pi} e^{-m\beta \cosh \theta} 2\pi \delta(\omega - m \cosh \theta) 2\pi \delta(q - m \sinh \theta), \end{aligned} \quad (\text{F4})$$

where the contours C_\pm are running above and below the real axis, respectively, to avoid the kinematical poles of the form factors. But $\theta = \theta_i$ ($i = 1, 2$) is impossible for $\omega < m$, so the integrals avoid the poles even for real rapidities and there is no need to

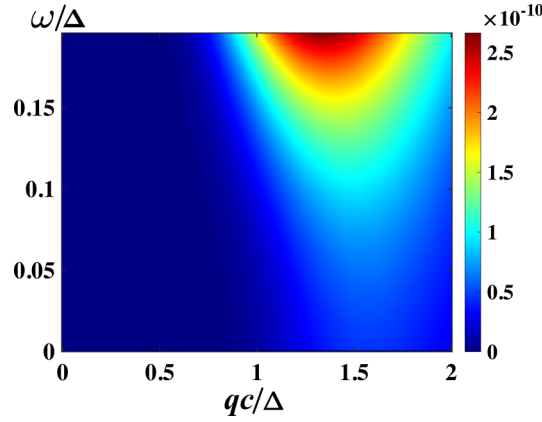


FIG. 5. Leading $O[e^{-2\Delta/(k_B T)}]$ contribution to the longitudinal dynamic structure factor in the scaling limit, $\Delta^2/(\hbar^2 c \bar{\sigma}^2) S^{zz}$, at $k_B T = \Delta/10$.

shift the contours off the real axis. The last term is proportional to D_{01} so it does not contribute for $\omega < m$ and we are left with

$$S_{12}^{zz}(\omega, q) = \frac{1}{2} \int \frac{d\theta}{2\pi} \int \frac{d\theta_1}{2\pi} \int \frac{d\theta_2}{2\pi} |F_3^{\sigma_c}(\theta + i\pi, \theta_1, \theta_2)|^2 e^{-\beta m \cosh \theta} \times 2\pi \delta[q - m(\sinh \theta_1 + \sinh \theta_2 - \sinh \theta)] 2\pi \delta[\omega - m(\cosh \theta_1 + \cosh \theta_2 - \cosh \theta)]. \quad (\text{F5})$$

Exploiting the Dirac deltas we perform the integrals over rapidities $\theta_{1,2}$. The Jacobian of the transformation is $m^2 \sinh(\theta_1 - \theta_2)$. The set of two constraint equations coming from the Dirac deltas has two solutions, $\{\theta_1, \theta_2\} = \{\theta_+, \theta_-\}$ and $\{\theta_1, \theta_2\} = \{\theta_-, \theta_+\}$, where

$$\theta_{\pm} = \ln \left[\frac{1}{2} \left(\omega_{\theta} + q_{\theta} \pm \frac{\sqrt{(\omega_{\theta}^2 - p_{\theta}^2)(\omega_{\theta}^2 - q_{\theta}^2 - 4)}}{\omega_{\theta} - q_{\theta}} \right) \right], \quad (\text{F6})$$

with $q_{\theta} \equiv q/m + \sinh \theta$, $\omega_{\theta} \equiv \omega/m + \cosh \theta$. The rapidities $\theta_{1,2}$ must be real, which gives restrictions on the remaining rapidity θ . The reality condition of $\theta_{1,2}$ is equivalent to the

condition that $e^{\theta_1} + e^{\theta_2}$ and $e^{\theta_1} e^{\theta_2}$ must be positive, which gives $\omega_{\theta} + q_{\theta} > 0$, $\omega_{\theta} - q_{\theta} > 0$. Moreover, the combination under the square root must also be positive, $\omega_{\theta}^2 - q_{\theta}^2 > 4$. One of the first two conditions, e.g., $\omega_{\theta} - q_{\theta} > 0$, can then be dropped, which leaves us with two conditions. The solution of $\omega_{\theta}^2 - q_{\theta}^2 > 4$ for $|\omega| < m$ is the following:

$$\theta < \theta^{(-)}, \quad |\omega| < q, \quad (\text{F7a})$$

$$\theta > \theta^{(+)}, \quad -|\omega| > q, \quad (\text{F7b})$$

$$\theta < \theta^{(-)} \text{ or } \theta > \theta^{(+)}, \quad -\omega < q < \omega, \quad (\text{F7c})$$

and for $\omega < q < -\omega$ ($\omega < 0$) there is no solution. Here

$$\theta^{(\pm)} = \ln \left[\frac{q^2 - \omega^2 + 3m^2 \pm \sqrt{(q^2 - \omega^2 + m^2)(q^2 - \omega^2 + 9m^2)}}{2m(\omega - q)} \right]. \quad (\text{F8})$$

It turns out that the other condition, $\omega_{\theta} + q_{\theta} > 0$, is automatically satisfied, so Eqs. (F7) give the integration domain of θ in the various cases depending on ω and q . Thus we find

$$S_{12}^{zz}(\omega, q) = 2 \int_D \frac{d\theta}{2\pi} \frac{e^{-\beta m \cosh \theta} |F_3^{\sigma}[\theta + i\pi, \theta_+(\theta), \theta_-(\theta)]|^2}{m^2 \sqrt{(\omega_{\theta}^2 - q_{\theta}^2)(\omega_{\theta}^2 - q_{\theta}^2 - 4)}}, \quad (\text{F9})$$

where D denotes the domain given in Eqs. (F7) and we used $\sinh(\theta_1 - \theta_2) = \sqrt{(\omega_{\theta}^2 - q_{\theta}^2)(\omega_{\theta}^2 - q_{\theta}^2 - 4)}/2$. It is easy to see that $S_{21}(\omega, q) = e^{\beta\omega} S_{12}(-\omega, q)$, so we have the total leading $O(e^{-2m\beta})$ contribution to the DSF. The result $S_{12}^{zz}(\omega, q) + S_{21}^{zz}(\omega, q)$ is plotted in Fig. 5.

The corresponding local DSF reads

$$\begin{aligned} S_{12}^{zz}(\omega) &= \frac{1}{2} \int \frac{d\theta}{2\pi} \int \frac{d\theta_1}{2\pi} \int \frac{d\theta_2}{2\pi} e^{-\beta m \cosh \theta} |F_3^{\sigma}(\theta + i\pi, \theta_1, \theta_2)|^2 2\pi \delta[\omega - m(\cosh \theta_1 + \cosh \theta_2 - \cosh \theta)] \\ &= \frac{1}{2} \int \frac{d\theta_1}{2\pi} \int \frac{d\theta_2}{2\pi} \frac{e^{\beta\omega - \beta m(\cosh \theta_1 + \cosh \theta_2)}}{\sqrt{(m \cosh \theta_1 + m \cosh \theta_2 - \omega)^2 - m^2}} [|F_3^{\sigma}(\theta_0 + i\pi, \theta_1, \theta_2)|^2 + \{\theta_0 \rightarrow -\theta_0\}], \end{aligned} \quad (\text{F10})$$

where $\theta_0 = \text{arccosh}(\cosh \theta_1 + \cosh \theta_2 - \omega/m) > 0$. At the second order we also need $S_{21}(\omega) = e^{\beta\omega} S_{12}(-\omega)$.

We can give approximate expressions for S_{12} and S_{21} . For $\beta m \gg 1$ only a small region around the origin in the (θ_1, θ_2) plane contributes, so we can expand both the exponent and the rest of the integrand to second order using the explicit form factors. Performing the resulting Gaussian integrals, and expanding the result in ω/m (with $T/m \ll 1$) we obtain the result in Eq. (12):

$$\begin{aligned} S^{zz}(\omega) &\approx S_{12}^{zz}(\omega) + S_{21}^{zz}(\omega) \approx \frac{\bar{\sigma}^2}{m} \frac{3\sqrt{3}}{4\pi} \left(\frac{1}{m\beta}\right)^2 e^{-2m\beta} \left[e^{\beta\omega} \left(1 + 2\frac{\omega}{m}\right) + \left(1 - 2\frac{\omega}{m}\right) \right] \\ &\approx \frac{\bar{\sigma}^2}{m} \frac{6\sqrt{3}}{4\pi} \left(\frac{T}{m}\right)^2 e^{-2\frac{m}{T}} = \frac{\bar{\sigma}^2}{\Delta} \frac{3\sqrt{3}}{2\pi} \left(\frac{k_B T}{\Delta}\right)^2 e^{-2\frac{\Delta}{k_B T}}. \end{aligned} \quad (\text{F11})$$

The correction terms to this result are the third order $S_{23} + S_{32}$. However, these terms contain singularities for which the regularization has not yet been worked out explicitly. But as we discussed, unlike the case of the broadening of the Dirac delta in the zero temperature DSF, there is no physical reason why unexpected singularities should show up in the higher terms; thus we stop at the second order.

APPENDIX G: EXACT TRANSVERSE DSF IN THE FIELD THEORY

Using the plane wave expansion Eq. (A3) and $\varepsilon = i\bar{\psi}\psi$, the connected correlation function

$$C^\varepsilon(x, t) = \langle \varepsilon(x, t) \varepsilon(0, 0) \rangle_T - \langle \varepsilon(x, t) \rangle \langle \varepsilon(0, 0) \rangle_T \quad (\text{G1})$$

can be written as a fourfold rapidity integral of a linear combination of thermal expectation values of products of four creation/annihilation operators. Using the thermal Wick's theorem,

$$\langle a^\pm(\theta) b_1 b_2 b_3 \rangle_T = f^\pm(\theta) (\langle a, b_1 \rangle \langle b_2 b_3 \rangle_T - \langle a, b_2 \rangle \langle b_1 b_3 \rangle_T + \langle a, b_3 \rangle \langle b_1 b_2 \rangle_T), \quad (\text{G2})$$

where $a^+ = a^\dagger$, $a^- = a$ and $f^+(\theta) = (1 + e^{\beta\varepsilon_\theta})^{-1} = f(\theta)$, $f^-(\theta) = (1 + e^{-\beta\varepsilon_\theta})^{-1} = 1 - f(\theta)$, one arrives at

$$\begin{aligned} C^\varepsilon(x, t) &= \frac{m^2}{4} \int \frac{d\theta}{2\pi} \int \frac{d\theta'}{2\pi} [f(\theta)f(\theta')(e^{\theta-\theta'} - 1)e^{i(p+p')\cdot x} + [1 - f(\theta)][1 - f(\theta')](e^{\theta-\theta'} - 1)e^{-i(p+p')\cdot x} \\ &\quad + f(\theta)[1 - f(\theta')](e^{\theta-\theta'} + 1)e^{i(p-p')\cdot x} + [1 - f(\theta)]f(\theta')(e^{\theta-\theta'} + 1)e^{-i(p-p')\cdot x}], \end{aligned} \quad (\text{G3})$$

where we used the Lorentz product notation, $p \cdot x = \varepsilon t - px$. At zero temperature $T = 0$, $f(\theta) = 0$ and we obtain the closed form result

$$\begin{aligned} C(x, t) &= \frac{m^2}{4} \int \frac{d\theta}{2\pi} \int \frac{d\theta'}{2\pi} (e^{\theta-\theta'} - 1) e^{-i(p+p')\cdot x} = \frac{m^2}{4} \int \frac{d\theta}{2\pi} e^\theta e^{-ip\cdot x} \int \frac{d\theta'}{2\pi} e^{-\theta'} e^{-ip'\cdot x} - \frac{m^2}{4} \left(\int \frac{d\theta}{2\pi} e^{-ip\cdot x} \right)^2 \\ &= m^2 K_0^2(m\sqrt{x^2 - t^2}) - m^2 K_1^2(m\sqrt{x^2 - t^2}). \end{aligned} \quad (\text{G4})$$

Note that since $(p + p') \cdot x = (\varepsilon_\theta + \varepsilon_{\theta'})t - (p_\theta + p_{\theta'})x$ and $\varepsilon_\theta + \varepsilon_{\theta'} \geq 2\Delta$, after Fourier transformation $S(\omega, q)|_{T=0} = 0$ for $0 < \omega < 2\Delta$. At low temperature, the leading order can be obtained by approximating $f(\theta) \approx e^{-\beta\varepsilon(\theta)}$ and keeping only first powers of $f(\theta)$:

$$\begin{aligned} C(x, t) &\approx \frac{m^2}{4} \int \frac{d\theta}{2\pi} \int \frac{d\theta'}{2\pi} [[1 - f(\theta) - f(\theta')](e^{\theta-\theta'} - 1) e^{-i(p+p')\cdot x} \\ &\quad + f(\theta)(e^{\theta-\theta'} + 1) e^{i(p-p')\cdot x} + f(\theta')(e^{\theta-\theta'} + 1) e^{-i(p-p')\cdot x}]. \end{aligned} \quad (\text{G5})$$

Taking the Fourier transform, for frequencies $|\omega| < m$ only the second line gives nonzero contribution and it recovers the expression Eq. (10).

APPENDIX H: ASYMPTOTIC ANALYSIS OF THE INTEGRAL EQ. (E12)

In this Appendix we report the details of the asymptotic analysis of Eq. (E12) for the local transverse DSF. We approximate the integral by dividing it into two integrals at the extreme point $q_m = \sqrt{\frac{\omega\Delta}{J(\Delta+2J)}}$ of the exponent:

$$\begin{aligned} S^{xx}(\omega) &\approx \int_{q_c}^{\pi} \frac{dq}{\pi} \left| \frac{\sqrt{1 + g^2 - 2g \cos \frac{q}{2}}}{gJ \sin \frac{q}{2}} \right| e^{-\varepsilon_{k_- + q/2}/(k_B T)} \\ &\approx \int_{q_c}^{\pi} \frac{dq}{\pi} \frac{\frac{\Delta}{Jq} + q\left(\frac{J}{2\Delta} + \frac{\Delta}{24J} + \frac{1}{2}\right)}{\frac{\Delta}{2} + J} \exp \left\{ -\frac{1}{k_B T} \left[\Delta + \frac{\Delta}{4J(\Delta + 2J)} \frac{\omega^2}{q^2} + q^2 J \left(\frac{J}{2\Delta} + \frac{1}{4} \right) \right] \right\} \\ &\approx \int_{q_c}^{q_m} \frac{dq}{\pi} \frac{\frac{\Delta}{Jq} + q\left(\frac{J}{2\Delta} + \frac{\Delta}{24J} + \frac{1}{2}\right)}{\frac{\Delta}{2} + J} \exp \left\{ -\frac{1}{k_B T} \left[\Delta + \frac{\Delta}{4J(\Delta + 2J)} \frac{\omega^2}{q^2} \right] \right\} \end{aligned}$$

$$\begin{aligned}
 & + \int_{q_m}^{\pi} \frac{dq}{\pi} \frac{\frac{\Delta}{Jq} + q \left(\frac{J}{2\Delta} + \frac{\Delta}{24J} + \frac{1}{2} \right)}{\frac{\Delta}{2} + J} \exp \left\{ -\frac{1}{k_B T} \left[\Delta + q^2 J \left(\frac{J}{2\Delta} + \frac{1}{4} \right) \right] \right\} \\
 & = \frac{1}{\pi} \frac{e^{-\frac{1}{k_B T} \left(\Delta + \frac{\Delta J}{\Delta + 2J} + \frac{\omega}{4} \right)}}{96 \Delta J^3 (\Delta + 2J)^2} \left\{ \omega (\Delta^2 + 12J^2 + 6\Delta J) \left(4\Delta J e^{\frac{\Delta J}{k_B T (\Delta + 2J)}} - \omega e^{\frac{\omega}{4k_B T}} (\Delta + 2J) \right) \right. \\
 & \quad - \Delta J e^{\frac{\omega}{4k_B T} + \frac{\Delta J}{k_B T (\Delta + 2J)}} \left(96 \Delta J (\Delta + 2J) - \frac{\omega^2}{k_B T} (\Delta^2 + 12J^2 + 6\Delta J) \right) \left[\Gamma \left(0, \frac{J\Delta}{k_B T (2J + \Delta)} \right) - \Gamma \left(0, \frac{\omega}{4T} \right) \right] \\
 & \quad + \frac{1}{\pi} \frac{e^{-\frac{1}{k_B T} \left(\Delta + \frac{\pi^2 J (\Delta + 2J)}{4\Delta} + \frac{\omega}{4} \right)}}{6J^2 (\Delta + 2J)^2} \left\{ 6\Delta J (\Delta + 2J) e^{\frac{1}{k_B T} \left(\frac{\pi^2 J (\Delta + 2J)}{4\Delta} + \frac{\omega}{4} \right)} \left[\text{Ei} \left(-\frac{J\pi^2 (2J + \Delta)}{4\Delta T} \right) - \text{Ei} \left(-\frac{\omega}{4k_B T} \right) \right] \right. \\
 & \quad \left. + k_B T (\Delta^2 + 12J^2 + 6\Delta J) \left(e^{\frac{\pi^2 J (\Delta + 2J)}{4\Delta k_B T}} - e^{\frac{\omega}{4k_B T}} \right) \right. \\
 & \quad \approx \frac{1}{\pi} e^{-\frac{\Delta}{k_B T}} \left\{ -\frac{2\Delta}{J(\Delta + 2J)} \left[\ln \left(\frac{\omega}{4k_B T} \right) + \gamma_E \right] + \frac{\Delta^2 + 12J^2 + 6\Delta J}{6J^2 (\Delta + 2J)^2} k_B T \right\} + \dots \\
 & \quad \approx \frac{\Delta}{\pi J^2} e^{-\frac{\Delta}{k_B T}} \left[-\ln \left(\frac{\omega}{4k_B T} \right) + \frac{k_B T}{2\Delta} - \gamma_E \right] + \dots, \tag{H1}
 \end{aligned}$$

with the incomplete gamma function $\Gamma(a, z) = \int_z^{\infty} dt t^{a-1} e^{-t}$ and the exponential integral function $\text{Ei}(z) = -\int_{-z}^{\infty} \frac{e^{-t}}{t} dt$. The last line is obtained by taking scaling limit $\Delta/J \rightarrow 0$, namely, $g \rightarrow g_c$, and the result agrees with field theory result Eq. (11).

APPENDIX I: NMR RELAXATION RATES FOR LARGE NUCLEAR SPIN

For nuclear spin $I > 1/2$, the nuclear quadrupole interaction splits the nuclear spin energy levels and Eq. (14a) needs to be evaluated based on Bloch-Wangsness-Redfield theory using the density matrix for nuclear spin $\rho_{\alpha\alpha'}$ [40–43],

$$\frac{d\rho_{\alpha\alpha'}}{dt} = \sum_{\beta\beta'} R_{\alpha\alpha',\beta\beta'} \rho_{\beta\beta'}, \tag{I1}$$

where α, α', β , and β' specify the nuclear spin energy levels and $R_{\alpha\alpha',\beta\beta'}$ is the element of the relaxation matrix R . In this approach, $1/T_2 = R_{\alpha\alpha-1,\alpha\alpha-1}$ for the $I_z = \alpha$ to $\alpha - 1$ transition of a given nuclear spin I [40] and

$$\frac{1}{T_2} = A \frac{1}{T_1} + \gamma_n^2 \overline{h^2} \tau_0, \tag{I2}$$

where the prefactor A is a constant that depends on I , γ_n is the nuclear gyromagnetic ratio of the observed nuclear spin, $\overline{h^2}$ represents the averaged fluctuating hyperfine magnetic field along the direction of the external magnetic field (i.e., x axis in the present case of TFIC), τ_0 is the correlation time ($\omega_n \tau_0 \ll 1$), and the second term represents $1/T_2'$ within the framework of Redfield's theory. In the case of nuclear spin $I = 1/2$ with no nuclear quadrupole splitting, $A = 1/2$ [40]. For the $I_z = +1/2$ to $-1/2$ central transition of $I = 3/2$, earlier work showed that $A = 7/2$ [41,42]. In the case of $I = 9/2$ at ^{93}Nb sites in the TFIC candidate material CoNb_2O_6 , the calculations of A are straightforward but rather tedious, and we obtained $A = 49/2$.

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