Excitation Spectrum Gap and Spin-Wave Velocity of XXZ Heisenberg Chains:
Global Renormalization-Group Calculation

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The anisotropic XXZ spin-$\frac{1}{2}$ Heisenberg chain is studied using renormalization-group theory. The specific heats and nearest-neighbor spin-spin correlations are calculated throughout the entire temperature and anisotropy ranges in both ferromagnetic and antiferromagnetic regions, obtaining a global description and quantitative results. We obtain, for all anisotropies, the antiferromagnetic spin-liquid spin-wave velocity and the Isinglike ferromagnetic excitation spectrum gap, exhibiting the spin-wave to spinon crossover. A number of characteristics of purely quantum nature are found: The in-plane interaction $s_i^x s_j^x + s_i^y s_j^y$ induces an antiferromagnetic correlation in the out-of-plane $s_i^z$ component, at higher temperatures in the antiferromagnetic XXZ chain, dominantly at low temperatures in the ferromagnetic XXZ chain, and, in-between, at all temperatures in the XY chain. We find that the converse effect also occurs in the antiferromagnetic XXZ chain: an antiferromagnetic $s_i^x s_j^x$ interaction induces a correlation in the $s_i^{xy}$ component. As another purely quantum effect, (i) in the antiferromagnet, the value of the specific heat peak is insensitive to anisotropy and the temperature of the specific heat peak decreases from the isotropic (Heisenberg) with introduction of either type (Ising or XY) anisotropy; (ii) in complete contrast, in the ferromagnet, the value and temperature of the specific heat peak increase with either type of anisotropy.

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I. INTRODUCTION

The quantum Heisenberg chain, including the possibility of spin-space anisotropy, is the simplest nontrivial quantum spin system and has thus been widely studied since the very beginning of the spin concept in quantum mechanics $[1, 2, 3]$. Interest in this model continued since the very beginning of the spin concept in quantum mechanics $[1, 2, 3]$. The XXZ Heisenberg chain is studied using renormalization-group theory. The $s_i^x s_j^x$ and dimer-cluster $[20]$ expansions, quantum decimation $[21]$, decoupled Green’s functions $[22]$, quantum transfer matrix $[23, 24]$, high-temperature series expansion $[25]$, and numerical evaluation of multiple integrals $[26]$. The XXZ Heisenberg chain retains high current interest as a theoretical model $[27, 28]$ with direct experimental relevance $[29]$. In the present paper, a position-space renormalization-group method introduced by Suzuki and Takano $[30, 31]$ for $d = 2$ dimensions and already applied to a number of $d > 1$ systems $[30, 31, 32, 33, 34, 35, 36]$ is used to compute the spin-spin correlations and the specific heat of the $d = 1$ anisotropic quantum XXZ Heisenberg model, easily resulting in a global description and detailed quantitative information for the entire temperature and anisotropy ranges including the ferromagnetic and antiferromagnetic, the spin-liquid and Isinglike regions. We obtain, for all anisotropies, the antiferromagnetic spin-liquid spin-wave velocity and the Isinglike ferromagnetic excitation spectrum gap, exhibiting the spin-wave to spinon crossover. A number of other characteristics of purely quantum nature are found: The in-plane interaction $s_i^x s_j^x + s_i^y s_j^y$ induces an antiferromagnetic correlation in the out-of-plane $s_i^z$ component, at higher temperatures in the antiferromagnetic XXZ chain, dominantly at low temperatures in the ferromagnetic XXZ chain, and, in-between, at all temperatures in the XY chain. We find that the converse effect also occurs in the antiferromagnetic XXZ chain: an antiferromagnetic $s_i^x s_j^x$ interaction induces a correlation in the $s_i^{xy}$ component. As another purely quantum effect, (i) in the antiferromagnet, the value of the specific heat peak is insensitive to anisotropy and the temperature of the specific heat peak decreases from the isotropic (Heisenberg) with introduction of either type (Ising or XY) anisotropy; (ii) in complete contrast, in the ferromagnet, the value and temperature of the specific heat peak increase with either type of anisotropy. This purely quantum effect is a precursor to different phase transition temperatures in three dimensions $[32, 33, 34, 35]$. Our calculational method is relatively simple, readily yields global results, and is overall quantitatively successful.
II. THE ANISOTROPIC QUANTUM HEISENBERG MODEL AND THE RENORMALIZATION-GROUP METHOD

A. The Anisotropic Quantum Heisenberg Model

The spin-$\frac{1}{2}$ anisotropic Heisenberg model (XXZ model) is defined by the dimensionless Hamiltonian

$$-\beta H = \sum_{\langle ij \rangle} \left\{ [J_{xy} (s_i^x s_j^y + s_i^y s_j^x)] + J_z s_i^z s_j^z \right\} + G,$$  \hspace{1cm} (1)

where $\beta = 1/k_B T$ and $\langle ij \rangle$ denotes summation over nearest-neighbor pairs of sites. Here the $s_i^\alpha$ are the quantum mechanical Pauli spin operators at site $i$. The additive constant $G$ is generated by the renormalization-group transformation and is used in the calculation of thermodynamic functions. The anisotropy coefficient is $R = J_z/J_{xy}$. The model reduces to the isotropic Heisenberg model (XXX model) for $|R| = 1$, to the XY model for $R = 0$, and to the Ising model for $|R| \to \infty$.

B. Renormalization-Group Recursion Relations

The Hamiltonian in Eq. (1) can be rewritten as

$$-\beta H = \sum_{i} \{-\beta H(i, i + 1)\}.$$  \hspace{1cm} (2)

where $\beta H(i, i + 1)$ is a Hamiltonian involving sites $i$ and $i + 1$ only. The renormalization-group procedure, which eliminates half of the degrees of freedom and keeps the partition function unchanged, is done approximately [30, 31]:

$$\text{Tr}_{\text{old}} e^{-\beta H} = \text{Tr}_{\text{old}} e^{\sum_{i} \{-\beta H(i, i + 1)\}} = \text{Tr}_{\text{old}} e^{e_{\text{odd}} \sum_{i} \{-\beta H(i-1, i) - \beta H(i, i + 1)\}} \simeq \prod_{i} \text{Tr}_{i} e^{-\beta H(i-1, i) - \beta H(i, i + 1)} \simeq \prod_{i} e^{-\beta H'(i-1, i+1)} \simeq e^{\sum_{i} \{-\beta H'(i-1, i+1)\}} = e^{-\beta H'}.$$ \hspace{1cm} (3)

Here and throughout this paper, the primes are used for the renormalized system. Thus, at each successive length scale, we ignore the non-commutativity of the operators beyond three consecutive sites, in the two steps indicated by $\simeq$ in the above equation. Since the approximations are applied in opposite directions, one can expect some mutual compensation. Earlier studies [30, 31, 32, 33, 34] have been successful in obtaining finite-temperature behavior on a variety of quantum systems.

The transformation above is summarized by

$$e^{-\beta H'(i,k)} = \text{Tr}_{j} e^{\{-\beta H(i,j) - \beta H(j,k)\}},$$  \hspace{1cm} (4)

where $i, j, k$ are three successive sites. The operator $-\beta H'(i,k)$ acts on two-site states, while the operator $-\beta H(i,j) - \beta H(j,k)$ acts on three-site states, so that we can rewrite Eq. (4) in the matrix form,

$$\langle u_i v_j | e^{-\beta H'(i,k)} | u_i v_k \rangle = \sum_{w_j} \langle u_i w_j v_k | e^{-\beta H(i,j) - \beta H(j,k)} | u_i w_j v_k \rangle, \hspace{1cm} (5)$$

where state variables $u, v, w, \bar{u}, \bar{v}$ can take spin-up or spin-down values at each site. The unrenormalized $8 \times 8$ matrix on the right-hand side is contracted into the renormalized $4 \times 4$ matrix on the left-hand side of Eq. (5). We use two-site basis states vectors $\{|\phi_p\rangle\}$ and three-site basis states vectors $\{|\psi_q\rangle\}$ to diagonalize the matrices in Eq. (5). The states $\{|\phi_p\rangle\}$, given in Table I, are eigenstates of parity, total spin magnitude, and total spin z-component. These $\{|\phi_p\rangle\}$ diagonalize the renormalized matrix, with eigenvalues

$$\lambda_1 = \frac{1}{4} J_z' + G', \hspace{1cm} \lambda_2 = \frac{1}{2} J_{xy}' - \frac{1}{4} J_z' + G', \hspace{1cm} \lambda_4 = -\frac{1}{4} J_{xy}' - \frac{1}{4} J_z' + G'. \hspace{1cm} (6)$$

The states $\{|\psi_q\rangle\}$, given in Table II, are eigenstates of parity and total spin z-component. The $\{|\psi_q\rangle\}$ diagonalize the unrenormalized matrix, with eigenvalues

$$\lambda_1 = \frac{1}{2} J_z + 2G, \hspace{1cm} \lambda_2 = \frac{1}{4} \left( J_z + \sqrt{8 J_{xy}^2 + J_z^2} \right) + 2G, \hspace{1cm} \lambda_3 = \frac{1}{4} \left( J_z - \sqrt{8 J_{xy}^2 + J_z^2} \right) + 2G. \hspace{1cm} (7)$$

With these eigenstates, Eq. (5) is rewritten as

$$\gamma_p \equiv \langle \phi_p | e^{-\beta H'(i,k)} | \phi_p \rangle = \sum_{u_i,v_j,v_k} \langle \phi_p | u_i v_j v_k | \psi_q \rangle \langle u_i w_j v_k | \psi_q \rangle \langle \psi_q | \bar{u}_i \bar{w}_j \bar{v}_k \rangle \langle \bar{u}_i \bar{v}_j \bar{v}_k | \phi_p \rangle. \hspace{1cm} (8)$$

\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
$p$ & $m_s$ \\
\hline
+1 & $|\phi_1 \rangle = |\pm \rangle$ \\
0 & $|\phi_2 \rangle = \frac{1}{\sqrt{2}} (|\downarrow \rangle + |\uparrow \rangle)$ \\
-1 & $|\phi_3 \rangle = \frac{1}{\sqrt{2}} (|\downarrow \rangle - |\uparrow \rangle)$ \\
\hline
\end{tabular}
\caption{The two-site basis eigenstates that appear in Eq. (5). These are the well-known singlet and triplet states. The state $|\phi_3 \rangle$ is obtained by spin reversal from $|\phi_1 \rangle$, with the same eigenvalue.}
\end{table}
The renormalization-group transformation, Eq.(1), which yield the recursion relations

\[
\hat{M} = \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix},
\]

which yield the recursion relations

\[
J'_{xy} = \ln \left( \frac{\gamma_2}{\gamma_4} \right), \quad J'_{z} = \ln \left( \frac{\gamma_2^2}{\gamma_2 \gamma_4} \right), \quad G' = \frac{1}{4} \ln \left( \frac{\gamma_1^2}{\gamma_2 \gamma_4} \right).
\]

As expected, \( J'_{xy} \) and \( J'_{z} \) are independent of the additive constant \( G \) and the derivative \( \partial_G G' = b^d = 2 \), where \( b = 2 \) is the rescaling factor and \( d = 1 \) is the dimensionality of the lattice.

For \( J_{xy} = J_z \), the recursion relations reduce to the spin-\( \frac{1}{2} \) isotropic Heisenberg (XXX) model recursion relations, while for \( J_{xy} = 0 \) they reduce to spin-\( \frac{1}{2} \) Ising model recursion relations. The \( J_{xy} = 0 \) subspace (XY model) is not (and need not be) closed under these recursion relations \[30, 31\]: The renormalization-group transformation induces a positive \( J_x \) value, but the spin-space easy-plane aspect is maintained.

In addition, there exists a mirror symmetry along the \( J_z \)-axis, so that \( J'_{xy} (-J_{xy}, J_z) = J'_{xy} (J_{xy}, J_z) \) and \( J'_{z} (-J_{xy}, J_z) = J'_{z} (J_{xy}, J_z) \). The thermodynamics of the system remains unchanged under flipping the interactions of the \( x \) and \( y \) spin components, since the renormalization-group trajectories do not change. In fact, this is part of a more general symmetry of the XYZ model, where flipping the signs of any two interactions leaves the spectrum unchanged \[8\]. Therefore, with no loss of generality, we take \( J_{xy} > 0 \). Independent of the sign of \( J_{xy} \), \( J_z > 0 \) gives the ferromagnetic model and \( J_z < 0 \) gives the antiferromagnetic model.

\[\begin{array}{c|c}
p & m_j \\ \hline
1/2 & \psi_3 = \nu \{ | \uparrow \downarrow \downarrow \rangle + | \uparrow \downarrow \uparrow \rangle + | \uparrow \uparrow \downarrow \rangle \} \\
1/2 & \psi_4 = \nu \{ | \downarrow \uparrow \downarrow \rangle + | \downarrow \downarrow \uparrow \rangle - | \uparrow \downarrow \uparrow \rangle \} \\
3/2 & \psi_1 = | \uparrow \uparrow \uparrow \rangle \\
3/2 & \psi_2 = \mu \{ | \uparrow \uparrow \downarrow \rangle + | \uparrow \downarrow \uparrow \rangle + | \downarrow \uparrow \uparrow \rangle \} \\
\end{array}\]

TABLE II: The three-site basis eigenstates that appear in Eq.(8) with coefficients \( \sigma = (-J_z + \sqrt{8J_{xy}^2 + J_z^2})/2J_{xy} \), \( \tau = (J_x + \sqrt{8J_{xy}^2 + J_z^2})/2J_{xy} \) and normalization factors \( \mu, \nu \). The states \( \psi_{3-4} \) are obtained by spin reversal from \( \psi_{1-2} \), with the same respective eigenvalues.

Thus, there are three independent \( \gamma_p \) that determine the renormalized Hamiltonian and, therefore, three renormalized interactions in the Hamiltonian closed under renormalization-group transformation, Eq.(1). These \( \gamma_p \) are

\[
\gamma_1 = e^{\frac{1}{2} J'_{xy} + G'} = e^{2G - \frac{1}{4} J_x} \left[ e^{\frac{1}{4} J_z} + \cosh \left( \frac{1}{4} \sqrt{8J_{xy}^2 + J_z^2} \right) \right],
\]

\[
\gamma_2 = e^{\frac{1}{4} J'_{xy} - \frac{1}{2} J_z + G'} = 2 e^{2G - \frac{1}{4} J_x} \left[ \cosh \left( \frac{1}{4} \sqrt{8J_{xy}^2 + J_z^2} \right) + \frac{J_z \sinh \left( \frac{1}{4} \sqrt{8J_{xy}^2 + J_z^2} \right)}{\sqrt{8J_{xy}^2 + J_z^2}} \right],
\]

\[
\gamma_4 = e^{-\frac{1}{2} J'_{xy} - \frac{1}{2} J_z + G'} = 2 e^{2G},
\]
\( \hat{M}^{(0)} = b^{-n} \hat{M}^{(n)} \hat{T}^{(n)} \hat{T}^{(n-1)} \ldots \hat{T}^{(1)}, \)  

where the upper indices indicate the number of iteration (transformation), with \( \hat{M}^{(n)} \sim \hat{M}^n. \)

This method is applied on our model Hamiltonian. The sink of the system is at infinite temperature \( J_{xy} = J_x = 0 \) for all initial conditions \( \langle J_x, J_y \rangle. \)

Response functions are calculated by differentiation of densities. For example, the internal energy is \( U = -2 \langle \hat{s}_x \hat{s}_y \rangle - R \langle \hat{s}_z \hat{s}_y \rangle \), employing \( T = 1/J_{xy} \), and \( U = -2 \langle \hat{s}_x \hat{s}_y \rangle / R - \langle \hat{s}_z \hat{s}_y \rangle \), employing \( T = 1/|J_z| \). The specific heat \( C = \partial T U \) follows from the chain rule,

\[
C = J_{xy}^2 \frac{\partial \left( 2 \langle \hat{s}_x \hat{s}_y \rangle + R \langle \hat{s}_z \hat{s}_y \rangle \right)}{\partial J_{xy}}, \quad \text{for} \ T = 1/J_{xy},
\]

\[
C = J_z^2 \frac{\partial \left( 2 \langle \hat{s}_x \hat{s}_y \rangle / R + \langle \hat{s}_z \hat{s}_y \rangle \right)}{\partial |J_z|}, \quad \text{for} \ T = 1/|J_z|.
\]

III. CORRELATIONS SCANNED WITH RESPECT TO ANISOTROPY

The ground-state and excitation properties of the XXZ model offer a variety of behaviors: the antiferromagnetic model with \( R < -1 \) is Isinglike and the ground state has Néel long-range order along the \( z \) spin component with a gap in the excitation spectrum. For \( -1 \leq R \leq 1 \), the system is a "spin liquid," with a gapless spectrum and power-law decay of correlations at zero temperature. The ferromagnetic model with \( R > 1 \) is also Isinglike, the ground state is ferromagnetic along the \( z \) spin component, with an excitation gap.

Our calculated \( \langle \hat{s}_z \hat{s}_y \rangle \) and \( \langle \hat{s}_x \hat{s}_y \rangle \equiv \langle \hat{s}_x \hat{s}_y \rangle = \langle \hat{s}_y \hat{s}_y \rangle \) nearest-neighbor spin-spin correlations for the whole range of the anisotropy coefficient \( R \) are shown in Fig.1 for various temperatures. The \( xy \) correlation is always non-negative. Recall that we use \( J_{xy} > 0 \) with no loss of generality. In the Isinglike antiferromagnetic \( (R < -1) \) region, the \( z \) correlation is expectedly antiferromagnetic. As the \( \langle \hat{s}_z \hat{s}_y \rangle \) correlation saturates for large \( |R| \), the transverse \( \langle \hat{s}_x \hat{s}_y \rangle \) correlation is somewhat depleted. In the Isinglike ferromagnetic \( (R > 1) \) region, the \( \langle \hat{s}_z \hat{s}_y \rangle \) correlation is ferromagnetic, saturates quickly as the \( \langle \hat{s}_x \hat{s}_y \rangle \) correlation quickly goes to zero.

In the spin-liquid \( (|R| < 1) \) region, the \( \langle \hat{s}_z \hat{s}_y \rangle \) correlation monotonically passes through zero in the ferromagnetic side, while the \( \langle \hat{s}_x \hat{s}_y \rangle \) correlation is maximal. The remarkable quantum behavior of \( \langle \hat{s}_z \hat{s}_y \rangle \) around \( R = 0 \) is discussed in Sec.V below. It is seen in the figure that these cangovers are increasingly sharp as temperature is decreased and, at zero temperature, become discontinuous at \( R = 1 \). As seen in Fig.1(b), at zero temperature, our calculated \( \langle \hat{s}_z \hat{s}_y \rangle \) and \( \langle \hat{s}_x \hat{s}_y \rangle \) correlations show very good agreement with the known exact points \[4, 40, 42, 43, 44\]. Also, our results for \( R > 1 \) fully overlap the exact results of \( \langle \hat{s}_z \hat{s}_y \rangle = 0.25 \) and \( \langle \hat{s}_x \hat{s}_y \rangle = 0 \) \[40\]. We also note that zero-temperature is the limit in which our approximation is at its worst.
versely, an increase in \(|s^x_i s^y_j|\) (upper panels) and \(|s^z_i s^z_j|\) (lower panels) for the antiferromagnetic XXZ chain, as a function of temperature, for anisotropy coefficients \(R = 0, -0.25, -0.50, -0.75, -1, -2, -4, -8, -\infty\) spanning the spin-liquid (left panels) and Isinglike (right panels) regions. This remarkable quantum phenomenon is expected on the basis of spin-wave calculations for the antiferromagnetic XXZ model [45, 46]. This linear form of \(C(T)\) reflects the linear energy-momentum dispersion of the low-lying excitations, the magnons. The low-temperature magnon dispersion relation is \(\hbar \omega = c k^n\), where \(c\) is the spin-wave velocity and \(n = 1\) for the antiferromagnetic XXZ model in \(d = 1\) [40]. The internal energy, given by \(U = (1/2\pi) \int d\omega \omega (\cosh (\omega/\beta T) - 1)\), is dominated by the magnons at low temperatures, yielding \(U \sim T^2\) and \(C \sim T\) for \(n = 1\) in the dispersion relation. From this relation, our calculated spin-wave velocity \(c\) as a function of anisotropy \(R\) is given in Fig. 4 and compares well with the also shown exact result [41]. A simultaneous fit to the dispersion relation exponent \(n\), expected to be \(1\), yields \(1.00 \pm 0.02\). However, for the Isinglike \(-R > 1\), the unexpected linearity instead of an exponential form
FIG. 4: Calculated specific heats $C$ of the antiferromagnetic XXZ chain, as a function of temperature for anisotropy coefficients $R = 0, -0.25, -0.50, -0.75, -1, -2, -4, -8, -\infty$ spanning the spin-liquid (upper panel) and Isinglike (lower panel) regions.

caused by a gap in the excitation spectrum, points to the approximate nature of our renormalization-group calculation. The correct exponential form is obtained in the large $-R$ limit, where the renormalization-group calculation becomes exact.

Rojas et al. [25] have obtained the high-temperature expansion of the free energy of the XXZ chain to order $\beta^3$, where $\beta$ is the inverse temperature. The specific heat from this expansion is

$$ C = \frac{2 + R^2}{16} J_{xy} - \frac{3R}{32} J_{xy}^3 + \frac{6 - 8R^2 - R^4}{256} J_{xy}^4. \quad (17) $$

This high-temperature specific heat result is also compared with our results, in Fig. 5, and very good agreement is seen. In fact, when in the high-temperature region of $0 < \beta < 0.1$, we fit our numerical results for $C(\beta)$ to the fourth degree polynomial $C = \Sigma_{i=0}^4 A_i \beta^i$, and we do find (1) the vanishing $A_0 < 10^{-5}$ and $A_1 < 10^{-7}$ for all $R$ and (2) the comparison in Fig. 5 between our results for $A_2$ and $A_3$ and those of Eq. (17) from Ref. [25], thus obtaining excellent agreement for all regions of the model.

V. FERROMAGNETIC XXZ CHAIN

For the ferromagnetic (i.e., $R > 0$) systems in Fig. 1, the $\langle s_i^z s_j^z \rangle$ expectation value becomes rapidly negative at lower temperatures for $R < 1$, even though for $R \geq 0$ all couplings in the Hamiltonian are ferromagnetic. This is actually a real physical effect, not a numerical anomaly. In fact, we know the spin-spin correlations for the ground state of the one-dimensional XY model (the $R = 0$ case of our Hamiltonian), and we can compare our low-temperature results with these exact values. The ground-state properties of the spin-$\frac{1}{2}$ XY model are studied by making a Jordan-Wigner trans-
formation, yielding a theory of non-interacting spinless fermions. Analysis of this theory yields the exact zero-temperature nearest-neighbor spin-spin correlations [4] shown in Table III. Our renormalization-group results in the zero-temperature limit, also shown in this table, compare quite well with the exact results, as with the other exact points in Fig.1(b), although in the worst region for our approximation. Finally, by continuity, it is reasonable that for a range of \( R \) positive but less than one, the \( z \) component correlation function is as we find, intriguingly but correctly negative at low temperatures. Thus, the interaction \( s_i^x s_j^z + s_i^y s_j^y \) (irrespective of its sign, due to the symmetry mentioned at the end of Sec.IIB) induces an antiferromagnetic correlation in the \( s_i^z \) component, competing with the \( s_i^z s_j^z \) interaction when the latter is ferromagnetic.

For finite temperatures, our calculated nearest-neighbor spin-spin correlations are shown in Figs.9, 10, for different values of \( R \). These results are compared with Green’s function calculations [22] in Fig.11. As expected from the discussion at the beginning of this section, in the spin-liquid region, the correlation \( \langle s_i^z s_j^z \rangle \) is negative at low temperatures. Thus, a competition occurs in the...
FIG. 11: Comparison of our ferromagnetic $R = 1, \frac{5}{3}$ results with Green’s function calculations \[22\].

FIG. 12: Calculated specific heats $C$ of the ferromagnetic XXZ chain, as a function of temperature for anisotropy coefficients $R = 0, 0.25, 0.50, 0.75, 1, 2, 4, 8, \infty$ spanning the spin-liquid (upper panel) and Isinglike (lower panel) regions.

FIG. 13: Comparison of our ferromagnetic specific heat results (thick lines) with the high-temperature $J \to 0$ behaviors (thin lines) obtained from series expansion \[25\], for anisotropy coefficients $R = 0.25, 0.50, 0.75, 1, 2, \infty$ spanning the spin-liquid and Isinglike regions.

TABLE III: Zero-temperature nearest-neighbor correlations of the spin-$\frac{1}{2}$ XY chain.

correlation $\langle s^z x_j \rangle$ is zero. Our calculated $T_0(R)$ curve is shown in Fig.10 and has very good agreement with the exact result $T_0 = (\sqrt{3} \sin \gamma/4\gamma) \tan[\pi(\pi - \gamma)/2\gamma]$ where $\gamma \equiv \cos^{-1}(-R) \[22\].

The calculated ferromagnetic specific heats are shown in Fig.12 for various anisotropy coefficients and compared, in Figs.13 and 14, with finite-lattice expansion \[6\], quantum decimation \[21\], decoupled Green’s functions \[22\], transfer matrix \[23, 24\], high-temperature series expansion \[25\] results and, for the $R = 0$ case, namely the XY model, with the exact result \[5\] $C = (1/4\pi T) \int_0^\infty (\cos \omega / \cosh (\cos \omega))^2 d\omega$. In sharp contrast to the antiferromagnetic case in Sec.IV, the peak $C(T)$ temperature is highest for the most anisotropic cases (XY or Ising) and decreases with anisotropy decreasing from either direction (towards Heisenberg). In the same contrast, the peak value of $C(T)$ is dependent on anisotropy, decreasing, eventually to a flat curve, as anisotropy is decreased. This contrast between the ferromagnetic and antiferromagnetic systems is a purely quantum phenomenon. Specifically, the marked contrast between the specific heats of the isotropic antiferromagnetic and ferromagnetic systems, seen in the full curves of Figs.4 and 12 respectively, translates into the different critical temperatures of the respective three-dimensional systems \[32, 33, 37, 38\]. Classical ferromagnetic and anti-
ferromagnetic systems are, on the other hand, identically mapped onto each other.

The low-temperature specific heats are discussed in detail and compared to other results in Sec.VI.

VI. LOW-TEMPERATURE SPECIFIC HEATS

Properties of the low-temperature specific heat of the ferromagnetic XXZ chain have been derived from the thermodynamic Bethe-ansatz equations [40]. For anisotropy coefficient $|R| \leq 1$, the model is gapless [11, 12] and, except at $R = 1$, the specific heat is linear in $T = J_{xy}$ in the zero-temperature limit, $C/T = 2\gamma/(3\sin\gamma)$ where again $\gamma \equiv \cos^{-1}(-R)$. Note that this result contradicts the spin-wave theory prediction of $C \sim T^{1/2}$ for the ferromagnetic chain ($n = 2$ for the ferromagnetic magnon dispersion relation of the kind given above in Sec.IV). The spin-wave result is valid only for $R = 1$, the isotropic Heisenberg case. From the expression given above, we see that $C/T$ diverges as $R \to 1^-$, and at exactly $R = 1$ it has been shown that $C \sim T^{1/2}$ [40].

In the Isinglike region $R > 1$, the system exhibits a gap in its excitation spectrum and the specific heat behaves as $C \sim T^{-a} \exp(-\Delta/T)$, with $\Delta$ being the excitation spectrum gap [11, 12, 40]. There exist two gaps for the energy, called the spinon gap and the spin-wave gap, given by $\Delta_{\text{spinon}} = \frac{1}{2}\sqrt{1-R^{-2}}$ and $\Delta_{\text{spinwave}} = 1-R^{-1}$. These are the minimal energies of elementary excitations [10, 40]. A crossover between them occurs at $R = \frac{5}{3}$: below this value, the spinon gap is lower, while above this value the spin-wave gap is lower. We have double-fitted our calculated specific heats with respect to the gap $\Delta$ and the leading exponent $a$, for the entire range of anisotropy $R$ between $0 < R^{-1} < 1$ (Fig.16). Our calculated gap $\Delta$ behaves linearly in $R^{-1}$ for $R^{-1}$ close to 1, and crosses over to $1/2$ at $R^{-1} = 0$, as expected. We also obtain the exponent $a = 1.99 \pm 0.02$ in the Ising
FIG. 17: Calculated specific heat coefficient $C/T$ as a function of temperature for anisotropy coefficient $R = -5$ (thin grey), $R = -2$ (thick grey), -1 (dotted), -0.5 (dash-dotted), 0.5 (dashed), and 2 (thin black).

limit $R^{-1} \leq 0.2$ and $a = 1.52 \pm 0.10$ in the Heisenberg limit $R^{-1} \geq 0.9$. These exponent values are respectively expected to be 2 and 1.5 \[9, 10\].

We now turn to the discussion of our specific heat results for the entire ferromagnetic and antiferromagnetic ranges. Our calculated $C/T$ curves are plotted as a function of anisotropy and temperature in Figs. 16 and 17 respectively. We discuss each region of the anisotropy $R$ separately:

(i) $R > 1$: The specific heat coefficient $C/T$ vanishes in the $T \to 0$ limit and has the expected exponential form as discussed above in this section. The spin-wave to spinon excitation gap crossover is obtained.

(ii) $R \approx 1$: The double-peak structure of $C/T$ in Fig. 16 is centered at $R = 1$. As temperature goes to zero, the peaks narrow and diverge.

(iii) $-1 \leq R < 1$: The specific heat coefficient is $C/T = 2\gamma/(3\sin\gamma)$ in this region \[11, 40\], and our calculated specific heat is indeed linear at low temperatures. The $C/T$ curves for $R = -1, -0.5, 0.5$ in Fig. 17 all extrapolate to nonzero limits at $T = 0$. The spin-wave dispersion relation exponent and velocity, for the antiferromagnetic system, is correctly obtained for the isotropic case and for all anisotropies, as seen in Fig. 7. Fig. 18 directly compares $C/T = 2\gamma/(3\sin\gamma)$ with our results: The curves have the same basic form, gradually rising from $R = -1$, with a sharp divergence as $R$ nears 1. At $R = 1^+$, we expect $C/T = 0$. Our $T = 10^{-10}$ curve diverges at $R = 1$ and indeed returns to zero at $R = 1.0000001$.

(iv) $R < -1$: We expect a vanishing $C/T$, which we do find as seen in Fig. 16 and in the insets of Fig. 17. The exponential behavior of the specific heat is clearly seen in the Ising limit.

VII. CONCLUSION

A detailed global renormalization-group solution of the XXZ Heisenberg chain, for all temperatures and anisotropies, for both ferromagnetic and antiferromagnetic couplings, has been obtained. In the spin-liquid region, the linear low-temperature specific heat and, for the antiferromagnetic chain, the spin-wave dispersion relation exponent $n$ and velocity $c$ have been obtained. In the Isinglike region, the spin-wave to spinon crossover of the excitation spectrum gap of the ferromagnetic chain has been obtained from the exponential specific heat, as well as the correct leading algebraic behaviors in the Heisenberg and Ising limits. Purely quantum mechanical effects have been seen: We find that the $xy$ correlations and the antiferromagnetic $z$ correlations mu-

FIG. 18: Calculated specific heat coefficient $C/T$ as a function of anisotropy coefficient $R$ in the spin-liquid region, $-1 \leq R \leq 1$, at constant temperature $T = 10^{-10}$. Our renormalization-group result (grey curve) is compared to the zero-temperature Bethe-Ansatz result (black curve). Inset: our calculation (grey curve) at constant $T = 10^{-2}$ is again compared to the zero-temperature Bethe-Ansatz result (black curve).
ally reinforce each other, for different ranges of temperatures and anisotropies, in ferromagnetic, antiferromagnetic, and XY systems. The behaviors, with respect to anisotropy, of the specific heat peak values and locations are opposite in the ferromagnetic and antiferromagnetic systems. The sharp contrast found in the specific heats of the isotropic ferromagnetic and antiferromagnetic systems is a harbinger of the different critical temperatures in the respective three-dimensional systems. When compared with existing calculations in the various regions of the global model, good quantitative agreement is seen. Even at zero temperature, where our approximation is at its worst, good quantitative agreement is seen with exact data points for the correlation functions (Fig. 11b), which we extend to all values of the anisotropy. Finally, the relative ease with which the Suzuki-Takano decimation procedure is globally and quantitatively implemented should be noted.

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