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 Ising-like 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 $s_i^x s_j^y$ interaction induces a correlation in the $s_i^y$ 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 $XY$) of anisotropy; and (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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PACS number(s): 67.10.Fj, 75.10.Pq, 64.60.Cn, 05.10.Cc
we ignore the noncommutativity of the operators beyond renormalized system. Thus at each successive length scale
\[ \beta \mathcal{H} = \sum_{(i)} \{ J_{ij}(s_i^x s_j^x + s_i^y s_j^y) + J_{ij} s_i^z s_j^z + G \}, \]
where \( \beta = 1/k_B T \) and \( \langle ij \rangle \) denotes summation over nearest-neighbor pairs of sites. Here the \( s_i^a \) 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 \( R = J_x/J_{xy} \). 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
\[ - \beta \mathcal{H} = \sum_i \{ - \beta \mathcal{H}(i,i+1) \}, \]
where \( \beta \mathcal{H}(i,i+1) \) 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 as
\[ \text{Tr}_{\text{odd}} e^{-\beta \mathcal{H}} = \text{Tr}_{\text{odd}} e^{\sum_i \{- \beta \mathcal{H}(i,i+1) \}} \]
\[ = \text{Tr}_{\text{odd}} e^{\sum_{i=1}^N \{- \beta \mathcal{H}(i,i+1) \}} \]
\[ = \prod_i \text{Tr}_i e^{-\beta \mathcal{H}(i,i+1)} \]
\[ = e^{\sum_{i=1}^N \{- \beta \mathcal{H}(i,i+1) \}} = e^{-\beta \mathcal{H}^\prime}. \]

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

The transformation above is summarized by
\[ e^{-\beta \mathcal{H}^\prime(i,i+1)} = \text{Tr}_i e^{-\beta \mathcal{H}(i,i+1)} \],
where \( i,j,k \) are three successive sites. The operator \(-\beta \mathcal{H}^\prime(i,i+1)\) acts on two-site states, while the operator \(-\beta \mathcal{H}(i,j) - \beta \mathcal{H}(j,k)\) acts on three-site states, so that we can rewrite Eq. (4) in the matrix form
\[ \langle u | e^{-\beta \mathcal{H}^\prime(i,i+1)} | \bar{u} \rangle = \sum_{w_j} \langle u | w_j | e^{-\beta \mathcal{H}(i,i+1)} | w_j | \bar{u} \rangle, \]
where state variables \( u, v, w, \bar{u} \) and \( \bar{v} \) 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 \( \{| \phi \rangle \} \) and three-site basis states vectors \( \{| \psi \rangle \} \) to diagonalize the matrices in Eq. (5). The states \( \{| \phi \rangle \} \), given in Table I, are eigenstates of parity, total spin magnitude, and total spin \( z \) component. These \( \{| \phi \rangle \} \) diagonalize the renormalized matrix, with eigenvalues
\[ \lambda_1 = \frac{1}{4} J_z + G', \quad \lambda_2 = \frac{1}{2} J_{xy} - \frac{1}{4} J_x + G', \]
\[ \lambda_3 = -\frac{1}{2} J_{xy} - \frac{1}{4} J_x + G'. \]

With these eigenstates, Eq. (5) is rewritten as
\[ \gamma_p = \sum_{u,v,w} \langle \phi | u | v | w | \phi \rangle \]
\[ = \sum_{u,v,w} \langle \phi | u | v | w | \phi \rangle \]
\[ \times \langle \psi | e^{-\beta \mathcal{H}(i,j) - \beta \mathcal{H}(i,k)} | \psi \rangle | \psi | \bar{u} | \bar{v} | \phi \rangle. \]
Thus there are three independent \( \gamma_p \) that determine the renormalized Hamiltonian and, therefore, three renormalized in-

### TABLE I. The two-site basis eigenstates that appear in Eq. (8).
These are the well-known singlet and triplet states. The state \( \{| \phi \rangle \} \) is obtained by spin reversal from \( \{| \psi \rangle \} \), with the same respective eigenvalues.

<table>
<thead>
<tr>
<th>( p )</th>
<th>( s )</th>
<th>( m_s )</th>
<th>Two-site basis eigenstates</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>1</td>
<td>1</td>
<td>(</td>
</tr>
<tr>
<td>+</td>
<td>1</td>
<td>1</td>
<td>(</td>
</tr>
<tr>
<td>−</td>
<td>0</td>
<td>0</td>
<td>(</td>
</tr>
</tbody>
</table>

### TABLE II. The three-site basis eigenstates that appear in Eq. (8).

<table>
<thead>
<tr>
<th>( p )</th>
<th>( m_s )</th>
<th>Three-site basis eigenstates</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>3/2</td>
<td>(</td>
</tr>
</tbody>
</table>
interactions in the Hamiltonian closed under renormalization-group transformation, Eq. (1). These $\gamma_p$ are
\[
  \gamma_1 = e^{(1/4)J_x^* + G'}, \\
  \gamma_2 = e^{(1/2)J_{xy}^* + (1/4)J_z^* + G'}, \\
  \gamma_3 = e^{(1/4)J_x^* + G'}, \\
  \gamma_4 = e^{(1/2)J_{xy}^* + (1/4)J_z^* + G'} = 2e^{2G},
\]
which yield the recursion relations
\[
  J_{xy}^* = \ln \left( \frac{\gamma_2}{\gamma_3} \right), \quad J_z^* = \ln \left( \frac{\gamma_4}{\gamma_2 \gamma_3} \right), \quad G' = \frac{1}{4} \ln (\gamma_1^2 \gamma_2 \gamma_4).
\]

As expected, $J_{xy}^*$ and $J_z^*$ are independent of the additive constant $G$ and the derivative $\partial G = b = 2$, 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 the spin-$\frac{1}{2}$ Ising model recursion relations. The $J_z = 0$ subspace (XY model) is not (and need not be) closed under these recursion relations. The renormalization-group transformation induces a positive $J_z$ 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. 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.

C. Calculation of densities and response functions by the recursion-matrix method

Just as the interaction constants of two consecutive points along the renormalization-group trajectory are related by the recursion relations, the densities are connected by a recursion matrix $\tilde{T}$, which is composed of derivatives of the recursion relations. For our Hamiltonian, the recursion matrix and density vector $M$ are
\[
  \tilde{T} = \begin{pmatrix}
  \frac{\partial G'}{\partial G} & \frac{\partial G'}{\partial J_{xy}} & \frac{\partial G'}{\partial J_z} \\
  0 & \frac{\partial J_{xy}'}{\partial J_{xy}} & \frac{\partial J_{xy}'}{\partial J_z} \\
  0 & \frac{\partial J_z'}{\partial J_{xy}} & \frac{\partial J_z'}{\partial J_z}
\end{pmatrix}, \\
  \tilde{M} = \begin{pmatrix}
  1 & 2(\langle s^y x^y \rangle) & \langle s^z x^z \rangle
\end{pmatrix}.
\]

These are densities $M_{\alpha}$ associated with each interaction $K_{\alpha}$,
\[
  M_{\alpha} = \frac{1}{N_{\alpha}} \frac{\partial \ln Z}{\partial K_{\alpha}},
\]

where $N_{\alpha}$ is the number of $\alpha$–type interactions and $Z$ is the partition function for the system, which can be expressed both via the unrenormalized interaction constants $Z(K)$ or via the renormalized interaction constants $Z(\tilde{K})$. By using these two equivalent forms, one can formulate the density recursion relation
\[
  M_{\alpha} = b^{-d} \sum_{\beta} M_{\beta}^* T_{\beta \alpha}, \quad T_{\beta \alpha} = \frac{N_{\beta} \partial K_{\beta}}{N_{\alpha} \partial K_{\alpha}},
\]

Since the interaction constants, under renormalization-group transformation, stay the same at fixed points such as critical fixed points or sinks, the above Eq. (13) takes the form of a solvable eigenvalue equation,
\[
  b^{d} \tilde{M}^* = \tilde{M}^* \cdot \tilde{T},
\]

at fixed points, where $\tilde{M} = \tilde{M}^* = \tilde{M}^*$. The fixed point densities are the components of the left eigenvector of the recursion matrix with eigenvalue $b^{d}$. At ordinary points, Eq. (13) is iterated until a sink point is reached under successive renormalization-group transformations. In algebraic form, this means
\[
  \tilde{M}^{(0)} = b^{-d} \tilde{M}^{(n)} \tilde{T}^{(n-1)} \cdots \tilde{T}^{(1)},
\]

where the upper indices indicate the number of iteration (transformation), with $\tilde{M}^{(0)} = \tilde{M}^*$. This method is applied on our model Hamiltonian. The sink of the system is at infinite temperature $J_{xy}^* = J_z^* = 0$ for all initial conditions $(J_{xy}, J_z)$.

Response functions are calculated by differentiation of densities. For example, the internal energy is $U = -2(\langle s^y x^y \rangle) - R(\langle s^z x^z \rangle)$, employing $T = 1/J_{xy}$, and $U = -2(\langle s^y x^y \rangle)/R - (\langle s^z x^z \rangle)$, employing $T = 1/|J_z|$. The specific heat $C = \partial U/\partial T$ follows from the chain rule,
\[
  C = J_{xy}^* \frac{\partial (2(\langle s^y x^y \rangle) + R(\langle s^z x^z \rangle))}{\partial J_{xy}}, \quad \text{for } T = 1/J_{xy},
\]
The system is a \textit{spin liquid}, with a gapless spectrum and upper limit going from ferromagnetic to the exact result of constant zero \( R \). At \( R=1 \), the calculated \( (s_i^x s_j^z) \) discontinuously goes from antiferromagnetic to the exact result of 0.25 (Ref. 40) of saturated ferromagnetism and the calculated \( (s_i^x s_j^y) \) discontinuously goes from ferromagnetic to the exact result of constant zero (Ref. 40).

\[
C = J_z^2 \frac{\partial^2 (s_i^x s_j^y) / \partial (s_i^x s_j^y)}{\partial (s_i^x s_j^z)}, \quad \text{for } T = 1/|J_z|. \quad (16)
\]

\section*{III. Correlations Scanned with Respect to Anisotropy}

The ground-state and excitation properties of the XXZ model offer a variety of behaviors.\textsuperscript{11,12,40,41} The antiferromagnetic model with \( R<-1 \) is Ising-like 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 Ising-like, the ground state is ferromagnetic along the \( z \) spin component, with an excitation gap.

Our calculated \( (s_i^x s_j^z) \) and \( (s_i^x s_j^z) \) 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 Ising-like antiferromagnetic \( (R<-1) \) region, the \( z \) correlation is expectedly antiferromagnetic. As the \( (s_i^x s_j^z) \) correlation saturates for large \( |R| \), the transverse \( (s_i^x s_j^y) \) correlation is somewhat depleted. In the Ising-like ferromagnetic \( (R>1) \) region, the \( (s_i^x s_j^z) \) correlation is ferromagnetic and saturates quickly as the \( (s_i^x s_j^y) \) correlation quickly goes to zero. In the spin-liquid \((|R|<1) \) region, the \( (s_i^x s_j^y) \) correlation monotonically passes through zero in the ferromagnetic side, while the \( (s_i^x s_j^y) \) correlation is maximal. The remarkable quantum behavior of \( (s_i^x s_j^y) \) around \( R=0 \) is discussed in V below. It is seen in the figure that these changes lead to 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 \( (s_i^x s_j^y) \) and \( (s_i^x s_j^y) \) correlations show very good agreement with the known exact points.\textsuperscript{42,44} Also, our results for \( R>1 \) fully overlap the exact results of \( (s_i^x s_j^y)=0.25 \) and \( (s_i^x s_j^y)=0.40 \). We also note that zero temperature is the limit in which our approximation is at its worst.

\section*{IV. Antiferromagnetic XXZ Chain}

For the antiferromagnetic XXZ chain, our calculated \( (s_i^x s_j^z) \) and \( (s_i^x s_j^z) \) nearest-neighbor spin-spin correlations as a function of temperature are shown in Fig. 2 for various anisotropy coefficients \( R \). We find that when \( J_{xy} \) is the dominant interaction (spin liquid), the correlations are weakly dependent on anisotropy \( R \). When \( J_z \) is the dominant interaction (Ising-like), the correlations are weakly dependent on anisotropy \( R \) only at the higher temperatures. Our results are com-
FIG. 3. Comparison of our results (thick lines) for the correlation functions of the antiferromagnetic XXZ chain, with the multiple-integral results of Ref. 26 (thin lines), for various anisotropy coefficients $R$ spanning the spin-liquid and Ising-like regions.

In every one of the panels of Fig. 2, the correlation curves cross each other, revealing a remarkable quantum phenomenon. In a classical system, the correlation between a given spin and another spin component (e.g., $\langle s_x s_y \rangle$) is expected to decrease when the coupling of another spin component (e.g., $|J_z| > 0$) is increased. It is found from the antiferromagnetic XXZ chain in Fig. 2 that the opposite may occur in a quantum system: In this figure, an increase in $|J_z|$ causes an increase in $\langle s_x s_y \rangle$ for $1/|J_z| > 0.9$ and $0.4$ in the spin-liquid and Ising-like regions, respectively. Conversely, an increase in $|J_z|$ causes an increase in $\langle s_y s_y \rangle$ for $1/|J_z| > 0.4$ and $2.1$ in the spin-liquid and Ising-like regions, respectively. This quantum effect can be called cross-component spin correlation.

The antiferromagnetic specific heats calculated with Eq. (16) are shown in Fig. 4 for various anisotropy coefficients and compared, in Figs. 5 and 6, with finite-lattice expansion results of Ref. 26 in Fig. 3.

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

FIG. 5. Comparison of our antiferromagnetic specific heat results (thick lines) with the results of Refs. 5 (open circles), 6 (dotted line), 19 (thin line), 21 (dash-dotted lines), and 24 (dashed lines), for anisotropy coefficients $R=0, -0.5, -1,$ and $-2$ spanning the spin-liquid and Ising-like regions.
regions of the model.

In the Hamiltonian are ferromagnetic. This is actually a real

polynomial

we fit our numerical results for

A

with our results, in Fig. 6, and very good agreement is seen.

This high-temperature specific heat result is also compared

temperatures for

R

/H20849

versus the anisotropy coefficient

s

result is also compared

Fig. 8 between our results for

R

10−5 and

R

obtained from series expansion in Ref. 25 for anisotropy co-

efficients

R

= 0, −0.50, −0.75, −1, −2, and −∞ spanning the spin-

liquid and Ising-like regions.

V. FERROMAGNETIC XXZ CHAIN

For the ferromagnetic (i.e., R > 0) systems in Fig. 1, the

⟨sxj⟩

expectation value becomes rapidly negative at lower

temperatures for R < 1, even though for R ≈ 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-1/2 XY

model are studied by making a Jordan-Wigner transforma-
tion, yielding a theory of noninteracting spinless fermions.

Analysis of this theory yields the exact zero-temperature

nearest-neighbor spin-spin correlations4 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

continuity, it is reasonable that for a range of R positive

but less than one, the z component correlation function is as

we find, intrinsically but correctly negative at low tempera-

tures. Thus the interaction sxj sxj (irrespective of its sign,

due to the symmetry mentioned at the end of Sec. II B) in-
duces an antiferromagnetic correlation in the xj component,

competing with the xj xj interaction when the latter is ferro-

magnetic.

For finite temperatures, our calculated nearest-neighbor

spin-spin correlations are shown in Figs. 9 and 10 for dif-

erent values of R. These results are compared with Green’s

function calculations25 in Fig. 11. As expected from the dis-

cussion at the beginning of this section, in the spin-liquid

region, the correlation ⟨sxj⟩ is negative at low temperatures.

Thus a competition occurs in the correlation ⟨sxj⟩ between

the XY-induced antiferromagnetism and the ferromagnetism
due to the direct coupling between the s^z spin components. In

TABLE III. Zero-temperature nearest-neighbor correlations of

the spin-1/2 XY chain.

<table>
<thead>
<tr>
<th>Zero-temperature correlations of the spin-1/2 XY chain</th>
<th>Exact values from Ref. 4</th>
<th>Our renormalization-group theory results</th>
</tr>
</thead>
<tbody>
<tr>
<td>⟨sxj⟩sxj⟩</td>
<td>0.15915</td>
<td>0.17678</td>
</tr>
<tr>
<td>⟨sxj⟩sxj⟩</td>
<td>−0.10132</td>
<td>−0.12500</td>
</tr>
</tbody>
</table>

FIG. 6. Comparison of our antiferromagnetic specific heat re-

sults (thick lines) with the high-temperature J → 0 behaviors (thin

lines) obtained from series expansion in Ref. 25 for anisotropy co-

efficients

R

=0, −0.50, −0.75, −1, −2, and −∞ spanning the spin-

liquid and Ising-like regions.

\[
C = \frac{2 + R^2}{16} f^2 - \frac{3R}{32} f^3 + \frac{6 - 8R^2 - R^4}{256} f^4.
\]

This high-temperature specific heat result is also compared

with our results, in Fig. 6, 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

\[
C = \sum_{i=0}^{4} A_i \beta^i,
\]

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. 8 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.

FIG. 7. Our calculated antiferromagnetic spin-wave velocity \(c\)

versus the anisotropy coefficient \(R\). The dashed line, \(2\pi \sin(\gamma) / \gamma\)

where \(\gamma = \cos^{-1}(-R)\), is the exact result (Ref. 47).

FIG. 8. Comparison of our results with the high-temperature

expansion of Ref. 25 for all regions: antiferromagnetic (outer pan-
els) and ferromagnetic (inner panels), spin-liquid (left panels) and

Ising-like (right panels). Triangles and circles denote our results,

while solid and dashed lines denote the results of Ref. 25 for \(A_2\) and

\(A_3\), respectively. The error bars, due to the statistical fitting proce-
dure of the coefficients \(A_2\) and \(A_3\), have half-heights of \(1.7 \times 10^{-4}\)

and \(2.6 \times 10^{-3}\), respectively.

FIG. 9. Nearest-neighbor spin-spin correlations \(s_i s_j\) for

the spin-1/2 XXZ chain.

FIG. 10. Nearest-neighbor spin-spin correlations \(s_i s_j\) for

the spin-1/2 XXZ chain.

FIG. 11. Comparison of our renormalization-group results in the

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the XY-induced antiferromagnetism and the ferromagnetism
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In the ferromagnetic XXZ chain, as a consequence of the competition mentioned above, a sign reversal in $\langle s_i^x s_j^x \rangle$ occurs from negative to positive correlation, at temperatures $J_{xy}^1 = T_0(R)$. At this temperature, by cancellation of the competing effects, the nearest-neighbor correlation $\langle s_i^x s_j^x \rangle$ is zero. Our calculated $T_0(R)$ curve is shown in Fig. 10 and has very good agreement with the exact result $T_0 = (\sqrt{3}\sin\gamma/4)\tan[\pi(\pi-\gamma)/2\gamma]$ where $\gamma = \cos^{-1}(-R)$.

The calculated ferromagnetic specific heats are shown in Fig. 12 for various anisotropy coefficients and compared, in fact, the reinforcement of antiferromagnetic correlations of $\langle s_i^x s_j^x \rangle$ by increasing $J_{xy}$ (and also its converse) was seen in the antiferromagnetic XXZ chain discussed in the previous section. Thus we see that whereas this cross-component effect is dominant at low temperatures in the ferromagnetic XXZ chain, it is seen at higher temperatures in the antiferromagnetic XXZ chain and, in-between, throughout the temperature range in the XY chain.

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FIG. 9. Calculated nearest-neighbor spin-spin correlations $\langle s_i^x s_j^x \rangle$ (upper panels) and $\langle s_i^x s_j^x \rangle$ (lower panels) for the ferromagnetic XXZ chain, as a function of temperature, for anisotropy coefficients $R=0, 0.25, 0.50, 0.75, 1, 2, 4, 8,$ and $\infty$ spanning the spin-liquid (left panels) and Ising-like (right panels) regions.

FIG. 10. Left panel: Calculated nearest-neighbor spin-spin correlations $\langle s_i^x s_j^x \rangle$ for the ferromagnetic XXZ chain, as a function of temperature $1/J_{xy}$ in the spin liquid, for anisotropy coefficients $R=0, 0.25, 0.50, 0.75, 1, 2, 4, 8,$ and $\infty$ spanning the spin-liquid (upper panel) and Ising-like (lower panel) regions.

FIG. 11. Comparison of our ferromagnetic $R=1/3$ results with Green’s function calculations (Ref. 22).

Figs. 13 and 14, with finite-lattice expansion, quantum decimation, decoupled Green’s functions, transfer matrix, high-temperature series expansion results and, for the $R=0$ case, namely the XY model, with the exact result $C=(1/4\pi T)\int_0^\infty[\cosh(\omega T/2)+\omega T/2]^2 d\omega$. 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. Classical ferromagnetic and antiferromagnetic systems are, on the other hand, identically mapped onto each other.

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

FIG. 12. Calculated specific heats $C$ of the ferromagnetic XXZ chain, as a function of temperature for anisotropy coefficients $R=0, 0.25, 0.50, 0.75, 1, 2, 4, 8,$ and $\infty$ spanning the spin-liquid (upper panel) and Ising-like (lower panel) regions.
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. For anisotropy coefficient $|R| \leq 1$, the model is gapless 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 $\gamma=\cos^{-1}(-R)$. 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 $R \rightarrow 1^-$, and at exactly $R=1$ it has been shown that $C \sim T^{1/2}$. In the Ising-like region $R > 1$, the system exhibits a gap in its excitation spectrum and the specific heat behaves as $C \sim T^{-\alpha} \exp(-\Delta/T)$, with $\Delta$ being the excitation spectrum gap. 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 $\Delta_{\text{spin wave}} = 1 - R^{-1}$. These are the minimal energies of elementary excitations. A crossover between them occurs at $R=\frac{1}{2}$; 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 $\alpha$, for the entire range of anisotropy $R$ between $0 < R^{-1} < 1$ (Fig. 15). 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 $\alpha=1.99 \pm 0.02$ in the Ising limit $R^{-1}=0.2$, and $\alpha=1.52 \pm 0.10$ in the Heisenberg limit $R^{-1}=0.9$. These exponent values are, respectively, expected to be 2 and 1.5.

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 $T \rightarrow 0$ 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) $-1 < R < 1$: The specific heat coefficient is $C/T = 2 \gamma/(3 \sin \gamma)$ in this region, and our calculated specific heat is indeed linear at low temperatures. The $C/T$ curves for $R=-1$, $-0.5$, and 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. Figure 18 directly compares $C/T = 2/9253/20849 \times 3 \sin R/20850$ 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 $R = 1.000 000 1$.

(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 Ising-like 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 mutually 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. 1(b)], 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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