General Quantum Fidelity Susceptibilities for the $J_1-J_2$ Chain

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We study slightly generalized quantum fidelity susceptibilities where the difference in the change of fidelity is measured with respect to a different term than the one used for driving the system towards a quantum phase transition. As a model system we use the spin-1/2 $J_1-J_2$ antiferromagnetic Heisenberg chain. For this model, we study three fidelity susceptibilities, $\chi_\rho$, $\chi_c$, and $\chi_{AF}$, which are related to the spin stiffness, the dimer order and antiferromagnetic order, respectively. All these ground-state fidelity susceptibilities are sensitive to the phase diagram of the $J_1-J_2$ model. We show that they all can accurately identify a quantum critical point in this model occurring at $J_2^c \sim 0.241J_1$ between a gapless Heisenberg phase for $J_2 < J_2^c$ and a dimerized phase for $J_2 > J_2^c$. This phase transition, in the Berezinskii-Kosterlitz-Thouless universality class, is controlled by a marginal operator and is therefore particularly difficult to observe.

I. INTRODUCTION

The study of quantum phase transitions, especially in one and two dimensions, is a topic of considerable and ongoing interest. Recently the utility of a concept with its origin in quantum information, the quantum fidelity and the related fidelity susceptibility, was demonstrated for the study of quantum phase transitions (QPT). It has since then been successfully applied to a great number of systems. In particular, it has been applied to the $J_1-J_2$ model that we consider here. For a recent review of the fidelity approach to quantum phase transitions, see Ref. 12. Most of these studies consider the case where the system undergoes a quantum phase transition as a coupling $\lambda$ is varied. The quantum fidelity and fidelity susceptibility is then defined with respect to a coupling different than $\lambda_c$ from Eq. (4) that the appropriate finite-size scaling form

$$\chi_\lambda(\lambda, \delta) = 2(1 - F(\lambda)) (\lambda)^2$$

where $\partial^2 F = \chi_\lambda$ is called the fidelity susceptibility. For a discussion of sign conventions and a more complete derivation see the topical review by Gu, Ref. 13. If the higher-order terms are taken to be negligibly small then the fidelity susceptibility is defined as:

$$\chi_\lambda(\lambda) = \frac{2(1 - F(\lambda))}{(\lambda)^2}$$

The scaling of $\chi_\lambda$ at a quantum critical point, $\lambda_c$, is often of considerable interest and has been studied in detail and previous studies, have shown that

$$\chi_\lambda \sim L^{2/\nu}, \quad \chi_\lambda/N \sim L^{2/\nu - d},$$

with $N = L^d$ the number of sites in the system. An easy way to re-derive this result is by envoking finite-size scaling. Since $1 - F$ obviously is dimensionless it follows from Eq. (9) that the appropriate finite-size scaling form for $\chi_\lambda$ is

$$\chi_\lambda \sim (\delta \lambda)^{-2} f(L/\xi).$$

If we now consider the case where the parameter $\lambda$ drives the transition we may at the critical point $\lambda_c$ identify $\delta \lambda$ with $\lambda - \lambda_c$. It follows that $\xi \sim (\delta \lambda)^{-\nu}$. As usual, we can then replace $f(L/\xi)$ by an equivalent function $f(L^{1/\nu} \delta \lambda)$. The requirement that $\chi_\lambda$ remains finite for a finite system when $\delta \lambda \to 0$ then implies that to leading order $f(x) \sim x^2 \sim L^{2/\nu}(\delta \lambda)^2$, from which Eq. (9) follows.

Here we shall consider a slightly more general case where the term driving the quantum phase transition is not the same as the one with respect to which the fidelity and fidelity susceptibility are defined. That is, one considers

$$H(\lambda, \delta) = H_1 + \delta H_1, \quad H_1 = H_0 + \lambda H_\lambda.$$

The fidelity and the related susceptibility is then defined as

$$F(\lambda, \delta) = |\langle \Psi_0(\lambda, 0)|\Psi_0(\lambda, \delta)\rangle|,$$

$$\chi_\delta(\lambda) = \frac{2(1 - F(\lambda, \delta))}{\delta^2}$$

A series expansion of the GS fidelity in $\delta \lambda$ yields

$$F(\lambda) = 1 - \frac{(\delta \lambda)^2}{2} \frac{\partial^2 F}{\partial \lambda^2} + \ldots$$

where $\partial^2 F = \chi_\lambda$ is called the fidelity susceptibility. For a discussion of sign conventions and a more complete derivation see the topical review by Gu, Ref. 13. If the higher-order terms are taken to be negligibly small then the fidelity susceptibility is defined as:

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$$H(\lambda, \delta) = H_1 + \delta H_1, \quad H_1 = H_0 + \lambda H_\lambda.$$
The scaling of $\chi_\delta$ at $\lambda_c$ for this more general case was derived by Venuti et al.\textsuperscript{15} where it was shown that:

$$\chi_\delta \sim L^{2d+2z-2\Delta_\nu}, \quad \chi_\delta/N \sim L^{d+2z-2\Delta_\nu}. \quad (10)$$

Here, $z$ is the dynamical exponent, $d$ the dimensionality and $\Delta_\nu$, the scaling dimension of the perturbation $H_\nu$. In all cases that we consider here $z = d = 1$. We note that Eq. (10) assumes $[H_1, H_\nu] \neq 0$, if $H_1$ commutes with $H_\nu$ then $F = 1$ and $\chi_\delta = 0$. The case where $H_\lambda$ and $H_\nu$ coincide is a special case of Eq. (10) for which $\Delta_\nu = d + z - 1/\nu$ and one recovers Eq. (13).

A particular appealing feature of Eq. (5) is that when $\Delta_\psi = 2$, field theory\textsuperscript{18} becomes exact and $\chi_\nu$ can be calculated through numerical exact diagonalization.\textsuperscript{21,22} On the other hand, if a phase transition is expected one might then use the fidelity susceptibility as a very sensitive probe of the quantum phase transition.\textsuperscript{18} On the other hand, if a phase transition is expected one might then use the fidelity susceptibility as a very sensitive probe of the quantum phase transition.\textsuperscript{18}

The spin-1/2 Heisenberg $J_1 - J_2$ chain is a very well studied model. The Hamiltonian is:

$$H = \sum_i S_i \cdot S_{i+1} + J_2 \sum_i S_i \cdot S_{i+2} \quad (11)$$

where $J_2$ is understood to be the ratio of the next-nearest neighbor exchange parameter over the nearest neighbor exchange parameter ($J_2 = J_2/J_1$). This model is known to have a quantum phase transition of the Berezinskii-Kosterlitz-Thouless (BKT) universality class occurring at $J_2$ between a gapless 'Heisenberg' (Luttinger liquid) phase for $J_2 < J_2$ and a dimerized phase with a two-fold degenerate ground-state for $J_2 > J_2$. Field theory\textsuperscript{19,20} and exact diagonalization\textsuperscript{21,22} and DMRG\textsuperscript{23,24} have yielded very accurate estimates of the Luttinger Liquid-Dimer phase transition, the most accurate of these being due to Eggert\textsuperscript{22} which yielded a value of $J_2 = 0.241167$. Previous studies by Chen et al.\textsuperscript{12} of this model using the fidelity approach used the same term for the driving and perturbing part of the Hamiltonian as in Eq. (11) with the correspondence $H_0 = \sum_i S_i \cdot S_{i+1}$, $H_\lambda = \sum_i S_i \cdot S_{i+2}$, $\lambda = J_2$. Chen et al. demonstrated that, though no useful information about the Luttinger Liquid-Dimer phase transition could be obtained directly from the ground-state fidelity (and similarly the fidelity susceptibility), a clear signature of the phase transition was present in the fidelity of the first excited state.\textsuperscript{22} Sometimes this is taken as an indication that ground-state fidelity susceptibilities are not useful for locating a quantum phase transition in the BKT universality class. Here we show that more general ground-state fidelity susceptibilities indeed can locate this transition.

Specifically, we will study three fidelity susceptibilities, $\chi_\rho$, $\chi_D$ and $\chi_{AF}$, which are coupled to the spin stiffness, a staggered interaction term and a staggered field term, respectively. In section \textbf{III} we present our results for $\chi_\rho$ while section \textbf{IV} is focused on $\chi_D$ and section \textbf{V} on $\chi_{AF}$.

\section{The Spin Stiffness Fidelity Susceptibility, $\chi_\rho$}

We begin by considering the $J_1 - J_2$ model with $J_2 = 0$ but with an anisotropy term $\Delta$, what is usually called the XXZ model:

$$H_{XXZ} = \sum_i [\Delta S_i^z S_{i+1}^z + \frac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)]. \quad (12)$$

The Heisenberg phase of this model, occurring for $\Delta \in [-1, 1]$, is characterized by a non-zero spin stiffness\textsuperscript{25,26} defined as:

$$\rho(L) = \frac{\partial^2 e(\phi)}{\partial \phi^2} \bigg|_{\phi=0}. \quad (13)$$

Here, $e(\phi)$ is the ground-state energy per spin of the model where a twist of $\phi$ is applied at every bond:

$$H_{XXZ}(\Delta, \phi) = \sum_i [\Delta S_i^z S_{i+1}^z + \frac{1}{2}(S_i^+ S_{i+1}^- e^{i\phi} + S_i^- S_{i+1}^+ e^{-i\phi})]. \quad (14)$$

The spin stiffness can be calculated exactly for the XXZ model for finite $L$ using the Bethe ansatz\textsuperscript{27} and exact expressions in the thermodynamic limit are available.\textsuperscript{25,26} Interestingly the usual fidelity susceptibility with respect to $\Delta$ can also be calculated exactly\textsuperscript{28,29}.

Since the non-zero spin stiffness defines the gapless Heisenberg phase it is therefore of interest to define a fidelity susceptibility associated with the stiffness. This can be done through the overlap of the ground-state with $\phi = 0$ and a non-zero $\phi$. With $\Psi_0(\Delta, \phi)$ the ground-state of $H_{XXZ}(\Delta, \phi)$ we can define the fidelity and fidelity susceptibility with respect to the twist in the limit where $\phi \rightarrow 0$:

$$F(\Delta, \phi) = |\langle \Psi_0(\Delta, 0) | \Psi_0(\Delta, \phi) \rangle|, \quad (15)$$

$$\chi_\rho(\Delta) = \frac{2(1 - F(\Delta, \phi))}{\phi^2}. \quad (16)$$

To calculate $\chi_\rho$ the ground-state of the unperturbed Hamiltonian was calculated through numerical exact diagonalization. The system was then perturbed by adding a twist of $e^{i\phi}$ at each bond and recalculating the ground-state. From the corresponding fidelity, $\chi_\rho$ was calculated using Eq. (16). Our results for $\chi_\rho/L$ versus $\Delta$ are shown in Fig. 1. For all data $\phi$ was taken to be $10^{-3}$ and periodic boundary conditions were assumed. In all cases it was verified that the finite value of $\phi$ used had no effect on the final results. The numerical diagonalizations were done using the Lanczos method as outlined by Lin et al.\textsuperscript{20} Total $S^z$ symmetry and parallel programming techniques
we note that, when $\Delta = 0$ both tors $(\phi)$ corrections to arise from the presence of the operator $J$ and kinetic energy $T$ commute with the XXZ Hamiltonian and thus such a perturbation does not change the ground-state, and the fidelity is one. Thus, $\chi_J$ is zero at this point.

At the $\Delta = 0$ point the spin-current operator $\chi_J$ is therefore independent of $\phi$. Thus, $\chi_J$ versus $\Delta$: The spin stiffness fidelity $\chi_J$ was employed to make computations feasible. Numerical errors are small and conservatively estimated to be on the order of $10^{-10}$ in the computed ground-state energies.

In order to understand the results in Fig. 1 in more detail we expand Eq. (14) for small $\Delta$ and $\theta$.

$$H_{\text{XXZ}}(\Delta, \phi) \sim H_{\text{XXZ}}(\Delta) + \phi J - \frac{\phi^2}{2} T + \ldots, \quad (17)$$

$$J = \frac{i}{2} \sum_i (S_i^+ S_{i+1}^- - S_i^- S_{i+1}^+), \quad (18)$$

$$T = \frac{1}{2} \sum_i (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+). \quad (19)$$

Here, $J$ is the spin current and $T$ a kinetic energy term. The first thing we note is that, when $\Delta = 0$ both $J$ and $T$ commute with $H_{\text{XXZ}}(\Delta = 0)$. The ground-state wavefunction is therefore independent of $\phi$ (for small $\phi$) and $\chi_J \equiv 0$. This can clearly be seen in Fig. 1.

In the continuum limit the spin current $J$ can be expressed in an effective low energy field theory with scaling dimension $\Delta_J = 1$. However, we expect subleading corrections to arise from the presence of the operators $(\partial \phi)^2$ with scaling dimension 2 and $\cos(\sqrt{16\pi} K \Phi)$ with scaling dimension 4K. Here, $K$ is given by $K = \pi/(2(\pi - \arccos(\Delta)))$. For $\Delta \neq 0$ both these terms will be generated by the term $T$ in Eq. (17). With these scaling dimensions and with the use of Eq. (19) we then find:

$$\chi_J/L = A_1 L + A_2 + A_3 L^{-1} + A_4 L^{3-sK} \quad (20)$$

In Fig. 2 a fit to this form is shown for 3 different values of $\Delta = 0.25, 0.5$ and 0.75 in all cases do we observe an excellent agreement with the expected form with corrections arising from the last term $L^{3-sK}$ being almost unnoticeable until $\Delta$ approaches 1. We would expect the sub-leading corrections $L^{-1}$ and $L^{3-sK}$ to be absent if the perturbative term is just $\phi J$.

We now turn to a discussion of a definition of $\chi_{\rho}$ in the presence of a non-zero $J$. In this case we define:

$$H(\phi) = \sum_i [S_i^z S_{i+1}^z + \frac{1}{2}(S_i^+ S_{i+1}^- e^{i \phi} + S_i^- S_{i+1}^+ e^{-i \phi})] + J_2 \sum_i [S_i^+ S_{i+1}^z e^{i \phi} + S_i^- S_{i+1}^z e^{-i \phi}] + \ldots, \quad (21)$$

That is, we simply apply the twist $\phi$ at every bond of the Hamiltonian. As before we can expand:

$$H(\phi) \sim H(0) + \phi J_1 + J_2 - \frac{\phi^2}{2} (T_1 + T_2) + \ldots, \quad (22)$$

$$J_1 = \frac{i}{2} \sum_i (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+), \quad (23)$$

$$J_2 = \frac{i}{2} \sum_i (S_i^+ S_{i+2}^- + S_i^- S_{i+2}^+), \quad (24)$$

$$T_1 = \frac{1}{2} \sum_i (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+), \quad (25)$$

$$T_2 = \frac{1}{2} \sum_i (S_i^+ S_{i+2}^- + S_i^- S_{i+2}^+). \quad (26)$$

Our results for $\chi_{\rho}/L$ versus $J_2$ using this definition are shown in Fig. 3 for a range of $L$ from 10 to 32. In the region of the critical point at $J_2 = 0.241167$ the size dependence of $\chi_{\rho}/L$ vanishes yielding near scale invariance. How well this works close to $J_2^c$ is shown in the inset of...
is that another noteworthy feature of the results in Fig. 3 is a clear size invariant form in the vicinity of the critical point \( J_2 \sim 0.24 \) as well as tending to a global minima. Inset shows the the minima for system sizes \( L=16,20,24,28,32 \) with \( J_2 \) indicated as the vertical dashed line. A clear dependence of the \( J_2 \) value of \( \chi_\rho/L \) minima on the system size can be seen.

As can be seen in the inset of Fig. 3 \( \chi_\rho/L \) reaches a minimum slightly prior to \( J_2 \). The \( J_2 \) value at which this minimum occurs has a clear system size dependence which can be fitted to a power-law and extrapolated to \( L=\infty \) yielding a value of \( J_{2c} = 0.24077 \). Hence, the minimum coincides with \( J_{2c} \) in the thermodynamic limit. This is shown in Fig. 4A. Comparison of this value with the accepted \( J_{2c} = 0.241167 \) reveals impressive agreement. Another noteworthy feature of the results in Fig. 3 is that \( \chi_\rho/L \) is non-zero at the critical point, \( J_{2c} \). This value is very small but we have verified in detail that numerically it is non-zero.

The scale invariance of \( \chi_\rho/L \) is clearly induced by the disappearance of the marginal operator \( \cos(\sqrt{16\pi}K\Phi) \) at \( J_{2c} \). We expect that in the continuum limit the absence of this operator implies that the spin current commutes with the Hamiltonian resulting in \( \chi_\rho \) being effectively zero at \( J_{2c} \). The observed non-zero value of \( \chi_\rho/L \) would then arise from short-distance physics.

Note that, as mentioned previously, we take the spin stiffness to be represented by a twist on every bond, both first and second nearest neighbor and not merely on the boundary as is sometimes done. This choice is not just a matter of taste. Imposing a twist only on the boundary (usually) breaks the translational invariance of the ground-state and, through extension, effects the value and behavior of the fidelity itself. Another point of note is the use of a twist of only \( \phi \) between next-nearest neighbors. Geometric intuition would suggest that a twist of \( 2\phi \) should be applied between next-nearest neighbor bonds. However, for the small system sizes available for exact diagonalization it is found that a simple twist of \( \phi \) on both bonds yields significantly better scaling.

### III. THE DIMER FIDELITY SUSCEPTIBILITY, \( \chi_\rho \)

We now turn to a discussion of a fidelity susceptibility associated with the dimer order present in the \( J_1 - J_2 \) model for \( J_2 > J_{2c} \). This susceptibility, which we call \( \chi_D \), is coupled to the order parameter of the dimerized phase by design. Usually in the fidelity approach to quantum phase transitions one considers the case where the ground-state is unique in the absence of the perturbation. This is not the case here, leading to a diverging \( \chi_D/L \) in the dimerized phase even in the presence of a gap. Specifically, we consider a Hamiltonian of the form:

\[
H = \sum_i [S_i \cdot S_{i+1} + J_2 S_i \cdot S_{i+2} + \delta h(-1)^i S_i \cdot S_{i+1}]
\]

(27)

Thus, in correspondence with Eq. (7) we have \( H_\rho = (-1)^i S_i \cdot S_{i+1} \) and we choose the driving coupling to be
J. This perturbing Hamiltonian represents a conjugate field for the dimer phase. The scaling dimension of \( H_I \) is known\(^{22} \), \( \Delta_D = \frac{1}{2} \), and from Eq. (19) we therefore find:

\[
\chi_D \sim L^{4-2\Delta_D} = L^3 \quad \text{(at } J_2^c) \tag{28}
\]

Due to the presence of the marginal coupling we cannot expect this relation to hold for \( J_2 < J_2^c \). However, the marginal coupling changes sign at \( J_2^c \) and is therefore absent at \( J_2^c \) where Eq. (28) should be exact.\(^{20} \) For \( J_2 < 0.241167 \) it is known\(^{22} \) that logarithmic corrections arising from the marginal coupling for the small system sizes considered here lead to an effective scaling dimension \( \Delta_D > \frac{1}{2} \). At \( J_2 = 0 \) Affleck and Bonner\(^{22} \) estimated \( \Delta_D = 0.71 \). Hence, using this results at \( J_2 = 0 \), we would expect that \( \chi_D \sim L^{2.58} \) which we find is in good agreement with our results at \( J_2 = 0 \).

We now need to consider the case \( J_2 > 0.241167 \). At \( J_2 = 1/2 \) the model is exactly solvable\(^{33} \) and the two dimerized ground-states are exactly degenerate even for finite \( L \). For \( J_2^c < J_2 < 1/2 \) the system is gapped with a unique ground-state but with an exponentially low-lying excited state. In the thermodynamic limit the two-fold degeneracy of ground-state is recovered, corresponding to the degeneracy of the two dimerization patterns. From this it follows that \( \chi_D \) is formally infinite at \( J_2 = 0 \) and as \( L \to \infty \) for \( J_2 < J_2^c < 1/2 \) we expect \( \chi_D \) to diverge exponentially with \( L \). At \( J_2^c \) we expect \( \chi_D \) to exactly scale as \( L^3 \) and for \( J_2 < J_2^c \) we expect \( \chi_D \sim L^{\alpha_{\text{eff}}} \) with \( \alpha_{\text{eff}} < 3 \). Hence, if \( \chi_D/L^3 \) is plotted for different \( L \) we would expect the curves to cross at \( J_2^c \). However, the crossing might be difficult to observe since it effectively arise from logarithmic corrections.

Our results for \( \chi_D/L^3 \) are shown in Fig. 5 where a crossing of the curves are visible around \( J_2 \sim 0.2 - 0.25 \).

As an illustration, the inset of Fig. 5 shows the crossing of \( L = 12 \) and \( L = 24 \). In order to obtain a more precise estimate of \( J_2^c \) the intersection of each curve and the curve corresponding to the next largest system were tabulated \( (L = L + 2) \). These intersection points as a function of system size were then plotted Fig. 6A and found to obey a power-law of the form \( a - bL^{-\alpha} \) with \( \alpha \sim 1.8 \) and \( a = 0.241 \). This estimate of the critical coupling is in good agreement with the value of \( J_2^c = 0.241167 \).\(^{22} \)

To further verify the scaling of \( \chi_D \) at \( J_2^c \) we show in Fig. 6B \( \chi_D \) at \( J_2^c \) as a function of the cubed system size, \( L^3 \). The strong linear scaling is in contrast to the scaling a small distance away from the critical point (not shown) where the scaling was found to be distorted by logarithmic corrections.

IV. THE AF FIDELITY SUSCEPTIBILITY, \( \chi_{AF} \)

Finally, we briefly discuss another fidelity susceptibility very analogous to \( \chi_D \). We consider a perturbing term in the form of a staggered field of the form \( \sum_i (-1)^i S_i^z \) with an associated fidelity susceptibility, \( \chi_{AF} \). The scaling dimension of such a staggered field is \( \Delta_{AF} = \frac{1}{2} \) and as for \( \chi_D \) we therefore expect that \( \chi_{AF} \sim L^3 \). However, in this case it is known\(^{22} \) that the effective scaling dimension for \( J_2 < J_2^c \) is smaller than \( \frac{1}{2} \) resulting in \( \chi_{AF} \sim L^{\alpha_{\text{eff}}} \) with \( \alpha_{\text{eff}} > 3 \) for \( J_2 < J_2^c \). On the other hand, in the dimerized phase \( \chi_{AF} \) must clearly go to zero exponentially with \( L \). Hence, if \( \chi_{AF} \) is plotted for different \( L \) as a function of \( J_2 \) a crossing of the curves should occur.

Our results are shown in Fig. 7 where \( \chi_{AF}/L^3 \) is plotted versus \( J_2 \) for a number of system sizes. It is clear...
from these results that $\chi_{AF}$ indeed goes to zero rapidly in the dimerized phase as one would expect. Close to $J_2^*$ the scaling is close to $L^3$ where as for $J_2 < J_2^*$ it is faster than $L^3$. Hence, as can be seen in Fig. 7 a crossing occurs close to $J_2^*$.

V. CONCLUSION AND SUMMARY

In this paper we have demonstrated the potential benefits of extending the concept of a fidelity susceptibility beyond a simple perturbation of the same term that drives the quantum phase transition. By using the spin-1/2 Heisenberg spin chain as an example we first created a susceptibility which was directly coupled to the spin stiffness but of increased sensitivity. This fidelity susceptibility, which we labelled $\chi_{AF}$, can be used to successfully estimate the transition point at $J_2 \sim 0.241$. Next we constructed another fidelity susceptibility, $\chi_D$, this time coupled to the order parameter susceptibility of the dimer phase. Again, we were able to estimate the critical point at a value of 0.241. Finally, we discussed an anti ferromagnetic fidelity susceptibility that rapidly approaches zero in the dimerized phase but diverges in the Heisenberg phase. Although susceptibilities linked to these quantities appeared the most useful for the $J_1 - J_2$ model we considered here, it is possible to define many other fidelity susceptibilities that could provide valuable insights into the ordering occurring in the system being studied.

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FIG. 7. (Color online.) $\chi_{AF}/L^3$ versus $J_2$. $\chi_{AF}$ is expected to approach zero exponentially with the system size for $J_2 > J_2^*$, to scale as $L^3$ at $J_2^*$ and to scale as $L^{\alpha_{eff}}$ with $\alpha_{eff} > 3$ for $J_2 < J_2^*$. A crossing close to the critical point $J_2^*$ (dashed vertical line) is then visible.
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