Magnetic susceptibilities of finite Ising chains in the presence of defect sites

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Any antiferromagnet with zero net magnetic moment exhibits limited response to an external homogeneous magnetic field. This changes dramatically in the presence of defect sites, even those that carry no spin. We examine the excess susceptibilities, longitudinal and transverse, due to one or more defects at arbitrary separations in a finite Ising chain with nearest-neighbor couplings. Adapting matrix methods to finite chains we derive exact formulas valid at all $T \geqslant 0$.

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I. INTRODUCTION

Antiferromagnets generally have a $S_{\text{tot}}=0$ ground state[1] and are insensitive to weak external fields at finite temperatures. This is not the case for defective antiferromagnets including those with rough surfaces or spin vacancies in the bulk. In principle, a detailed study of the anomalous magnetization of defective antiferromagnets should be capable of yielding important information on the nature and positions of the defects.

Experimental evidence from Knight shift data and numerical calculations using Monte Carlo methods for sampling large numbers of spins have shown that any missing spin in an antiferromagnet generates a "ghost" spin distributed among a large number of neighbors.[2–4] Regardless of whether the original spins are quantum or classical, the ghost acts like a classical dipole centered at the defect site, satisfying a Curie law $\chi = C/T$ at low temperatures. If the defects lie on distinct sublattices, the ghosts tend to cancel one another, while if they lie on the same sublattice, the net magnetization is enhanced. Thus they carry both a magnitude and a phase.

Clearly the most interesting applications are to isotropic antiferromagnets in three dimensions, in which long-range ordering occurs below some Néel temperature T_N. The magnetization of one or more defects in such lattices should illuminate the short- and long-range orderings of the host spins and should be quite interesting in the neighborhood of the critical point. But the theory of such systems is notoriously difficult even in the absence of any defects. The only statement one can make with certainty is that the total ground-state spin in a Heisenberg antiferromagnet on a bipartite lattice must be $s|N_A - N_B|$, given s the magnitude of an individual spin and N_j their number on the j sublattice ($j=A$ or B).[1] It would be nice to be able to generalize this to finite T and obtain the response to homogeneous fields, $\chi_0(T)$, as a function of the number and placement of missing spins.

Before undertaking this task we have worked out exact results in one dimension for an idealized antiferromagnetic polymer. One-dimensional (1D) *isotropic* models have been studied before,[5–8] exhibiting some interesting and somewhat surprising features. In particular, nonmagnetic defects (such as magnetic ion vacancies) exhibited a Curie-like susceptibility at low temperatures, with a Curie constant that in fact was *not* constant but logarithmically dependent on T. Our exact calculations do not show this effect. However, the Ising model for which we obtain an exact solution does not have continuous symmetry.

In our model, the magnetic degrees of freedom are those of an Ising chain. Our study involves, first, a simple adaptation of the transfer matrix method to obtain the thermodynamic properties of a finite chain in a magnetic field. Second, we make use of the Jordan-Wigner transformation[9] to obtain the transverse susceptibility. For a given distribution of defects there are differences and similarities between the longitudinal and transverse susceptibilities. The principal results of this paper concern single defects and pairs of defects whether on the same or on opposite sublattices. Generalization to more than two defects involves a simple extension of the methods that are outlined below.

II. ISING CHAIN IN LONGITUDINAL FIELDS

A. Susceptibility of a chain with free ends in a *longitudinal* field

Let us consider an Ising chain of N spins with an external magnetic field parallel to the axis of quantization. The system's Hamiltonian is given by

$$\hat{H} = -J\sum_{n=1}^{N-1} \sigma_n \sigma_{n+1} - H\sum_{n=1}^{N} \sigma_n,$$

with $\sigma_n = \pm 1$. We are mainly interested in the antiferromagnetic case, $J<0$, where even the smallest numbers of defects can have a large effect on the over-all susceptibility. This is not the case in ferromagnetism ($J>0$). The partition function is most conveniently written in terms of the transfer matrix

$$\hat{V} = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix},$$

where $K=\frac{J}{T}$, $h=\frac{H}{T}$, and $T \equiv \beta^{-1}$ is the temperature. The last spin "connects" to the first one by the following matrix obtained as the limiting case of $\hat{V}$ at $K=0$:

$$\hat{D} = \begin{pmatrix} e^{h} & 1 \\ 1 & e^{-h} \end{pmatrix}.$$

The partition function is then given by

$$Z_N = \mathrm{Tr}[\hat{V}^{N-1}\hat{D}].$$

If, instead of a chain with free ends, cyclic boundary conditions are imposed, one just replaces $\hat{D}$ by $\hat{V}$ to obtain the usual expression. In either case, the trace is most conveniently evaluated if we first diagonalize the matrix $\hat{V}$:

$$\hat{X}^{-1}\hat{V}\hat{X} = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}, \quad \hat{X} = \begin{pmatrix} c_{1+} & c_{1-} \\ c_{2+} & c_{2-} \end{pmatrix}.$$

Here

$$\lambda_\pm = e^K \cosh h \pm \sqrt{e^{2K}\sinh^2 h + e^{-2K}},$$

$$c_{1\pm} = \frac{1}{\sqrt{1 + e^{2K}(\lambda_\pm - e^{K+h})^2}},$$

$$c_{2\pm} = \frac{e^K(\lambda_\pm - e^{K+h})}{\sqrt{1 + e^{2K}(\lambda_\pm - e^{K+h})^2}}.$$

When $h \to 0$, $\lambda_\pm \to e^K \pm e^{-K}$, $c_{1\pm} \to \frac{1}{\sqrt{2}}$, and $c_{2\pm} \to \pm\frac{1}{\sqrt{2}}$. Note that, for $T \to 0$ and $h \to 0$, $|\lambda_+|$ and $|\lambda_-|$ are of the same order of magnitude.

The matrix $\hat{D}$ in the basis, where $\hat{V}$ is diagonal, takes the form

$$\hat{X}^{-1}\hat{D}\hat{X} = \begin{pmatrix} a_+ & b \\ b & a_- \end{pmatrix},$$

with

$$a_\pm = e^h c_{1\pm}^2 + 2c_{1\pm}c_{2\pm} + e^{-h}c_{2\pm}^2,$$

$$b = e^h c_{1+}c_{1-} + c_{1-}c_{2+} + c_{1+}c_{2-} + e^{-h}c_{2+}c_{2-}.$$

When $h \to 0$, $a_\pm \to 1 \pm 1$ and $b \to 0$.

The partition function is given by

$$Z_N = a_+\lambda_+^{N-1} + a_-\lambda_-^{N-1},$$

whereas for cyclic boundary conditions one would have $Z_N^c = \lambda_+^N + \lambda_-^N$. The magnetic susceptibility is defined as

$$\chi_N = -\frac{1}{T^2}\left.\frac{\partial^2 F_N}{\partial h^2}\right|_{h=0}, \quad (1)$$

where $F_N = -T\ln Z_N$ is the free energy. In order to evaluate χ_N we will need to know the following derivatives:

$$\left.\frac{\partial\lambda_\pm}{\partial h}\right|_{h=0} = 0,$$

$$\left.\frac{\partial^2\lambda_\pm}{\partial h^2}\right|_{h=0} = (e^{-K} \pm e^K)e^{2K},$$

$$\left.\frac{\partial a_\pm}{\partial h}\right|_{h=0} = 0,$$

$$\left.\frac{\partial^2 a_\pm}{\partial h^2}\right|_{h=0} = \pm e^{2K}(2 - e^{2K} \pm e^{-2K}).$$

Then we will have

$$\chi_N^{\|} = \left.\frac{1}{T}\frac{\lambda_+^{N-1}\frac{\partial^2 a_+}{\partial h^2} + (N-1)a_+\lambda_+^{N-2}\frac{\partial^2\lambda_+}{\partial h^2} + \lambda_-^{N-1}\frac{\partial^2 a_-}{\partial h^2}}{a_+\lambda_+^{N-1}}\right|_{h=0}$$

and, finally,

$$\chi_N^{\|} = \frac{e^{2K}}{T}(N - \sinh 2K + 2\sinh^2 K[\tanh K]^{N-1}). \quad (2)$$

This result is to be compared with the susceptibility for cyclic boundary conditions:

$$\chi_N^{\|c} = \frac{e^{2K}}{T}N\frac{1-(\tanh K)^N}{1+(\tanh K)^N}.$$

In particular, we have $\chi_{N=0}^{\|} = \chi_{N=0}^{\|c} = 0$, $\chi_{N=1}^{\|} = \chi_{N=1}^{\|c} = 1/T$, and $\chi_{N=2}^{\|}(K) = \chi_{N=2}^{\|c}(K/2)$. The latter equality shows that, for the chain with $N=2$, the cyclic boundary condition is equivalent to taking into account the coupling between spins twice. When $K \to 0$ and the chain behaves as N independent spins, both $\chi_N^{\|}$ and $\chi_N^{\|c}$ tend to N/T.

B. Ising chain with *one* defect in a longitudinal field

The change in susceptibility caused by the introduction of a defect at site i $(1 \leq i \leq N)$ is given by

$$\Delta\chi_{i,N}^{\|} = \chi_{i-1}^{\|} + \chi_{N-i}^{\|} - \chi_N^{\|} = \frac{e^{2K}}{T}\{-1 - \sinh 2K + 2\sinh^2 K([\tanh K]^{i-2} + [\tanh K]^{N-i-1} - [\tanh K]^{N-1})\}. \quad (3)$$

Let us specialize to antiferromagnetic coupling $J = -|J|$. At $T=0$ the analysis is straightforward. We distinguish special cases. When both i and N are odd, $T\Delta\chi_{i,N}^{\|} = -1$. In this case the defect separates two spin segments with even numbers of spins, while the defectless chain has an uncompensated spin (susceptibility of a single spin is $\chi_{N=1}^{\|} = 1/T$). In all other cases, $T\Delta\chi_{i,N}^{\|} = 1$. When N is odd and i is even, then each of the two spin segments contains uncompensated spin and so does the defectless chain. When N is even, then, independent of the parity of i, only one of the segments has an uncompensated spin, while the defectless chain does not have one. Therefore, in this model, the single-defect-induced change in susceptibility of an antiferromagnetic chain equals the susceptibility of a single spin—provided N is even.

The same results hold for an odd-length "defect cluster" (an odd-numbered sequence of contiguous missing spins) in an even-length chain. However, if the length of such a cluster is even, there is no defect-induced change in susceptibility, provided the defects separate two spin segments also of even lengths. But with equal likelihood, if the two spin segments each contain odd numbers of spins, the net change in $T\chi^{\|}$ will be 2.

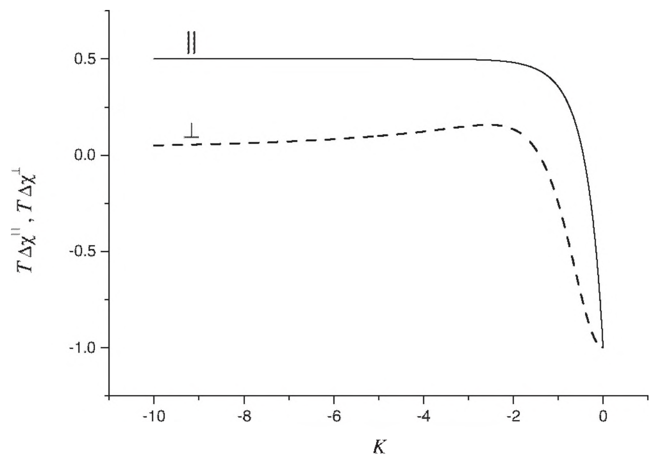

FIG. 1. Changes in longitudinal ($\Delta\chi^{\parallel}_{i,N}$, solid line) and transverse ($\Delta\chi^{\perp}_{i,N}$, dashed line) susceptibilities (multiplied by temperature, T) induced by introduction of a defect at site i into Ising chain consisting of N spins ($N \gg i \gg 1$) as functions of $K=J/T$.

Now we turn to finite temperature $T>0$. Then, if $N \gg i \gg 1$, Eq. (3) reduces to

$$\Delta\chi^{\parallel}_{i,N} = \frac{e^{2K}}{T}\{-1 - \sinh 2K\}.$$

Now, the product $T\Delta\chi^{\parallel}_{i,N}$, which measures the Curie constant (itself proportional to the square of the effective dipole constant of the defect, as a function of T), turns out to be the most informative quantity to plot. In Fig. 1 the solid line indicates this product $T\Delta\chi^{\parallel}_{i,N}$ as a function of K for the interesting regime of antiferromagnetic coupling, $K<0$. At high temperature, when the coupling is weak compared to the temperature ($K\to 0$) all spins behave independently of one another and $\Delta\chi^{\parallel}_{i,N} \to -1/T$ simply because the defectless chain contains one more spin compared to the chain with a defect. It must be noted that the low-temperature limit can differ in detail from the case $T=0$ analyzed above, because $T=0$ is the critical point at which the one-dimensional system undergoes a phase transition.

C. Ising chain with *two* defects in a longitudinal field

Consider two defects at sites i and $i+m$, respectively. The change in the chain's succeptibility due to the defects is

$$\Delta\chi^{\parallel}_{\{i,i+m\},N} = \chi^{\parallel}_{i-1} + \chi^{\parallel}_{m-1} + \chi^{\parallel}_{N-i-m} - \chi^{\parallel}_{N} = \frac{e^{2K}}{T}\{-2 - 2\sinh 2K + 2\sinh^2 K([\tanh K]^{i-2} + [\tanh K]^{m-2} + [\tanh K]^{N-i-m-1} - [\tanh K]^{N-1})\}.$$

When $T>0$, $m \ll i$, and $N \gg i \gg 1$, this expression reduces to

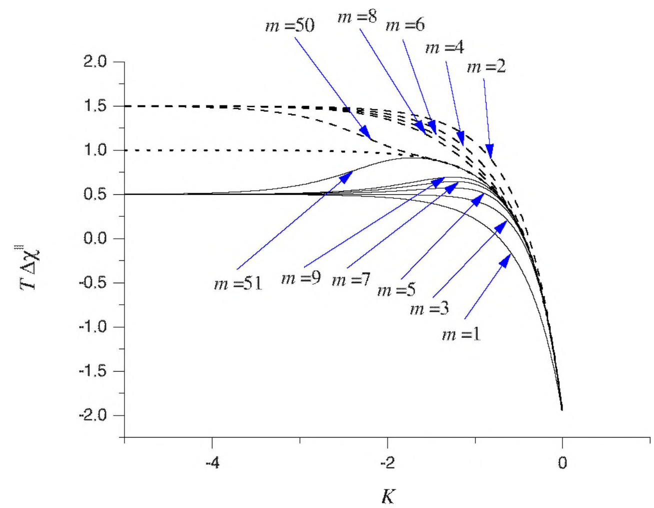

FIG. 2. (Color online) Changes in longitudinal susceptibilities (multiplied by temperature T) induced by introduction of two defects at sites i and $i+m$, respectively, into Ising chain consisting of N spins ($N \gg i \gg 1$) as functions of $K=J/T$ for odd (solid lines) and even (dashed lines) m. Dotted line shows $2T\Delta\chi^{\parallel}_{i,N}(K)$.

$$\Delta\chi^{\parallel}_{\{i,i+m\},N} = \frac{e^{2K}}{T}\{-2 - 2\sinh 2K + 2\sinh^2 K[\tanh K]^{m-2}\}. \tag{4}$$

In Fig. 2 is shown $T\Delta\chi^{\parallel}_{\{i,i+m\},N}$ as a function of K for negative K (antiferromagnetic coupling). When $K\to 0$ (high temperatures), this magnitude tends to -2. This limit is obvious, as all spins behave independently of one another. When $|K| \gg 1$, $T\Delta\chi^{\parallel}_{\{i,i+m\},N} \to 1+(-1)^m/2$. One can see that the larger is m, the wider is the temperature range, where the change in susceptibility does not depend on the parity of m such that the changes in susceptibility for m and for $m\pm 1$ coincide. In this range the dependence of $T\Delta\chi^{\parallel}_{\{i,i+m\},N}$ on K approaches $2T\Delta\chi^{\parallel}_{i,N}(K)$ (cf. Fig. 1) shown in Fig. 2 by the dotted line. The interpretation is straightforward: when the distance separating the two defects exceeds the correlation distance in the spin chain, they become independent. Thus, one can consider Fig. 2 as an illustration of the fact that the correlation distance in the system is increasing as the system is approaching the critical point at $T=0$.[10,11]

III. ISING CHAIN IN TRANSVERSE FIELDS

A. Susceptibility of a chain with free ends in a *transverse* field

Next we consider a one-dimensional Ising chain of N atoms with free ends, subject to an external magnetic field perpendicular to the axis of quantization. Following Ref. 12, we start with the Hamiltonian

$$\hat{H} = -J\sum_{n=1}^{N-1} S^x_n S^x_{n+1} + B\sum_{n=1}^{N} S^z_n.$$

Using the Jordan-Wigner transformation[9,12]

$$S_j^- = c_j \exp\left(i\pi \sum_{r<j} n_r\right), \quad S_j^+ = (S_j^-)^\dagger,$$

$$S_j^z = 2n_j - 1, \quad n_j = c_j^\dagger c_j,$$

the Hamiltonian is rewritten in terms of spinless fermion operators $c_n^\dagger$ and c_n:[12]

$$\hat{H} = -J\sum_{n=1}^{N-1} (c_n^\dagger c_{n+1}^\dagger + c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n + c_{n+1} c_n)$$

$$+ B\sum_{n=1}^{N} (2c_n^\dagger c_n - 1).$$

This Hamiltonian is a special case of the quadratic form

$$\hat{H} = \sum_{n,m=1}^{N} \left[c_n^\dagger A_{nm} c_m + \frac{1}{2}(c_n^\dagger B_{nm} c_m^\dagger + \text{H.c.}) \right] - BN,$$

with

$$\hat{A} = \begin{pmatrix} 2B & -J & 0 & 0 & \dots & 0 & 0 \\ -J & 2B & -J & 0 & \dots & 0 & 0 \\ 0 & -J & 2B & -J & \dots & 0 & 0 \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & \cdot \\ & & & & & -J & 2B \end{pmatrix},$$

$$\hat{B} = \begin{pmatrix} 0 & -J & 0 & 0 & \dots & 0 & 0 \\ J & 0 & -J & 0 & \dots & 0 & 0 \\ 0 & J & 0 & -J & \dots & 0 & 0 \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & \cdot \\ & & & & & J & 0 \end{pmatrix}.$$

Diagonalization of this quadratic form proceeds through diagonalization of the matrix $\hat{D} = (\hat{A} - \hat{B})(\hat{A} + \hat{B})$:[12,13]

$$\hat{D} = \begin{pmatrix} 4B^2 & -4BJ & 0 & 0 & \dots & 0 & 0 \\ -4BJ & 4(B^2+J^2) & -4BJ & 0 & \dots & 0 & 0 \\ 0 & -4BJ & 4(B^2+J^2) & -4BJ & \dots & 0 & 0 \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & \cdot \\ & & & & & -4BJ & 4(B^2+J^2) \end{pmatrix}. \tag{5}$$

Consider first the case $N=2$. The eigenvalues of the matrix (5) give squares of the normal-mode energies

$$E_\pm^2 = 2(J^2 + 2B^2) \pm 2|J|\sqrt{J^2 + 4B^2}.$$

In terms of the new operators describing fermionic excitations in the system, the Hamiltonian takes the form

$$\hat{H} = E_+\left(b_+^\dagger b_+ - \frac{1}{2}\right) + E_-\left(b_-^\dagger b_- - \frac{1}{2}\right).$$

The partition function is given by

$$Z_2 = 2\cosh\beta\frac{E_+ + E_-}{2} + 2\cosh\beta\frac{E_+ - E_-}{2}.$$

According to Eq. (1), magnetic susceptibility is defined through the second derivative of the free energy with respect to magnetic field:

$$\frac{d^2F_2}{dB^2} = -T\frac{\frac{d^2Z_2}{dB^2}Z_2 - \left(\frac{dZ_2}{dB}\right)^2}{Z_2^2}.$$

We then have

$$\left.\frac{dE_\pm}{dB}\right|_{B=0} = 0,$$

$$\left.\frac{d^2E_\pm}{dB^2}\right|_{B=0} = \frac{4}{|J|},$$

$$\frac{dZ_2}{dB} = \beta\left(\frac{dE_+}{dB} + \frac{dE_-}{dB}\right)\sinh\beta\frac{E_+ + E_-}{2}$$
$$+ \beta\left(\frac{dE_+}{dB} - \frac{dE_-}{dB}\right)\sinh\beta\frac{E_+ - E_-}{2},$$

$$\left.\frac{d^2Z_2}{dB^2}\right|_{B=0} = \frac{8\sinh\beta J}{TJ}.$$

Thus, the susceptibility is given by

$$\chi_{N=2}^{\perp} = \frac{2\tanh\beta J}{J}. \qquad (6)$$

When $\beta J \to 0$, the two spins become independent from one another and $\chi_{N=2}^{\perp} \to 2/T$.

Now consider the case $N>2$. Then, as shown in the Appendix, the eigenvectors of the matrix (5) are

$$\phi_q = \begin{pmatrix} \sin Nq \\ \sin(N-1)q \\ \cdot \\ \cdot \\ \sin q \end{pmatrix}.$$

Its eigenvalues give squares of the normal-mode energies

$$E_q^2 = 4(B^2+J^2) - 8BJ\cos q.$$

The allowed values of the quantum number q are to be found by solving the following equation:

$$\sin Nq = \frac{B}{J}\sin(N+1)q.$$

As $B\to 0$, the allowed values of q become $q=\pi l/N$, where $l=1,\ldots,N-1$. In terms of the new operators describing fermionic excitations in the system, the Hamiltonian takes the form

$$\hat{H} = \sum_q E_q\left(b_q^\dagger b_q - \frac{1}{2}\right).$$

The free energy is given by

$$F_N = -T\sum_q \ln\left(2\cosh\frac{\beta E_q}{2}\right).$$

In order to calculate the magnetic susceptibility, we need to know its derivatives with respect to magnetic field. We thus obtain

$$\frac{dF_N}{dB} = -\sum_q \frac{1}{2}\tanh\frac{\beta E_q}{2}\left(\frac{\partial E_q}{\partial B} + \frac{\partial E_q}{\partial q}\frac{dq}{dB}\right),$$

$$\frac{d^2F_N}{dB^2} = -\sum_q \frac{\beta}{4\cosh^2\frac{\beta E_q}{2}}\left(\frac{\partial E_q}{\partial B} + \frac{\partial E_q}{\partial q}\frac{dq}{dB}\right)^2 - \sum_q \frac{1}{2}\tanh\frac{\beta E_q}{2}\left[\frac{\partial^2 E_q}{\partial B^2} + 2\frac{\partial^2 E_q}{\partial B\partial q}\frac{dq}{dB} + \frac{\partial^2 E_q}{\partial q^2}\left(\frac{dq}{dB}\right)^2 + \frac{\partial E_q}{\partial q}\frac{d^2q}{dB^2}\right],$$

$$\left.\frac{\partial E_q}{\partial B}\right|_{B=0} = -\frac{2J\cos q}{|J|},$$

$$\left.\frac{\partial^2 E_q}{\partial B^2}\right|_{B=0} = \frac{2\sin^2 q}{|J|},$$

$$\left.\frac{\partial E_q}{\partial q}\right|_{B=0} = 0,$$

$$\left.\frac{\partial^2 E_q}{\partial q^2}\right|_{B=0} = 0,$$

$$\left.\frac{\partial^2 E_q}{\partial B\partial q}\right|_{B=0} = \frac{2J\sin q}{|J|},$$

and[14]

$$\left.\frac{dq}{dB}\right|_{B=0} = \frac{\sin q}{NJ}.$$

The susceptibility is given by

$$\chi_N^{\perp} = \frac{1}{T\cosh^2\beta J}\sum_q \cos^2 q + \frac{N+2}{N}\frac{\tanh\beta J}{J}\sum_q \sin^2 q. \qquad (7)$$

For $B\to 0$ the summations in Eq. (7) can be evaluated exactly:

$$\sum_q \cos^2 q = \sum_{l=1}^{N-1}\cos^2\frac{\pi l}{N} = \frac{N-2}{2},$$

$$\sum_q \sin^2 q = \sum_{l=1}^{N-1}\sin^2\frac{\pi l}{N} = \frac{N}{2}.$$

Therefore, the susceptibility is given by

$$\chi_N^{\perp} = \frac{N-2}{2}\frac{\beta}{\cosh^2\beta J} + \frac{N+2}{2}\frac{\tanh\beta J}{J}. \qquad (8)$$

Note that Eq. (6) turns out to be a special case of Eq. (8). This latter can be compared with the transverse susceptibility of a chain with cyclic boundary condition[12]

$$\chi_N^{\perp c} = \frac{N}{2}\frac{\beta}{\cosh^2\beta J} + \frac{N}{2}\frac{\tanh\beta J}{J}. \qquad (9)$$

Equations (8) and (9) are both $O(N)$ in the limit $N\gg 1$. Furthermore, when $\beta J\to 0$ and the chain behaves as N independent spins, both $\chi_N^{\perp}$ and $\chi_N^{\perp c}$ tend to N/T. The difference in Eqs. (8) and (9) reflects the contributions of the two ends of the finite chain.

B. Ising chain with *one* defect in a transverse field

The change in susceptibility caused by an introduction of a defect at site i $(2<i<N-1)$ is given by

$$\Delta\chi_{i,N}^{\perp} = \chi_{i-1}^{\perp} + \chi_{N-i}^{\perp} - \chi_{N}^{\perp} = -\frac{3}{2}\frac{\beta}{\cosh^2 \beta J} + \frac{1}{2}\frac{\tanh \beta J}{J}. \quad (10)$$

In Fig. 1 by dashed line is shown $T\Delta\chi_{i,N}^{\perp}$ as a function of $K \equiv \beta J$ for $K<0$ (antiferromagnetic coupling) and $2<i<N-1$. When the coupling is weak compared to the temperature ($K \to 0$) all spins behave independently of one another and $\Delta\chi_{i,N}^{\perp} \to -1/T$, just as in the case of longitudinal susceptibility. When $T \to 0$, the susceptibility of each defectless segment is finite and $T\Delta\chi_{i,N}^{\perp} \to 0$.

C. Ising chain with *two* defects in a transverse field

Consider two defects at sites i and $i+m$, respectively. The change in the chain's susceptibility is

$$\Delta\chi_{\{i,i+m\},N}^{\perp} = \chi_{i-1}^{\perp} + \chi_{m-1}^{\perp} + \chi_{N-i-m}^{\perp} - \chi_{N}^{\perp}.$$

When $m>2$, this expression reduces to

$$\Delta\chi_{\{i,i+m\},N}^{\perp} = -3\frac{\beta}{\cosh^2 \beta J} + \frac{\tanh \beta J}{J}. \quad (11)$$

In the range $m>2$ this result is independent of m. It is instructive to compare this observation with the case of longitudinal susceptibility. While in the case of the longitudinal succeptibility the two defects behave as independent only for relatively weak coupling, in the transverse case the defects are independent for every $m>2$ in the entire range of K.

As Eq. (8) is not valid for $N<2$, the cases $m=1$ and $m=2$ need special consideration. For $m=1$, we get

$$\Delta\chi_{\{i,i+1\},N}^{\perp} = -2\frac{\beta}{\cosh^2 \beta J},$$

while, for $m=2$,

$$\Delta\chi_{\{i,i+2\},N}^{\perp} = -\frac{5}{2}\frac{\beta}{\cosh^2 \beta J} + \beta - \frac{1}{2}\frac{\tanh \beta J}{J}.$$

In Fig. 3 we exhibit $T\Delta\chi_{\{i,i+m\},N}^{\perp}$ as a function of $K \equiv \beta J$ for negative K (antiferromagnetic coupling). When $m=2$, there is a single spin in the middle of the chain disconnected to all the other spins. The behavior of this single, decoupled, spin determines the limit of $T\Delta\chi_{\{i,i+m\},N}^{\perp}$ for $|K| \gg 1$. All other limits are analyzed in the same way as was done in the case of a single defect.

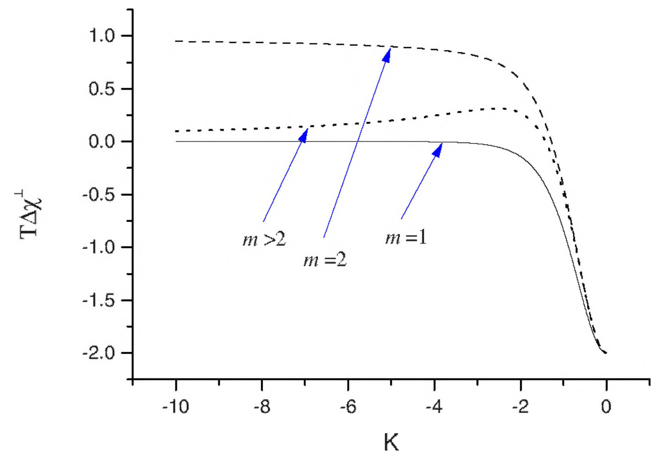

FIG. 3. (Color online) Changes in transverse susceptibilities (multiplied by temperature $T=\beta^{-1}$) induced by introduction of two defects at sites i and $i+m$, respectively, into Ising chain consisting of N spins ($2<i<i+m<N-1$) as functions of $K=\beta J$ for $m=1$ (solid line), $m=2$ (dashed line), and $m>2$ (dotted line). The dotted line also corresponds to the dependence $2T\Delta\chi_{i,N}^{\perp}(K)$ (cf. Fig. 1).

IV. DEFECTS: ADDITIONAL CONSIDERATIONS

Thus far, we have been interested in changes in magnetic susceptibilities induced by defects placed at fixed positions in the chain. Now suppose that the defects are mobile. Then the question arises: what is the most favorable configuration of n defects which yields the minimum of the free energy? In an external magnetic field this will be determined by a competition between the tendency to minimize the number of the broken bonds and that to minimize magnetic energy in an external field. If the defects are charged, one has also to take into account the electrostatic energy of their interaction.

If the defects carry no charge, then it does not take a calculation to see that, in zero external field and at arbitrary T, all defects would migrate to one end or the other of the chain to minimize the number of broken bonds. Thus the chain again becomes compact but shorter by n. However, if each defect carries a charge q, such phase separation increases the electrostatic energy greatly.

Now let us show that the magnetic energy, although much smaller, favors configurations in which the defects are all next-nearest neighbors. One can think of the magnetic energy (in an external field $V=-1/2\Delta\chi H^2$) as a temperature-dependent potential energy. Figure 2 for longitudinal fields shows that even spacings m minimize V compared to odd m's. Moreover, $m=2$ yields the lowest V at any fixed T. From this we infer that the minimum magnetic energy of n defects occurs when they are situated at $j, j+2, \ldots, j+2(n-1)$, for any j far from the ends ($N \gg j \gg 1$). This result is quite intuitive, as it also yields $n-1$ isolated spins embedded between the defects and all lying on the same sublattice, a configuration with the maximal possible Curie constant for n defects. The transverse case is very much the same: although Fig. 3 for transverse fields shows no generalized magnetic force between any pair of defects separated by more than two sites, nearest-neighbor positioning of defect sites ($m=1$) is disfavored. The lowest magnetic energy is therefore, once again, achieved when the separations are precisely 2. Thus the n defects would minimize the transverse magnetic energy by positioning themselves at $j, j+2, \ldots, j+2(n-1)$, with $n-1$ free spins embedded within. But do recall that this particular configuration of n defects has the greatest number of broken bonds, and hence in vanishing magnetic field $H=0$, it has the highest possible free energy.

V. DISCUSSION

Recently the literature on the Knight shift in defective antiferromagnets was nicely summarized by Anfuso and

Eggert[3] in their Letter concerning vacancies in the 2D (and 1D) Heisenberg models. These authors examined the deviations in sublattice magnetization surrounding the impurities by means of quantum Monte Carlo calculations.

The present paper is limited to 1D. The calculations were nontrivial, as first it was necessary to adapt the formulas in the transfer matrix formulation to free-ends boundary conditions and to do the same in the fermionic normal-mode analysis for the transverse susceptibility. Our formulas are in closed form on an anisotropic model, as opposed to numerical results on an isotropic model. Despite these differences, our calculations do confirm Refs. 2 and 3 on the whole and do shed some additional light on this interesting physical situation. In our model, with its discrete symmetry, the nonmagnetic defects also produce ghost spins. These satisfy Curie's law, with Curie's constants being truly constant at low temperatures.

Unfortunately neither the transfer matrix formalism nor the Jordan-Wigner transformation can be extended to point defects in 2D and 3D. In ongoing work we are utilizing an entirely different approach based on the isotropic *spherical model* of Berlin and Kac,[16] after noting that their method has proved useful in the study of the closely related spin glasses[12] and that it also correctly predicts the lack of long-range order in 1D and 2D, while yielding a mean-field-like phase transition in 3D antiferromagnets that are devoid of frozen-in defects.

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APPENDIX: EIGENVALUE PROBLEM

(i) Define the symmetric cyclic matrix as follows:

$$C_{nm} = c_{n-m}, \quad m,n = 1, \ldots, N,$$

$$c_{-k} = c_k, \quad k = 1-N, \ldots, N-1,$$

$$c_k = c_{N-k}, \quad k = 1, \ldots, N-1,$$

$$c_k = c_{k+N}, \quad k = 1-N, \ldots, -1.$$

Then the eigenvalue problem

$$\sum_{m=1}^{N} C_{nm}\phi_m = \lambda\phi_n$$

reduces to

$$\sum_{k=n-N}^{n-1} c_k\phi_{n+k} = \lambda\phi_n,$$

which has solutions of the type $\phi_n = ae^{iqn}$ with the eigenvalues

$$\lambda_q = \sum_{k=n-N}^{n-1} c_k e^{iqk}. \tag{A1}$$

(ii) For a symmetric cyclic matrix with $c_0 = 4(B^2+J^2)$, $c_1 = -4BJ$, and $c_2 = \cdots = c_{N-2} = 0$,[15] Eq. (A1) with $n = 2, \ldots, N-1$ yields

$$\lambda_q = 4(B^2+J^2) - 8BJ\cos q.$$

Equation (A1) with $n=1$, N gives the allowed values of q:

$$q_l = \frac{2\pi l}{N}.$$

(iii) Let C_{nm} be the symmetric cyclic matrix defined above. Define D_{nm} as

$$D_{nm} = C_{nm}, \quad n = 2, \ldots, N-1, \quad m = 1, \ldots, N,$$

$$D_{11} = 4B^2,$$

$$D_{12} = D_{NN-1} = -4BJ,$$

$$D_{1m} = 0, \quad m = 3, \ldots, N,$$

$$D_{Nm} = 0, \quad m = 1, \ldots, N-2,$$

$$D_{NN} = 4(B^2+J^2).$$

The eigenvalue equations

$$\sum_{m=1}^{N} D_{nm}\phi_m = \lambda\phi_n,$$

with $n = 2, \ldots, N-1$, are equivalent to those for C_{nm} and have solutions of the type $\phi_n = ae^{iqn} + be^{-iqn}$ with the eigenvalue $\lambda_q = 4(B^2+J^2) - 8BJ\cos q$. The same equation with $n=N$ yields $a/b = -e^{-2iq(N+1)}$, or $\phi_n = \tilde{a}\sin q(N+1-n)$, whereas from the equation with $n=1$ we get the condition for allowed values of q:

$$\sin qN = \frac{B}{J}\sin q(N+1).$$

The eigenvectors are enumerated by positive quantum numbers q. When $B \to 0$, the allowed values of q become $q = \pi l/N$, where $l = 1, \ldots, N-1$. In this case the first row as well as the first column of the matrix $\hat{D}$ becomes trivial [cf. Eq. (5)] and we obtain $N-1$ nontrivial eigenvalues and 1 zero eigenvalue.

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