

## Field-theory treatment of the Heisenberg spin-1 chain

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We suggest a new field-theory treatment of the Heisenberg spin-1 chain with a single-ion anisotropy as a theory of three Majorana (real) fermions. We calculate the static and dynamic magnetic susceptibilities. We show that our results are in a good agreement with the experimental data for NENP [ $\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2\text{ClO}_4$ ] compound. In particular, we eliminate the reported contradiction between excitation gaps deduced from high-field magnetization measurements and neutron scattering.

### I. INTRODUCTION

According to Haldane's prediction,<sup>1</sup> the one-dimensional Heisenberg antiferromagnetic with integer spin  $S$  should have an excitation gap and finite correlation length. This prediction has been confirmed both theoretically (see Ref. 2 for a review) and experimentally. The neutron-scattering data and measurements of magnetic susceptibility for several spin-1 systems (see Ref. 3 for a review) give evidence of an excitation gap. The most studied compound is  $\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2(\text{ClO}_4)$  (NENP) (Refs. 4–6) to which we shall refer throughout the paper.

Explaining the experiments qualitatively, the theory nevertheless cannot explain details. To discuss the reasons for this, we should remind ourselves of some basic ideas of Haldane's approach. The main idea is to deduce an effective field theory instead of the initial lattice Hamiltonian and then apply to this theory all field-theoretical machinery. This was done in the semiclassical approximation  $S \gg 1$  and the resulting theory is the  $\text{O}(3)$  nonlinear  $\sigma$  model which is known to be exactly solvable. The quantity  $1/S$  plays the role of a bare coupling constant in this theory. At  $S = 1$  the coupling constant is not small and such a description seems to be too crude. It does not mean, however, that one cannot find in this case another continuous description. The Monte Carlo simulations<sup>7</sup> give, for the spin-1 Heisenberg spin chain, the correlation length  $\xi = 6.2$ . In such a case a continuous description is still reasonable. The experimental data for such materials as  $\text{Ni}(\text{C}_3\text{H}_{10}\text{N}_2)_2\text{NO}_2\text{ClO}_4$  and  $\text{AgVP}_2\text{S}_6$  (see Ref. 3 for references) show that the ratio  $E/J$  ( $E$  is the gap) may be smaller than in the Heisenberg chain, which means that the correlation length in these compounds is even larger than 6.2.

In any case, the nonlinear  $\sigma$  model is actually difficult to use for practical calculations. Such calculations are needed, however, for a proper treatment of anisotropy, which is always present in real systems. In particular, NENP is found to have a significant single-ion anisotropy. It is well known that particles of the  $\text{O}(3)$  nonlinear  $\sigma$  model are triplets. According to general symmetry arguments, this triplet should be split in the presence of planar anisotropy into a singlet and doublet. From the

present knowledge of the nonlinear  $\sigma$  model, one cannot provide any more detailed information. But one actually needs extra information to explain the high-field magnetization<sup>4</sup> and the neutron-scattering measurements.<sup>5,6</sup> Both types of experiments demonstrate this splitting, but there is an apparent contradiction in the values of gaps deduced from these experiments. The authors of Ref. 4 define the excitation gaps as the critical magnetic fields  $E_{\perp, \parallel}^{(H)} = g_{\perp, \parallel} \mu_B H_c^{\perp, \parallel}$  for perpendicular and parallel directions to the chain axis. They find  $E_{\parallel}^{(H)} = 14.2$  K,  $E_{\perp}^{(H)} = 19.5$  K. In neutron-scattering experiments one observes peaks in the differential scattering cross section of neutrons moving in a given direction. The measurements of scattering in the direction of the chain give  $E_{\parallel}^{(N)} = 30$  K, and, for the perpendicular direction,  $E_{\perp}^{(N)} = 14$  K.<sup>5</sup> To eliminate this apparent contradiction, the authors of Ref. 4 have been forced to use some uncontrolled suggestions about the excitation spectrum.

Recently a semiquantitative theory of the anisotropic spin-1 chain was proposed by Affleck.<sup>8</sup> Instead of the  $\text{O}(3)$  nonlinear  $\sigma$  model, he used the theory of three bosons with  $\phi^4$  interaction. Affleck succeeded in explaining the small finite susceptibility at zero field, but the above-mentioned paradox has been left unresolved.

In the present paper we suggest an alternative field theory for the spin-1 Heisenberg model with the additional quadratic exchange

$$H_b = J \sum_{n=1}^N [(\mathbf{S}_n \cdot \mathbf{S}_{n+1}) - b(\mathbf{S}_n \cdot \mathbf{S}_{n+1})^2 + D(S_n^z)^2] \quad (1)$$

in the vicinity of the integrable point  $b = 1$ ,  $D = 0$ . The ordinary Heisenberg model with the single-ion anisotropy will be treated as a limiting case. Model (1) with  $D = 0$  has been extensively studied by many authors (see Ref. 9 and references therein). Therefore, our results may be interesting independently of the practical reasons concerning analysis of the experimental data for spin-1 Heisenberg chains.

In the framework of our approach, we eliminate the above contradiction in a self-consistent way. We show that the neutron scattering in the perpendicular direction and the high-field magnetization experiments in the parallel direction measure the mass of the doublet:

$E_{\perp}^{(N)} = E_{\parallel}^{(H)} = m_1$ . The neutron scattering in the parallel direction measures the mass of the singlet  $m_2$  and the critical magnetic field in the perpendicular direction is  $E_{\perp}^{(H)} = \sqrt{m_1 m_2}$ .

Rigorously speaking, the fields  $E_{\perp}^{(H)}$  and  $E_{\parallel}^{(H)}$  are not critical fields because the finite magnetic susceptibility survives until  $H=0$ , but up to the critical fields it is very small (8–10 % and less than 3–4 % of a high-field susceptibility for the transverse and longitudinal susceptibilities, respectively). The origin of this effect lies in the presence of anisotropy. We succeed in getting estimates for  $\chi$  ( $H=0$ ) which agree with experimental data.

The paper is organized as follows. In Sec. II we describe the continuous limit of the model (1) in the integrable point  $b=1$ ,  $D=0$  which will be used as a reference point. In Sec. III we derive a model describing a vicinity of the integrable point. In Sec. IV this model is quantized and the magnetization is calculated. The dynamical spin susceptibility is calculated in Sec. V.

## II. DESCRIPTION OF THE INTEGRABLE POINT

For  $D=0$ , model (1) is known to be integrable at  $b=1$  (Ref. 10) and  $b=-1$  (Ref. 11) where it possesses the SU(3) symmetry. The excitation spectrum is gapless in both points. At  $b=-\frac{1}{3}$ , the ground state is known exactly; the correlation length is found to be very short,  $\lambda=1/\ln 3$ .<sup>12</sup> There is a general belief that the excitation gap is present in the whole region  $-1 < b < 1$ .

The point  $b=0$  is especially interesting because it represents the Heisenberg chain. It seems to be closer to the point  $b=-\frac{1}{3}$  than to the point  $b=1$  which we are going to use as reference. However, for  $b=-\frac{1}{3}$  only the ground-state wave function is known which is not enough to elaborate any kind of perturbation theory. In addition, as we have mentioned above, the correlation length for the  $b=0$  case is not so short as for  $b=-\frac{1}{3}$ .

At  $b=1$ ,  $D=0$ , model (1) has a gapless spectrum<sup>9</sup> and therefore possesses conformal symmetry (for more details about this notion see Ref. 13). According to Ref. 14, its central charge [a ratio of the number of degrees of freedom of the given theory and the number of degrees of freedom of the free fermionic (bosonic) field theory;  $C$  characterizes the universality class] is  $C=\frac{3}{2}$ . The presence of conformal symmetry has principal consequences because it allows the classification of all operators presented in the theory and the calculation of all their scaling dimensions. The model possesses the SU(2) symmetry as well. To get a theory with  $C=\frac{1}{2}$  one may consider, instead of Dirac fermions, Majorana fermions whose spectrum  $\varepsilon(k)=|k|$  represents only the positive part of the Dirac spectrum  $\varepsilon(k)=\pm k$ .

The model possesses the SU(2) symmetry as well. To satisfy this symmetry and to get the correct  $C$ , we consider the model of three Majorana fermions belonging to the adjoint representation of the SU(2) group. The corresponding Lagrangian is

$$L = i\bar{\chi}_a \gamma_{\mu} \partial_{\mu} \chi_a, \quad a = 1, 2, 3, \quad (2)$$

where

$$\chi_a = \begin{pmatrix} \chi_{+,a} \\ \chi_{-,a} \end{pmatrix}$$

is a real spinor,  $\bar{\chi} = \chi^T \gamma_0$ , and  $\gamma_{\mu}$  ( $\mu=0,1$ ) are one-dimensional  $\gamma$  matrices. We will explain the further details concerning the Majorana representation below when we calculate the magnetic moment of our system.

## III. CONTINUOUS DESCRIPTION OF A REGION AROUND THE INTEGRABLE POINT

The conformal group theory provides us an operator basis for each universality class. Any perturbation may be expressed in terms of this basis. For model (1) we have

$$H_b = H_{b=1} + (1-b)J \sum_{n=0}^N (\mathbf{S}_n \cdot \mathbf{S}_{n+1})^2 + JD \sum_{n=0}^N (S_n^z)^2. \quad (3)$$

In the continuous limit one should save only relevant perturbations which break the conformal invariance. It is very important that we are able to enumerate all possible relevant operators as long as we know the universality class of the theory. This universality class is completely specified by the symmetry group and the central charge. The operator content for model (2) was described in Ref. 15. It includes, in our case, only two primary (relevant) fields: the field

$$\Phi_{\alpha\beta}^{(1/2)}(z, \bar{z}), \quad \alpha, \beta = 1, 2 \quad (4)$$

( $z = x + vt$ ,  $\bar{z} = x - vt$ ,  $v$  is the velocity of magnons), which transforms according to the fundamental representation of the SU(2) group and has the scaling dimension  $\Delta = \frac{3}{16}$  and the field

$$\Phi_{ab}^{(1)}(z, \bar{z}) = \chi_{+,a}(\bar{z}) \chi_{-,b}(z) \quad (5)$$

with the scaling dimension  $\frac{1}{2}$  transforming according to the adjoint representation. The signs  $+$  and  $-$  correspond to chiralities of fermions. There is also one marginal operator with dimension 1:  $J_{\mu}^a J_{\mu}^a$  where  $J_{\mu}^a = \epsilon^{abc} \bar{\chi}_b \gamma_{\mu} \chi_c$ .

Therefore, treating model (1) perturbatively, one may obtain, in the continuous limit, only the following Lagrangian:

$$L = i\bar{\chi}_a \gamma_{\mu} \partial_{\mu} \chi_a - m_a \bar{\chi}_a \chi_a + g_a J_{\mu}^a J_{\mu}^a. \quad (6)$$

The anisotropy creates the difference between fermionic masses and coupling constants:  $m_1 = m_3 < m_2$ ,  $g_1 = g_3 \neq g_2$ .

The field  $\Phi^{(1,2)}$  which is nonlocal with respect to the  $\chi$  field cannot be present because it breaks the time invariance. It is clear because this field enters into the expression for the staggered magnetization of model (1) at  $b=1$  (see, for example, Ref. 16):

$$(-1)^n S^a(x, t) = \text{Tr}[\sigma^a \Phi^{(1/2)}(x, t)] + \dots, \quad (7)$$

where the ellipsis represents fields with higher dimensions. At  $|1-b| \ll 1$ ,  $m_a \sim |1-b|$  at  $b \sim 1$  one should consider the parameters of model (6) as phenomenological.

We have one additional argument in favor of model (6). According to the Zamolodchikov theorem,<sup>17</sup> if we perturb the conformally invariant theory, then the specific-heat curve of the perturbed theory would lie below the curve of the original theory. In the integrable limit  $b=1$ ,  $D=0$ , model (1) exhibits a linear specific heat at  $T \ll J$ :<sup>10,14</sup>

$$\frac{C_v}{T} = \frac{\pi}{6v} C, \quad C = \frac{3}{2}, \quad (8)$$

which coincides with the specific heat of model (2). The  $C_v(T)$  curve for model (6) definitely lies below (8) which satisfies the claim of the Zamolodchikov theorem.

Let us consider the  $O(3)$  nonlinear  $\sigma$  model:

$$L = \frac{1}{2g} \int [(\partial_\mu \theta)^2 + \sin^2 \theta (\partial_\mu \psi)^2] dx. \quad (9)$$

At temperatures higher than mass scale ( $T \gg m$ ), one may substitute  $\sin^2 \theta$  in (9) by unity which gives us the Lagrangian of two free bosonic fields. Thus, the heat capacity at  $T \gg m$  is given by expression (8), but with  $C=2$ , which is higher than the upper bound  $C = \frac{3}{2}$ .

#### IV. CALCULATION OF THE MAGNETIZATION

In this section we quantize model (6) and calculate its magnetization. As we have already mentioned above, the masses are not very small in comparison with the bandwidth and therefore one can neglect the interaction giving only small corrections  $\sim g_a \ln(J/m)$ . After omitting the interaction, model (6) is easily quantized.

To add to the magnetic field acting in the  $a$  direction means to add to the Lagrangian the integral of motion

$$h_a i \int dx \epsilon^{abc} \bar{\chi}_b(x) \gamma_0 \chi_c(x). \quad (10)$$

Let us introduce the Fourier-transformed fields

$$\chi_{\pm,a}(k,t) = \int dx e^{ikx} \chi_{\pm,a}(x,t), \quad (11)$$

where the sign  $+$  ( $-$ ) corresponds to the right (left) movers. After this transformation the kinetic part of the Lagrangian (6) becomes

$$L_0 = \sum_{k>0, r=\pm} [i \chi_{\tau,a}(-k,t) \partial_t \chi_{\tau,a}(k,t)]. \quad (12)$$

To quantize the model one should introduce the commutation relations between the  $\chi$  field and the momentum canonically conjugated to it:

$$\begin{aligned} \pi(k) &= \frac{\partial L_0}{\partial \dot{\chi}(k,t)} = i \chi(-k,t), \\ [\pi(k), \chi(p)]_+ &= i \delta(k-p). \end{aligned} \quad (13)$$

From (13) it is clear that the creation and annihilation operators are defined as follows:

$$a_{\pm,b}^*(k) = \chi_{\pm,b}(-k), \quad a_{\pm,b}(k) = \chi_{\pm,b}(k) \quad (k>0), \quad (14)$$

and it follows from (6) and (10) that the corresponding Hamiltonian is

$$\begin{aligned} H = \sum_{k>0, r=\pm} \{ & (k \tau \delta_{bc} + i h_a \epsilon_{abc}) a_{\tau,b}^*(k) a_{\tau,b}(k) \\ & + m_b [a_{\tau,b}^*(k) a_{-\tau,b}(k)] \}, \end{aligned} \quad (15)$$

where we choose  $\gamma_0 = \sigma_x$ ,  $\gamma_1 = i \sigma_y$ .

Diagonalizing this quadratic Hamiltonian we obtain the following energy spectrum:

$$H_0 + H_{\text{mag}} = \sum_{k,a=1,2,3} [\epsilon_a(k) c_a^*(k) c_a(k)], \quad (16a)$$

$$c(k>0) = c_+(k), \quad c(k<0) = c_-(k),$$

where

$$\epsilon_a(k) = (m_a^2 + k^2)^{1/2} - (2-a)h \quad \text{for } \mathbf{h} \parallel \hat{\mathbf{z}}, \quad (16b)$$

$$\begin{aligned} \epsilon_{\pm}^2(k) &= k^2 + h^2 + (m_1^2 + m_2^2)/2 \\ &\pm \left[ \left( \frac{m_1^2 - m_2^2}{2} \right)^2 + h^2 (m_1 + m_2)^2 + 4k^2 h^2 \right]^{1/2}, \end{aligned} \quad (16c)$$

$$\epsilon_3(k) = (m_1^2 + k^2)^{1/2} \quad \text{for } \mathbf{h} \parallel \hat{\mathbf{x}} \text{ or } \hat{\mathbf{y}} (1 \leftrightarrow 3)$$

(remember that  $m_1 = m_3$  and, therefore, the index 2 stands for  $z$  and the indices 1 and 3 for  $x$  and  $y$ ).

The expression (16c) differs from the expression obtained in Ref. 8. Therefore, we obtain a different answer for the behavior of magnetization. Namely, we get  $\epsilon_-(k=0, h)=0$  at  $h = \sqrt{m_1 m_2}$  instead of  $h = m_1$  according to Ref. 8.

The gaps for the case  $\mathbf{h} \parallel \hat{\mathbf{z}}$  are equal to

$$\begin{aligned} (E_{\pm;1,2}^{(N)})^2 &= h^2 + \frac{(m_1^2 + m_2^2)}{2} \pm (m_1 + m_2) \\ &\times \left[ \left( \frac{m_1 - m_2}{2} \right)^2 + h^2 \right]^{1/2}, \end{aligned} \quad (17)$$

$$E_{\pm;3}^{(N)} = m_1.$$

This almost hyperbolic dependence of the gaps from magnetic field was observed by neutrons.<sup>6</sup>

The magnetic moment is equal to

$$M_a = i h_a \epsilon_{abc} \int_{-\infty}^{\infty} \frac{dk}{2\pi} \langle a_b^+(k) a_c(k) \rangle. \quad (18)$$

Using the results of diagonalization we obtain

$$M = \frac{1}{\pi v} [(h^2 - m_1^2)]^{1/2} \quad \text{for } \mathbf{h} \parallel \hat{\mathbf{z}} \quad (19)$$

and

$$\begin{aligned} M &= \frac{h}{2\pi v} \int_{-\infty}^{\infty} dk \frac{-k^2 - m_1 m_2 + h^2 + \epsilon_+(k) \epsilon_-(k)}{\epsilon_+(k) \epsilon_-(k) [\epsilon_+(k) + \epsilon_-(k)]} \\ &\quad \text{for } \mathbf{h} \parallel \hat{\mathbf{z}}. \end{aligned} \quad (20)$$

Rigorously speaking, in case  $\mathbf{h} \parallel \hat{\mathbf{z}}$  the magnetization is never equal to zero. At zero magnetic field there is still a finite magnetic susceptibility:

$$\chi(0) = \frac{1}{v} \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{[(k^2 + m_1^2)(k^2 + m_2^2)]^{1/2} - k^2 - m_1 m_2}{[(k^2 + m_1^2)(k^2 + m_2^2)]^{1/2} [(k^2 + m_1^2)^{1/2} + (k^2 + m_2^2)^{1/2}]}$$

$$\approx \chi(\infty) \frac{2}{3} \left[ \frac{m_1 - m_2}{m_1 + m_2} \right]^2. \quad (21)$$

The latter estimate is valid for  $|(m_1 - m_2)/m_2| < 2$ .

At  $m_2/m_1 = 2$  we obtain, from (21),  $\chi(0)/\chi(\infty) \approx 0.077$ , which is in an excellent agreement with the experimental value 0.08–0.1.<sup>5</sup>

The analysis of the integral (21) shows that the sharp increase in the magnetization happens if  $h \gtrsim \sqrt{m_1 m_2}$ . The latter quantity might be considered as the critical field.

Thus, the previous analysis shows that the critical magnetic fields are  $E_{\parallel}^{(H)} = g_{\parallel} H_c^{\parallel} = m_1$  and  $E_{\perp}^{(H)} = g_{\perp} H_c^{\perp} = \sqrt{m_1 m_2}$ . Using the values of  $E_{\perp}^{(H)}$ ,  $E_{\parallel}^{(H)}$  given in Ref. 4, we obtain

$$m_1 = E_{\parallel}^{(H)} = 14.2 \text{ K}$$

and

$$m_2 = (E_{\perp}^{(H)})^2 / E_{\parallel}^{(H)} = 26.7 \text{ K},$$

which are rather close to the masses observed in neutron-scattering experiments.<sup>5,6</sup>

## V. CALCULATION OF THE DYNAMICAL MAGNETIC SUSCEPTIBILITY

The differential cross section of inelastic neutron scattering is directly proportional to the imaginary part of ac magnetic susceptibility. Our approach provides us an ability to calculate the ac magnetic susceptibility. It follows from (7) that

$$\chi(x, t) = \langle S^+(x, t) S^-(0, 0) \rangle$$

$$\sim (-1)^{x/a} \langle \text{Tr}[\sigma^+ \Phi^{(1/2)}(x, t)]$$

$$\times \text{Tr}[\sigma^- \Phi^{1/2}(0, 0)] \rangle, \quad (22)$$

where  $a$  is a lattice spacing.

It is well known that the two-dimensional (2D) Ising model is equivalent to the model of free massive Majorana fermions with mass equal to  $m = a(T - T_c)$  (see Ref. 13). Model (6), in the absence of interactions, may be considered as a collection of three Ising models each at its own temperature, relating with the masses of Majorana fermions. According to Ref. 15, the following relation between the components of the matrix field  $\Phi$  and the order and disorder fields  $\sigma$  and  $\mu$  takes place at  $T = T_c$ :

$$\text{Tr}(\sigma^+ \Phi^{(1/2)}) = \sigma^1 \mu^2 \mu^3 + i \mu^1 \sigma^2 \sigma^3,$$

$$\text{Tr}(\sigma^- \Phi^{(1/2)}) = \sigma^1 \mu^2 \mu^3 - i \mu^1 \sigma^2 \sigma^3. \quad (23)$$

In the absence of interactions, these relations are still valid beyond the critical point. To write down the expression for the spin-spin correlation function in the anisotropic case one should specify the correspondence between the labels 1, 2, 3 in expressions (22) and the labels of

the fermionic fields in (6). It is important because fermions with different labels have different masses. Each possible arrangement of labels corresponds to a spin susceptibility  $\chi$  along the appropriate direction of the ac magnetic field. There are two arrangements giving the same expression for  $\chi$ :

$$\sigma^1 \Longleftrightarrow \chi_1,$$

$$\sigma^2 \Longleftrightarrow \chi_3 \text{ (masses } m_1), \quad (24a)$$

$$\sigma^3 \Longleftrightarrow \chi_2 \text{ (mass } m_2),$$

and

$$\sigma^1 \Longleftrightarrow \chi_1,$$

$$\sigma^3 \Longleftrightarrow \chi_3 \text{ (mass } m_1), \quad (24b)$$

$$\sigma^2 \Longleftrightarrow \chi_2 \text{ (mass } m_2).$$

(An arrow shows that fields belong to the same Ising model.)

In these cases one gets, from (22) and (23),

$$\chi_{\perp}(x, t) = \langle S^+(x, t) S^-(0, 0) \rangle$$

$$= (-1)^{x/a} F_+(m_1 r) F_-(m_1 r)$$

$$\times [F_+(m_2 r) + F_-(m_2 r)]$$

$$r = (x^2 + v^2 t^2)^{1/2}, \quad (25)$$

where  $t$  is the Matsubara time. The correlation functions  $F_+(\mathbf{x}) = \langle \sigma(\mathbf{x}) \sigma(0) \rangle$  and  $F_-(\mathbf{x}) = \langle \mu(\mathbf{x}) \mu(0) \rangle$  are calculated in Ref. 18.

The third arrangement is

$$\sigma^2 \Longleftrightarrow \chi_1, \quad \sigma^3 \Longleftrightarrow \chi_3, \quad \sigma^1 \Longleftrightarrow \chi_2, \quad (26)$$

which gives

$$\chi_{\parallel}(x, t) = (-1)^{x/a} [F_+(m_2 r) F_-^2(m_1 r)$$

$$+ F_-(m_2 r) F_+^2(m_1 r)]. \quad (27)$$

For expression (23) there are two possible arrangements (24a) and (24b) and for (27), only one, (26). Therefore, it follows from the symmetry arguments that (23) corresponds to the spin-spin correlation functions along the directions transverse to the  $z$  axis and (27) gives the longitudinal susceptibility.

Using the explicit expressions for the  $F$  functions from Ref. 18 we get, for the imaginary parts of the ac susceptibilities, the following:

$$\begin{aligned}
\text{Im}\chi_{\perp}^{(R)}(\omega, k) &= f_{\perp}(s) = \delta(s^2 - m_1^2) \\
&\quad + 2[(s - m_2)^2 - m_1^2]^{-1/2} \\
&\quad \times [(s + m_2)^2 - m_1^2]^{-1/2} + \dots, \\
\text{Im}\chi_{\parallel}^{(R)}(\omega, k) &= f_{\parallel}(s) = \delta(s^2 - m_2^2) \\
&\quad + 2|s|^{-1}[s^2 - 4m_1^2]^{-1/2} + \dots, \\
s^2 &= \omega^2 - v^2(k - \pi/a)^2,
\end{aligned} \tag{28}$$

From (27) one sees that the neutron-scattering measurements along the  $z$  direction should exhibit the strongest singularity at the largest mass  $m_2$ . One should remember that the high-field magnetization measurements along this axis give the critical field proportional to the smallest mass  $m_1$ . Thus, the above-mentioned contradiction is removed.

The  $\delta$ -functional term in (28) gives the largest contribution into the space dependence of spin-spin correlation function at large distances. For the isotropic case we get, from (28),

$$\begin{aligned}
\langle \mathbf{S}(t=0, \mathbf{x}) \cdot \mathbf{S}(0, 0) \rangle &= \frac{i}{(2\pi)^2} \int d\omega dk \frac{e^{-ikx}}{\omega^2 - v^2 k^2 - m^2} \\
&\sim e^{-m|x|} |x|^{-1/2},
\end{aligned} \tag{29}$$

which is in a perfect agreement with the Monte Carlo results.<sup>7</sup>

Another quantity usually measured in neutron-scattering experiments is the integrated intensity

$$I(k) = \int d\omega \text{Im}\chi^{(R)}(\omega, k).$$

Usually in experiments only broadened  $\delta$ -functional peaks are seen. According to (27) the integrated intensity corresponding to them is

$$I_{\perp, \parallel}(k) = \frac{1}{(k^2 + m_{1,2}^2)^{1/2}}. \tag{30}$$

Instead of (30), experimentalists usually use the Lorentzian function which leads to larger estimates for mass gaps. Fitting the data for the integrated intensity for the NENP exhibited in Ref. 3 to the expression (30), we get the estimate  $m_2 \approx 20-30$  K.

## VI. CONCLUSION

In summary, we have suggested the continuous field theory (6) for the 1D spin-1 chain in the vicinity of the integrable point. This model is a simple theory of free fermions. Using fermions for the description of spin systems is the usual trick in one dimension and therefore the choice of description is a matter of convenience. Actually, we use some variant of the Jordan-Wigner transformation. The equivalence of bosonic and fermionic descriptions means that, for a given model, correlation functions of bosonic fields may be rewritten via fermionic ones and vice versa. Such expressions may be quite complicated, such as the expression for the spin operator (22) described in Sec. V.

In principle, the proposed model should work well if the correlation length is large. But it seems that it describes the ordinary Heisenberg chain where  $\xi = 6.2$  because our results are in good agreement with all present experimental data for the NENP compound including the critical magnetic fields and dynamical magnetic susceptibility. We hope to have an even better agreement for such substances as  $\text{Ni}(\text{C}_3\text{H}_{10}\text{N}_2)_2\text{NO}_2(\text{ClO}_4)$  (NINO), and  $\text{AgVP}_2\text{S}_6$  where magnetization measurements show larger correlation lengths. The correlation length may be increased by an interchain coupling or by the  $(\mathbf{S}_n \cdot \mathbf{S}_{n+1})^2$  interaction. A realization of the latter variant would abolish the monopoly of the ordinary Heisenberg model on the theory of one-dimensional magnetism.

Returning to the theoretical aspects of the problem it is worth it to notice that the present description of model (3) forms a bridge between its gapless phase ( $b=1$ ) and the Affleck-Kennedy-Lieb-Tasaki (AKLT) point ( $b=-\frac{1}{3}$ ).<sup>12</sup> The latter point has attracted a considerable interest as an example of a valence-bond solid. We think that our description is qualitatively valid near the AKLT point.

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