# Spinon Attraction in Spin-1/2 Antiferromagnetic Chains

B. A. Bernevig,[1] D. Giuliano,[1,2] and R. B. Laughlin[1]
[1]*Department of Physics, Stanford University, Stanford, California 94305*
[2]*Istituto Nazionale di Fisica della Materia (INFM), Unitá di Napoli, via Cintia, I-80126 Napoli, Italy*
(Received 6 November 2000)

We derive the representation of the two-spinon wave function for the Haldane-Shastry model in terms of the spinon coordinates. This result allows us to rigorously analyze spinon interaction and its physical effects. We show that spinons attract one another. The attraction gets stronger as the size of the system is increased and, in the thermodynamic limit, determines the power law with which the susceptibility diverges.

DOI: 10.1103/PhysRevLett.86.3392 PACS numbers: 75.10.Jm, 05.30.Pr, 75.40.Gb

Several properties of interacting spin-1/2 antiferromagnetic spin chains can be figured out by means of the Bethe-ansatz (BA) technique, developed by Bethe in his pioneristic paper [1]. From the dispersion relation of low-lying excitations [2], it has been figured out that low-energy excitations in spin-1/2 antiferromagnets have spin-1/2 [3]. Later on they were called spinons [4,5]. The Brillouin zone for one spinon is halved [3,4,6], and spinons are semions, i.e., particles with statistics half that of regular fermions [5,7].

Low-energy excitations of BA-solvable models are in the same universality class as excitations of the Haldane-Shastry model (HSM) [8]. The HSM is a system of spins on a circular lattice interacting via an antiferromagnetic interaction inversely proportional to the square of the chord between the corresponding sites. The Hamiltonian is given by

$$\mathcal{H}_{\mathrm{HS}} = J\left(\frac{2\pi}{N}\right)^2 \sum_{\alpha<\beta}^{N} \frac{\vec{S}_\alpha \cdot \vec{S}_\beta}{|z_\alpha - z_\beta|^2}, \tag{1}$$

where $z_\alpha = \exp(2\pi i\alpha/N)$ and $\alpha$ is the lattice site. The HSM is one of the simplest exactly solvable interacting antiferromagnets in 1D. It is the prototype of a 1D spinon gas [5] since it does not take marginal logarithmic corrections, in contrast, for instance, with the behavior of the Heisenberg model [4,6]. Hence, in this Letter we focus on the dynamics of spinon excitations in the HSM.

$L$-spinon solutions of the HSM have been constructed [5] in analogy to the corresponding spinless continuum version of the model [9]. When expressed in terms of Bethe-ansatz such as "pseudomenta," the energy of a many-spinon solution in the corresponding "plane wave" representation in the thermodynamic limit appears to be given by the energy of a set of noninteracting particles, often referred to as "free spinon gas" [10,11]. However, from the representation of the many-spinon wave function, the persistence of a spinon interaction in the thermodynamic limit is not at all transparent. Indeed, the interaction between spinons is encoded in the definition of the pseudomomenta, which enter the formula for the energy of a many-spinon solution [5,7].

In this paper we analyze carefully the nature of spinon interaction and its persistence in the thermodynamic limit, by working out the real-space coordinate representation for two-spinon eigenstates of $\mathcal{H}_{\mathrm{HS}}$ and the corresponding Schrödinger equation. The spinon interaction and its nature follow straightforwardly from the behavior of the exact solution of this equation. In Fig. 1 we plot the result. While at large separations the probability amplitude is independent of spinon separation, as it is appropriate for noninteracting particles, at short separations there is a huge enhancement. Such an enhancement is a clear evidence for a short range, attractive interaction between spinons. As we show in Fig. 1, this enhancement gets sharpened as the number of sites increases, at odds with the conclusion that spinon interaction and its effects disappear in the thermodynamic limit, which could be derived from the additivity of the energy.

Spinon dynamics determines the low-energy physics of the HSM. 1D interacting antiferromagnets do not order and, accordingly, the spin-1 spin wave (SW) is an unstable excitation of the HSM. The SW is unstable at any energy and momentum against decay into a spinon pair [3]. This causes nonanalyticities in the SW propagator, the

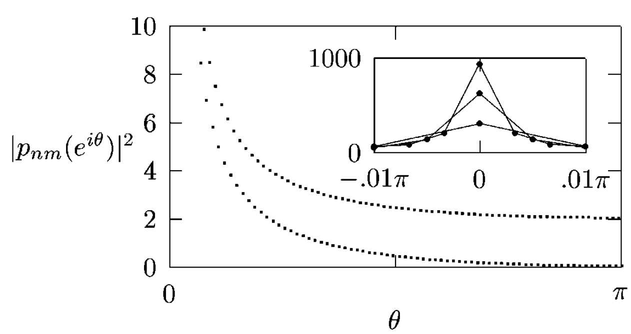


FIG. 1. Square of the two-spinon wave function $|p_{mn}(z)|^2$ defined by Eq. (22) for the case of $N = 300$, $m = N/2 - 1$, and $n = 0$. At large separations the probability oscillates between 0 and 2 and averages to 1. The inset shows this function close to the origin for $N = 200$, 400, and 600. The value at the origin diverges in the thermodynamic limit.

 0031-9007/01/86(15)/3392(4)$15.00 

dynamical spin susceptibility (DSS) $\chi_q(\omega)$. $\chi_q(\omega)$ develops a branch cut at the threshold energy for a SW and a broad continuum above this threshold. Broad spectra have been observed by means of neutron scattering on quasi 1D samples [12], which experimentally substantiates this scenario. However, the continuum is not flat, as would be the case if it were a spinon joint density of states, but rather has a divergent square-root edge. We show that it is the spinon interaction which makes the matrix element for the decay of the spin wave into spinon pairs huge at threshold and causes this divergence. We explicitly prove that, in the thermodynamic limit, the spinon attraction turns into the square-root divergence in the DSS. Spinon interaction and its relation to the DSS are the main result of our work.

Let us begin with some basic results from the HSM. In the even-$N$ case the ground state of $\mathcal{H}_{\mathrm{HS}}$ [Eq. (1)] is a disordered spin singlet, whose wave function is given by

$$\Psi_{\mathrm{GS}}(z_1,\ldots,z_M) = \prod_{i<j}^{M}(z_i - z_j)^2 \prod_{j}^{M} z_j\,, \qquad (2)$$

where $M = N/2$ and the $\{j\}$'s denote the positions of $\uparrow$ spins, all the others being $\downarrow$. The corresponding energy is given by $E_{\mathrm{GS}} = -J(\pi^2/24)(N + 5/N)$ [4,6,13]. Elementary excitations above $\Psi_{\mathrm{GS}}$ are spinons–spin-1/2 defects in the otherwise featureless disordered sea. A $\downarrow$ spinon localized at $\alpha$ can be thought of as a singlet sea where the spin at $\alpha$ is constrained to be $\downarrow$. The corresponding wave function is

$$\Psi_\alpha(z_1,\ldots,z_M) = \prod_{j}^{M}(z_\alpha - z_j)\prod_{i<j}^{M}(z_i - z_j)^2\prod_{j}^{M} z_j\,, \qquad (3)$$

where now $N$ is odd and $M = (N-1)/2$. A one-spinon eigenstate of $\mathcal{H}_{\mathrm{HS}}$ is constructed by making the plane-wave superposition

$$\Psi_m(z_1,\ldots,z_M) = \frac{1}{N}\sum_{\alpha=1}^{N}(z_\alpha^*)^m\Psi_\alpha(z_1,\ldots,z_M)\,. \qquad (4)$$

The corresponding energy is

$$E_m = -J\frac{\pi^2}{24}\left(N - \frac{1}{N}\right) + \frac{J}{2}\left(\frac{2\pi}{N}\right)^2 m(M-m)\,. \qquad (5)$$

$\Psi_m$ also has a well-defined crystal momentum: $q_m = (\pi/2)N - (2\pi/N)(m + 1/4)$ (mod$2\pi$). In terms of $q_m$ the energy with respect to the ground state is $E(q_m) = (J/2)[(\pi/2)^2 - q_m^2]$ (mod$\pi$) [4,6,13].

Spinons do not lose their identity when many of them are present. $L$ spinons can be thought of as a disordered sea with the spin at $L$ sites constrained to be $\downarrow$ [4]. For two spinons this means that the corresponding wave function for a pair of localized spinons at $\alpha$ and $\beta$ is given by ($M = N/2 - 1$)

$$\Psi_{\alpha\beta}(z_1,\ldots,z_M) = \prod_{j}^{M}(z_\alpha - z_j)(z_\beta - z_j) \times \prod_{i<j}^{M}(z_i - z_j)^2\prod_{j}^{M} z_j\,. \qquad (6)$$

$\Psi_{\alpha\beta}$ can be analytically extended to any value of $z_\alpha, z_\beta$ on the unit circle. As $z_\alpha, z_\beta$ are lattice sites, they are interpreted as locations of $\downarrow$ spins [5].

States with two spinons carrying well-defined crystal momentum are given by the lattice plane waves which have the expression

$$\Psi_{mn}(z_1,\ldots,z_M) = \sum_{\alpha,\beta}^{N}\frac{(z_\alpha^*)^m(z_\beta^*)^n}{N^2}\Psi_{\alpha\beta}(z_1,\ldots,z_M)\,. \qquad (7)$$

The total crystal momentum of $\Psi_{mn}$ is $q = (\pi/2)(N-2) + q_m + q_n$ (mod$2\pi$) and $q_m, q_n$ are the momenta of each spinon. The $\Psi_{mn}$ are an overcomplete set. A set of linearly independent states is constructed by taking only the $\Psi_{mn}$ with $M \ge m \ge n \ge 0$. Two-spinon energy eigenstates are linear superpositions of these:

$$\Phi_{mn} = \sum_{l=0}^{\ell_M} a_\ell^{mn}\Psi_{m+\ell,n-\ell}\,, \qquad (8)$$

where $\ell_M = n$ if $m + n < M$, $\ell_M = M - m$ otherwise. The coefficients $a_\ell^{mn}$ are [9,13]

$$a_\ell^{mn} = -\frac{(m - n + 2\ell)}{2\ell(\ell + m - n + \frac{1}{2})}\sum_{k=1}^{\ell} a_{k-1}^{mn} \qquad (a_0 = 1)\,, \qquad (9)$$

and the corresponding eigenvalue is

$$E_{mn} = -J\left(\frac{\pi^2}{24}\right)\left(N + \frac{5}{N}\right) + \left[E(q_m) + E(q_n) - \frac{\pi J}{N}\frac{|q_m - q_n|}{2}\right] \qquad (q_m \le q_n)\,. \qquad (10)$$

$E_{mn}$ is the sum of the ground-state contribution, $E_{\mathrm{GS}} = -J(\pi^2/24)(N + 5/N)$, and $E(q_m, q_n)$, which is the two-spinon energy above the ground state. $E(q_m, q_n)$ is the sum of the energies of two isolated spinons plus a negative interaction contribution that becomes negligibly small in the thermodynamic limit [4,6].

The norm of $\Phi_{mn}$ can be computed by means of a recursive procedure, based on the operator $e_1(z_1,\ldots,z_M) = z_1 + \cdots + z_M$. For any wave function of the form $\Phi \times \Psi_{\mathrm{GS}}$, where $\Phi$ is a symmetric polynomial, we have

$$\mathcal{H}\Phi\Psi_{\mathrm{GS}} = E_{\mathrm{GS}}\Phi\Psi_{\mathrm{GS}} + \frac{J}{2}\left(\frac{2\pi}{N}\right)^2\Psi_{\mathrm{GS}}\left\{\frac{1}{2}\left[\sum_j z_j^2\frac{\partial^2}{\partial z_j^2} + 4\sum_{j\neq k}\frac{z_j^2}{z_j - z_k}\frac{\partial}{\partial z_j}\right] - (M-1)\sum_j z_j\frac{\partial}{\partial z_j}\right\}\Phi\,, \qquad (11)$$

and thus

$$\mathcal{H} e_1 \Phi \Psi_{\mathrm{GS}} - e_1 \mathcal{H} \Phi \Psi_{\mathrm{GS}} = \frac{J}{2}\left(\frac{2\pi}{N}\right)^2 \Psi_{\mathrm{GS}}\Big[\sum_j z_j^2 \frac{\partial}{\partial z_j} + (M-1)e_1\Big]\Phi\,. \tag{12}$$

From the matrix elements of the commutator between $\mathcal{H}_{\mathrm{HS}}$ and $e_1$ under the inner product $\langle f \,|\, g\rangle = \sum_{z_1,\ldots,z_M} f^*(z_1,\ldots,z_M) g(z_1,\ldots,z_M)$ we find that

$$\frac{\langle \Phi_{m-1,n}|e_1|\Phi_{mn}\rangle}{\langle \Phi_{m-1,n} \,|\, \Phi_{m-1,n}\rangle} = \frac{-(M-m+1)}{2(M-m+\frac{1}{2})}, \tag{13}$$

$$\frac{\langle \Phi_{m-1,n}|e_1|\Phi_{mn}\rangle}{\langle \Phi_{mn} \,|\, \Phi_{mn}\rangle} = \frac{-(m+\frac{1}{2})(m-n)^2}{2(m-n+\frac{1}{2})m(m-n-\frac{1}{2})}, \tag{14}$$

$$\frac{\langle \Phi_{m,n-1}|e_1|\Phi_{mn}\rangle}{\langle \Phi_{mn}|\Phi_{mn}\rangle} = \frac{-n}{2(n-\frac{1}{2})}, \tag{15}$$

$$\frac{\langle \Phi_{m,n-1}|e_1|\Phi_{mn}\rangle}{\langle \Phi_{m,n-1} \,|\, \Phi_{m,n-1}\rangle} = \frac{-(M-n+\frac{3}{2})(m-n+1)^2}{2(m-n+\frac{3}{2})(m-n+\frac{1}{2})(M-n+1)}. \tag{16}$$

Combining these expressions, one then finds by induction that

$$\frac{\langle \Phi_{mn} \,|\, \Phi_{mn}\rangle}{\langle \Psi_{\mathrm{GS}} \,|\, \Psi_{\mathrm{GS}}\rangle} = \frac{\Gamma[m-n+\frac{1}{2}]\Gamma[m-n+\frac{3}{2}]}{2\pi N(M+1)\Gamma^2[m-n+1]} \times \frac{\Gamma[m+1]\Gamma[M-m+\frac{1}{2}]}{\Gamma[m+\frac{3}{2}]\Gamma[M-m+1]} \times \frac{\Gamma[n+\frac{1}{2}]\Gamma[M-n+1]}{\Gamma[n+1]\Gamma[M-n+\frac{3}{2}]}, \tag{17}$$

where $\langle \Psi_{\mathrm{GS}} \,|\, \Psi_{\mathrm{GS}}\rangle = N^{M+1}(2M+2)!/2^{M+1}$ [14].

The definition of the wave function for two spinons in real space is now straightforward. $\Psi_{\alpha\beta}$ is the state of two localized spinons at $z_\alpha$ and $z_\beta$. The states $\Phi_{mn}$ have been classified in [10] as highest-weight states of a Yangian algebra. They provide a basis for the fully polarized two-spinon states, as $\Psi_{\alpha\beta}$. Hence, we define the two-spinon wave function $z_\alpha^m z_\beta^n p_{mn}(z_\alpha/z_\beta)$ from

$$\Psi_{\alpha\beta} = \sum_{m=0}^{M}\sum_{n=0}^{m} (-1)^{m+n} z_\alpha^m z_\beta^n p_{mn}\left(\frac{z_\alpha}{z_\beta}\right)\Phi_{mn}\,. \tag{18}$$

It is, in principle, possible to invert Eq. (8) and to obtain $p_{mn}$ algebraically. However, we developed a much simpler approach, which makes use of the fact that $\Psi_{\alpha\beta}$ is perfectly defined for any $z_\alpha, z_\beta$ on the unit circle. Because $|\Phi_{mn}\rangle$ is an eigenstate of $\mathcal{H}_{\mathrm{HS}}$, one obtains

$$\langle \Phi_{mn}|\mathcal{H}_{\mathrm{HS}}|\Psi_{\alpha\beta}\rangle = E_{mn}\langle \Phi_{mn} \,|\, \Psi_{\alpha\beta}\rangle\,. \tag{19}$$

On the other hand, by standard manipulations [5,9,13], one can also show that

$$\langle \Phi_{mn}|\mathcal{H}_{\mathrm{HS}}|\Psi_{\alpha\beta}\rangle = E_{\mathrm{GS}}\langle \Phi_{mn} \,|\, \Psi_{\alpha\beta}\rangle + \frac{J}{2}\left(\frac{2\pi}{N}\right)^2\Big\{\Big(M - z_\alpha\frac{\partial}{\partial z_\alpha}\Big)z_\alpha\frac{\partial}{\partial z_\alpha} + \Big(M - z_\beta\frac{\partial}{\partial z_\beta}\Big)z_\beta\frac{\partial}{\partial z_\beta} - \frac{1}{2}\,\frac{z_\alpha+z_\beta}{z_\alpha-z_\beta}\Big(z_\alpha\frac{\partial}{\partial z_\alpha} - z_\beta\frac{\partial}{\partial z_\beta}\Big)\Big\} \times \langle \Phi_{mn} \,|\, \Psi_{\alpha\beta}\rangle\,. \tag{20}$$

Note the last term in this equation, which is the spinon interaction, is *large* and diverges as the first power of the spinon separation. Upon equating Eq. (19) to Eq. (20) we finally derive the differential equation

$$z(1-z)\frac{d^2 p_{mn}}{dz^2} + \left[\frac{1}{2} - m + n - \left(-m+n+\frac{3}{2}\right)z\right]\frac{dp_{mn}}{dz} + \frac{m-n}{2}\,p_{mn} = 0\,. \tag{21}$$

The solution to Eq. (21) is the hypergeometric polynomial [15]

$$p_{mn}(z) = \frac{\Gamma[m-n+1]}{\Gamma[\frac{1}{2}]\Gamma[m-n+\frac{1}{2}]} \times \sum_{k=0}^{m-n}\frac{\Gamma[k+\frac{1}{2}]\Gamma[m-n-k+\frac{1}{2}]}{\Gamma[k+1]\Gamma[m-n-k+1]}\,z^k. \tag{22}$$

In Fig. 1 we plot $|p_{mn}(z_\alpha/z_\beta)|$ vs $\alpha-\beta$. The sharp maximum at small spinon separation is a direct consequence of the strong attractive interaction between the spinons seen in Eq. (20).

We now prove rigorously that this enhancement is responsible for the square-root singularity in the DDS. The susceptibility is defined by

$$\chi_q(\omega) = \sum_X \frac{|\langle X|S_q^-|\Psi_{\mathrm{GS}}\rangle|^2}{\langle X \,|\, X\rangle\langle \Psi_{\mathrm{GS}} \,|\, \Psi_{\mathrm{GS}}\rangle} \times \frac{2(E_X - E_{\mathrm{GS}})}{(\omega+i\eta)^2 - (E_X - E_{\mathrm{GS}})^2}, \tag{23}$$

where $|X\rangle$ denotes an exact eigenstate of $\mathcal{H}$, $E_X$ denotes its eigenvalue, and

$$S_q^- = \sum_\alpha (z_\alpha^*)^k (S_\alpha^x - iS_\alpha^y) \qquad (q = 2\pi k/N). \tag{24}$$

However, since the act of flipping an ↑ spin to ↓ at site $\alpha$ is the same as creating two ↓ spinons on top of each other at site $\alpha$ we have by virtue of Eq. (18)

$$\begin{aligned} S_q^- \Psi_{\mathrm{GS}} &= \sum_\alpha (z_\alpha^*)^k \Psi_{\alpha\alpha} \\ &= N \sum_{m=0}^{M} \sum_{n=0}^{m} (-1)^{m+n} p_{mn}(1) \delta(m+n-k) \Phi_{mn}. \end{aligned} \tag{25}$$

Thus the set of two-spinon eigenstates exhausts the excited states coupled to $\Psi_{\mathrm{GS}}$ by $S_q^-$, and we have

$$\begin{aligned} \chi_q(\omega) = N^2 \sum_{m=0}^{M} \sum_{n=0}^{m} \frac{\langle \Phi_{mn} | \Phi_{mn} \rangle}{\langle \Psi_{\mathrm{GS}} | \Psi_{\mathrm{GS}} \rangle} p_{mn}^2(1) \\ \times \delta(m+n-k) \frac{2(E_{mn} - E_{\mathrm{GS}})}{(\omega + i\eta)^2 - (E_{mn} - E_{\mathrm{GS}})^2}. \end{aligned} \tag{26}$$

This proves that the enhancement is *entirely* due to the functional form of $p_{mn}(z)$ shown in Fig. 1.

The thermodynamic limit is defined as $M \to \infty$, with $m/M$ and $n/M$ held constant. From general properties of the hypergeometric functions [15] we obtain $p_{mn}(1) = \Gamma[1/2]\Gamma[m - n + 1]/\Gamma[m - n + 1/2]$. Then approximating all the gamma functions using Stirling's formula and converting the sums on $n$ and $m$ to integrals over the 1-spinon Brillouin zone, we obtain the Haldane-Zirnbauer formula for the DSS [8]

$$\begin{aligned} \chi_q(\omega) = \frac{J}{2} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} dq_1 \int_{-\frac{\pi}{2}}^{q_1} dq_2 \frac{|q_1 - q_2| \delta(q_1 + q_2 - q)}{\sqrt{E(q_1)E(q_2)}} \\ \times \frac{2E(q_1, q_2)}{(\omega + i\eta)^2 - E^2(q_1, q_2)}, \end{aligned} \tag{27}$$

where $E(q)$ and $E(q_1, q_2)$ are the one-spinon and the two-spinon energies, respectively. This may be exactly integrated over $q_1$ and $q_2$, and the result is

$$\chi_q(\omega) = \frac{J}{4} \frac{\Theta[\omega_2(q) - \omega]\Theta[\omega - \omega_{-1}(q)]\Theta[\omega - \omega_{+1}(q)]}{\sqrt{\omega - \omega_{-1}(q)}\sqrt{\omega - \omega_{+1}(q)}}, \tag{28}$$

where $\omega_{-1}(q) = (J/2)q(\pi - q)$, $\omega_{+1}(q) = (J/2)(2\pi - q)(q - \pi)$, and $\omega_2(q) = (J/2)q(2\pi - q)$.

We see that, in the thermodynamic limit, the enhancement in $p_{mn}$ turns into the square-root divergence in $\chi_q(\omega)$ at threshold. The origin of the branch cut is the threshold energy for the creation of a spinon pair with total momentum $q$. The physical meaning of this branch cut is that the spin wave is unstable versus decay into a spinon pair. Hence, no sharp poles, corresponding to possible low-energy spin-1 stable excitations, develop, but, on the contrary, the spinon-pair threshold is the same as the spin-wave threshold. This last observation points toward the main conclusion of our work: spinon attraction is of fundamental importance for understanding relevant low-energy properties of spin-1/2 antiferromagnets. It generates an enhancement of the probability for two spinons to be at the same site. The enhancement greatly increases the amplitude for a spin-1 excitation to break into a spinon pair, on top of a uniform two-spinon joint density of states. This effect is evident in the thermodynamic limit of our formulas, where we show that the enhancement turns into the branch cut in the DSS.

We thank A. Tagliacozzo and D. I. Santiago for numerous useful discussions. This work was supported primarily by the National Science Foundation under Grant No. DMR-9813899. Additional support was provided by the U.S. Department of Energy under Contract No. DE-AC03-76SF00515 and by the Bing Foundation.

[1] H. A. Bethe, Z. Phys. **71**, 205 (1931).
[2] J. des Cloizeaux and J. J. Pearson, Phys. Rev. **128**, 2131 (1962).
[3] L. A. Takhtadzhan and L. D. Fadeev, Russ. Math. Surv. **34**, 11 (1979); Phys. Lett. **85A**, 375 (1981).
[4] F. D. M. Haldane, Phys. Rev. Lett. **60**, 635 (1988).
[5] F. D. M. Haldane, Phys. Rev. Lett. **66**, 1529 (1991).
[6] B. S. Shastry, Phys. Rev. Lett. **60**, 639 (1988).
[7] C. Nayak and F. Wilczek, Phys. Rev. Lett. **73**, 2740 (1994).
[8] F. D. M. Haldane and M. R. Zirnbauer, Phys. Rev. Lett. **71**, 4055 (1993).
[9] B. Sutherland, Phys. Rev. A **4**, 2019 (1971); **5**, 1372 (1972); F. Calogero, J. Math. Phys. (N.Y.) **10**, 2197 (1969).
[10] F. D. M. Haldane, Z. N. C. Ha, J. C. Talstra, D. Bernard, and V. Pasquier, Phys. Rev. Lett. **69**, 2021 (1992).
[11] J. C. Talstra and S. P. Strong, Phys. Rev. B **56**, 6094 (1997).
[12] D. A. Tennant *et al.,* Phys. Rev. B **52**, 13 368 (1995).
[13] R. B. Laughlin *et al.,* in *Field Theory for Low-Dimensional Systems,* edited by G. Morandi *et al.,* Springer Series in Solid State Physics Vol. 131 (Springer, Berlin, 2000).
[14] K. G. Wilson, J. Math. Phys. **3**, 1040 (1962).
[15] M. Abramowitz, *Handbook of Mathematical Functions,* Applied Mathematics Series Vol. 55 (U.S. GPO, Washington, DC, 1964).