Tracking the Effects of Interactions on Spinons in Gapless Heisenberg Chains

Jean-Sébastien Caux,[1] Hitoshi Konno,[2] Mark Sorrell,[3] and Robert Weston[4]

[1]*Institute for Theoretical Physics, Universiteit van Amsterdam, Science Park 904, Amsterdam, The Netherlands*
[2]*Department of Mathematics, Hiroshima University, Higashi-Hiroshima 739-8521, Japan*
[3]*Department of Mathematics and Statistics, The University of Melbourne, Parkville VIC 3010, Australia*
[4]*Department of Mathematics, Heriot-Watt University, Edinburgh EH14 4AS, United Kingdom*

We consider the effects of interactions on spinon excitations in Heisenberg spin-1/2 chains. We compute the exact two-spinon part of the longitudinal structure factor of the infinite chain in zero field for all values of anisotropy in the gapless antiferromagnetic regime, via an exact algebraic approach. Our results allow us to quantitatively describe the behavior of these fundamental excitations throughout the observable continuum, for cases ranging from free to fully coupled chains, thereby explicitly mapping the effects of "turning on the interactions" in a strongly correlated system.

PACS numbers: 75.10.Jm

Interactions in one-dimensional (1D) systems are known to lead to collective quantum liquid states with low-energy excitations described by the theory of Tomonaga-Luttinger liquids [1]. While the "universal" physics of 1D systems is phenomenologically well understood [2], it is almost always impossible to track the effects of "turning on interactions" on the constituent particles, as one does for Fermi liquids. In this respect, our general understanding of 1D systems can benefit from nonperturbative solutions of microscopic models, a fundamental example being the Heisenberg spin-1/2 anisotropic chain, whose Hamiltonian is (we take $J > 0$)

$$H = J \sum_{j=1}^{N} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z). \quad (1)$$

This system is a Tomonaga-Luttinger liquid for anisotropy (i.e., interaction) values Δ in the range $-1 < \Delta \leq 1$ (in zero field). Its fundamental excitations are spinons [3]: spin-1/2 fractionalized objects which can be viewed as domain walls dressed by quantum fluctuations.

A way to probe the nature of excitations is to determine how they carry observable correlations, an interesting example here being the longitudinal structure factor

$$S^{zz}(k, \omega) = \frac{1}{N} \sum_{j,j'} e^{-ik(j-j')} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle S_j^z(t) S_{j'}^z(0) \rangle. \quad (2)$$

At $\Delta = 0$, this can be written as a density correlator of free Jordan-Wigner fermions. Only single particle-hole excitations contribute, the exact structure factor being proportional to their density of states. For $\Delta > 0$, this picture breaks down [4] due to nonperturbative effects of the interactions.

It is the purpose of this Letter to track in detail the effects of "turning on" $\Delta \neq 0$ interactions on the spinon quasi-particles and their ability to carry correlations, throughout the gapless antiferromagnetic regime $0 \leq \Delta \leq 1$, which can be realized by closing the triplet gap in frustrated spin ladder systems [5,6] (the anisotropy being determined by the values of the frustrated couplings; for example, in $(C_5H_{12}N)_2CuBr_4$ [7,8], this leads to a $\Delta = 0.5$ *XXZ* chain with tunable field), or using optical lattices [9], in which the tuning of the anisotropy is now possible using photon-assisted superexchange processes [10]. Focusing on zero temperature, we will compute the exact two-spinon contribution to (2) directly in the thermodynamic limit $N \to \infty$, using an adaptation of the "vertex operator approach" [11]. Our results provide a strict lower bound and (for practical purposes) an extremely accurate representation for the complete correlator of the infinite system (more that 99% for $\Delta < 0.5$) throughout the observable excitation continuum. They provide a robust benchmark for assessing the line shapes obtained for finite systems directly from integrability [12] or using variants of the density matrix renormalization group (DMRG) [13] or quantum Monte Carlo (QMC) [14] calculations, and confirm the threshold behavior predicted using field theory [15–17], complementing it with exact prefactors. Our results, which unlike the latter are valid for general energies and momenta, should be more directly comparable to finite-resolution experimental (e.g., inelastic neutron scattering) measurements.

The vertex operator approach was originally developed for $\Delta \geq 1$ where the Hamiltonian commutes with the action of the quantum group $U_q(\widehat{sl}_2)$. The representation theory of this quantum group leads to explicit expressions for states, physical operators and their matrix elements [11], providing building blocks for correlations in terms of contributions from intermediate states made of increasing numbers of pairs of spinons, $S^{zz}(k, \omega) = \sum_{m=1}^{\infty} S_{(2m)}^{zz}(k, \omega)$. The calculation of (2) was treated using the vertex operator approach at $\Delta = 1$ for two [18,19] and four spinons [20], the combination being shown to yield

about 99% overall accuracy. The $\Delta > 1$ regime was also considered [21]. The physically more interesting quantum critical gapless regime ($0 \leq \Delta \leq 1$) remains however largely unexplored by these exact thermodynamic methods. Our Letter aims to fill this gap.

Spinon excitations.—The ground state of the gapless *XXZ* antiferromagnet supports spinon excitations [3] with exact zero-field dispersion relation $e(p) = v_F|\sin p|$, $p \in [-\pi, 0]$, where the Fermi velocity is $v_F(\Delta) = \frac{\pi J}{2} \frac{\sqrt{1-\Delta^2}}{\arccos\Delta}$. Spinons always appear in pairs, so the simplest states which contribute to the structure factor are made of 2 spinons. Parametrizing their momentum by p_1 and p_2, momentum and energy conservation impose $k = -p_1 - p_2$, $\omega = e(p_1) + e(p_2)$. The two-spinon states thus form a continuum in k-ω defined by lower and upper boundaries

$$\omega_{2,l}(k) = v_F|\sin k|, \qquad \omega_{2,u}(k) = 2v_F \sin(k/2). \quad (3)$$

Matrix elements.—The vertex operator approach is also applicable, albeit indirectly, to the gapless region $0 \leq \Delta \leq 1$. The strategy [22,23] is to first generalize to the completely anisotropic Heisenberg model $\sum_j (J_x S_j^x S_{j+1}^x + J_y S_j^y S_{j+1}^y + J_z S_j^z S_{j+1}^z)$ in the principal regime $|J_y| \leq J_x \leq J_z$ [24] for which matrix elements of local operators between the vacuum and excited states can be computed using a variant of the vertex operator approach [25]. These results can then be mapped to the disordered regime $|J_z| \leq J_y \leq J_x$ [23,26] before taking the $J_x \rightarrow J_y$ limit to reconstruct the matrix elements for (1) with $0 \leq \Delta \leq 1$. In this way we find the following exact expression for the two-spinon contribution to $S^{zz}(k, w)$:

$$S_2^{zz}(k, \omega) = \frac{\Theta(\omega_{2,u}(k) - \omega)\Theta(\omega - \omega_{2,l}(k))}{\sqrt{\omega_{2,u}^2(k) - \omega^2}}(1 + 1/\xi)^2$$
$$\times \frac{e^{-I_\xi(\rho(k,\omega))}}{\cosh\frac{2\pi\rho(k,\omega)}{\xi} + \cos\frac{\pi}{\xi}}, \quad (4)$$

in which $\xi = \frac{\pi}{\arccos\Delta} - 1$, Θ is the Heaviside function, and

$$I_\xi(\rho) \equiv \int_0^\infty \frac{dt}{t} \frac{\sinh[(\xi+1)t]}{\sinh(\xi t)} \frac{[\cosh(2t)\cos(4\rho t) - 1]}{\cosh(t)\sinh(2t)} \quad (5)$$

in which the parameter ρ is defined as

$$\cosh(\pi\rho(k, \omega)) = \sqrt{\frac{\omega_{2,u}^2(k) - \omega_{2,l}^2(k)}{\omega^2 - \omega_{2,l}^2(k)}}. \quad (6)$$

Results.—In Fig. 1, we plot the two-spinon part of the structure factor (4) for values of Δ between weak and strong coupling. A few striking things are worth mentioning concerning the influence of interactions on the correlations. Most noticeably, the upper threshold divergence disappears immediately upon turning interactions on. The correlation weight also starts flowing around the edges of

the continuum, mostly via the wings at $k \simeq 0, 2\pi$ (see, e.g., the $\Delta = 0.2$ plot), and thereafter starts accumulating at the antiferromagnetic point $k = \pi$ (see the $\Delta = 0.4$ plot). The lower threshold divergence starts carrying more weight from $\Delta \simeq 0.5$ onwards, and becomes increasingly sharp as one approaches the isotropic point. Within the two-spinon continuum, the weight quickly changes shape as Δ is turned on: from a pure $[\omega_{2,u}(k) - \omega]^{-1/2}$ form at $\Delta = 0$, it becomes almost uniform in frequency for $\Delta \simeq 0.2$; it then becomes a rapidly decreasing function of frequency for higher interactions. Turning interactions on thus leads to a remarkable collapse of correlation weight from *high* to *low* energies.

Sum rules.—To quantify the importance of the two-spinon contribution to the full structure factor, we use two useful sum rules, namely, the integrated intensity

$$I^{zz} = \int_0^{2\pi} \frac{dk}{2\pi} \int_0^\infty \frac{d\omega}{2\pi} S^{zz}(k, \omega) = 1/4, \quad (7)$$

and the *f* sum rule (at fixed momentum) [27],

$$I_1^{zz}(k) = \int_0^{2\pi} \frac{d\omega}{2\pi} \omega S^{zz}(k, \omega) = -2X^x(1 - \cos k), \quad (8)$$

where $X^x \equiv \langle S_j^x S_{j+1}^x \rangle$ is the ground-state expectation value of the in-plane exchange term. This can be obtained from the ground-state energy density e_0 [28] and its derivative, namely $X^x = \frac{1}{2J}(1 - \Delta\frac{\partial}{\partial\Delta})e_0$, with $e_0 = \frac{-J(\xi+1)}{2\pi} \times \sin[\frac{\pi}{\xi+1}]\int_{-\infty}^\infty dt(1 - \frac{\tanh t}{\tanh[(\xi+1)t]})$. We provide the explicit values of the sum rule saturations coming from two-spinon contributions in Table I (for the *f* sum rule, the saturation is the same at all momenta). The two-spinon states carry the totality of the correlation at $\Delta = 0$, and this remains approximately true up to surprisingly large values of interactions $\Delta \sim 0.8$, above which four, six, ... spinon states become noticeable. Interestingly, this level of saturation from few spinon states does not hold for the transverse (in-plane) structure factor for $\Delta < 1$, for which (as anticipated earlier [29]) the two-spinon states have a vanishing contribution [30]; our method is thus not directly applicable to this correlation.

Threshold behavior.—The behavior of the longitudinal structure factor in the vicinity of thresholds can be determined analytically from (4)–(6), allowing us to make contact with and complement recent field theory predictions [17,31] (the former giving the correct exponent).

The structure factor near the upper threshold.—The upper threshold $\omega \rightarrow \omega_{2,u}(k)$ is approached by the limit $\rho \rightarrow 0$ as can be seen from (6). A careful evaluation shows that the integral (5) then behaves according to $I_\xi(\rho) \overset{\rho \rightarrow 0}{\rightarrow} -2\ln\rho + O(1)$. We thus have from (4) and (6) that the structure factor vanishes as a square root,
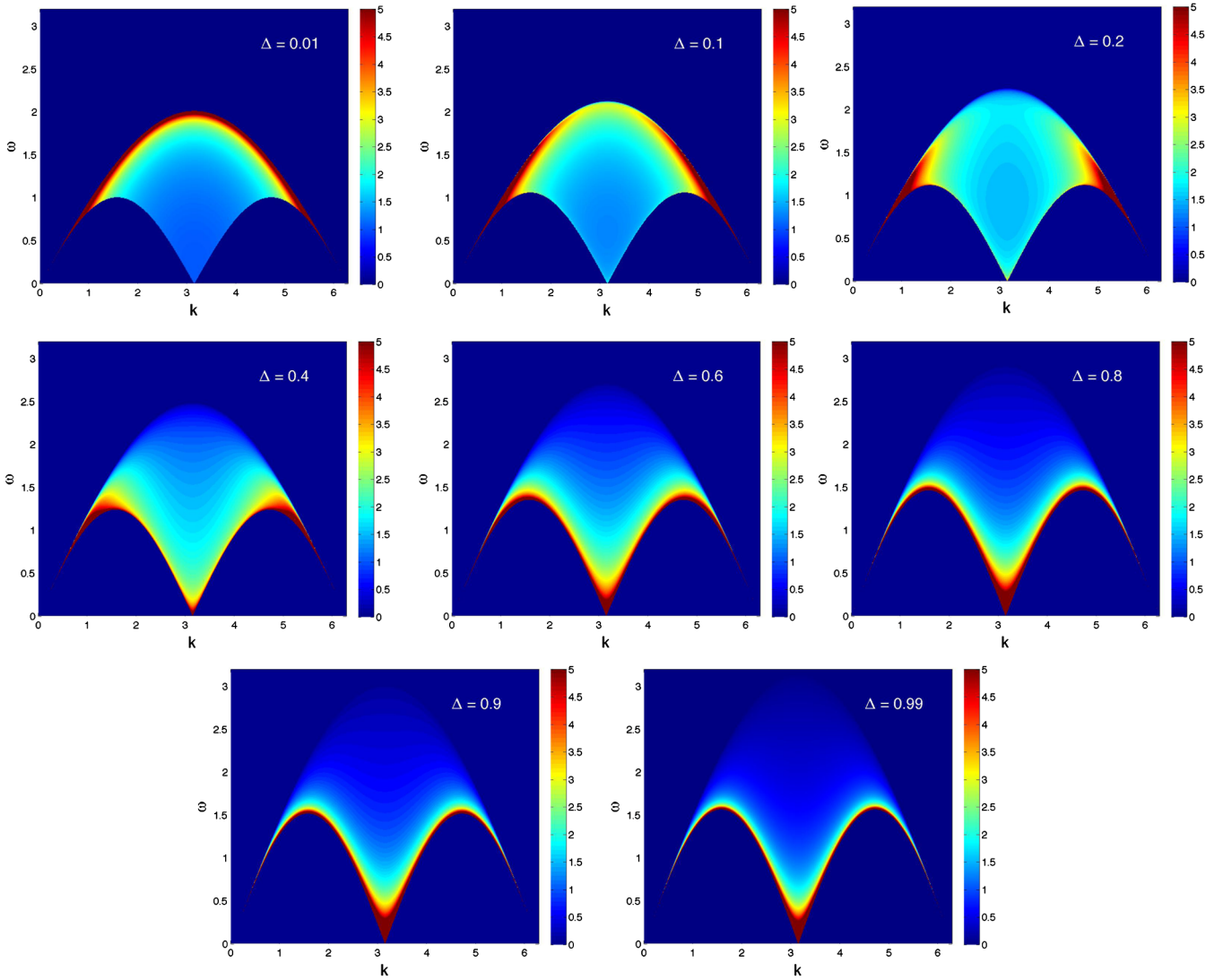
FIG. 1 (color online).   Two-spinon part of the longitudinal structure factor of the infinite Heisenberg chain, for different values of the anisotropy parameter Δ. For $\Delta \to 0$, the correlation follows the density of states, and has a square-root singularity at the upper threshold for all values of momenta. Increasing the anisotropy shifts the weight progressively towards the lower boundary. The lower boundary becomes increasingly sharp as the $\Delta \to 1$ limit is approached.

$$S_2^{zz}(k, \omega) \overset{\omega \to \omega_{2,u}(k)}{\to} f_u(\xi)\left(\sin\frac{k}{2}\right)^{-7/2}\sqrt{\omega_{2,u}(k) - \omega} \quad (9)$$

in which $f_u(\xi)$ is a momentum-independent function of anisotropy. The anisotropy-independent square-root cusp at the threshold (for $0 < \Delta \leq 1$) confirms the field theory predictions [17], and at $\Delta \to 1$ matches the same limit known to apply for the *XXX* case [19]. The prefactor we obtain here varies quickly with momentum, showing strong enhancement of the upper threshold singularity when taking the momentum towards the $k = 0$, 2π zone boundaries (as can be seen in Fig. 1, most clearly at small anisotropies). For the $\Delta \to 0$ limit (so $\xi \to 1$), the $\cosh\frac{2\pi\rho}{\xi} + \cos\frac{\pi}{\xi}$ in the denominator of (4) vanishes when $\rho \to 0$. Overall, in this case one rather obtains a square-root divergence,

$S_2^{zz}(k, \omega) \overset{\omega \to \omega_{2,u}(k)}{\to} f_u(1)\dfrac{(\sin\frac{k}{2})^{-1/2}}{\sqrt{\omega_{2,u}(k) - \omega}}$, which follows the singularity of the density of states (the matrix elements are then energy independent). This discontinuous in Δ threshold

TABLE I.   Sum rule saturations as a function of anisotropy: two-spinon contribution to the integrated intensity I^{zz} (7) and first frequency moment I_1^{zz} (8).

Δ	I_{2sp}^{zz}/I^{zz}	$I_{1,2sp}^{zz}/I_1^{zz}$	Δ	I_{2sp}^{zz}/I^{zz}	$I_{1,2sp}^{zz}/I_1^{zz}$
0	1	1	0.6	0.9778	0.9743
0.1	0.9997	0.9997	0.7	0.9637	0.9578
0.2	0.9986	9.9984	0.8	0.9406	0.9314
0.3	0.9964	9.9959	0.9	0.8980	0.8844
0.4	0.9927	0.9917	0.99	0.7918	0.7748
0.5	0.9869	0.9849	0.999	0.7494	0.7331

exponent behavior is also consistent with field theory [17]. We notice further that the momentum dependence of the prefactor is changed to a much weaker one than that at $\Delta \neq 0$.

The structure factor near the lower threshold.—The limit $\omega \rightarrow \omega_{2,l}(k)$ is obtained via $\rho \rightarrow \infty$. Evaluating (5) yields $I_\xi(\rho) \overset{\rho \rightarrow \infty}{\rightarrow} -\pi(1 + \frac{1}{\xi})\rho + O(1)$. The structure factor then obeys

$$S_2^{zz}(k, \omega) \overset{\omega \rightarrow \omega_{2,l}(k)}{\rightarrow} f_l(\xi) \frac{|\sin k|^{-(1/2)(1-1/\xi)}(\sin \frac{k}{2})^{-2/\xi}}{[\omega - \omega_{2,l}(k)]^{(1/2)(1-1/\xi)}}, \quad (10)$$

where $f_l(\xi)$ is again a momentum-independent function of anisotropy. The singularity exponent reproduces an early conjecture [4] and field theory predictions [17]; the momentum-dependent part of the prefactor shows an even more complicated behavior than that of the upper threshold, being enhanced (though differently) both at the zone boundaries $k = 0, 2\pi$ as well as near $k = \pi$. As a final detail, the $\Delta \rightarrow 0$ limit (so $\xi \rightarrow 1$) yields the expected behavior, $S_2^{zz}(k, \omega) \overset{\omega \rightarrow \omega_{2,l}(k)}{\rightarrow} O(1)$.

Conclusions.—In summary, we have tracked how spinons in Heisenberg antiferromagnets contribute to the longitudinal structure factor (2), as a function of anisotropy (i.e., interaction). We obtained the two-spinon part of (2) exactly in the zero field, infinite-size chain throughout the gapless antiferromagnetic regime, using the vertex operator approach. Our results provide an exact lower bound for and an extremely accurate description of the full correlator (as shown by sum rules) throughout the observable continuum (i.e., not only at low energies or near thresholds), provide a resilient check for alternate methods and give a nonperturbative derivation of threshold exponents, complementing these with exact prefactors. The precise functional form we obtained also allows us to determine the region of validity of the threshold behavior; we will address this and other issues in future work.

[1] F. D. M. Haldane, J. Phys. C **14**, 2585 (1981).
[2] T. Giamarchi, *Quantum Physics in One Dimension* (Oxford University Press, Oxford, 2004).
[3] L. D. Faddeev and L. A. Takhtajan, Phys. Lett. A **85**, 375 (1981).
[4] G. Müller, H. Thomas, H. Beck, and J. C. Bonner, Phys. Rev. B **24**, 1429 (1981); G. Müller, H. Thomas, M. W. Puga, and H. Beck, J. Phys. C **14**, 3399 (1981).
[5] K. Totsuka, Phys. Rev. B **57**, 3454 (1998).
[6] F. Mila, Eur. Phys. J. B **6**, 201 (1998).
[7] B. C. Watson et al., Phys. Rev. Lett. **86**, 5168 (2001).
[8] B. Thielemann et al., Phys. Rev. Lett. **102**, 107204 (2009).
[9] A. B. Kuklov and B. V. Svistunov, Phys. Rev. Lett. **90**, 100401 (2003); L.-M. Duan, E. Demler, and M. D. Lukin, Phys. Rev. Lett. **91**, 090402 (2003); J. J. Garcia-Ripoll and J. I. Cirac, New J. Phys. **5**, 76 (2003); M. Lewenstein et al., Adv. Phys. **56**, 243 (2007).
[10] Y.-A. Chen, S. Nascimbène, M. Aidelsburger, M. Atala, S. Trotzky, and I. Bloch, arXiv:1104.1833.
[11] M. Jimbo and T. Miwa, *Algebraic Analysis of Solvable Lattice Models* (American Mathematical Society, Providence, RI, 1995).
[12] J.-S. Caux and J. M. Maillet, Phys. Rev. Lett. **95**, 077201 (2005); J.-S. Caux, R. Hagemans, and J. M. Maillet, J. Stat. Mech. (2005) P09003.
[13] S. R. White and A. E. Feiguin, Phys. Rev. Lett. **93**, 076401 (2004); A. J. Daley, C. Kollath, U. Schollwöck, and G. Vidal, J. Stat. Mech. (2004) P04005; J. Sirker, Phys. Rev. B **73**, 224424 (2006).
[14] O. F. Syljuåsen, Phys. Rev. B **78**, 174429 (2008).
[15] M. Pustilnik, M. Khodas, A. Kamenev, and L. I. Glazman, Phys. Rev. Lett. **96**, 196405 (2006).
[16] R. G. Pereira et al., Phys. Rev. Lett. **96**, 257202 (2006).
[17] R. G. Pereira, S. R. White, and I. Affleck, Phys. Rev. Lett. **100**, 027206 (2008); R. G. Pereira, S. R. White, and I. Affleck, Phys. Rev. B **79**, 165113 (2009).
[18] A. H. Bougourzi, M. Couture, and M. Kacir, Phys. Rev. B **54**, R12 669 (1996).
[19] M. Karbach et al., Phys. Rev. B **55**, 12510 (1997).
[20] A. Abada, A. H. Bougourzi, and B. Si-Lakhal, Nucl. Phys. B **497**, 733 (1997); J.-S. Caux and R. Hagemans, J. Stat. Mech. (2006) P12013.
[21] A. H. Bougourzi, M. Karbach, and G. Müller, Phys. Rev. B **57**, 11 429 (1998); J.-S. Caux, J. Mossel, and I. P. Castillo, J. Stat. Mech. (2008) P08006.
[22] M. Jimbo and T. Miwa, J. Phys. A **29**, 2923 (1996).
[23] M. Jimbo, H. Konno, and T. Miwa, in *Deformation Theory and Symplectic Geometry*, edited by D. Sternheimer, J. Rawnsley, and S. Gutt (1997), No. 20 in Math. Phys. Studies, p. 117, proceedings of the Ascona Meeting, 1996.
[24] R. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic Press, London, 1982).
[25] M. Lashkevich and Y. Pugai, Nucl. Phys. **B516**, 623 (1998); M. Lashkevich and Y. Pugai, JETP Lett. **68**, 257 (1998); M. Lashkevich, Nucl. Phys. **B621**, 587 (2002); T. Kojima, H. Konno, and R. Weston, Nucl. Phys. **B720**, 348 (2005).
[26] S. Lukyanov and V. Terras, Nucl. Phys. **B654**, 323 (2003).
[27] P. C. Hohenberg and W. F. Brinkman, Phys. Rev. B **10**, 128 (1974).
[28] C. N. Yang and C. P. Yang, Phys. Rev. **150**, 327 (1966).
[29] M. Arikawa, M. Karbach, G. Müller, and K. Wiele, J. Phys. A **39**, 10623 (2006).
[30] J.-S. Caux, H. Konno, M. Sorrell, and R. Weston (to be published).
[31] V. V. Cheianov and M. Pustilnik, Phys. Rev. Lett. **100**, 126403 (2008).