Magnetization plateaus and Luttinger liquid behavior in *XXZ* chains with superlattice structure

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We study spin superlattices composed of a repeated pattern of two long spin-$\frac{1}{2}$ *XXZ* chains with different anisotropy parameters. They can be viewed as the limit of *p*-merized chains when the number of sites per cluster is very large. Magnetization plateaus are found, with magnetization values that depend on the relative sizes of the subchains. In certain regions of parameter space, the low-energy properties are described in terms of a Luttinger liquid superlattice parametrized by an effective velocity and an effective compactification radius.

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Quantum magnetism in one dimension (1D) has revealed a number of surprises in the last two decades that can be partly associated with an interplay of fluctuations and topology.[1] One example is the conjecture due to Haldane[2–7] that isotropic Heisenberg half-integer spin chains are gapless, whereas integer spin ones are gapful. Related to the Haldane gaps are the magnetization plateaus, which are essentially macroscopic quantum phenomena in which the magnetization in an external magnetic field is quantized to fractions of the saturated value. Following up on initial studies on organic compounds,[8,9] Oshikawa, Yamanaka, and Affleck[10] extended the Lieb-Schultz-Mattis theorem[11] to systems in a magnetic field, thus arriving at a necessary condition for the appearance of magnetization plateaus in 1D systems, namely,

$$p(S-m^z)=(\text{integer}). \tag{1}$$

Here, p is the number of sites in the unit cell of the magnetic ground state, S is the magnitude of the spin, and m^z is the magnetization per site (taken to be in the z direction). The plateau state can be viewed as a spin gapped state with nonzero magnetization, the Haldane systems being a special case where $p=1$ and $m^z=0$. In the particular case of spin ladders in a magnetic field, for example, the phase diagram has been thoroughly mapped and it has been discovered that the necessary condition (1) becomes also sufficient.[12–14] Moreover, the existence of real dimerized[15] and trimerized[16,17] systems has lent a great impetus to the studies of *p*-merized chains and ladders.[12,13,18–27] Despite the existence of considerable theoretical insight, a satisfactory understanding of the experimental situation is still lacking.

Thus motivated, we focus here on a different limit of the problem of *p*-merized chains, namely, the case where the repeated pattern consists of *two long anisotropic spin-*$\frac{1}{2}$ *XXZ chains*. In this case, each uniform stretch of the chain can be treated in the continuum limit and a Luttinger liquid (LL) description[28–36] becomes possible in some parameter ranges. We, therefore, view the *p*-merized spin chain as a *spin superlattice* (SS) and its description can then be framed in terms of a LL superlattice.[37]

Consider a SS whose unit cell consists of two $S=1/2$ *XXZ* chains with different anisotropy parameters Δ_λ and sizes L_λ ($\lambda=1,2$) (but the same planar coupling) in the presence of a magnetic field h applied along the anisotropy (z) axis. Its Hamiltonian is

$$H=J\sum_{n=1}^{L}\left(S_n^xS_{n+1}^x+S_n^yS_{n+1}^y+\Delta_\lambda S_n^zS_{n+1}^z\right)-h\sum_{n=1}^{L}S_n^z, \tag{2}$$

where S^x, S^y, and S^z denote the spin-$\frac{1}{2}$ operators and $L=N_c(L_1+L_2)$ is the superlattice size. Here, N_c is the number of unit cells, each of which has a basis with L_1+L_2 sites. We assume the chain is subjected to periodic boundary conditions.

In the homogeneous situation ($\Delta_\lambda=\Delta$, independent of the position), the Hamiltonian (2) is exactly solvable by the Bethe Ansatz.[38–41] Furthermore, for $\Delta>-1$ and a range of h values (see below), its low-energy properties can be described in terms of a LL with velocity u and interaction parameter K (or, equivalently, compactification radius R, with $2\pi KR^2=1$).[13,42,43]

We then take advantage of the fact that *each subchain is a* LL *connected at its ends to reservoirs* (the rest of the lattice) to describe the low-energy properties of the SS in terms of a LL superlattice (LLSL)[37] with Hamiltonian

$$H=\frac{1}{2\pi}\int dx\left\{u(x)K(x)(\partial_x\Theta)^2+\frac{u(x)}{K(x)}(\partial_x\Phi)^2\right\}. \tag{3}$$

Here, we have introduced the subchain-dependent parameters $u(x)$ and $K(x)$. For x on the sublattice λ, one has $K(x)=K(J,\Delta_\lambda,h)$ and $u(x)=u(J,\Delta_\lambda,h)$, i.e., the usual uniform LL parameters for each subchain, which can be obtained directly from the Bethe Ansatz solution.[13,42]

In the Hamiltonian (3), $\partial_x\Theta$ is the momentum field conjugate to Φ: $[\Phi(x),\partial_y\Theta(y)]=i\delta(x-y)$. Φ and Θ are dual fields, since they satisfy both

$$\partial_t\Phi=u(x)K(x)\partial_x\Theta \tag{4}$$

and the equation obtained through the replacements $\Phi\rightarrow\Theta$, $\Theta\rightarrow\Phi$, and $K\rightarrow1/K$. These equations can be uncoupled to yield

$$\partial_{tt}\Phi-u(x)K(x)\partial_x\left(\frac{u(x)}{K(x)}\partial_x\Phi\right)=0, \tag{5}$$

and a dual equation for Θ.

The equations of motion are subject to the continuity of Φ and Θ.[44–47] This guarantees the continuity of the spin field. Since the time derivatives of these functions are continuous, the right-hand side of Eq. (4) and its dual yield, as additional conditions, the continuity of $(u/K)\partial_x\Phi$ and $uK\partial_x\Theta$ at the contacts. Physically, this reflects the conservation of the z-axis magnetization current density $j=\sqrt{2}\partial_t\Phi/\pi$ at the interfaces between the subchains, see, Eq. (4).

We diagonalize the Hamiltonian (3) through a normal-mode expansion of the phase fields[37]

$$\Phi(x,t)=-i\sum_{p\neq 0}\ \mathrm{sgn}(p)\,\frac{\phi_p(x)}{2\sqrt{\omega_p}}[b_{-p}e^{i\omega_p t}+b_p^\dagger e^{-i\omega_p t}] -\phi_0(x)+\gamma_\lambda t, \tag{6}$$

$$\Theta(x,t)=i\sum_{p\neq 0}\frac{\theta_p(x)}{2\sqrt{\omega_p}}[b_{-p}e^{i\omega_p t}-b_p^\dagger e^{-i\omega_p t}]+\theta_0(x)-\tau_\lambda t, \tag{7}$$

where $b_p^\dagger$ are boson creation operators $(p>0)$. Plugging Eq. (6) into Eq. (5) we obtain an eigenvalue problem for $\phi_p(x)$ with eigenvalues ω_p, and similarly for $\theta_p(x)$. In Eqs. (6) and (7), $\phi_0(x)$ and $\theta_0(x)$ are the zero-mode functions which, in the homogeneous case, are given by $\phi_0(x)=N(\pi x/L)$, $\theta_0(x)=J(\pi x/L)$, where N and J are the number and current operators.[35,36] Besides, in this case $\gamma=\pi uKJ/L$ and $\tau=\pi(u/K)N/L$. In the superlattice case, there will be, in general, a nonuniform magnetization profile. This will be captured by a subchain-dependent number operator N_λ. Introducing also subchain-dependent currents J_λ, we have

$$\phi_0(x)=A_{j,\lambda}+\frac{\pi N_\lambda x}{L_\lambda}, \tag{8}$$

$$\theta_0(x)=B_{j,\lambda}+\frac{\pi J_\lambda x}{L_\lambda}. \tag{9}$$

$A_{j,\lambda}$ and $B_{j,\lambda}$ are given by

$$A_{j,\lambda}=(j-1)\pi L_2\left(\frac{N_2}{L_2}-\frac{N_1}{L_1}\right) \tag{10}$$

with an analogous expression for $B_{j,\lambda}$ obtained with the replacement of N_λ by J_λ. Here, $j=1,2,3,\ldots$ labels the unit cell. The ground state for a given magnetic field h has $J_\lambda=0$ and N_λ can be determined from the equation of state obtained from the exact solution[13,38–41]

$$h=h(J,\Delta_1,M_1)=h(J,\Delta_2,M_2). \tag{11}$$

Note that here, $M_\lambda=2m_\lambda^z=1-2N_\lambda/L_\lambda$ is the magnetization per site of subchain λ normalized to the saturation value. Then, the total magnetization of the SS is simply the weighted average

$$M_s=\frac{L_1M_1+L_2M_2}{L_1+L_2}. \tag{12}$$

We stress that Eqs. (11) and (12) are valid also in the regions where the LL description no longer applies. These are (i) the ferromagnetic region (FMR) for $\Delta<-1$ and for any Δ at high enough fields and (ii) the antiferromagnetic region (AFMR) at small fields and $\Delta>1$ (see, e.g., Fig. 1 of Ref. 13). In the AFMR, the system is described by a sine-Gordon theory and has a gap, whereas in the FMR the system is fully magnetized and cannot be described by a Lorentz-invariant field theory.[43]

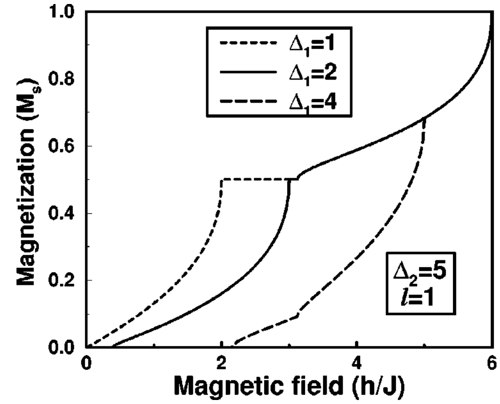

FIG. 1. Magnetization curve of the spin superlattice with $\Delta_2=5$ and $\Delta_1=1$, 2, 4 $(l=1)$.

Figure 1 shows the magnetization of the SS $(L_2/L_1\equiv l=1)$ as a function of the external magnetic field for $\Delta_2=5$ and $\Delta_1=1$, 2, 4. We can see the existence of magnetization plateaus at $M_s=0$ and $M_s=0.5=1/(1+l)$. The plateaus occur when the subchain magnetizations are either zero (AFMR) or one (FMR), where the LLSL description is not possible. Depending on the value of Δ_1, the system may exhibit one or both kinds of plateaus, as seen in Fig. 1. In Fig. 2, we show the magnetization of the SS with $\Delta_2=5$ and $\Delta_1=2$ for different values of l. There is a plateau with $M_s=0$ for magnetic fields smaller than $h_c=0.3898J$, for any l. For higher fields, another plateau is present at $M_s=1/(1+l)$, which corresponds to $M_1=1$ (FMR) and $M_2=0$ (AFMR). Thus, at this plateau, the SS exhibits a spatial modulation of the magnetization. Note that, whereas the width of the plateaus is always the same, the magnetization value *can vary continuously with l*. This feature is a macroscopic signature of the superlattice structure and is an extreme limit of the magnetization plateaus systematized in Ref. 10. Another feature also pointed out in the latter refer-

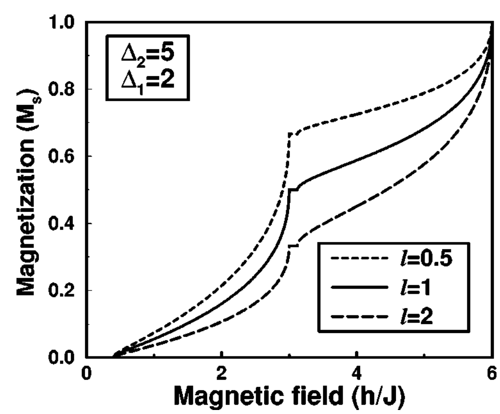

FIG. 2. Magnetization curve of the spin superlattice with $\Delta_2=5$ and $\Delta_1=2$ for different values of l.

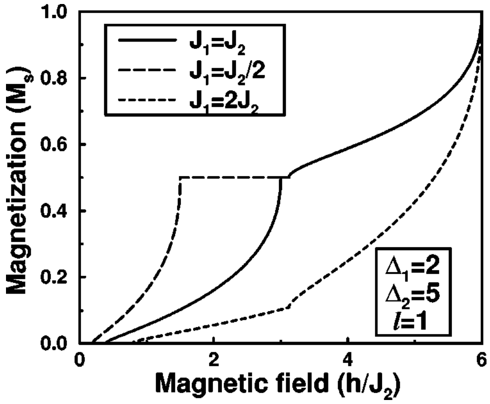

FIG. 3. Magnetization as a function of external field h for spin superlattices with different exchange coupling ratios and fixed anisotropy parameters.

ence is the field dependence of the magnetization as the plateau is approached: $M_s \propto \sqrt{|h-h_c|}$, typical of this universality class.[48–50] In this case, this is due to the weighted average nature of M_s [Eq. (12)] and the individual square-root dependences of both M_1 and M_2 upon approaching their plateau values. By contrast, however, here the gap is not the consequence of a relevant perturbation,[10] as is usually the case, since the ferromagnetically saturated subchain simply cannot be described by a field theory.[43]

On the other hand, generalizing the model in Eq. (2) by allowing different values of the exchange constants J_λ of the subchains, but keeping the anisotropies fixed, one can tune the width of the plateaus (though not the magnetization values), as can be seen in Fig. 3. This happens because, by lowering the exchange coupling (long-dashed curve in Fig. 3), one lowers the magnetic-field scale and the subchain can then be more easily saturated. Likewise, by enhancing that scale, one can even get rid of the plateau altogether (short-dashed curve in Fig. 3).

The LLSL description is only possible away from the plateaus, since they reflect "spin incompressibility." The phase diagram for a SS with $\Delta_1 < \Delta_2 \neq 0$ and any l is shown in Fig. 4. The LLSL description is possible only for magnetic fields higher than $h_c(\Delta_2=5)=3.2182J$ (dashed line in Fig. 4). For

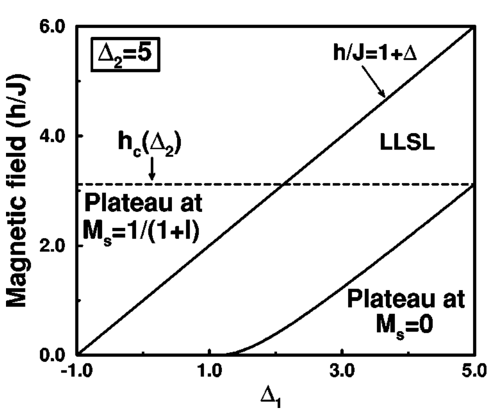

FIG. 4. Phase diagram for spin superlattice with $\Delta_2=5$.

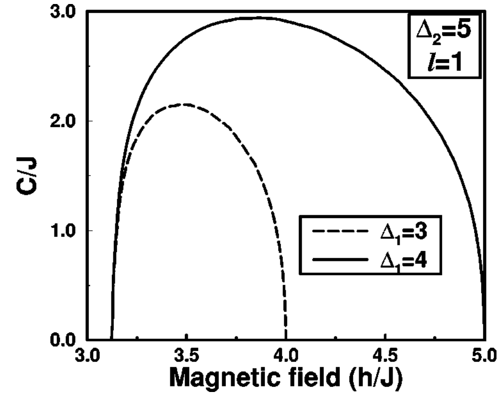

FIG. 5. The effective velocity of a spin superlattice as a function of magnetic field h for $l=1$, with $\Delta_2=5$ and $\Delta_1=3$ and 4.

smaller fields, we have plateaus at $M_s=1/(1+l)$ for $-1<\Delta_1<2.2182$ and antiferromagnetism with an $M_s=0$ plateau for $\Delta_1>1$. Therefore, in the interval $1<\Delta_1<2.2182$, there are two magnetization plateaus (cf., Fig. 1). The other regions in this phase diagram have magnetizations $M_s \neq 0$, 1 and no plateaus. Furthermore, the phase diagram is valid only for $\Delta_2>1$. For $-1<\Delta_1<\Delta_2<1$, no plateaus are possible due to the absence of subchain antiferromagnetism.

For $p \ll \pi/(L_2+L_1)$, $\omega_p \cong c|p|$, and the effective velocity for the SS is

$$c=\frac{u_1(1+l)}{\sqrt{1+\eta l u_1/u_2+(l u_1/u_2)^2}}, \tag{13}$$

where $\eta=K_1/K_2+K_2/K_1$. Clearly, $c \to u_2$ as $l \to \infty$, and $c \to u_1$ as $l \to 0$. The effective velocity is shown in Fig. 5, in the region where a LLSL description exists, namely, for magnetic fields between $h_c(\Delta_2=5)=3.2182J$ and $h/J=1+\Delta_1$. The important feature to notice in Eq. (13) is the spatial averaging of the velocities induced by the superlattice structure, a feature ubiquitous to LLSL's.[37]

In terms of the bosonic fields, the spin operators read[31]

$$S_x^z=\frac{M}{2}-\frac{1}{\sqrt{2\pi}}\partial_x\Phi+\frac{1}{\pi\alpha}\cos[2\Phi(x)-2\bar{\phi}(x)],$$

$$S_x^+=\frac{1}{\sqrt{2\pi\alpha}}\exp[-i\Theta(x)]\{1+e^{2i\bar{\phi}(x)}\cos[2\Phi(x)]\},$$

where $\bar{\phi}(x)=k_F x-\phi_0(x)$, the Fermi momentum k_F is related to the magnetization by $k_F=(1+M)\pi/2$ and α is a cutoff parameter.[36] Thus, the correlation functions of the SS (for well separated x and y) are given by

$$\langle S^z(y)S^z(x)\rangle \sim \frac{C}{2\pi^2|x-y|^2}+A\frac{\exp\{2i[\bar{\phi}(y)-\bar{\phi}(x)]\}}{|x-y|^{2K^*}} \tag{14}$$

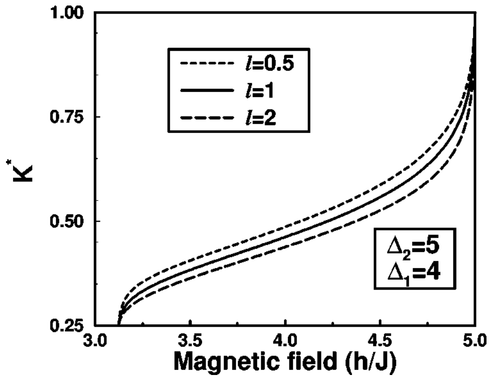

FIG. 6. The correlation exponent K^* of a spin superlattice as a function of magnetic field h with $\Delta_2=5$ and $\Delta_1=4$, for $l=0.5$, 1, 2.

$$\langle S^+(y)S^-(x)\rangle \sim \frac{B_1}{|x-y|^{K/2}} + B_2\frac{\exp\{2i[\overline{\phi}(y)-\overline{\phi}(x)]\}}{|x-y|^{K/2+2K^*}}, \tag{15}$$

where the LLSL effective exponent is

$$K^* = \frac{\sqrt{1+\eta l u_1/u_2+(l u_1/u_2)^2}}{\dfrac{1}{K_1}+l\dfrac{1}{K_2}\dfrac{u_1}{u_2}} \equiv f(K_1,K_2), \tag{16}$$

$\overline{K}=f(1/K_1,1/K_2)$ and C is a function of system parameters and the subchain lengths.[37] From Eqs. (14) and (15), we see how the correlation functions of the homogeneous system are recovered when $K_1=K_2$ and $u_1=u_2$.

In Fig. 6, the correlation exponent K^* of a SS is shown as a function of the magnetic field. We observe that $K^*<1$, as in the homogeneous case with anisotropy larger than one. Besides, K^* interpolates smoothly between K_1 and K_2 as l increases [cf., Eq. (16)], another manifestation of the spatial averaging due to the superlattice structure.

It is interesting to relate the above treatment to previous strong coupling analyses. It has been shown that the magnetization plateaus can be easily understood in terms of strongly coupled clusters of spins that are weakly coupled to each other. In this case, the clusters will tend to magnetize independently, leading to the quantized magnetization values.[12,13,22,26] This is precisely what happens in the SS case. Because we focus on the limit of very long subchains, the boundary interactions between them is always a *weak perturbation* and the strong coupling argument holds.

We note, in passing, that certain boundary conditions can be frustrating and lead to important effects in small spin chains. One example is a Heisenberg chain with an odd number of sites and periodic boundary conditions (PBC).[13,14] Thus, an N-leg spin ladder with odd N and transverse PBC (a ''spin tube'') appears to have a gap at zero magnetic field (with a corresponding plateau), whereas the same system with open boundary conditions (OBC) is gapless. In Ref. 13, it was argued that even in the $N\to\infty$ limit, this gap may survive. The question of transverse boundary conditions does not arise in our case and we have kept to PBC along the chain. It does not appear that different boundary conditions would modify our plateau results, specially since we restrict ourselves to very long subchains. In particular, the condition for a magnetization plateau we find, namely, that the subchains are either in the AFMR or in the FMR should not depend on whether we impose PBC or OBC along the chain. We also do not expect the positions of these plateaus to change.

The current description can be easily extended to higher spin values, using the procedure introduced by Schulz,[51] where additional plateaus should occur. For half-integer SS's, there will be regions where a LLSL description is possible.

In summary, we have considered spin superlattices made up of a periodic arrangement two long *XXZ* chains with different parameters and sizes. Due to the space-dependent properties of the system, an inhomogeneous magnetization profile ensues. The magnetization curve presents plateaus whose magnetization value depends on the relative size of subchains l and is given by $M_s=1/(1+l)$. We also found a massless region in which a description in terms of Luttinger liquid superlattices is possible.

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[1] See, for example, J. Phys. Soc. Jpn. **69**, (2000), Special issue on *Frontiers in Magnetism-Nanoscale, Glassy and Quantum Magnetism*, edited by Y. Miyako, H. Takayama, and S. Miyashita.
[2] F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983).
[3] F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983).
[4] T. Ziman and H. J. Schulz, Phys. Rev. Lett. **59**, 140 (1987).
[5] M. Takahashi, Phys. Rev. Lett. **62**, 2313 (1989).
[6] S. White, Phys. Rev. Lett. **69**, 2863 (1992).
[7] K. Hallberg, X. Q. G. Wang, P. Horsch, and A. Moreo, Phys. Rev. Lett. **76**, 4955 (1996).
[8] K. Hida, J. Phys. Soc. Jpn. **63**, 2359 (1994).
[9] K. Okamoto, Solid State Commun. **98**, 245 (1996).
[10] M. Oshikawa, M. Yamanaka, and I. Affleck, Phys. Rev. Lett. **78**, 1984 (1997).
[11] E. H. Lieb, T. Schultz, and D. J. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).
[12] D. C. Cabra, A. Honecker, and P. Pujol, Phys. Rev. Lett. **79**, 5126 (1997).
[13] D. C. Cabra, A. Honecker, and P. Pujol, Phys. Rev. B **58**, 6241 (1998).
[14] R. Citro, E. Orignac, N. Andrei, C. Itoi, and S. Qin, J. Phys.: Condens. Matter **12**, 3041 (2000).
[15] W. Shiramura, K. Takatsu, B. Kurniawan, H. Tanaka, H. Uekusa, Y. Ohashi, K. Takizawa, H. Mitamura, and T. Goto, J. Phys. Soc. Jpn. **67**, 1548 (1998).
[16] Y. Ajiro, T. Asano, T. Inami, H. Aruga-Katori, and T. Goto, J. Phys. Soc. Jpn. **63**, 859 (1994).

[17] D. D. Swank, C. P. Landee, and R. D. Willet, J. Magn. Magn. Mater. **15**, 319 (1980).
[18] W. Chen, K. Hida, and H. Nakano, J. Phys. Soc. Jpn. **68**, 625 (1999).
[19] W. Chen, K. Hida, and B. C. Sanctuary, Phys. Rev. B **63**, 134427 (2001).
[20] D. C. Cabra and M. D. Grynberg, Phys. Rev. Lett. **82**, 1768 (1999).
[21] D. C. Cabra and M. D. Grynberg, Phys. Rev. B **59**, 119 (1999).
[22] A. Honecker, Phys. Rev. B **59**, 6790 (1999).
[23] D. C. Cabra and M. D. Grynberg, Phys. Rev. B **62**, 337 (2000).
[24] R. M. Wiessner, A. Fledderjohann, K.-H. Mütter, and M. Karbach, Eur. Phys. J. B **15**, 475 (2000).
[25] D. C. Cabra, A. de Martino, M. D. Grynberg, S. Peysson, and P. Pujol, Phys. Rev. Lett. **85**, 4791 (2000).
[26] D. C. Cabra, A. de Martino, A. Honecker, P. Pujol, and P. Simon, Phys. Lett. A **268**, 418 (2000).
[27] D. C. Cabra, A. de Martino, A. Honecker, P. Pujol, and P. Simon, Phys. Rev. B **63**, 094406 (2001).
[28] J. M. Luttinger, J. Math. Phys. **4**, 1154 (1963).
[29] D. C. Mattis and E. H. Lieb, J. Math. Phys. **6**, 304 (1965).
[30] D. C. Mattis, J. Math. Phys. **15**, 609 (1974).
[31] A. Luther and I. Peschel, Phys. Rev. B **12**, 3908 (1975).
[32] J. Sólyom, Adv. Phys. **28**, 201 (1979).
[33] V. J. Emery, in *Highly Conducting One-Dimensional Solids*, edited by J. Devreese, R. Evrard, and V. van Doren (Plenum, New York, 1979), Chap. 6, pp. 247–303.
[34] R. Heidenreich, R. Seiler, and A. Uhlenbrock, J. Stat. Phys. **22**, 27 (1980).
[35] F. D. M. Haldane, J. Phys. C **14**, 2585 (1981).
[36] J. Voit, Rep. Prog. Phys. **57**, 977 (1994).
[37] J. Silva-Valencia, E. Miranda, and R. R. dos Santos, J. Phys.: Condens. Matter **13**, L619 (2001).
[38] C. N. Yang and C. P. Yang, Phys. Rev. **147**, 303 (1966).
[39] C. N. Yang and C. P. Yang, Phys. Rev. **150**, 321 (1966).
[40] C. N. Yang and C. P. Yang, Phys. Rev. **150**, 327 (1966).
[41] C. N. Yang and C. P. Yang, Phys. Rev. **151**, 258 (1966).
[42] F. D. M. Haldane, Phys. Rev. Lett. **45**, 1358 (1980).
[43] I. Affleck, in *Fields, Strings And Critical Phenomena*, edited by E. Brézin and J. Zinn-Justin (North-Holland, Amsterdam, 1988), pp. 563–640.
[44] I. Safi and H. J. Schulz, Phys. Rev. B **52**, 17 040 (1995).
[45] I. Safi and H. J. Schulz, Phys. Rev. B **59**, 3040 (1999).
[46] D. L. Maslov and M. Stone, Phys. Rev. B **52**, 5539 (1995).
[47] V. V. Ponomarenko, Phys. Rev. B **52**, 8666 (1995).
[48] G. I. Dzhaparidze and A. A. Nersesyan, Pis'ma Zh. Eksp. Teor. Fiz. **27**, 356 (1978) [JETP Lett. **27**, 334 (1978)].
[49] V. L. Pokrovsky and A. L. Talapov, Phys. Rev. Lett. **42**, 65 (1979).
[50] H. J. Schulz, Phys. Rev. B **22**, 5274 (1980).
[51] H. J. Schulz, Phys. Rev. B **34**, 6372 (1986).