Ground-state magnetization of polymerized spin chains

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We investigate the ground-state magnetization plateaus appearing in spin-1/2 polymerized Heisenberg chains under external magnetic fields. The associated fractional quantization scenario and the exponents which characterize the opening of gapful excitations are analyzed by means of Abelian bosonization methods. Our conclusions are fully supported by the extrapolated results obtained from Lanczos diagonalizations of finite systems. [S0163-1829(99)03401-3]

Models of low-dimensional magnets, such as strongly correlated quantum spin chains[1] and ladders,[2] are currently receiving renewed and systematic attention for a variety of reasons. Amongst the most remarkable are the spin-Peierls dimerization instability,[3,4] the Haldane conjecture,[5] and concepts such as fractional quantization and topological energy gaps.[1,6] These rather complex phenomena are largely owing to quantum fluctuations of individual spins which tend to restore the rotational symmetry of the ground state. Depending on the exchange interactions, fluctuations can manifest themselves collectively into many possible ground states, particularly in lower dimensions where their effects are most severe.[7]

A wealth of issues have been addressed experimentally to confirm these expectations in a series of quasi-one-dimensional compounds.[8] After a vast body of research, it is by now well established that half-integer-spin chains are massless whereas integer ones are gapful (see, also Ref. 9). In spite of the availability of a number of excellent realizations of one-dimensional Heisenberg antiferromagnets,[4,8] detailed measurements of spin excitations, however, have remained confined within the limits of applied magnetic fields which are low with respect to the exchange interactions thus, precluding a comparison with theory. Nevertheless, advanced neutron-scattering experiments spanning large magnetic fields regions in relatively low exchange coupling materials, e.g., Cs_2CuCl_4, are now beginning to appear (see, e.g., Ref. 10).

Magnetization properties of spin chains have been the subject of intensive investigations for quite a while. Important work includes that of Parkinson and Bonner,[11] and has recently gained new interest due to the appearance of magnetization plateaus studied by several authors in a variety of systems.[12–18] As a contribution to the understanding of massive spin excitations in high magnetic fields, here we consider an alternative scenario for their low-temperature realization. Specifically, we study the interplay between explicit breaking of full translational symmetry and applied magnetic fields, say along the z direction, in spin-1/2 Heisenberg chains at $T=0$. This can be conveniently described by a set of Heisenberg antiferromagnets in which the exchange coupling interactions J_n are all equal but one every p sites, i.e.,

$$J_n=\begin{cases} J(1-\delta), & n/p\in\mathcal{Z}, \\ J, & \text{otherwise.} \end{cases} \tag{1}$$

It should be stressed that periodic arrays of couplings are relevant to the study of ferrimagnetic materials[19] and that also one-dimensional dimerized and trimerized materials are known to exist.[3,12]

The Hamiltonians of our polymerized chains in the presence of a (dimensionless) magnetic field h applied along the z axis are thus given by

$$H_p=\sum_{n=1}^{L} J_n\vec{S}_n\cdot\vec{S}_{n+1}-h/2\sum_{n=1}^{L} S_n^z. \tag{2}$$

Here, the $\vec{S}_n$ are spin-1/2 operators, whereas periodic boundary conditions are assumed along the L sites of the chain $[(L/p)\in\mathcal{Z}]$. Despite their simplicity, we will show however that these Hamiltonians entail a highly nontrivial magnetic behavior controlled solely by the chain periodicity p and the external field h.

As is known,[20] the full translationally invariant (FTI) $S=\frac{1}{2}$ chain remains gapless for all magnetizations $\langle M\rangle \equiv 2/L\,\langle\Sigma_n S_n^z\rangle$, up to a saturation field where each of the L individual spins becomes fully polarized. On general grounds however, the Lieb-Schultz-Mattis theorem[14,21] indicates that FTI Hamiltonians of arbitrary spin S, can be gapful provided the magnetization per spin $\langle M\rangle$ satisfies $(S-\frac{1}{2}\langle M\rangle)\in\mathcal{Z}$. Such gapful excitations should be reflected through the presence of magnetization plateaus, in principle at these special values of $\langle M\rangle$. However, notice that the above theorem *does not prove* the existence of this quantization scenario as it refers to nonmagnetic excitations, i.e., modes which preserve the total magnetization. Nevertheless, magnetization plateaus have been extensively conjectured and observed in both Peierls dimerized[3,15] and trimerized[12] spin chains, as well as in frustrated,[17,18] anisotropic spin-1 systems[13] and ladders models.[16] They all are examples of a

rather subtle phenomenon namely, fractional quantization of a macroscopic physical quantity under external varying fields. Here, we examine this situation for the whole class of nonhomogeneous chains (2), attempting to extend and systematize aspects of quantization emphasized in those studies.

Following a recent analysis discussed as in Refs. 15,16,18 and comprehensively accounted in Refs. 6,22, we will apply the by now standard method of Abelian bosonization to Eq. (2). It is well known that the low-energy properties of the FTI Heisenberg chain, ($\delta=0$), are described by a $c=1$ conformal field theory of a free bosonic field compactified at radius R for any given magnetization $\langle M\rangle$ (see, e.g., Ref. 23). The functional dependence of R can be obtained from the exact Bethe ansatz solution by solving a set of differential equations obtained in Refs. 24 and 25 (for a fuller derivation consult, for instance, Ref. 16). Exploiting this knowledge, the bosonized expression of the low-energy effective Hamiltonian (2) in the homogeneous case $\delta=0$, can be readily shown to adopt the form

$$\overline{H}=\int dx\,\frac{\pi}{2}\left\{\frac{1}{R^2(\langle M\rangle)}(\Pi^2(x)+R^2(\langle M\rangle)[\partial_x\phi(x)]^2\right\}, \tag{3}$$

with $\Pi=(1/\pi)\partial_x\tilde{\phi}$, and $\phi=\phi_L+\phi_R$, $\tilde{\phi}=\phi_L-\phi_R$. Here, the effect of the magnetic field h enters through the radius of compactification $R(\langle M\rangle)$. This radius governs the conformal dimensions, in particular the conformal dimension of a vertex operator $e^{i\beta\phi}$ is given by $(\beta/4\pi R)^2$. Within the framework of the theory of Luttinger liquids, it is worth pointing out also that the compactification radius is related to the parameter K by $R^2=K/4\pi$.

The bosonized expressions for the spin operators read

$$S_i^z(x)\approx\frac{1}{\sqrt{2\pi}}\frac{\partial\phi_i}{\partial x}+\text{const:}\cos(2k_Fx+\sqrt{4\pi}\phi_i)\text{:}+\frac{\langle M\rangle}{2}, \tag{4}$$

and

$$S_i^-(x)\approx e^{-i\sqrt{\pi}\tilde{\phi}_i}[1+\text{const:}\cos(2k_Fx+\sqrt{4\pi}\phi_i)\text{:}], \tag{5}$$

where the colons denote normal ordering with respect to the ground state with magnetization $\langle M\rangle$. Now we apply this methodology to compute the effective form of the interaction. After some algebra, in the limit of weak polymerization $\delta\ll 1$, it can be readily shown that the most relevant perturbation term is given by

$$H_{\text{int}}\approx\delta\sum_{x'=1}^{L/p}\cos\left[2k_F\left(px'+\frac{1}{2}\right)\sqrt{4\pi}\,\phi\right]. \tag{6}$$

This operator will survive in passing from the lattice to the continuum model, assuming that the fields vary slowly, only when the oscillating factor $\exp(i2px'k_F)$ equals one. Since the Fermi level is given by $k_F=(\pi/2)(1-\langle M\rangle)$, this in turn will happen when the condition

$$\frac{p}{2}(1-\langle M\rangle)\in\mathcal{Z} \tag{7}$$

is satisfied.

We can now study when a plateau will appear in the magnetization curve for the polymerized chain (2). To do that, we first have to see which are the values for the magnetization where there could be a plateau, for a given value of the period p [i.e., solve for Eq. (7)] and then we need to evaluate the scaling dimension of the operator (6), which at zero loop is given by

$$d=\frac{1}{4\pi R^2}, \tag{8}$$

which is in turn governed by the radius of compactification as we already stressed. By virtue of the lower bound of the compactification radius,[24,25] namely $R(\langle M\rangle)\geqslant R(\pm 1)=1/(2\sqrt{\pi})$, it follows from Eq. (8) that $d<2$ for all magnetizations $|\langle M\rangle|<1$. This ensures the *relevant* character of the operator (6) which in turn survives in the continuum limit whenever Eq. (7) is satisfied. Therefore, we can conclude that constraint (7) constitutes a *sufficient condition* ultimately responsible for the appearance of magnetization plateaus and massive spin excitations. This is our main result.

We now turn to a numerical finite-size analysis. In Figs. 1(a)–1(e) we display a variety of magnetization regimes as a function of both polymerization parameters $J'/J\equiv 1-\delta$ and applied magnetic fields h. This is a rather compact form of representing conventional magnetization curves for different polymerization strengths. Here, each line is associated to successive values of $\langle M\rangle$ which decrease monotonically from top to bottom, as they should for a nonfrustrated system. The results were obtained from exact diagonalization of finite systems via a recursion type Lanczos algorithm[26] applied on each magnetization subspace $S^z=\{0,1,\ldots,L/2\}$. To avoid the formation of spurious interfaces, even multiple lengths of the lattice periodicity were taken throughout. Using fully isotropic chains up to $L=24$ sites with periodic boundary conditions, our numerical analysis supports entirely the quantization constraint (7).

As expected, the ground-state ''phase diagrams'' exhibit bands of empty regions corresponding to the magnetization plateaus of S^z referred to above, while regions filled with magnetization lines reflect smooth magnon excitations arising in the thermodynamic limit $L\to\infty$. It can be readily observed that for chains of periodicity $p>1$ (dimers, trimers, etc.), a plateaulike structure emerges precisely at the *rational* magnon densities $\langle M\rangle=1-2q/p$, $(q=0,1,\ldots,p)$, implicit in the general scenario of Eq. (7). It is worth remarking on the robustness of this topological constraint as similar results continue to hold for anisotropic (XXZ) chains, the plateaus always appearing at the *same* values of $\langle M\rangle$.

We can also predict the behavior of the mass gap (width of the plateau), with the polymerization strength δ by means of a simple zero-loop computation.[27] Aside logarithmic corrections to the case $\langle M\rangle=0$, this yields

$$g\propto\delta^{1/(2-d)}, \tag{9}$$

with d given as in Eq. (8).

To enable an independent check of this result, we now turn to the issue of extrapolating the numerical finite-size estimates of the mass gaps g_L towards their corresponding

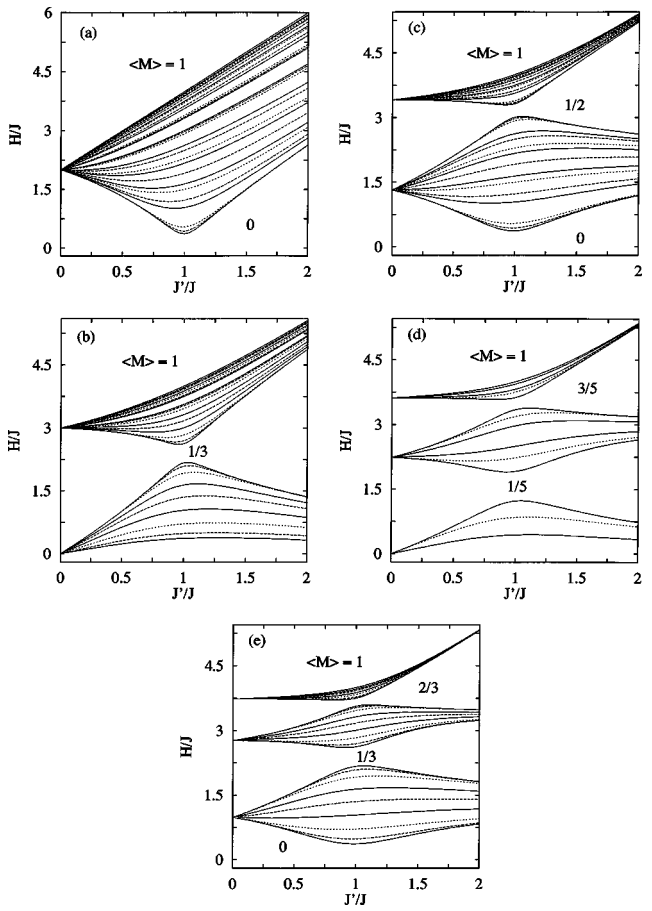

FIG. 1. Magnetization contours of finite polymerized chains for (a) $p=2$, $L=24,20,16$; (b) $p=3$, $L=24,18,12$; (c) $p=4$, $L=24,20,16$; (d) $p=5$, $L=20,10$ (full and dotted lines, respectively) and (e) $p=6$, $L=24,18,12$. Except for (d), full, dashed, and dotted lines stand, respectively, for large, medium, and small sizes. They denote all accessible magnetizations, whereas their values decrease from top to bottom. Though numerical accuracy in h/J is bounded by 10^{-7}, size effects become evident for $J'=J$, as no plateaus (empty wide bands), should occur in the thermodynamic limit.

thermodynamic limits. Note, on one hand, that *any* extrapolation procedure by necessity assumes that the asymptotic behavior applies to the values of L within reach. However, it is known[20] that finite-size corrections to the gap in the excitation spectrum of the homogeneous Heisenberg chain vary slowly as $\ln(\ln L)/\ln^2(L)$, thus affecting the results over a wide range of sizes. In fact, as can be seen in Fig. 2, this turns out to be the case also for weak polymerization regimes, $\delta\to 0$, where finite-size effects are more pronounced. Therefore, in studying numerically the mass gap behavior obtained in Eq. (9), we are confronted with restricting considerations to the noncritical region $0<|\delta|\leqslant 1$, which is, however, suitable to test independently the correctness of our bosonization approach.

To estimate the actual masses in the limit $L\to\infty$, we fitted the whole set of finite-size results (even integer multiples of p within the range $4\leqslant L\leqslant 24$), using both linear, and logarithmic type methodologies of convergence,[28] i.e.,

$$g_L \simeq g + Ae^{-BL}, \quad g_L \simeq g + A/L^B. \tag{10}$$

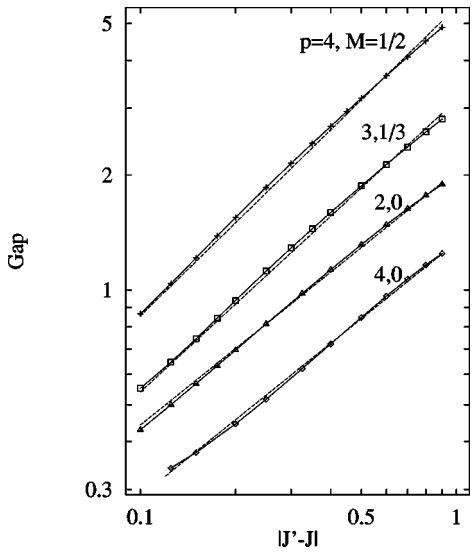

FIG. 2. Extrapolated values of the gap for $p=2$ around $\langle M\rangle=0$, $p=3$ for $\langle M\rangle=1/3$ and, $p=4$ with $\langle M\rangle=0,1/2$. Solid lines are guides to the eye whereas slopes of dashed lines denote the estimated opening exponents, namely (in descending order), 0.8(1), 0.77(10) and, 0.66(10), ($\langle M\rangle=0$). To improve the clarity of the figure, the uppermost curve was shifted multiplying the gap by a scale factor 2.5.

Either extrapolation procedure yields basically the same result with at least three significant digits. This latter variation ultimately gives an estimative idea of the lower bound of the extrapolation error. The reliability of our results was checked also by comparing the trend arising from *smaller* systems ($L\leqslant 20$). When the critical region is approached however, the accuracy differs widely, particularly for $|\delta|<0.2$.

Although there are alternative extrapolation algorithms which do not involve fits to specific forms[28] we should hasten to add however, that their efficiency depends strongly on the abundance of data. In our case, this is translated in the availability of matching sizes, already constrained by both the periodicity p and the antiferromagnetism. Nevertheless, we were able to find a remarkable agreement with the compactification radius comprehended in Eq. (8) and the exponents of Eq. (9). The results are shown in Fig. 2 where we display, respectively, the gap openings around $\langle M\rangle=0$, 1/3, 1/2, for $p=2$, 3, and 4. The dimerized case reproduces the well-known 2/3 exponent predicted in Ref. 3 and corroborated subsequently by diverse numerical studies.[29] To our knowledge however, opening exponents for $p\geqslant 3$ (see Fig. 2), have not been elucidated yet by other investigations.

Finally, it is instructive to comment further on the role of *quantum* fluctuations namely, the tendency of spins to spontaneously tilt occasionally due to the Heisenberg uncertainty relations, and their relevance to our results.[7] For classical spins, e.g., Ising and n-vector models, the interplay between dimensionality and *statistical* fluctuations, though crucial in determining phase transitions, is not sufficient to entail the fractional behavior studied so far. In fact, an elementary transfer-matrix calculation shows that the Ising equivalent of Eq. (2) wipes out all but two magnetization plateaus, namely $\langle M\rangle=0,2/p$, (even $p>2$), their widths behaving linearly with δ. Thus, it is worth pointing out that Eqs. (7) and (9), in contrast, constitute a genuine macroscopic quantum effect.

In summary, we have presented a bosonization picture that accounts for the fractional quantization observed in a class of nonhomogeneous Heisenberg antiferromagnets. All low-energy exponents which characterize the opening of gapful excitations have been obtained and treated on an equal footing while checked with Lanczos diagonalizations of finite systems. Aside from these theoretical pursuits, we trust our study will help to convey a clearer understanding of the many characteristics present in *real* low dimensional magnets. A similar analysis in polymerized ladder systems is in progress.

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[1] For a comprehensive account, consult I. Affleck, J. Phys.: Condens. Matter **1**, 3047 (1989).

[2] The current status of the field has been reviewed by T. M. Rice, Z. Phys. B **103**, 165 (1997); E. Dagotto and T. M. Rice, Science **271**, 618 (1996).

[3] M. C. Cross and D. S. Fisher, Phys. Rev. B **19**, 402 (1979); M. P. M. den Nijs, Physica A **95**, 449 (1979).

[4] Recent studies of the Peierls transition in $CuGeO_3$ compounds have been reported by G. Castilla, S. Chakravorty, and V. J. Emery, Phys. Rev. Lett. **75**, 1823 (1995).

[5] F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983).

[6] I. Affleck, in *Fields, Strings and Critical Phenomena, Les Houches, Session XLIX*, edited by E. Brezin and J. Zinn-Justin (North-Holland, Amsterdam, 1988).

[7] The role of quantum fluctuations and their particular relevance to massive spin phases have been stressed by M. Sigrist and A. Furusaki, J. Phys. Soc. Jpn. **65**, 2385 (1996); Y. Motome *et al.*, *ibid.* **65**, 1949 (1996).

[8] G. Chaboussant *et al.*, Phys. Rev. Lett. **79**, 925 (1997); Phys. Rev. B **55**, 3046 (1997).

[9] D. C. Cabra, P. Pujol, and C. von Reichenbach, Phys. Rev. B **58**, 65 (1998).

[10] R. Coldea *et al.*, Phys. Rev. Lett. **79**, 151 (1997); J. Phys.: Condens. Matter **40**, 7473 (1996).

[11] J. B. Parkinson and J. C. Bonner, Phys. Rev. B **32**, 4703 (1985).

[12] K. Hida, J. Phys. Soc. Jpn. **63**, 2359 (1994); K. Okamoto, Solid State Commun. **98**, 245 (1995).

[13] T. Tonegawa *et al.*, J. Phys. Soc. Jpn. **65**, 3317 (1996).

[14] M. Oshikawa, M. Yamanaka, and I. Affleck, Phys. Rev. Lett. **78**, 1984 (1997).

[15] K. Totsuka, Phys. Lett. A **228**, 103 (1997).

[16] D. C. Cabra, A. Honecker, and P. Pujol, Phys. Rev. Lett. **79**, 5126 (1997); Phys. Rev. B **58**, 6241 (1998).

[17] T. Tonegawa *et al.*, Physica B **246-247**, 368 (1998); B. S. Shastry and B. Sutherland, Phys. Rev. Lett. **47**, 964 (1981).

[18] K. Totsuka, Phys. Rev. B **57**, 3454 (1998).

[19] S. Yamamoto, S. Brehmer, and H.-J. Mikeska, Phys. Rev. B **57**, 13 610 (1998), and references therein.

[20] R. B. Griffiths, Phys. Rev. **133**, A768 (1964); C. N. Yang and C. P. Yang, *ibid.* **150**, 321 (1966).

[21] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. **16**, 407 (1961); I. Affleck and E. H. Lieb, Lett. Math. Phys. **12**, 57 (1986).

[22] H. J. Schulz, Phys. Rev. B **34**, 6372 (1986).

[23] F. D. M. Haldane, Phys. Rev. Lett. **45**, 1358 (1980).

[24] V. E. Korepin, N. M. Bogoliubov, and A. G. Izergin, *Quantum Inverse Scattering Method and Correlation Functions* (Cambridge University Press, Cambridge, 1993).

[25] N. M. Bogoliubov, A. G. Izergin, and V. E. Korepin, Nucl. Phys. B **275**, 687 (1986).

[26] See, for example, G. H. Golub and C. F. Van Loan, *Matrix Computations*, 3rd ed. (Johns Hopkins University Press, Baltimore, 1996).

[27] I. Affleck *et al.*, J. Phys. A **22**, 511 (1989).

[28] For a review, consult A. J. Guttmann, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. Lebowitz (Academic Press, New York, 1990), Vol. 13; see, also, C. J. Hamer and M. N. Barber, J. Phys. A **14**, 2009 (1981).

[29] G. Spronken, B. Fourcade, and Y. Lépine, Phys. Rev. B **33**, 1886 (1986), and references therein.