

Magnetization Plateaus in Spin Chains: “Haldane Gap” for Half-Integer Spins

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We discuss zero-temperature quantum spin chains in a uniform magnetic field, with axial symmetry. For integer or half-integer spin, S , the magnetization curve can have plateaus and we argue that the magnetization per site m is topologically quantized as $n(S - m) = \text{integer}$ at the plateaus, where n is the period of the ground state. We also discuss conditions for the presence of the plateau at those quantized values. For $S = 3/2$ and $m = 1/2$, we study several models and find two distinct types of massive phases at the plateau. One of them is argued to be a “Haldane gap phase” for half-integer S . [S0031-9007(97)02624-0]

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One-dimensional antiferromagnets are expected not to have long-range magnetic order in general. It was argued by Haldane [1], in 1983, that for integer, but not half-integer spin, S , there is a gap to the excited states. In the presence of a magnetic field, the $S = 1/2$ Heisenberg antiferromagnetic (AF) chain remains gapless from zero field up to the saturation field, where the ground state is fully polarized [2]. For integer S , the gap persists up to a critical field, equal to the gap, where Bose condensation of magnons occurs [3]. The $S = 1$ Heisenberg AF chain is known to be gapless from the critical field up to the saturation field [4]. Recently Hida observed that an $S = 1/2$ antiferromagnetic chain with period 3 exchange coupling shows a plateau in the magnetization curve at magnetization per site $m = 1/6$ ($1/3$ of the full magnetization) [5]. Related works on bond-alternating chains have also been reported [6–9] including experimental observation [10].

In this Letter, we consider the zero-temperature behavior of general quantum spin chains, including chains with periodic structures, in a uniform magnetic field pointing along the direction of the axial symmetry (z axis) (i.e., the total S^z is conserved). We argue that, in quantum spin chains, there is a phenomenon which is strikingly analogous to the quantum Hall effect—topological quantization of a physical quantity under a changing magnetic field [11]. We first consider an extension of the Lieb-Schultz-Mattis (LSM) theorem [12] to the case with an applied field. This indicates that translationally invariant spin chains in an applied field can be gapful without breaking translation symmetry, *only when* the magnetization per spin, m , obeys $S - m = \text{integer}$. We expect such gapped phases to correspond to plateaus at these quantized values of m . “Fractional quantization” can also occur, if accompanied by (explicit or spontaneous) breaking of the translational symmetry. The generalized LSM theorem does not prove the presence of the plateau, however. Thus we construct a corresponding argument using Abelian bosonization, which is in complete agree-

ment with the generalized LSM theorem, and also gives a condition for the presence of the plateau. As simplest examples, we study translationally invariant $S = 3/2$ chains at $m = 1/2$. We present numerical diagonalization and density matrix renormalization group (DMRG) [13] calculations, which demonstrate the existence of the two distinct types of gapped phases for generalized models. They are related to the $S = 1$ large- D phase and the $S = 1$ Haldane phase, respectively. On the other hand, our study shows that the standard $S = 3/2$ Heisenberg model is gapless with no plateau at $m = 1/2$. Details and further results, including the effect of the axial symmetry breaking, will be presented in a longer paper [14].

The LSM theorem [12] proves the existence of at least one low-energy, $O(1/L)$ excited state for even length L half-integer S AF chains with periodic boundary conditions and general, translationally invariant Hamiltonians. It is expected that this implies either gapless excitations or spontaneously broken translational symmetry in the $L \rightarrow \infty$ limit. The failure of this proof for the integer- S case is necessary for the existence of the Haldane phase with no broken translational symmetry and a gap. We observe that the original version of this proof also works in a magnetic field *except for integer* $S - m$. Thus only in this case is a massive phase without spontaneously broken translational symmetry possible. The proof consists of making a slow rotation on the ground state, $|\psi\rangle$, assumed to be unique, and observing that the resulting low-energy state is orthogonal to the ground state. The rotation operator is $U \equiv \exp[-i \sum_{j=1}^L (2\pi j/L) S_j^z]$. For any Hamiltonian H , including a magnetic field term, with short-range interactions which is invariant under rotation about z axis and either reflection about a link or time reversal (S^x, S^y, S^z) \rightarrow ($S^x, -S^y, S^z$),

$$\langle \psi | U^\dagger H U - H | \psi \rangle = O(1/L). \quad (1)$$

This implies the existence of an excited state with excitation energy of $O(1/L)$, if we can show that $U|\psi\rangle$ is

orthogonal to $|\psi\rangle$. To this end, we use the invariance of H under translation by one site, T . This operation maps U into

$$U \rightarrow TUT^{-1} = Ue^{i2\pi S_1^z - i(2\pi/L)\sum_{j=1}^L S_j^z}. \quad (2)$$

Namely, the operation of U changes the eigenvalue of T by a factor $e^{i2\pi(S-m)}$, where $m = \sum_{j=1}^L S_j^z/L$. Thus $U|\psi\rangle$ must be orthogonal to $|\psi\rangle$ except when $(S-m)$ is an integer. We note that this is consistent with previous results for translationally invariant $S=1/2$ and 1 AF chains, where no gap is found at partial magnetization. However, for higher spin, gapped phases at partial magnetization are possible without breaking the translational symmetry, when $S-m$ is an integer.

When $S-m$ is not an integer, there is a low-lying state with energy of $O(1/L)$. This means either a massless phase with a continuum of low-energy states or spontaneous symmetry breaking in the thermodynamic limit. Following the above proof, when $S-m = p/q$ where p and q are coprimes, $U^k|\psi\rangle$ for $k=0, 1, \dots, q-1$ have different eigenvalues of T . Thus these q states have low energy of $O(1/L)$. If these are related to a spontaneous breaking of the symmetry, the ground states in the thermodynamic limit should be q -fold degenerate. Since they have q different eigenvalues of T , they can be related to a spontaneous breaking of the translation symmetry to period of q sites in the thermodynamic limit. It is natural to expect a gap and plateau in this case. As in the case of quantum Hall effect, "fractional quantization" is therefore possible, accompanying the spontaneous breaking of the translation symmetry in the present case. We may compare this to a hidden symmetry breaking in fractional quantum Hall effect [15].

Our generalization of LSM theorem is easily extended to Hamiltonian with spatial structures: bond-alternating chains [5,8], spin-alternating chains [16], spin ladders, etc. For example, Hida's model [5] is only invariant under a three-site translation T^3 ; a massive phase without spontaneous symmetry breaking is possible for $3(S-m) = \text{integer}$. Thus a quantized plateau is possible at $m = 1/6$ as he observed. In general, the quantization condition is given by $S_u - m_u = \text{integer}$, where S_u and m_u are, respectively, the sum of S and m over all sites in the unit period of the ground state. The period of the ground state is determined by the explicit spatial structure of the Hamiltonian, and also by spontaneous symmetry breakings.

The low-energy state $U|\psi\rangle$ appearing in the LSM theorem has the same total magnetization as in the ground state. It does not directly contradict the existence of a plateau, which is determined by the gap to states with other total magnetizations. However, we expect that, in general, a gapless phase has low-energy states in both fixed and different magnetization sector, as can be seen in the following Abelian bosonization approach. Schulz [17] explained the difference between integer and half-integer spin by Abelian bosonization. We show

that his result can be understood more simply as a consequence of symmetries. At the same time, we generalize the discussion to the case with a nonvanishing magnetization. Following Schulz [17], we start from Abelian bosonization of $2S$ spin-1/2 chains and then couple them to form a spin- S chain. First, each spin-1/2 chain is fermionized by Jordan-Wigner transformation. The z component of each spin-1/2 is related to the fermion number as $\sigma_n^z = 1 - 2\psi_n^\dagger\psi_n$. Then the low-energy excitations are treated by continuous fermion fields. Let us denote the lattice spacing as a and the spatial location $x = na$. The continuous fermion fields ψ_R and ψ_L are defined by

$$\psi_n^j \sim e^{ik_F x} \psi_R^j(x) + e^{-ik_F x} \psi_L^j(x), \quad (3)$$

where $j = 1, \dots, 2S$ is the "flavor" index to distinguish $2S$ spin-1/2's. They are bosonized in a standard way: $\psi_R^j = e^{i\varphi_R^j/R}$ and $\psi_L^j = e^{-i\varphi_L^j/R}$, where φ_R^j and φ_L^j are chiral bosons and R is the compactification radius of the boson. R will be renormalized by interactions [18], and will eventually depend on the model and on the magnetization m . (For an isotropic model, R is fixed by the symmetry at $m=0$, but the magnetic field breaks the symmetry and thus R will depend on m .) We define the nonchiral bosonic field $\varphi^j = \varphi_L^j + \varphi_R^j$ and its dual $\tilde{\varphi}^j = \varphi_L^j - \varphi_R^j$.

Interactions among bosonic fields are also generated during the mapping from the original spin problem. In general, we expect any interaction would be generated if not forbidden by a symmetry. Thus we analyze symmetries of the system, following the treatment of spin-1/2 chains in Ref. [18]. The original problem has a $U(1)$ symmetry: rotational invariance about the z axis. Rotation of each spin-1/2 is given by the phase transformation $\psi_{L,R}^j \rightarrow e^{i\theta} \psi_{L,R}^j$ of the corresponding fermion. In bosonic language, this corresponds to a shift of the dual field $\tilde{\varphi}^j \rightarrow \tilde{\varphi}^j + \text{const}$. Since we have coupled $2S$ spin-1/2 chains into a spin- S chain, only the simultaneous rotation of $2S$ spin-1/2's is a symmetry of the system. If we define a new bosonic field $\phi = \sum_j \varphi^j$ (and similarly for $\tilde{\varphi}^j$), the $U(1)$ symmetry is written as $\tilde{\phi} \rightarrow \tilde{\phi} + \text{const}$. Thus all the interactions of the form $e^{\pm 2n\pi i R \tilde{\phi}}$ are prohibited by the symmetry. The remaining $2S-1$ fields, which are defined by linear combinations of original $\tilde{\varphi}^j$ fields, are not protected by the symmetry. Thus all fields except ϕ are expected to become massive by interactions, as Schulz observed by an explicit calculation. The remaining ϕ field is also subject to $e^{\pm in\phi/R}$ type interactions. Let us consider another symmetry of the system: one-site translation. By definition (3), it actually corresponds to a transformation of the continuum field $\psi_R^j \rightarrow e^{ik_F a} \psi_R^j$ and $\psi_L^j \rightarrow e^{-ik_F a} \psi_L^j$. Again, only the simultaneous translation of all flavors is a symmetry of the system. Thus the one-site translation T is written as $\phi \rightarrow \phi + 4S(k_F a)R$, in the bosonic language.

Since all of the $2S$ flavors are equivalent, the magnetization should be equally distributed among them. Thus the Fermi momentum k_F is determined as $k_F a = (S - m)\pi/2S$. As a consequence, the one-site translation T is given by

$$\phi \rightarrow \phi + 2(S - m)\pi R. \quad (4)$$

Thus the leading operator $\cos(\phi/R)$ is permitted only if $S - m$ is an integer. For m satisfying the quantization condition, the leading operator $\cos(\phi/R)$ should be relevant in order to produce a gap. Thus R must be larger than $R_c = 1/\sqrt{8\pi}$ for the presence of the plateau. If $S - m = p/q$ where p and q are coprimes, the operator $\cos(q\phi/R)$ is permitted. It can be relevant if $R \geq q/\sqrt{8\pi}$ (this is a severe condition for a large q); if it is, a ground state in the thermodynamic limit corresponds to a potential minimum of $\cos(q\phi/R)$. There are q such ground states, and they are mapped to each other by applying the translation operator T^k ($k < q$). Thus the ground states have spontaneously q -fold broken translation symmetry. These results are in agreement with the generalized LSM theorem, and also give conditions for a finite plateau at the quantized values.

Our bosonization argument is also readily generalized to models with spatial structures. Our picture is consistent with Okamoto's analysis [6] of Hida's plateau [5]. For $S = 1$ AF chains, Tonegawa *et al.* [8] obtained an $m = 1/2$ plateau as soon as they introduced a small bond alternation. In our approach, the leading operator is expected to appear as soon as the translational symmetry is broken. Thus we expect a plateau for any finite amount of bond alternation, if the radius exceeds the critical value, in agreement with Ref. [8]. This is also in agreement with an explicit bosonization calculation by Totsuka [9] for $S = 1$ bond-alternating chains.

Now let us discuss some examples of translationally invariant $S = 3/2$ chains. It is interesting both from an experimental and conceptual point of view to add an easy-plane crystal field term,

$$H = \sum_j \vec{S}_j \cdot \vec{S}_{j+1} + D(S_j^z)^2 - hS_j^z. \quad (5)$$

Clearly, if $D \gg 1$, all the spins are first fixed to $S^z = 1/2$ with increasing field before any of the spins go into the $S^z = 3/2$ state, corresponding to a gapped $m = 1/2$ plateau. The presence of finite gap and plateau is proved rigorously for a sufficiently large but finite D [19], by applying the general theorem in Ref. [20]. This situation is reminiscent of that which occurs in the large- D phase in a zero field $S = 1$ chain. Numerically, we found a finite $m = 1/2$ plateau at least for $D \geq 2$.

Another kind of trial ground state for an $S = 3/2$ chain, corresponding to an $m = 1/2$ plateau is shown in Fig. 1 in the valence bond notation [21]. Regarding each $S = 3/2$ operator as being a symmetrized product of three $S = 1/2$'s, one $S = 1/2$ is polarized by the applied field at each site while the other two form a valence-bond-

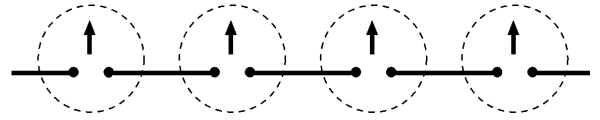


FIG. 1. The partially magnetized VBS state for $S = 3/2$. A solid line denotes a valence bond (singlet formed from two spin-1/2's). An up arrow denotes a spin-1/2 with $S^z = 1/2$. A dashed circle represents the symmetrization of spin-1/2 variables at each site.

solid (VBS) ground state as occurs for an $S = 1$ chain in zero field. In Ref. [22], this partially magnetized VBS state was proposed and the relevance to the magnetization process was suggested. A generalization of this kind of VBS-type state and further analysis were later done in Ref. [23]. (See also [16].) Clearly this sort of VBS-type state exists for all S and m such that $S - m$ is an integer.

We can construct a model to realize the $S = 3/2$ VBS-type state in Fig. 1 as a ground state,

$$H = \sum_j P_3^{(j,j+1)} + \alpha \vec{S}_j \cdot \vec{S}_{j+1} - hS_j^z, \quad (6)$$

where $P_3^{(j,j+1)}$ is the projection operator onto the space with total spin 3 for sites j and $j + 1$. At $\alpha = 0$, any state constructed with one valence bond between neighboring sites is a ground state. The ground state is thus infinitely degenerate due to the "free" spin-1/2 at each site. Applying an infinitesimal magnetic field, the degeneracy is lifted and the ground state is the above-mentioned VBS-type state (Fig. 1). Thus the model with $\alpha = 0$ has an $m = 1/2$ plateau starting from zero magnetic field. Turning on the Heisenberg term, α , the degeneracy at $h = 0$ is lifted and a finite magnetic field is required to reach $m = 1/2$. For small value of α , however, we might still expect a finite $m = 1/2$ plateau. We studied this model with periodic boundary conditions by numerical diagonalization for up to 12 sites and found the $m = 1/2$ plateau exists at least for $\alpha \leq 0.06$. In contrast to the plateau at large positive D , which is related to the large- D phase in $S = 1$ chains, it is natural to relate this state to the $S = 1$ Haldane phase.

For $S = 1$, the Haldane phase is known to be distinct from the large- D phase; these two massive phases are separated by a critical point D_c , where the gap vanishes [17,24]. The Haldane phase is characterized by the existence of a topological long-range order [25], and gapless edge excitations in the open boundary conditions [26]. These are understood as consequences of a hidden symmetry breaking [20]. One might suspect that the two types of $S = 3/2$ massive phases at the $m = 1/2$ plateaus discussed above, correspond to distinct phases.

If they are distinct, there should be a phase transition between them. In terms of Abelian bosonization, this phase transition may be understood as the vanishing of the coefficient of the allowed relevant operator $\cos(\phi/R)$, as in the case of $S = 1$ [17]. We numerically measured the

gap (width of the plateau) for the model

$$H = \sum_j \alpha \vec{S}_j \cdot \vec{S}_{j+1} + D(S_j^z)^2 + P_3^{(j,j+1)} - hS_j^z, \quad (7)$$

which interpolates between (5) and (6). For $\alpha = 0.03$ (fixed), we find the plateau vanishes at $D \sim 4.5$, separating the “Haldane gap” type plateau and the “large- D ” type plateau. Moreover, we compared the spectrum at $\alpha = 0.03$ and $D = 0$ between open and periodic boundary conditions, and found evidence for edge states. In the large- D region, there are no such edge states. These indicate that the “Haldane phase” at $m = 1/2$ plateau, which accompanies the edge states, is distinct from the “large- D phase.”

We also numerically examined the standard $S = 3/2$ Heisenberg AF chain with open boundary conditions, by DMRG up to 100 sites. We did not find an $m = 1/2$ plateau in this case, in agreement with Refs. [5–7]. We emphasize that the absence is not *a priori* obvious. As we have shown, in terms of the free boson theory, the plateau would be present if the compactification radius R is greater than the critical value R_c and the coefficient of the most relevant operator $\cos(\phi/R)$ is nonvanishing. We have determined the compactification radius from the spectrum for the open boundary condition obtained by DMRG, as $R = 0.95R_c < R_c$. We note that R is rather close to the critical value, and possibly we can realize a plateau by a small perturbation of the standard Heisenberg Hamiltonian [14]. On the other hand, while the radius is not completely well defined at the *massive* $D = 2$ plateau, a similar analysis gives the estimate $R \sim 1.2R_c > R_c$. This result is consistent with the presence of the plateau.

The plateaus that we have found are closely related [14] to Mott insulating (or charge density wave) phases in models of interacting fermions or bosons [27,28]. Similarly to those cases [14,29], we have found that the singular part of the magnetization curve near a plateau is proportional to $\sqrt{|h - h_c|}$ where h_c is the critical field at (either) edge of a plateau, at least for examples we have studied. Our approach will also give new insights into models of interacting fermions or bosons [14].

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a substantial enhancement of his presentation [9] at Japanese Physical Society meeting Fall 1996, and contains some of our general arguments using bosonization.

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- [1] F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983).
 - [2] R. B. Griffiths, Phys. Rev. **133**, A768 (1964).
 - [3] I. Affleck, Phys. Rev. B **43**, 3215 (1991).
 - [4] T. Sakai and M. Takahashi, Phys. Rev. B **43**, 13383 (1991).
 - [5] K. Hida, J. Phys. Soc. Jpn. **63**, 2359 (1994).
 - [6] K. Okamoto, Solid State Commun. **98**, 245 (1996).
 - [7] M. Roji and S. Miyashita, J. Phys. Soc. Jpn. **65**, 1994 (1996).
 - [8] T. Tonegawa, T. Nakao, and M. Kaburagi, J. Phys. Soc. Jpn. **65**, 3317 (1996).
 - [9] K. Totsuka, contribution to the JPS meeting Fall 1996, at Yamaguchi University.
 - [10] Y. Narumi, K. Kindo, and M. Hagiwara, contribution to the JPS meeting Fall 1996 at Yamaguchi University; (private communication).
 - [11] R. B. Laughlin, Phys. Rev. B **23**, 5632 (1981); D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982).
 - [12] E. H. Lieb, T. Schultz, and D. J. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961); I. Affleck and E. H. Lieb, Lett. Math. Phys. **12**, 57 (1986).
 - [13] S. R. White, Phys. Rev. B **48**, 10345 (1993).
 - [14] M. Oshikawa, M. Yamanaka, and I. Affleck (to be published).
 - [15] R. Tao and Y.-S. Wu, Phys. Rev. B **30**, 1097 (1984).
 - [16] S. K. Pati, S. Ramasesha, and D. Sen, cond-mat/9610080; A. K. Kolezhuk, H.-J. Mikeska, and S. Yamamoto, cond-mat/0610097.
 - [17] H. J. Schulz, Phys. Rev. B **34**, 6372 (1986).
 - [18] I. Affleck, in *Fields, Strings and Critical Phenomena*, Proceedings of the Les Houches Summer School, Session XLIX, edited by E. Brezin and J. Zinn-Justin (North-Holland, Amsterdam, 1988).
 - [19] H. Tasaki (private communication).
 - [20] T. Kennedy and H. Tasaki, Commun. Math. Phys. **147**, 431 (1992).
 - [21] I. Affleck, T. Kennedy, E. Lieb, and H. Tasaki, Commun. Math. Phys. **115**, 477 (1988).
 - [22] M. Oshikawa, J. Phys. Condens. Matter **4**, 7469 (1992).
 - [23] H. Niggemann and J. Zittartz, Z. Phys. B **101**, 289 (1996).
 - [24] R. Botet, R. Julien, and M. Kolb, Phys. Rev. B **28**, 3914 (1983).
 - [25] M. den Nijs and K. Rommelse, Phys. Rev. B **40**, 4709 (1989); S. M. Girvin and D. P. Arovas, Phys. Scr. **T27**, 156 (1989); Y. Hatsugai and M. Kohmoto, Phys. Rev. B **44**, 11789 (1991).
 - [26] T. Kennedy, J. Phys. Condens. Matter **2**, 5737 (1990).
 - [27] T. Giamarchi, in the Proceedings of the SCES96 conference (cond-mat/9609114) (to be published), and references therein.
 - [28] P. Niyaz, R. T. Scalettar, C. Y. Fong, and G. G. Batrouni, Phys. Rev. B **50**, 362 (1994), and references therein.
 - [29] H. J. Schulz, Phys. Rev. B **22**, 5274 (1980).