Bloch Walls and Macroscopic String States in Bethe's Solution of the Heisenberg Ferromagnetic Linear Chain

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We present a calculation of the lowest excited states of the Heisenberg ferromagnet in 1D for any wave vector. These turn out to be string solutions of Bethe's equations with a macroscopic number of particles in them. They are identified as generalized quantum Bloch wall states, and a simple physical picture is provided for the same.

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Introduction.—The question of elementariness of excitations in low dimensional magnetic systems is receiving much attention currently. It was perhaps first addressed in the seminal work of Bethe in 1931 [1]. In addition to providing the celebrated *ansatz* named after him, Bethe asked if Bloch's magnons are the "most elementary" excitations in 1D. He came to the conclusion that they were not, and instead found that the bound states of spin reversals were. After the original paper of Bethe, the ferromagnet has received [2–4] comparatively less attention than its antipode, namely the antiferromagnet [5–7]. One source of revival of interest in the ferromagnet is in connection with stochastic dynamical systems, albeit with a complex Aharonov Bohm magnetic flux [8,9]. Another notable recent exception is a work by Sutherland [4], who shows that the excited states of the ferromagnet contain a singlet state at momentum π, with an excitation energy (EE) that is very low, of $O(1/N)$, where N is the length of the ring.

At the semiclassical level, domain wall arguments [10] lead one to expect in dimensions d (with volume $= N^d$) the *Bloch wall* excitations to be of $O(N^{d-2})$, and hence to be among contenders for the lowest EE in $d = 1$. Such "large deviation" excitations carry spin as well as momentum as we show below. These configurations of spins will be discussed within the context of Bethe's ansatz (BA) for the $s = 1/2$ ferromagnet presently.

In this work we ask (and answer) the following question: *For a given value of the total momentum of the Bethe ferromagnet, what is the lowest excited state?* The nontriviality of the question arises from the fact that within the famous Bethe formula for the bound state of n magnons, $\omega_{\rm Bethe}(q) = J\frac{2}{n}[1 - \cos(q)]$, the lower limit on the total momentum q [11] depends implicitly upon n. Its dependence has not been fully explicated earlier, at least as far as we could find in the literature. In this work, we use a combination of exact diagonalization and analytic methods to attack the problem. A new and essential tool that we develop is the argument of continuity of certain regular root solutions with respect to the density, regarded as a continuous variable, leading to a differential equation formulation of Bethe's equations (BE) that bypasses the knowledge (or otherwise) of the quantum numbers.

Our findings are readily stated: The lowest excitations for any momentum q arise from special string solutions of BE. These special string solutions involve *a macroscopic number of particles* in a given string, and hence we call them macroscopic strings. Sutherland's solution at momentum π is a particular case of these. We have found the lowest solution for every value of the total momentum; these correspond to a definite value of total spin as well. Such states are of the type that one would expect from Bethe's formula for n magnon bound states, with n of the size of the lattice. The formula of Bethe cannot, however, be used for such large bound states since we show that there are significant corrections to the traditional assumption of a uniformly spaced vertical Bethe string in the complex plane: The curvature and nonuniformity of spacing produces essential differences. Our states can be represented by a new formula: $\omega_{BW}(q) = \frac{2\pi}{N}Jq[1 - q/(2\pi)]$ for $0 \leq q \leq \pi$. We find that the solution for a given q corresponds to a particular value of total spin, $S_{\rm tot} = N(1/2 - q/2\pi)$. If we write n the spin deviation from the saturated ferromagnet ($S^z = N/2 - n$) in terms of the density d as $n = d\,N$, the spectrum can be written as $\omega_{BW} = \frac{4\pi^2}{N}Jd(1 - d)$ with $q = 2\pi d$ and $S_{\rm tot} = N(1/2 - d)$. We show finally that these states correspond to generalized quantum Bloch walls [12]: *thus the states with lowest EE at any wave vector of $O(1)$ are Bloch walls* [13].

Before presenting our calculations, we note that the bound states of Bethe for $s = 1/2$ have been identified with solitonic excitations [14] of the nonlinear classical, i.e., large s, Landau Lifschitz equations $\dot{\vec{S}}(x) = \vec{S}(x) \times \partial^2/\partial x^2 \vec{S}(x)$. Several explicit solutions of these are known [15,16]. We note that Bloch walls form a certain class of exact solutions [14,16] of the nonlinear classical equations, namely nonlinear spin waves.

Calculations.—We consider the ferromagnetic Heisenberg Hamiltonian: $\mathcal{H} = 2J\sum_{l=1,N}[s^2 - \vec{S}_l \cdot \vec{S}_{l+1}]$, with periodic boundary conditions, and where for the most part we consider $s = 1/2$ and $\vec{S}_l = \frac{1}{2}\vec{\sigma}_l$, in terms of the usual Pauli spin operators.

Our first result is from observations on wave functions of the energy eigenstates obtained from exact numerical diagonalization of chains up to length $N = 16$ in a momentum resolved basis. We observed that in all cases, the lowest state at momentum $q = 2\pi n/N$ has total angular momentum $S = N/2 - n$. This implies that this state can be obtained in the n particle sector where it is a "maximal," i.e., highest weight state. The corresponding Bethe wave function has all pseudomomenta nonvanishing, and the momentum and particle density related as $q = 2\pi d$.

We next write the BE for the Heisenberg chain in the Orbach parametrization as

$$Nf(\alpha_l) = 2\pi I_l + \sum_{m \neq l} f[(\alpha_l - \alpha_m)/2]$$
$$l = 1, 2 \ldots n, \tag{1}$$

where $f(x) = \frac{1}{i}\log(\frac{x+i}{x-i}) = 2\,\mathrm{arccot}(x)$, $\alpha_l = \cot(k_l/2)$ and $\{I_l\}$ are the Bethe integers, and k_l the Bethe pseudomomenta. We take the branch cut of $f(x)$ to be on the imaginary axis running from $-i$ to $+i$. The energy and total momentum are given, respectively, by $\epsilon = J\sum_{l=1,n}\frac{4}{1+\alpha_l^2}$ and $q = \frac{2\pi}{N}\sum_{l=1,n} I_l$. Let us note that we are interested in the lowest energy states for a given q, requiring a knowledge of the integers I_l. These integers, as shown by Bethe, differ by 2 for scattering states, and by either one or zero for bound states in general. Eliminating the integer sets with zeros in them, a very plausible state is one with $I_l = 1$ for $1 \leq l \leq n$, and we found from numerical studies of BE for small N and small n (with $n \ll N$), that this was indeed so: The resulting state is invariably the lowest energy state for small q. Emboldened by this exercise we found the following exact solution analytically in the limit of a thermodynamic n as well as N, but at low density, i.e., $d = n/N \ll 1$. Since we are interested in excitation energies that are vanishing in the thermodynamic limit, the corresponding variables α_l scale with system size and it is convenient to introduce new scaled variables $z_l = \alpha_l/n$. In terms of these, the left-hand side of Eq. (1) becomes $2/(z_l d)$ on using the large x expansion of $f(x)$ and ignoring terms of size $O(1/N^2)$. On the right-hand side we cannot make the expansion in general since, at high densities, a core is formed [4] where the separations $n(z_l - z_m)/2$ between pairs of particles can become arbitrarily close to the branch points of $f(x)$. In the low density limit we find it is possible to obtain a perturbative solution, using the crucial observation that the typical interparticle separation $\sim 1/\sqrt{d}$, and hence we can use the smallness of d as an expansion parameter in a perturbative sense. Setting $I_l = 1$ we find the approximate equation:

$$\frac{1}{z_l} = \pi d + \frac{2d}{n}\sum_{m \neq l}\frac{1}{z_l - z_m}. \tag{2}$$

Note that Eq. (2) has corrections from the expansion of the phase shift, that is typically of $O(d)$ smaller than the least term retained. The solution of the system Eq. (2) can actually be found exactly [17], but we save it for a future publication. We find at low densities the following result:

$$z_l = \frac{1}{\pi d} + \frac{i\sqrt{2}}{\pi\sqrt{d}}x_l - \frac{2}{3\pi}\left(x_l^2 + 1 - \frac{1}{n}\right) + O(\sqrt{d}), \tag{3}$$

where x_l satisfy $H_n(\sqrt{n}\,x_l) = 0$, H_n being the nth order Hermite polynomial. In the limit of large n the x_j form a continuum stretching from $-\sqrt{2}$ to $\sqrt{2}$ with the familiar semicircular density of states $\rho(x) = \frac{1}{\pi}\sqrt{2 - x^2}$. This solution can be used to obtain the energy to order d^2. The energy $N\epsilon = 4J/(nd)\sum_i 1/z_i^2$ for low d can be found as $N\epsilon = 4J\pi^2[d + d^2\{3\langle(\beta_i^{(1)})^2\rangle - 2\langle\beta_i^{(2)}\rangle\} + O(d^3)]$, where the averages are normalized sums over the indicated variables. Using the explicit expression Eq. (3) and converting the sums to integrals over the semicircular density of states we get finally the low density formula: $N\epsilon = 4J\pi^2 d(1 - d) + O(d^3)$. Below we will argue that there are no corrections to the above formula beyond the first term: *it is exact*. Thus provisionally we write

$$N\epsilon = 4J\pi^2 d(1 - d) = 2J\pi q\left(1 - \frac{q}{2\pi}\right). \tag{4}$$

We note that the low density Eq. (2) must be abandoned once the minimum separation $n(z_i - z_j)$ hits the value $2i$, this happens at $2 = |n(z_0 - z_i)| = (\sqrt{2}/\sqrt{d}\pi)n|(x_0 - x_1)$. However, $n|(x_0 - x_1)| = 1/\rho(0) = \pi/\sqrt{2}$, thus $d \sim 1/4$. Indeed we found for small systems that $d \geq 1/4$ cannot be treated easily numerically: The new difficulty is that the quantum numbers are no longer simple as we discuss below. For $d \leq 1/4$ the low density result Eq. (3) and the full solution of Eq. (2) [17] are extremely close.

We now discuss the techniques used for solving Eq. (1) numerically at larger densities. There are two main problems. One is that the integers jump around in a complicated way that is not known beforehand, and it is clearly not feasible to try all combinations. The second problem is the formation of the core [4], i.e., successive roots that are placed very close to a separation $2i$, which causes singularities in the equation and results in numerical inaccuracies. Our strategy is to start from low densities where we know the roots, and change d slowly and study the evolution of the roots. For this we first convert Eq. (1) into a set of first order ordinary differential equations (ODE) with $\log(d)$ as a timelike flow parameter [18]. Taking the derivative of Eq. (1) with respect to d and defining new variables $t = \log d$ and $f_l = z_l e^t$ we obtain

$$\sum_m A_{lm}\dot{f}_m = -\pi f_l^2 \dot{I}_l - \sum_m A_{lm}(f_l - f_m), \tag{5}$$

where

$$A_{lm} = \frac{2e^t f_l^2}{n} \frac{1}{[4e^{2t}/n^2 + (f_l - f_m)^2]}, \qquad m \neq l,$$

$$A_{ll} = 1 - \sum_{m \neq l} A_{lm},$$

and the derivatives are with respect to the "time" variable t. The time derivatives of the integers are delta functions and hence drop out of the equations at almost all times. Also since the flow of the roots themselves is smooth, we expect the delta-function singularities to be *precisely canceled* by other terms in the equation. Hence in evolving the above ODE we can drop the first term on the right-hand side of the equation. This immediately solves the problem of our lack of knowledge of the integers since they do not occur anywhere else in the differential equations. From these solutions we can recover the integers and use them in the root finder to get more accurate solutions. We find that until densities around $d = 0.45$ the solutions obtained from the ODE are very accurate. At higher densities, significant numerical errors show up because of the singularities associated with the core. In these cases we correct our ODE solutions by fixing the core by hand and using the root finder to self-consistently solve for the roots outside the core. We plot in Fig. 1 the solutions, for a system of 16 particles, at different densities. The table below shows the integer sets at four different densities (since they occur in pairs we show only half of them).

$d = 0.2$	1	1	1	1	1	1	1	1
$d = 0.3$	1	1	1	0	1	1	2	1
$d = 0.4$	1	0	1	0	1	1	2	2
$d = 0.5$	0	0	0	0	0	0	0	8

We now discuss the energies that we obtain from the BA solutions. For $N \leq 16$, we have verified that all the solutions obtained from the numerical solutions of the BE using the above scheme, match with those obtained from exact numerical diagonalization. With the BE we can go to much larger system sizes. *We find that the gap vanishes at every finite q, with system size dependence* $\sim 1/N$. In Fig. 2 we plot the system size dependence of the gap at two densities, namely at quarter and half fillings. The latter case corresponds to the $q = \pi$ state considered by Sutherland and we verify his result $N\delta E = J\pi^2$. At $d = 1/4$ $N\delta E$ seems to asymptote to the value $3J\pi^2/4$. Remarkably both these asymptotic values of $N\delta E$ at densities 1/2 and 1/4 can be obtained from the low density formula in Eq. (4). In Fig. 2 we also plot the energy-wave-vector curve, obtained from the solution of the 16-particle problem, and compare it with Eq. (4). Note that the discrepancies at large q are finite size effects and would vanish in the $N \longrightarrow \infty$ limit.

Variational results.—Having found the excited states, we now turn to the explicit connection with Bloch wall states. We now show, remarkably enough, that the expression Eq. (4) for the gap can be obtained from a simple variational calculation. We work with arbitrary spin s of the particles. A neat way to generate Bloch walls is via a unitary rotation operator [19] $Q = \exp i \frac{2\pi}{N} \sum_m m S_m^z$ acting upon an appropriate state, $|0_n\rangle \equiv (\hat{S}_0^-)^n |\text{ferro}\rangle$, where $\hat{S}_q^- \equiv \sum_j \exp(iq \cdot r_j) S_j^-$ is a spin wave creation operator carrying momentum q and $|\text{ferro}\rangle$ is the state with all spins up. Using $[H, \hat{S}_0^-] = 0$, we see that $|0_n\rangle$ is the ground state in the n-particle sector with zero total momentum. Thus finally we write the variational Bloch wall state $|\text{BW}\rangle \equiv Q|0_n\rangle$. Using the quasicommutator $Q\hat{S}_q^- = \hat{S}_{q+2\pi/N}^- Q$, we find that $|\text{BW}\rangle = (\hat{S}_{2\pi/N}^-)^n |\text{ferro}\rangle$, and has total momentum $q = 2\pi d$. In the semiclassical limit, $s \gg 1$, the above state is readily visualized as classical spins that are tipped from the z axis and rotate along a cone. The variational calculation of the excitation energy δE, i.e., $\langle 0_n | Q^\dagger \mathcal{H} Q | 0_n \rangle$ can be done easily by transforming the rotation onto the spin operators. Writing $n = dN$, with

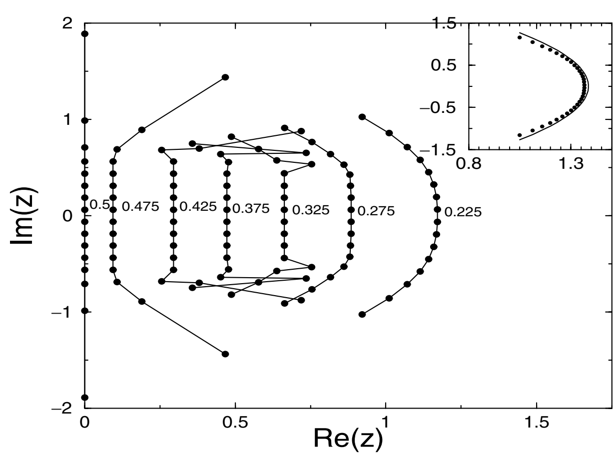

FIG. 1. The figure shows the Bethe curves for a 16-particle system at different densities (values indicated along each curve). The inset compares the numerically obtained roots (points), for a 32-particle system at $d = 0.2$, with the exact low-density result (solid line).

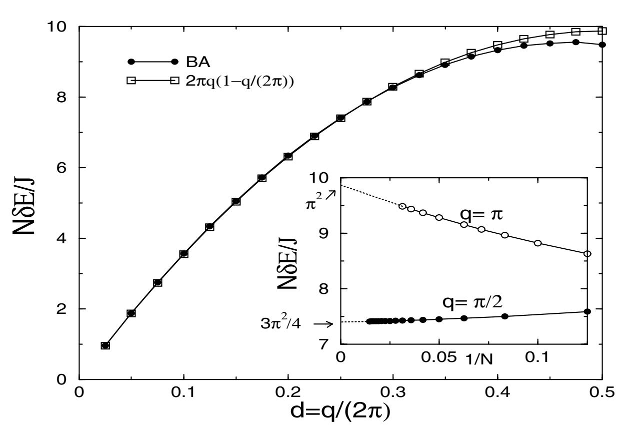

FIG. 2. The gaps at different wave vectors as obtained from the solution of the BA equations for 16 particles. The gap as given by Eq. (4) is also shown. The inset shows dependence of the gap on system size at two different wave vectors.

$0 \leq d \leq 2s$, we find $\delta E = \frac{4J\pi^2}{N} d(2s - d)$. At $s = 1/2$ *this is also the result of the calculation in* Eq. (4).

At this point we admit that we were surprised, as the reader might well be, that the results of an elaborate bound state calculation with a macroscopic number of complex roots agree with the result of a simple looking variational wave function that resembles a Bose condensate of spin waves. This phenomenon is presumably a consequence of the shallow nature of the bound state. We note that the variational states satisfy $\sqrt{\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2}/\langle \mathcal{H} \rangle \sim O(1/\sqrt{N})$ which shows that in the $N \rightarrow \infty$ limit, these become exact eigenstates, thereby providing independent evidence for the exactness of the main result of our work.

For large s, the energy as well as momentum of these states agrees with the semiclassical estimates [16] using a Poisson bracket structure to construct a semiclassical momentum operator. The variational results for all values of s thus collapse onto the same formula. The conjecture of [15,16] implies just this kind of a result, but for the solitons, i.e., for bound states with a small number of spin deviations. Needless to say, we believe that our variational results are exact (in the thermodynamic limit) for *all spin,* since we have established them at $s = 1/2$ and also for very large s.

We note that the Bloch wall states $|\text{BW}\rangle$ carry a total spin that is easy to calculate using simple extension of the above calculation: $\langle S_{\text{tot}}^2 \rangle = \langle S_z \rangle^2 = N^2(s - d)^2$. Finally we note that these variational results for Bloch walls are generalizable to higher dimensions.

Conclusion.—We finally note in summary that the Bethe formula for n magnon bound states: $\omega_{\text{Bethe}} = J\,\frac{2}{n}[1 - \cos(q)]$ is (a) exact for $q \gg 2\pi n/N$, (b) invalid for $q < 2\pi n/N$, and (c) has significant corrections when $q \sim 2\pi n/N$ [20]. The evidence for (a) is in Bethe's paper itself, the corrections to it are exponential in N, (b) is numerical. Evidence for (c) has been presented in this paper, where we find instead: $\omega_{BW} = 2\pi J/N|q|(1 - \frac{|q|}{2\pi})$.

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[11] The total momentum q and spin S_{tot} are found from the eigenvalues of the lattice translation operator T and total spin S^2 as $T \rightarrow e^{iq}$ and $S^2 \rightarrow S_{\text{tot}}(S_{\text{tot}} + 1)$.
[12] We use the term "Bloch wall" in a slightly generalized sense from the usual domain walls of [10]. In the latter, the magnetization rotates from up at $x = 0$ to down at $x = L$, thus defining spin-twisted boundary conditions. Our excitations satisfy periodic boundary conditions, with the magnetization rotating along a cone as we traverse the ring, and hence constitute $2, 4, 6, \ldots$ domain walls of the former.
[13] For wave vectors q of $O(1/N)$, spin wave energies are on a scale $O(1/N^2)$, and these are also obtained from our formula Eq. (4). We mention that the very lowest excited state (over all q) is the Bloch spin wave with $q = \frac{2\pi}{N}$, with the usual energy $J4\pi^2/N^2$, much above the lower bound $4J/N^2$ found in [9].
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[20] This is true even for small n. For example for $n = 2$, $q = 4\pi/N$ the roots, from Eq. (3), are at $\alpha_{1,2} = N/\pi \pm i\sqrt{N}/\pi$ instead of Bethe's $N/\pi \pm i$. As noted by Bethe, for 2 magnons the string solution holds for $q \gtrsim 1/\sqrt{N}$.