Low-Lying Eigenstates of the One-Dimensional Heisenberg Ferromagnet for any Magnetization and Momentum

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I present the exact dispersion relations for certain low-lying states of the one-dimensional Heisenberg ferromagnet. These states are bound complexes of M overturned spins, and in fact are the states with the lowest energy for given values of the total spin, z component of spin and momentum.

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Soon after the invention of quantum mechanics, Bloch and Slater proposed a mechanism for ferromagnetism based on a quantum mechanical Hamiltonian proposed earlier by Heisenberg. In a classic paper [1] published in 1931, Bethe studied the one-dimensional version of this Heisenberg ferromagnet, presenting the solution in the form of a guess—Bethe's ansatz—for the wave functions. He then verified that these wave functions in fact do obey the eigenvalue equation, and gave a counting scheme to show that they were a complete set. Of great interest was a set of low-lying states made up of plane waves with complex wave vectors—the so-called bound states. For bound states of small numbers of overturned spins, Bethe gave the explicit dispersion relation. However, when the number of overturned spins in a bound state is a finite fraction of the total number of spins making up the sample, then the situation is much more complicated. In particular, the question of the stability of a bound state—and so completeness— is subtle. They are precisely these states that we will study. (Our conclusion is that Bethe's original argument does not apply when the number of overturned spins is a finite fraction of the total lattice size.)

We wish to investigate certain low-lying states of the one-dimensional Heisenberg ferromagnet [2]. We take the lattice to be a ring of N sites, so an index j will be understood as modulo N. We will always write the quantum states in a basis of eigenstates of σ_j^z, where the z direction is "up." An operator $P_{j,k}$ permutes the spins on sites j and k. With these definitions, the Hamiltonian is given as

$$H = -\frac{1}{2}\sum_{j=1}^{N}\left[\boldsymbol{\sigma}_j \cdot \boldsymbol{\sigma}_{j+1} - 1\right] = -\sum_{j=1}^{N}\left[P_{j,j+1} - 1\right].$$

Clearly the absolute ground state is $\Psi_0 = 1$, with ground state energy $E_0 = 0$.

The Hamiltonian commutes with the total spin operator, and with the translation operator which translates by one site. Thus, we can specify the states by their total spin, the z component of spin—or, equivalently, M spins down, $N - M$ spins up—and the total momentum P, given modulo 2π.

It is convenient to take twisted boundary conditions [3,4], rather than the usual periodic boundary conditions. These are defined as follows: Let the M down spins be located at sites $\{x_1, \ldots, x_M\}$, so the wave function for a state is then written as $\Psi(x_1, \ldots, x_M)$, symmetric in permutations of the coordinates. Then the twisted boundary conditions are given as $\Psi(\ldots, x_j + N, \ldots) = e^{i\Phi}\Psi(\ldots, x_j, \ldots)$. The parameter Φ is the magnitude of the twist, and $\Phi = 0 \bmod 2\pi$ is the usual periodic boundary condition. We can then treat Φ as a continuous parameter for the wave function. If we increase Φ by 2π, the physical problem is obviously the same, although a twisted state will in general not be the same state. In particular, translating a state by N, we see that $e^{iNP} = e^{iM\Phi}$. Thus, we speak of boosting the momentum by $M\Phi/N$, and we can then usefully think of momentum as a continuous variable.

We obviously have in mind a lattice gas model, where the $N - M$ up spins are empty lattice sites or holes, and M down spins are particles, with a density $d = M/N$. Particle-hole symmetry allows us to restrict the density to $d \leq \frac{1}{2}$. Then the twist is supplied to the charged particles by means of a magnetic flux threading the ring—the Bohm-Aharonov effect.

This ability to boost the momentum has the added advantage of giving us a criterion for judging whether a given M-particle state is a bound complex of M particles acting as a single entity, or whether it is instead a coherent beam of M particles. This in general is a difficult question because we know that for a finite system a quantity like energy is an analytic function of any analytic parameter of the Hamiltonian, such as the coupling constant. Therefore, even if we obtain a bound state of two particles as we vary the coupling constant through a threshold value—meaning the asymptotic momenta of the particles become complex—there is no singularity in the energy to signal such a qualitative change. But, if we boost the momentum of an M-particle bound state through 2π by a twist of $2\pi N/M$, then the energy returns to its initial value. This is to be contrasted with the case of a coherent beam of M particles, when the momentum of each particle must be boosted through 2π— for a change in total momentum of $2\pi M$—before the energy returns to its initial value. This is accomplished by a twist of $2\pi N$. Thus, an M-particle state is a bound complex of M particles if the energy of the state is periodic in the twist with a period of

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$2\pi N/M$. This is no more than the familiar observation in superconductors that the periodicity is a half-flux quantum because the excitations are Cooper pairs.

As first discovered by Bethe, the energy eigenfunctions are given by

$$\Psi(\ldots,x_j,\ldots) = \sum_P A(P)\exp\left[i\sum_{j=1}^{M} x_j p_{Pj}\right],$$

with $x_1 < \ldots < x_M$. The summation is over all $M!$ permutations $\{P1,\ldots,PM\}$. The energy and momentum are given by $P = \sum p$, mod2π, and $E = 2\sum[1 - \cos p]$. The amplitudes $A(P)$ are related one to another by the two-body phase shifts. (For $M > N/2$, eigenstates are determined by particle-hole symmetry.) Then, upon imposing the twisted boundary conditions, we obtain M coupled transcendental equations for the asymptotic momenta $\{p_j\}$,

$$e^{ipN} = e^{i\Phi}\prod_{p'}\left[-\frac{1 + e^{i(p+p')} - 2e^{ip}}{1 + e^{i(p+p')} - 2e^{ip'}}\right],$$

the product being over all the $M - 1$ p's other than p. This is well known, and serves as our starting point.

We now make a change of variable, from p's to α's, given by $e^{ip} = (2\alpha + 1)/(2\alpha - 1)$, or $p = -2i\,\mathrm{arccoth}(2\alpha) \equiv -if(\alpha)$. Some care is needed in specifying the branch structure of $f(\alpha)$. We make the branch cut from $-\frac{1}{2}$ to $\frac{1}{2}$, and choose the branch so that $f(\alpha)$ is real for α real, and $|\alpha| > \frac{1}{2}$. The equations for the p's then become

$$\left[\frac{2\alpha + 1}{2\alpha - 1}\right]^N = e^{i\Phi}\prod_{\alpha'}\left[\frac{\alpha - \alpha' + 1}{\alpha - \alpha' - 1}\right].$$

Taking the logarithm of these equations, we obtain

$$Nf(\alpha) = 2\pi iI(\alpha) + i\Phi + \sum_{\alpha'} f((\alpha - \alpha')/2).$$

The numbers $I(\alpha)$ are integers from log(1). We shall refer to the α's as the roots, to distinguish them from the p's.

The energy as a function of the α's becomes $E = \sum f'(\alpha)$, $f'(\alpha)$ being the derivative of $f(\alpha)$, a single valued function. The momentum then is $P = -i\sum f(\alpha)$, mod2π. The solutions will all have p's in complex conjugate pairs, written as $\{p\}^* = \{p\}$, implying $\{\alpha\}^* = \{-\alpha\}$. We take $I(\alpha) = 0$, throughout. For $\Phi = 0$, the α's will be real, symmetric, and $|\Delta\alpha| \geq 1$. Thus, $|\alpha| > \frac{1}{2}$, with the exception of (i) $\alpha = 0$, for M odd; (ii) $\alpha = \pm\frac{1}{2}$, M even. For $\Phi = 0$, this gives the momentum of the state to be $P = \pi$, and hence for general Φ the momentum of the state to be $P = M\Phi/N + \pi$.

The case when $N \to \infty$, M finite has been previously discussed [1,4]. We see that if $N \to \infty$, then $e^{iNp} \to \infty$ or 0, according to whether Im$(p) <$ or > 0. Thus, we see that $\Delta\alpha =$ integer, and so $\alpha_j = j - (M + 1)/2 - ia$, $j = 1,\ldots,M$, with a real. These are the so-called bound states, or M strings, first found by Bethe. The energy is evaluated as $E = 4M/(M^2 + 4a^2)$. The momentum is evaluated as $e^{iP} = -(M - 2ia)/(M + 2ia)$, so $P = \pi - 2\arctan(2a/M)$. Thus, the momentum ranges between 0 and 2π. Eliminating a between the equations for E and P gives the dispersion relation for the M string $E = 2[1 - \cos(P)]/M$. Note that when $N \to \infty$ it requires $\Phi \to \infty$ to boost the momentum by a finite amount. These expressions will be useful when $M,N \to \infty$, $d = M/N$ fixed. For fixed M and large but finite N, the differences $\alpha_{j+1} - \alpha_j$ deviate from 1 by a positive term exponentially small in N.

For $M,N \to \infty$, we assume as before that the roots α distribute themselves along a curve in the complex α plane, symmetric about the imaginary axis. The α's cannot be closer to one another than $|\Delta\alpha| = 1$, a distance fixed by the branch points of $f(\Delta\alpha/2)$. Thus the end points will be of order N, and we rescale by choosing a new variable $x = \alpha/N$. We then assume that the x's distribute themselves along the curve in the complex x plane with a root density $\rho(x)$, so that $N\rho(x)\,|dx|$ is the number of x's in dx. Finally, we make the ansatz that in the central portion the x's are distributed with a maximum density $\rho(x) = 1$, along a straight curve Ω perpendicular to the imaginary axis, as for the finite M strings. We call these condensed roots the core, and they make a contribution to the energy and momentum identical to that of an M string. On the other hand, the remaining x's in the tails of the distribution have a density $\rho(x) < 1$, and lie along a more general curve Γ. Thus we can write $\int_{\Omega+\Gamma}\rho(x)\,|dx| = M/N = d$.

If we examine the function $f(\alpha)$ under the change of variable, we see $f(Nx) = 2\,\mathrm{arccoth}(2Nx) \to 1/Nx$, as $N \to \infty$. Inserting this expression into the transcendental equations, and replacing the summations by integrals along the curve $\Omega + \Gamma$ with the density $\rho(x)$, and assuming a core of condensed roots, we obtain the following singular integral equation:

$$\frac{1}{x} = i\Phi + 2\int_\Omega \frac{dy}{x - y} + 2\int_\Gamma \frac{\rho(y)\,|dy|}{x - y}, \qquad x \in \Gamma.$$

Let $\pm B_1 + iB_2$ be the end points of Ω, while $\pm A_1 + iA_2$ are the end points of $\Omega + \Gamma$. To reduce the number of parameters in the problem, let us once more change variables, moving the end points of Ω to ± 1 by $x = B_1 x' + iB_2$. This new scaled variable we will also call x and, in fact, will continue to use ρ for the original density considered as a function of the new scaled variable. With the definitions $a = A_1/B_1$, $b = A_2/B_1$, $c = -B_2/B_1$, the singular integral equation becomes

$$\frac{1}{2B_1(x - ic)} = \frac{i\Phi}{2} + \int_{-1}^{1}\frac{dy}{x - y} + \int_\gamma \frac{\rho(y)\,|dy|}{x - y}, \qquad x \in \gamma.$$

The contours are shown in Fig. 1(a). It is in this form that we will solve the equation.

Let us now derive expressions for the auxiliary quantities, starting with the particle density. We have

$$M/N = d = B_1\left[2 + \int_\gamma \rho(x)\,|dx|\right].$$

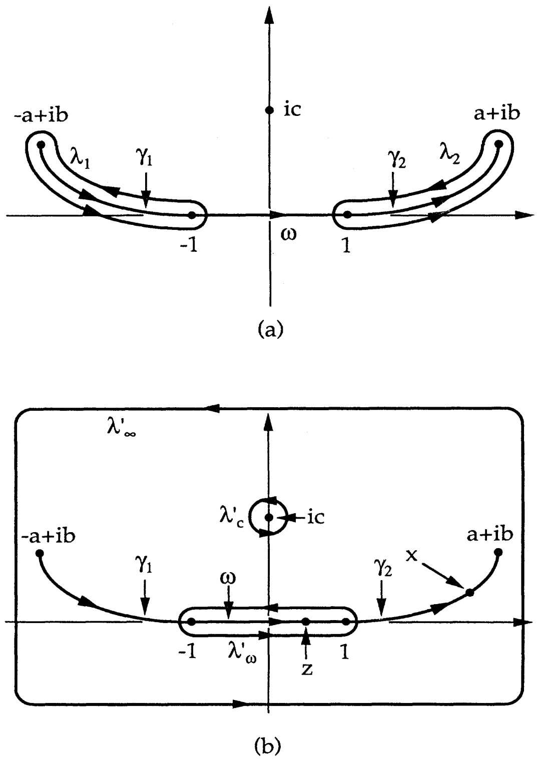

FIG. 1. Contours (a) and deformed contours (b) in the x plane, as explained in the text; we have $\gamma_1 + \gamma_2 = \gamma$ and $\lambda_1 + \lambda_2 = \lambda$.

Thus, there are $2B_1N$ condensed roots in the core, with the remaining roots in the tails. The energy of the core is identical to that of a $2B_1N$ string, while the energy of a single root in the tails becomes $-1/(Nx)^2$; so, combining the two contributions, we have for the energy

$$NE = \varepsilon = \frac{1}{B_1}\left[\frac{2}{1+c^2} - \int_\gamma \frac{\rho(x)\,|dx|}{(x-ic)^2}\right].$$

We shall treat Φ as a parameter of the equation, so the momentum can be written as

$$P - \pi = M\Phi/N = -2\arctan(c) - i\int_\gamma \frac{\rho(x)\,|dx|}{x-ic}.$$

Again, the first term is from the core, while the second is from the tails.

Our integral equation is of a classic form, and can be solved in full generality [5]. We first enclose the contour γ with a counterclockwise contour λ as in Fig. 1(a). The density ρ can then be found from a "field" $h(x)$ by $\rho(x)\,|dx| = [h(x+) - h(x-)]dx/2\pi i$. Define the function $r(x) = \{(x^2-1)[(x-ib)^2 - a^2]\}^{1/2}$, placing branch cuts on γ, and choosing the branch of r so that $r(0) = \sqrt{a^2+b^2}$, and $r(x) \to -x^2$ as $|x| \to \infty$.

Let us rewrite the integral equation as

$$\int_\gamma \frac{\rho(y)\,|dy|}{x-y} = \int_{\omega'} \frac{\sigma(y)\,|dy|}{x-y} - \frac{i\Phi}{2},\ x \in \gamma,$$

where ω' combines the contour $\omega = [-1,1]$ and the point ic. We now seek the field h in the form $h(x) = r(x)\int_{\omega'}\phi(y)dy/(x-y)$. By deforming the contour λ into the contour λ', as shown in Fig. 1(b), we see that to have a solution to our original equation we must choose $\phi(x) = \sigma(x)/r(x)$, with $\int_{\omega'}\phi(z)\,dz = 0$, and $\int_{\omega'} x\phi(x)\,dx = i\Phi/2$. Translating back, the condition on the zeroth moment of ϕ gives B_1, while the condition on the first moment of ϕ gives Φ. There is the one further constraint that $\mathrm{Re}\int_{\Delta\gamma} h(x)\,dx = 0$; this is the difficult one, and it will fix the contour γ.

It is convenient to define $g(x|a,b) \equiv \int_{-1}^{1} dy/r(y)(x-y)$ with moments $g_n(a,b) \equiv \int_{-1}^{1} y^n\,dy/r(y)$, related by $g(x|a,b) = \sum_{n=0}^{\infty} g_n(a,b)/x^{n+1}$. All of these expressions can be explicitly given in terms of elliptic integrals. We then summarize our results: $B_1 = 1/2\,r(ic)g_0$, $\Phi = 2[ig_1 + cg_0]$, $h(x) = r(x)[g_0/(x-ic) - g(x)]$.

We can derive expressions for the particle density $d = M/N$ and the energy $\varepsilon = NE$ that do not require us to integrate over the contour γ, since this is particularly difficult to determine. These are

$$d = \frac{1}{2} - \frac{g_2 - ibg_1 + c(c-b)g_0}{2g_0\sqrt{(1+c^2)[(c-b)^2 + a^2]}},$$

$$\varepsilon = 2g_0 r(ic)[r(ic)g'(ic) + r'(ic)g(ic)] - g_0^2 r(ic)r''(ic).$$

We save the details for a longer publication.

If the twist Φ is zero, then the equations simplify considerably, since we can conclude by symmetry that $c = 0$ and $b = 0$, and thus the curve γ of the roots lies entirely on the real axis. Then, we find that $g(x) = 2/ax\Pi(1/x^2, 1/a)$, $g_0 = 2aK(1/a)$, $g_1 = 2a/3[(2a^2+1)K(1/a) - 2(a^2+1)E(1/a)]$. [The functions $K(k)$, $E(k)$, and $\Pi(n,k)$ are the complete elliptic integral of the first, second, and third kinds.] Then $r(x) = [(x^2-1)(x^2-a^2)]^{1/2}$, so $r(0) = a$, $r'(0) = 0$, and $r''(0) = -(a + 1/a)$. We then use the previous expressions to find the actual range of the core of condensed roots B_1 to be $B_1 = 1/4K(1/a)$. The field h is given as

$$h(x) = 2[(x^2-1)(x^2-a^2)]^{1/2} \times [K(1/a) - \Pi(1/x^2, 1/a)]/ax.$$

Finally, the density of the roots ρ along the real axis, in terms of the scaled variable x, is

$$\rho(x) = \begin{cases} 1, & |x| \le 1, \\ 0, & |x| \ge a, \\ 2[(x^2-1)(a^2-x^2)]^{1/2}[\Pi(1/x^2, 1/a) - K(1/a)]/\pi|x|, & 1 \le |x| \le a. \end{cases}$$

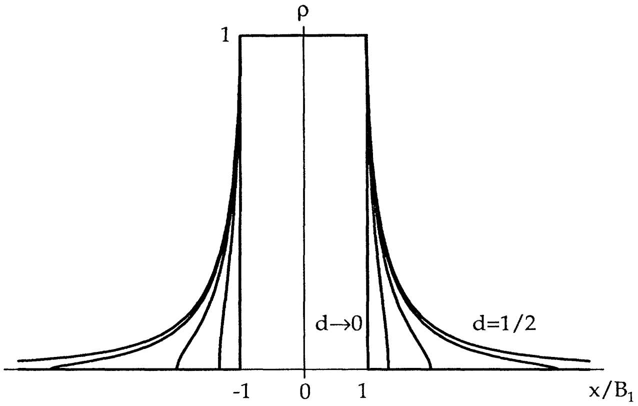

FIG. 2. The density of the roots as a function of the scaled variable, for typical values of particle density.

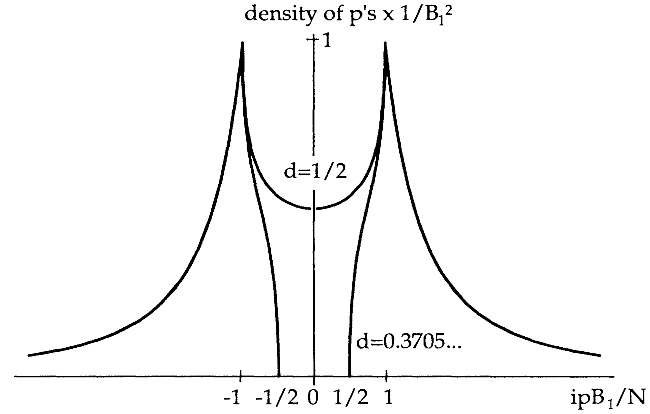

FIG. 3. The density of the asymptotic momenta, which occur in Bethe's wave function, for selected values of the particle density.

In Fig. 2 we show $\rho(x)$ for selected values of $a = A_1/B_1$. Note the sharp edges to the distribution. The original p's are distributed along the imaginary axis with a momentum density as shown in Fig. 3, for $a = 2$, corresponding to $d = 0.370\,51\ldots$, and for $a = \infty$ with $d = \frac{1}{2}$. Note that the "core" of α's with uniform density has become the "tails" of the p distribution.

Previous expressions give the particle density and energy

$$d = 1/2 + a[E(1/a)/K(1/a) - 1]/2,$$
$$\varepsilon = 4K(1/a)[2E(1/a) - (1 - 1/a^2)K(1/a)].$$

This then gives the energy ε parametrically as a function of the density d. The point $a \to \infty$ is a singular point, corresponding to the distribution of roots being unbounded. At this point $d = \frac{1}{2}$, so the lattice gas is half filled, and $\varepsilon = \pi^2$. The boundary of the core is $B_1 = \frac{1}{2}\pi$. The density of roots in the tails becomes $\rho(x) = 1 - (x^2 - 1)^{1/2}/|x|$, $|x| \geq 1$. Completing the energy versus density curve by symmetry, we find for d, near $\frac{1}{2}$, $\varepsilon = \pi^2[1 + 8(d - \frac{1}{2})^2 + \cdots]$. This then gives the spin susceptibility at the point $d = \frac{1}{2}$. (We note that this calculation, giving a weak paramagnetism for momentum π, is in direct contradiction to the string hypothesis.)

If the twist Φ is not zero, then the roots are no longer confined to the real axis. Since we have solved this problem in all generality, we can determine the full dispersion relation for the bound states, but this requires extensive numerical analysis, so I save this for a longer paper. Physically, we are most interested in dispersion curves of ε versus Φ or momentum $P = \pi + d\Phi$, for fixed density d, corresponding to an M complex, $M = dN$. In the limit as $a, b, c \to \infty$, the physical quantities d, Φ, ε approach limiting values, leading to end points for the dispersion curves. What happens at these points on the boundary curve? It is at precisely these points that the end points $\pm a + id$ of the contour γ extend to infinity, so that the roots become arbitrarily large. This leads to a finite density for the p's at the origin. We saw this for $\Phi = 0$. But p's at the origin play no point in the dynamics of the problem, make no contribution to the energy or momentum, and in fact are the source of the large degeneracies for large values of total spin, reflecting rotational invariance of our Hamiltonian.

If we examine the momentum π states for the periodic Heisenberg ferromagnet when $\Phi = 0$, the M-particle states we have studied have z component of spin S_z given by $2S_z = N - 2M$, but also they have a total spin quantum number $S = S_z$; they are the so-called "maximum weight" states. However, there are $N - 2M$ other states degenerate with this one; what is their nature? These other states have the same energy and momentum as our M-complex state, but contain $M' > M$ particles, so the additional $M' - M$ particles have $p = 0$. The tails of the M complex imbedded within the M' state do not extend to infinity, and so do not feed particles in and out of the $p = 0$ reservoir. This makes the two components dynamically independent, and so the M' complex with $|S_z| < S$ is composite, and this is reflected in the fact that the energy as a function of Φ has a period of $2\pi N$ rather than $2\pi N/M$.

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