No attraction between spinons in the Haldane-Shastry model

Martin Greiter and Dirk Schuricht

Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, Postfach 6980, D-76128 Karlsruhe, Germany

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While the Bethe ansatz solution of the Haldane-Shastry model appears to suggest that the spinons represent a free gas of half-fermions Bernevig, Giuliano, and Laughlin (BGL) [Phys. Rev. Lett. **86**, 3392 (2001); Phys. Rev. B **64**, 24425 (2001)] have concluded recently that there is an attractive interaction between spinons. We argue that the dressed scattering matrix obtained with the asymptotic Bethe ansatz is to be interpreted as the true and physical scattering matrix of the excitations, and hence, that the result by BGL is inconsistent with an earlier result by Essler [Phys. Rev. B **51**, 13357 (1995)]. We critically reexamine the analysis of BGL, and conclude that there is no interaction between spinons or spinons and holons in the Haldane-Shastry model.

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The Haldane-Shastry model (HSM)^{4–8} plays a unique role among the integrable models of spin $S=\frac{1}{2}$ chains. In what might be referred to as a brilliant theoretical coup, Haldane and Shastry discovered independently in 1988 that a trial wave function proposed by Gutzwiller⁹ in 1963 provides the exact ground state to a Heisenberg-type spin Hamiltonian whose interaction strength falls off as the inverse square of the distance between two spins on the chain. If one imposes periodic boundary conditions (PBCs), and embeds the onedimensional chain into a two-dimensional complex plane by mapping it onto the unit circle with the $S=\frac{1}{2}$ spins located at complex positions $\eta_{\alpha} = \exp[i(2\pi/N) \alpha]$, where N denotes the number of sites and $\alpha = 1, ..., N$, the Hamiltonian

$$H_{\rm HS} = J \left(\frac{2\pi}{N}\right)^2 \sum_{\alpha < \beta}^{N} \frac{S_{\alpha} \cdot S_{\beta}}{|\eta_{\alpha} - \eta_{\beta}|^2} \tag{1}$$

possesses the exact ground state

$$\Psi_0(z_1,...,z_M) = \prod_{i< j}^M (z_i - z_j)^2 \prod_{j=1}^M z_j,$$
(2)

for N even, M = N/2. The corresponding state vector is given by

$$|\Psi_0\rangle = \sum_{\{z_1,\dots,z_M\}} \Psi_0(z_1,\dots,z_M) S_{z_1}^+ \cdots S_{z_M}^+ |\downarrow\downarrow\dots\downarrow\rangle, \quad (3)$$

where the sum extends over all possible ways to distribute the positions z_i of the up spins over the *N* sites. The model is fully integrable even for a finite number of sites; the algebra of the (infinite number of) conserved quantities is generated by the total spin and rapidity operators

$$S = \sum_{\alpha=1}^{N} S_{\alpha}, \quad \Lambda = \frac{i}{2} \sum_{\alpha \neq \beta}^{N} \frac{\eta_{\alpha} + \eta_{\beta}}{\eta_{\alpha} - \eta_{\beta}} (S_{\alpha} \times S_{\beta}), \quad (4)$$

which both commute with the Hamiltonian but do not commute mutually. The unique feature of the model, from a practical point of view, is that in addition to its amenability to solution by the asymptotic Bethe ansatz (ABA),^{6,10–12} the ground state and many of the excited states (in principle, all the ones where the spins of the spinon excitations are fully polarized) can be written down in closed form, i.e., the wave functions are known explicitly. In particular, the wave function for an individual spinon excitation, which carries spin one-half but no charge, at site η_{α} is constructed in complete analogy to the wave function for a quasihole excitation in a fractionally quantized Hall liquid¹³

$$\Psi_{\alpha}(z_1,...,z_M) = \prod_{j=1}^{M} (\eta_{\alpha} - z_j) \prod_{i< j}^{M} (z_i - z_j)^2 \prod_{j=1}^{M} z_j, \qquad (5)$$

where *N* odd, M = (N-1)/2. The model may hence be used to illustrate the sense in which spinons are fractionally quantized excitations: the spin of the spinon is one-half, while the Hilbert space (3) is built up from spin flips, which carry spin one.

On a more profound level, the model is unique in that there is no spin exchange between spinon excitations,⁶ which follows directly from the commutativity of Λ with H_{HS} . Furthermore, the spinon excitations of the model have or had been considered to constitute an ideal gas of half-fermions, that is, an ideal gas of particles obeying fractional statistics.^{14,15} This view has received strong support from Essler,³ who calculated the dressed scattering matrix of the spinon excitations using the ABA, and found it to be $S=\pm i$. The fact that *S* does not depend on the spinon momenta implies that they are noninteracting or free; the phase *i* implies that they obey half-fermion statistics. This picture, and in particular the applicability of the ABA to the HSM, were commonly accepted until a few years ago.

In 2001, this picture was challenged by Bernevig, Giuliano, and Laughlin (BGL),^{1,2} who investigated the nature of the spinon interaction by working out the wave functions for the spin-polarized two-spinon eigenstates explicitly. They found "clear evidence for a short-range, attractive interaction between spinons."¹ Furthermore, they "prove rigorously that this enhancement"—meaning a probability enhancement as the spinons are close together—"is responsible for the square-root singularity in the dynamical spin susceptibility,"¹ which has been evaluated exactly in the thermodynamic limit for the HSM by Haldane and Zirnbauer,¹⁶ and experimentally observed in KCuF₃ by Tennant *et al.*¹⁷ According to BGL, "the experiments provide evidence that

spinons do interact and that the spinon interaction is what determines the peculiar low-energy physics of spin one-half antiferromagnetic chains." ² BGL attribute the apparent contradiction between their results and the ABA result to the fact that "the interaction between spinons is encoded in the definition of the pseudomomenta" which label the Bethe ansatz solutions.¹ In other words, they assert that it is a special feature of the ABA technique that the spinon excitations appear to be free, while there is in fact an attractive interaction between them.

This line of reasoning may sound convincing at first sight. Indeed, in models like the Sutherland-Calogero^{10,18} or the Haldane-Shastry model, the long-range interaction of the particles or spins, respectively, is encoded in the definition of the pseudomomenta. The interacting degrees of freedom the Hilbert space is built up from, the particles or spin flips, are mapped through a nonlocal and highly nontrivial transformation into a new set of degrees of freedom, the pseudomomenta, which do not interact. In a sense, in the HSM both the $1/r^2$ tail of the spin-flip terms $S^+_{\alpha}S^-_{\beta}$ as well as the "potential energy" term $S_{\alpha}^{z}S_{\beta}^{z}$ are encoded in the pseudomomenta. In the framework of the ABA, spinon excitations for the HSM correspond to fractional holes in the otherwise uniform distribution of pseudomomenta. Specifically, a pair of spinons is constructed by shifting the pseudomomenta quantum numbers I_i from integer to half-integer values or vice versa, and leaving the I_i 's or pseudomomenta associated with the spinons unoccupied. The energy of the state is given by a sum of "kinetic energies" of each occupied pseudomomentum, without an interaction between them. The information regarding the $1/r^2$ interaction between the original spins is no longer accessible in this framework.

What is still accessible, however, is the information regarding the energies of and the interaction between the spinon excitations. The energies of the spinons are given by the change in the kinetic energies associated with the occupied pseudomomenta as we shift them. The interaction between the spinons is encoded in the way this shift in the pseudomomenta induced by one spinon is affected by the existence of another. In the spin one-half Heisenberg chain, for example, there is a rather complicated change or "screening" of the pseudomomenta due to an interaction between the spinons. In the HSM, by contrast, the creation of a spinon only induces a constant shift of the pseudomomenta, which implies that the spinons are free. The most reliable way to extract this information, however, is to calculate the spinonspinon scattering matrix. If the ABA is applicable to the HSM at all, which is not garanteed a priori as the spin-spin interaction is long ranged, the result by Essler quoted above unambigously confirms that the spinons are free.

In the remainder of this paper, we resolve the contradiction between the conclusions reached by Essler³ and BGL.^{1,2} The result is that we find no reason to doubt the applicability of the ABA, and completely agree with Essler's conclusions. We also agree with the explicit calculations of BGL, but do not agree with their interpretation of the calculations. In particular, their conclusion that there is an attraction between spinons or spinons and holons in the HSM, title to several publications,^{1,2,19–21} is incorrect.

To begin with, it is worth noting that there is a physical reason to be suspicious of BGL's result. They conclude that there is an attractive interaction between spinons, but no bound state. If there was an arbitrarily weak attraction, however, it would presumably yield a bound state due to the Cooper instability.²² Cooper's argument was originally formulated for two electrons outside a completely occupied Fermi sphere, which are subject to an arbitrarily weak attraction. The argument is independent of the number of dimensions. The Fermi surface is only relevant in that it blocks certain states, and renders the density of states available to the two electrons at the point where their kinetic energy is minimal (i.e., at the Fermi surface) finite. The Fermi statistics of the electrons accounts for the formation of a spin singlet, but is not essential to the instability; for example, one would also find a bound state if one were to use spinless bosons instead. The only subtlety involved in applying the argument to spinons in the HSM is the half-fermi statistics of the spinons. It is not plausible to us, however, that this statistical interaction would preclude the pairing, as there is not even an angular momentum barrier associated with the statistical interaction in one dimension.

Let us now critically reexamine the arguments presented by BGL. We begin with a review of their analysis, and then explain why we disagree.

BGL construct exact two-spinon eigenstates for the HSM starting from basis states with the two spinons localized at sites η_{α} and η_{β}

$$\Psi_{\alpha\beta}(z_1,...,z_M) = \prod_{j=1}^M (\eta_{\alpha} - z_j)(\eta_{\beta} - z_j) \prod_{i< j}^M (z_i - z_j)^2 \prod_{j=1}^M z_j,$$
(6)

where M = (N-2)/2 denotes the number of up or down spins condensed in the uniform singlet sea. The momentum space basis states are obtained by Fourier transformation,

$$\Psi_{mn}(z_1,\ldots,z_M) = \sum_{\alpha,\beta}^N \frac{(\bar{\eta}_{\alpha})^m}{N} \frac{(\bar{\eta}_{\beta})^n}{N} \Psi_{\alpha\beta}(z_1,\ldots,z_M), \quad (7)$$

where $M \ge n \ge 0$. For *m* or *n* outside this range, Ψ_{mn} will vanish identically, reflecting the overcompleteness of the position space basis (6). Acting with the Haldane-Shastry Hamiltonian on Eq. (7) yields

$$H_{\rm HS}|\Psi_{mn}\rangle = E_{mn}|\Psi_{mn}\rangle + \sum_{l=1}^{l_M} V_l^{mn}|\Psi_{m+l,n-l}\rangle,\tag{8}$$

where

$$E_{mn} = -J \frac{\pi^2}{24} \left(N - \frac{19}{N} + \frac{24}{N^2} \right) + \frac{J}{2} \left(\frac{2\pi}{N} \right)^2 \left[m \left(\frac{N}{2} - 1 - m \right) + n \left(\frac{N}{2} - 1 - n \right) - \frac{m - n}{2} \right],$$
(9)

 $l_M = \min(M - m, n)$, and $V_l^{mn} = -(J/2)(2\pi/N)^2(m - n + 2l)$. Since the "scattering" of $H_{\rm HS}$ acting on the nonorthogonal basis states $|\Psi_{mn}\rangle$ only occurs in one direction, increasing the difference m - n while keeping the "total momentum" m + n fixed, the (unnormalized) eigenstates of $H_{\rm HS}$ have energy eigenvalues E_{mn} and are of the form

$$|\Phi_{mn}\rangle = \sum_{l=0}^{l_M} a_l^{mn} |\Psi_{m+l,n-l}\rangle \tag{10}$$

with $a_0^{mn} = 1$. A recursion relation for the coefficients a_l^{mn} is easily obtained from Eq. (8). Combining Eqs. (10) and (7), one thus obtains an expansion of the exact energy eigenstates $|\Phi_{mn}\rangle$ in terms of localized spinon states $|\Psi_{\alpha\beta}\rangle$.

In a technically truly remarkable analysis, BGL have further succeeded in obtaining the coefficients $p_{mn}(\eta_{\alpha-\beta})$ in the inverse expansion

$$|\Psi_{\alpha\beta}\rangle = \sum_{m=0}^{M} \sum_{n=0}^{m} (-1)^{m+n} \eta^{m}_{\alpha} \eta^{n}_{\beta} p_{mn}(\eta_{\alpha-\beta}) |\Phi_{mn}\rangle \quad (11)$$

of the localized spinon states in terms of the energy eigenstates by solving a hypergeometric differential equation. Since a spin flip S_{α}^{-} acting on the Haldane-Shastry ground state yields a state with a pair of spinons localized at $\eta_{\alpha}, S_{\alpha}^{-} |\Psi_{0}\rangle = \eta_{\alpha} |\Psi_{\alpha\alpha}\rangle$, the expansion of $S_{q}^{-} |\Psi_{0}\rangle$ in terms of $|\Phi_{mn}\rangle$ is determined by $p_{mn}(1)$,

$$S_{q}^{-}|\Psi_{0}\rangle = \sum_{\alpha=1}^{N} (\eta_{\alpha})^{k} S_{\alpha}^{-}|\Psi_{0}\rangle$$
$$= N \sum_{m=0}^{M} \sum_{n=0}^{m} (-1)^{m+n} \delta_{m+n+k+1,0} p_{mn}(1) |\Phi_{mn}\rangle, (12)$$

where $q=2\pi k/N$ and the Kronecker δ is defined modulo *N*. The explicit expression for $p_{mn}(1)$ enabled BGL to calculate the dynamical spin susceptibility (DSS)

$$\chi_{q}(\omega) \equiv -\operatorname{Im}\langle \Psi_{0} | S_{-q}^{+} \frac{1}{\omega - (H_{\mathrm{HS}} - E_{0}) + i0} S_{q}^{-} | \Psi_{0} \rangle, \quad (13)$$

for finite chains as well as in the thermodynamic limit, thus providing an alternative derivation of the Haldane-Zirnbauer formula.¹⁶ The DSS shows a square-root singularity at the lower threshold frequency of the two-spinon continuum, which is a characteristic feature of spin one-half chains.²³

As already mentioned, we completely agree with these calculations. We disagree, however, with BGL's interpretation of the results as evidence for a spinon attraction.

The first argument given by BGL in favor of a spinon interaction is based on a plot of $|p_{mn}(e^{i\theta})|^2$ for m=M, n=0, as a function of θ . They interpret $|p_{mn}(e^{i\theta})|^2$ as probability for finding the spinons at a distance θ along the circle from each other, and show it to be strongly enhanced at small θ . The problem with the argument is that, as one can easily see from Eq. (11), the $p_{mn}(\eta_{\alpha-\beta})$'s are the coefficients in the expansion of the overcomplete basis states $|\Psi_{\alpha\beta}\rangle$ at fixed α, β in terms of $|\Phi_{mn}\rangle$. Due to this overcompleteness, the $p_{mn}(\eta_{\alpha-\beta})$'s as functions of $\eta_{\alpha-\beta}$ have no direct physical interpretation. The actual relative spinon-spinon wave function $\varphi_{mn}(\eta_{\alpha-\beta})$ for given m and n provides the coefficients in

$$|\Phi_{mn}\rangle = \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} \varphi_{mn}(\eta_{\alpha-\beta})(\eta_{\alpha+\beta})^{(m+n)/2} \frac{|\Psi_{\alpha\beta}\rangle}{\||\Psi_{\alpha\beta}\rangle\|}.$$
 (14)

It is easily seen from Eqs. (10) and (7) that a possible choice for $\varphi_{mn}(\eta_{\alpha-\beta})$ is

$$\varphi_{mn}(\eta_{\alpha-\beta}) = \sum_{l=0}^{l_M} a_l^{mn}(\eta_{\alpha-\beta})^{(m-n+2l)/2} \||\Psi_{\alpha\beta}\rangle\|.$$
(15)

Depending on *m* and *n*, one finds that $\varphi_{mn}(e^{i\theta})$ is sometimes enhanced and sometimes suppressed for small θ , but even if there was a clear enhancement, it would not allow for a conclusion regarding a spinon attraction. The reason is simply that the overcompleteness of the basis states $|\Psi_{\alpha\beta}\rangle$ implies that $\varphi_{mn}(\eta_{\alpha-\beta})$ is not uniquely determined, i.e., there are infinitely many choices for $\varphi_{mn}(\eta_{\alpha-\beta})$ which yield the same $|\Phi_{mn}\rangle$ in Eq. (14).

The second argument of BGL is that the last term in the energy (9) of the two-spinon state $|\Phi_{mn}\rangle$ represents "a negative interaction contribution that becomes negligibly small in the thermodynamic limit."¹ The problem here is that BGL identify the momenta q_m and q_n of the individual spinons according to

$$q_m = \frac{\pi}{2} - \frac{2\pi}{N} \left(m + \frac{1}{2} \right), \quad q_n = \frac{\pi}{2} - \frac{2\pi}{N} \left(n + \frac{1}{2} \right), \quad (16)$$

and interpret the two preceding terms in Eq. (9) as the kinetic energies of the individual spinons. The correct identification of the spinon momenta for $m \ge n$, however, is

$$q_m = \frac{\pi}{2} - \frac{2\pi}{N} \left(m + \frac{3}{4} \right), \quad q_n = \frac{\pi}{2} - \frac{2\pi}{N} \left(n + \frac{1}{4} \right), \quad (17)$$

which implies that the kinetic energy of the spinons is given by all three terms in the square bracket in Eq. (9). With $E(q)=(J/2)[(\pi/2)^2-q^2]$, one finds

$$E_{mn} = -J\frac{\pi^2}{24} \left(N + \frac{5}{N} - \frac{6}{N^2} \right) + E(q_m) + E(q_n).$$
(18)

The alleged spinon interaction term has disappeared. Physically, the shift between q_m and q_n by one-half of a momentum spacing $2\pi/N$ is nothing but a manifestation of the half-fermi statistics of the spinons. While the allowed values for the total momenta q_m+q_n are those for PBCs, the allowed values for the difference in the momenta q_m-q_n are those for anti-PBCs, i.e., PBCs with the ring threaded by a flux π .

Finally, BGL claim to prove that the enhancement of $|p_{mn}(e^{i\theta})|^2$ they find when plotting it as a function of the spinon separation θ is responsible for the square-root singularity in the DSS.¹ Their proof then consists of the derivation of the Haldane-Zirnbauer formula sketched above. In their longer paper,² BGL conclude that their "analysis definitely proves that the square-root sharp edge on top of the broad spectrum is nothing but the interaction between spinons," and say that "this result is of the utmost importance, since it represents a way to experimentally test the interaction among spinons in one dimension."

There are several problems attached to this line of reasoning. First, the coefficients $|p_{mn}(e^{i\theta})|^2$ cannot be interpreted as a probability as a function of the spinon separation θ , as explained above. Second, it is not $p_{mn}(e^{i\theta})$ as a function of θ for fixed *m* and *n* which enters the derivation of the Haldane-Zirnbauer formula, but $p_{mn}(1)$ as a function of *m* and *n*, as one can directly see from Eq. (12).

The square-root singularity in the DSS is accordingly not due to an alleged spinon attraction, but a general consequence of the fractional quantization of spin excitations in spin one-half chains. The position space basis for these fractional excitations, the spinons, is necessarily overcomplete. The local creation of two spinons through a spin flip is in general not equivalent to a creation of all two-spinon energy eigenstates with the same relative weight. The process rather creates predominantly spinons with lower energies, which is reflected in the square-root singularity in the DSS. (These general considerations are of course not sufficient to explain the precise functional form of the DSS, but do provide an intuitive understanding of how a singularity can occur even though the spinons are free.) Since the fractional quantization of spin excitations is a generic feature of spin one-half chains, the square-root singularity in the DSS must be generic as well. It exists in the HSM, where spinons are free, but also in the Heisenberg model, where spinons are interacting. With the experimental observation of the square-root singularity in KCuF₃, Tennant et al.¹⁷ have indirectly observed fractional quantization in spin chains.

In the context of this analysis, it is worthwhile to mention a curiosity of the two-spinon eigenstates. In the evaluation reviewed above, BGL obtained the coefficients a_l^{mn} by explicitly solving the Sutherland equation (8) using the ansatz (10). The coefficients a_l^{mn} were hence determined by the Hamiltonian, and appear to contain information inflicted on the system by the Hamiltonian. In principle, this could include information regarding an interaction between spinons.

In fact, however, the Hamiltonian is not even required in determining the coefficients a_l^{mn} . If we wish to construct an orthogonal basis $|\Phi_{mn}\rangle$ according to Eq. (10) with $a_0^{mn}=1$ from the nonorthogonal basis $|\Psi_{mn}\rangle$, the overlaps $\langle \Psi_{mn} | \Psi_{m'n'} \rangle$ for all m, n, m', n' completely determine all the coefficients a_l^{mn} , as the reader will be able to verify easily for himself. The coefficients a_l^{mn} as well as $p_{mn}(\eta_{\alpha})$, and therefore also the "scattering amplitudes" V_l^{mn} in Eq. (8), hence contain no information except the one regarding the Hilbert space structure of the fractionally quantized excitations. Accordingly, it seems impossible as a matter of principle to reach a conclusion regarding an interaction between the spinons by studying these coefficients.

In conclusion, we have shown that the spinons in the HSM represent an ideal gas of half-fermions, and thereby dispersed all evidence that the ABA might not be applicable to the model. An analysis similar to the one presented here shows that there is likewise no interaction between spinons and holons in the HSM. The conclusions drawn by BGL with regard to this question^{19,20} are likewise incorrect.

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