Method to Characterize Spinons as Emergent Elementary Particles

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We develop a technique to directly study spinons (emergent spin $S = 1/2$ particles) in quantum spin models in any number of dimensions. The size of a spinon wave packet and of a bound pair (a triplon) are defined in terms of wave-function overlaps that can be evaluated by quantum Monte Carlo simulations. We show that the same information is contained in the spin-spin correlation function as well. We illustrate the method in one dimension. We confirm that spinons are well-defined particles (have exponentially localized wave packet) in a valence-bond-solid state, are marginally defined (with power-law shaped wave packet) in the standard Heisenberg critical state, and are not well defined in an ordered Néel state (achieved in one dimension using long-range interactions).

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Spinons are emergent spin $S = 1/2$ particles (fractional excitations) of quantum magnets [1–3] and potentially exist also in strongly correlated electron systems such as the high-T_c cuprate superconductors [4]. Their existence is well established in one-dimensional systems [1,2], where they correspond to kinks and antikinks (solitons). In higher dimensions, gapped magnons (''triplons'') can be viewed as bound states of spinons. Under some conditions, in spin liquid states [3] and at certain quantum-critical points [5], these spinons may become deconfined (unbound). Even in cases where the spinons are not completely deconfined, such as in a valence-bond-solid (VBS) state of a two-dimensional system close to a phase transition into the antiferromagnetic (Néel) state, the bound state can become very large [5]. The spinons can then be viewed as deconfined below the length scale of the pair size and above a corresponding (relatively low) energy scale. This is analogous to quarks, which are the elementary constituent particles of the baryons although they are, strictly speaking, always confined.

Observing deconfined or almost deconfined spinons in experiments is in general difficult [6]. In 1D systems, e.g., the Heisenberg chain, it is well understood (based on the exact Bethe ansatz solution and numerical calculations [2,7]) that spinons lead to a broad continuum in the dynamic spin structure factor $S(q, \omega)$. This continuum has been observed in neutron scattering experiments on quasi-1D quantum antiferromagnets [8]. In 2D systems, there is no known reference model with deconfined spinons in which $S(q, \omega)$ can be computed exactly. One nevertheless expects a broad continuum also in this case, and such experimental signatures have been claimed in some quasi-2D systems [9]. The issue is complicated, however, by the fact that a continuum is also expected due to multi-magnon processes [10].

In this Letter, we discuss spinon detection in numerical model calculations. This has also been a challenging problem, the solution of which will greatly help to understand the conditions under which spinons can exist as independent elementary particles. Recently, signatures in thermodynamic properties were observed [11] in a 2D J-Q model (a spin-1/2 Heisenberg model including four-spin interactions [12]) at the point separating its Néel and VBS ground states. This model may, thus, exhibit the deconfined quantum-criticality proposed by Senthil *et al.* [5]. It is still desirable to have a more direct way to unambiguously (independently of any phenomenological ansatz or theory) detect spinons in numerical studies of spin models (and eventually in doped systems). Here we introduce a method based on quantum Monte Carlo (QMC) simulations in the basis of valence bonds (singlet pairs) [13], generalized to include one or two unpaired spins [14,15]. We show that an unpaired spin can constitute the core of a spinon wave packet, the size of which can be computed with our method. Analyzing the separation of two such wave packets we obtain quantitative information on the confinement or deconfinement of spinons in a magnetically disordered state. Importantly, our definitions also reproduce the expectation that the spinon should not be a low-energy particle in the ordered Néel state.

Models.—The primary model we use to test our method is the J-Q_3 chain, a 1D member of the broad class of J-Q models introduced in Refs. [12,16]. Defining a two-spin singlet projector $C_{i,j} = 1/4 - \mathbf{S}_i \cdot \mathbf{S}_j$, the Hamiltonian is

$$H = -\sum_{i=1}^{N}(JC_{i,i+1} + Q_3 C_{i,i+1}C_{i+2,i+3}C_{i+4,i+5}), \qquad (1)$$

where $J, Q_3 \geq 0$ and we define $g = Q_3/J$. The ground state of this system is in the class of the standard critical Heisenberg chain for $g < g_c$ and is a doubly degenerate VBS for $g > g_c$. Using Lanczos diagonalization to extract the lowest singlet and triplet excitations and studying their crossings in the standard way for this kind of transition (see, e.g., [17]), we obtain $g_c \approx 0.1645$ (in agreement with a recent QMC study of the critical properties of the same model [18]). We have also studied the J-Q_2 model, i.e., using two singlet projectors in the Q term in (1), for which $g_c \approx 0.848\,31$. We focus here on the J-Q_3 model because it is more strongly VBS ordered at $J = 0$.

We also wish to study an ordered Néel state, which in an SU(2) invariant 1D system can only be achieved with long-range interactions. The Hamiltonian

$$H = \sum_{i=1}^{N} \sum_{r=1}^{N/2} (-1)^{r-1} J_r \mathbf{S}_i \cdot \mathbf{S}_{i+r}, \qquad J_r > 0 \tag{2}$$

was studied in [19]. With $J_r = 1/r^\alpha$, a quantum phase transition from the critical state for $\alpha > \alpha_c$ to a Néel state for $\alpha < \alpha_c$ was observed, with $\alpha_c \approx 2.2$. Here we use a slightly different model, with $J_r = 1/r^\alpha$ for odd r but $J_r = 0$ for even r, to make the system amenable to QMC simulations in the valence-bond basis [13]. We choose $\alpha = 3/2$, for which the system is Néel ordered.

To demonstrate the ground states of interest—VBS, critical, and Néel—in Fig. 1 we plot the spin and dimer correlation functions, defined by

$$C(r) = \langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle, \tag{3}$$

$$D(r) = \langle (\mathbf{S}_i \cdot \mathbf{S}_{i+1})(\mathbf{S}_{i+r} \cdot \mathbf{S}_{i+1+r}) \rangle, \tag{4}$$

and computed using the QMC method discussed below. We multiply $C(r)$ by $(-1)^r$ to cancel the signs of the correlations and graph $(-1)^r[D(r) - D(r+1)]$, which for large r can be regarded as the VBS order parameter.

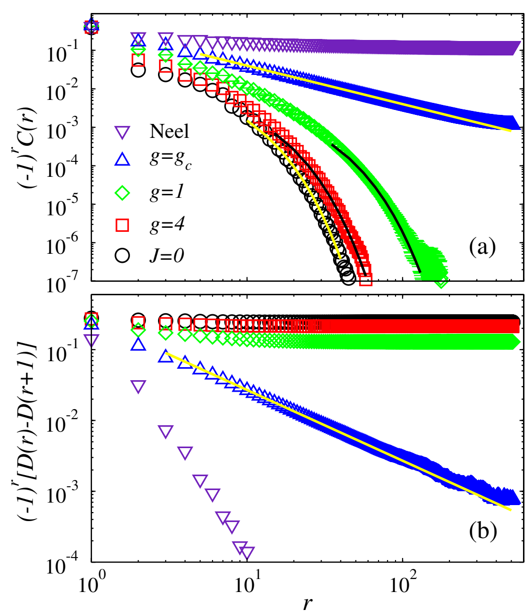

FIG. 1 (color online). Spin (a) and dimer (b) correlations of systems with $N = 1024$ spins. Results for the J-Q_3 model in the VBS phase ($J = 0$, $g = 4, 1$) and at criticality (g_c) are shown along with the behavior in the Néel state of the long-range model with $\alpha = 3/2$. The curves in (a) are fits to the form $\propto e^{-r/\xi}$ (with $\xi \approx 4$ at $J = 0$). The straight lines at the g_c data show the expected $\sim 1/r$ critical behavior [27].

QMC method.—The valence-bond QMC algorithm and its generalizations to $S > 0$ states have been discussed in several papers [13–15,20]. Here we review key aspects of the basis and the form of the generated ground states.

Acting with a high power of the Hamiltonian H^m on a trial state $|\Psi_t\rangle$, with H written as a sum of singlet projectors (individual ones and products of three, for J and Q interactions, respectively), the ground-state normalization $\langle\Psi_0|\Psi_0\rangle$ is sampled (for m large enough for $H^m|\Psi_t\rangle$ to be completely dominated by $|\Psi_0\rangle$). In an $S = 0$ state for even N, the states are expressed as superpositions of bipartite valence-bond states $|V_\alpha\rangle$, i.e., products of $N/2$ singlets $(a, b) = (\uparrow_a\downarrow_b - \downarrow_b\uparrow_a)/\sqrt{2}$, where a and b are sites on sublattice A and B, respectively. We use trial states of the amplitude-product form [21].

The valence-bond basis is nonorthogonal, and the normalization of the projected ground state is therefore of the form $\langle\Psi_0|\Psi_0\rangle = \sum_{\alpha\beta} f_\beta f_\alpha \langle V_\beta|V_\alpha\rangle$, where f_β, f_α are not known explicitly. Implicitly, the probability of generating a pair of states is $P(V_\alpha, V_\beta) = f_\beta f_\alpha \langle V_\beta|V_\alpha\rangle$. The overlap $\langle V_\beta|V_\alpha\rangle = 2^{N_0 - N/2}$, where N_0 is the number of loops in the transition graph of the two states. Figure 2(a) shows a case with $N_0 = 1$. Matrix elements of the form $\langle V_\beta|A|V_\alpha\rangle$ for many observables A of interest depend on the loop structure of the transition graph [21,22].

For $S > 0$ and magnetization $m_z = S$ the states have $2m_z$ unpaired $\uparrow$ spins and $(N - 2m_z)/2$ singlet bonds (as discussed, e.g., in [14,15]). For odd N, which we use for $S = 1/2$, the system is in principle frustrated by periodic boundaries. This is a finite-size effect, however, which vanishes when $N \to \infty$ (at least for observables probing distances $r \ll N$). The QMC loop updates [20] automatically exclude frustrated negative-sign configurations, and this should, thus, be the most rapid way to approach $N = \infty$. Configurations for $S = 1/2$ and $S = 1$ states are illustrated in Figs. 2(b) and 2(c). We note that the valence-bond basis with two unpaired spins was used in a pioneering variational study on spinon deconfinement in a VBS state of a 1D frustrated model [1].

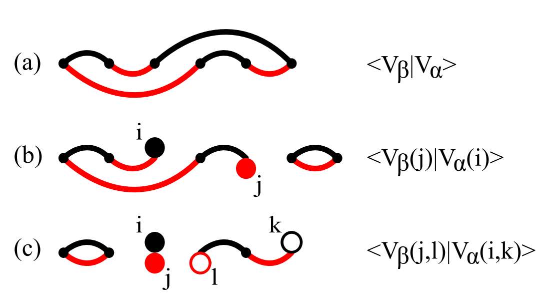

FIG. 2 (color online). Illustration of the basis for states with (a) $S = 0$ (even N), (b) $S = 1/2$ (odd N), and (c) $S = 1$ (even N). The bonds and unpaired spins of the bra and ket states are shown below and above the line of sites, respectively.

Spinon statistics.—The first aspect of our method relies on the representation of $S = 1/2$ states in terms of valence-bond states with an unpaired spin [15]. One can determine whether there is a well-defined wave packet (localizable particle) carrying the spin. The second aspect is to characterize the correlations of two spinons in an $S = 1$ state, to determine whether they are confined, and, if so, to extract the size of the bound state.

The $S = 1/2$ ground state (with momentum $k = 0$) can be written as $|\Psi_{1/2}\rangle = \sum_r |\psi_{1/2}(r)\rangle$, where r is the location of the unpaired spin [15]. Denoting a basis state with the spinon at r as $|V_\alpha(r)\rangle$, we have $|\psi_{1/2}(r)\rangle = \sum_\alpha f_r^\alpha |V_\alpha(r)\rangle$, and the overlap of two states with different location of their spinon cores is

$$\langle \psi_{1/2}(r')|\psi_{1/2}(r)\rangle = \sum_{\alpha\beta} f_{r'}^{\beta} f_r^{\alpha} \langle V_\beta(r')|V_\alpha(r)\rangle. \qquad (5)$$

What we propose is that this quantity allows for a generic way to test whether a spinon is a well-defined particle. Such a particle should have a finite wave packet (i.e., a minimum size of a region to which the $S = 1/2$ degree of freedom can be confined), which typically should lead to an exponential decay of the overlap with the separation $|r' - r|$ (with a power-law decay corresponding to a marginal case). This follows in a VBS state because the basis-state overlap $\langle V_\beta(r')|V_\alpha(r)\rangle$ is dictated by the number of loops in the transition graph. An $S = 1/2$ transition graph has a string of bonds terminating in unpaired spins [15], as seen in Fig. 2(b). In a VBS state, the loops are typically short, and the presence of a string will reduce the number of loops in proportion to the length of the string, and, thus, $\langle V_\beta(r')|V_\alpha(r)\rangle$ and (5) should decay exponentially with the separation $|r' - r|$. One can then also expect a power-law decay in a critical VBS state.

The overlap (5) can be computed by accumulating the distribution $P(r)$ of separations r of the unpaired spins in the $S = 1/2$ transition graphs. The above expected behaviors are indeed realized in the J-Q_3 model, as shown in Fig. 3. In VBS states for large N, the overlap vanishes for odd distances, implying that the bra and ket spinons are on the same sublattice in the infinite system. For the even distances the overlap is of the form $P(r) \propto e^{-r/\lambda}$, and λ is essentially the size of an exponentially decaying wave packet. The size λ is roughly twice the spin correlation length in the cases we have studied.

In the critical state, the overlap has the form $P(r) \sim 1/\sqrt{r}$ and the wave packet is only marginally defined. The Heisenberg chain is known to have spinon excitations [2] and, thus, it appears that one can still consider such a broad algebraic wave packet as a particle. The total weight of all odd-r overlaps is roughly constant, $\approx 1/4$.

In the Néel state $P(r)$ is almost flat and even and odd r have almost the same weight. The unpaired spin in the Néel state is, thus, not localizable within a wave packet, in agreement with the expectation that the spinon should not be an elementary excitation of this state. The unpaired spin is strongly aligned with the Néel order of the rest of the system [23] and cannot be regarded as an independent spatial $S = 1/2$ degree of freedom.

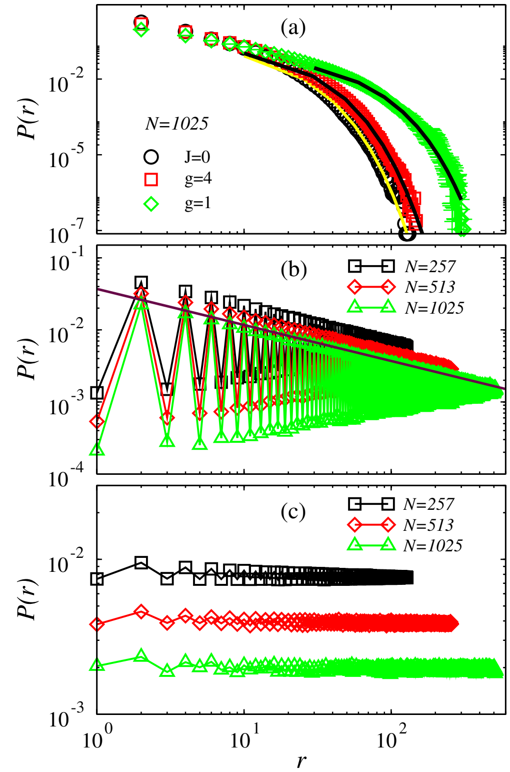

FIG. 3 (color online). Overlap $P(r) = \langle \psi_{1/2}(i+r)|\psi_{1/2}(i)\rangle$ for (a) different VBS states of the J-Q_3 model of size $N = 1025$, (b) at g_c for different N, and (c) in the Néel state of the long-range model ($\alpha = 3/2$) for different N. The curves in (a) are fits to $\propto e^{-r/\lambda}$ (with $\lambda \approx 9$ at $J = 0$) and the line in (b) shows the form $\propto 1/\sqrt{r}$.

For an $S = 1$ state with two unpaired spins, we have

$$\langle \psi_1(r_A', r_B')|\psi_1(r_A, r_B)\rangle = \sum_{\alpha\beta} f_{r_A' r_B'}^{\beta} f_{r_A r_B}^{\alpha} \langle V_\beta(r_A', r_B')|V_\alpha(r_A, r_B)\rangle, \qquad (6)$$

where, as indicated, in both the bra and the ket state one spinon is on sublattice A and one on B. Here we can define several probability distributions depending on a single distance, e.g., $|r_A - r_B|$ or $|r_A - r_B'|$, integrating over the remaining two free-spin locations. To investigate the confinement length we define $P_{AB}(r)$ as the average of the distributions of the above two distances. The results, shown in Fig. 4, indicate deconfined spinons with weak mutual repulsion, which makes the distribution broadly peaked at $r = N/2$. Size-scaled distributions $NP_{AB}(r)$ for different N fall almost on top of each other when graphed versus r/N. For confined spinons, the confinement length will be reflected in an asymptotic decay $P_{AB}(r) \sim e^{-r/\Lambda}$, where Λ is the size of the bound state.

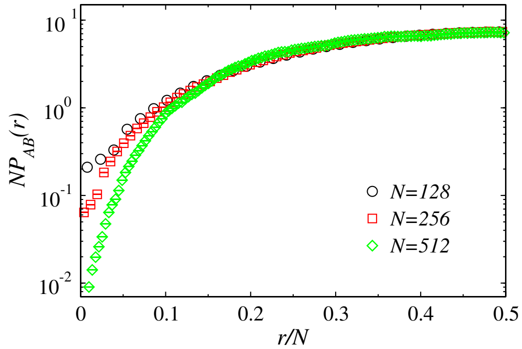

FIG. 4 (color online). Size-scaled distribution of the distance between two spinons in the $S = 1$ VBS state at $g = 4$.

The two length scales we have discussed—the size of the spinon wave packet λ and the bound state Λ (for confined spinons)—are also visible in the z-component spin correlation function $C_z(r) = \langle S_i^z S_{i+r}^z \rangle$. We demonstrate this for both $S = 1/2$ and $S = 1$ states in Fig. 5. The reason for the spinon contributions can be understood from Figs. 2(b) and 2(c). The unpaired spins in the $S = 1$ state [2(c)] dominate the long-distance correlation function if the confinement length is larger than the correlation length of the background VBS. In addition, the short-distance correlations of both the $S = 1/2$ and $S = 1$ states are modified by the presence of strings. Indeed, as we demonstrate in Fig. 5, by subtracting off $C_z(r)$ of the $S = 0$ state, the remaining short-distance correlations contain an exponentially decaying contribution which for both $S = 1/2$ and $S = 1$ is roughly twice the correlation length, i.e., similar to the wave packet size λ. In the $S = 1$ state, the correlation function remains nonzero, $\propto 1/N$, as $r \rightarrow \infty$, reflecting deconfined spinons. Note that there is a change in phase of $C_z(r)$, at some r which is related to N and λ (and hence depends on g).

Conclusions and discussion.—We have introduced a method to determine whether a spinon is a well-defined emergent particle (excitation) of a quantum spin system, and, if so, whether two spinons in an $S = 1$ excitation are deconfined or form a bound state (the size of which can be computed). The discussion was framed around the valence-bond basis and QMC simulations with it, but the definitions are independent of this basis. Our arguments only rely on the fact that one can write a state for, e.g., $S = 1/2$ as $\sum_r |\psi_0(r)\rangle \otimes |\uparrow_r\rangle$ (for momentum $k = 0$, with self-evident generalization to $k \neq 0$), where $|\psi_0(r)\rangle$ is an $S = 0$ state of all spins except the one at r (and similar decompositions for higher S). One can, thus, compute the quantities we have investigated here with other methods as well. The crucial observation is that states $|\psi_0(r)\rangle \otimes |\uparrow_r\rangle$ for different r are nonorthogonal. If the unpaired spin $\uparrow_r$ is localized within a spinon wave packet (by definition for a spinon), then the overlaps give direct information on the size of this wave packet. The spinon is not an independent particle if the wave packet is uniformly delocalized over the whole system as $N \rightarrow \infty$, as we have demonstrated here for a Néel state.

Our method does not rely on any knowledge or theory of the nature of the spinon (other than it carrying spin $S = 1/2$). The wave-function overlaps (5) and (6) are completely general and applicable to any system in any number of dimensions. For 1D systems there are alternative methods to study spinons using the fact that they are kink and antikink solitons [24], which can be created by boundary conditions. The spinon wave function, which is similar to that of a particle in a box [25], does not, however, contain any direct information on the intrinsic size of the spinon "particle." A criterion of deconfinement based on impurity (un)binding was also presented recently [26], but that approach cannot unambiguously determine whether a spinon is a well-defined particle. Our approach also avoids potential differences between spinon-spinon and spinon-impurity affinities.

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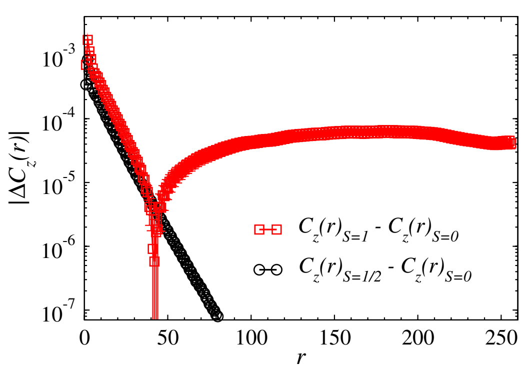

FIG. 5 (color online). Spin correlations in an $N = 513$ system with a single spinon ($S = 1/2$) and in $N = 512$ systems with two spinons ($S = 1$) in the $J = 0$ VBS state. The $N = 512$, $S = 0$ correlation has been subtracted off to isolate the spinon contributions. For $S = 1$ there is a phase change at $r \approx 42$.

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