S Matrix from Matrix Product States

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We use the matrix product state formalism to construct stationary scattering states of elementary excitations in generic one-dimensional quantum lattice systems. Our method is applied to the spin-1 Heisenberg antiferromagnet, for which we calculate the full magnon-magnon S matrix for arbitrary momenta and spin, the two-particle contribution to the spectral function, and higher order corrections to the magnetization curve. As our method provides an accurate microscopic representation of the interaction between elementary excitations, we envisage the description of low-energy dynamics of one-dimensional spin chains in terms of these particlelike excitations.

Theoretical studies have shown that, despite the exponential growth of Hilbert space, the low-energy physics of large one-dimensional quantum systems can be described efficiently. More specifically, the entanglement of the ground state and lowest-lying excitations obey an area law [1], which confines the low-lying physics of these systems to some small subspace of the complete Hilbert space. A natural and efficient parametrization of this subspace is provided by the class of matrix product states (MPS) [2] underlying the density matrix renormalization group (DMRG) [3]. While DMRG and MPS algorithms were initially focused on describing ground states, a lot of work has gone into extending the formalism to the calculation of dynamical properties [4,5].

One of these approaches towards the low-lying dynamics consists of finding accurate descriptions of elementary excitations variationally. By casting the Feynman-Bijl ansatz [6] into the MPS formalism, elementary excitation spectra of one-dimensional quantum spin systems [7] and quantum field theories [8] were obtained to an unprecedented precision. Recently, this approach has found its theoretical ground as it was shown that gapped elementary excitations are local in the sense that they can be created by a local operator acting on the ground state [9]. This result suggested that elementary excitations can be identified as particles on a nontrivial background and raises the question whether we can study their scattering. As the particle interactions are partly constituted by the strongly correlated background itself, this amounts to a highly nontrivial scattering problem (in contrast to Ref. [10], where scattering states were constructed on top of a product dimer state).

In many studies, interactions between elementary excitations are modeled by different effective field theories to capture, for example, the response of magnetic systems to external fields [11–14]. Lacking a microscopic description of the particles, the parameters in these effective theories

had to be determined from global properties of the system [15,16] and/or strong- or weak-coupling limits [17].

In this Letter, we present a variational study of the interactions between particlelike excitations in full microscopic detail. We construct stationary scattering states and calculate scattering phase shifts between particles with arbitrary individual momenta. Our method is applied to the spin-1 Heisenberg antiferromagnet, for which we calculate the full magnon-magnon S matrix, the two-particle contribution to the spectral function, and higher order corrections to the magnetization curve.

Variational method.—Consider a one-dimensional spin system with local dimension d in the thermodynamic limit, described by a local and translation invariant Hamiltonian $\hat{H} = \sum_{n\in\mathbb{Z}} \hat{h}_{n,n+1}$, where we restrict to nearest neighbour interaction. The translation invariant ground state of this system can be accurately described by a uniform matrix product state [18,19]

$$|\Psi[A]\rangle = \sum_{\{s\}=1}^{d} \mathbf{v}_{\mathbf{L}}^{\dagger} \left[\prod_{m\in\mathbb{Z}} A^{s_m} \right] \mathbf{v}_{\mathbf{R}} |\{s\}\rangle,$$

where the $D \times d \times D$ tensor A^s contains all variational parameters.

Having found the ground state (by, e.g., simulating imaginary time evolution using the time-dependent variational principle [18]), the variational ansatz for an elementary excitation with definite momentum κ is given by [7,20]

$$
\begin{aligned}
|\Phi_\kappa[B]\rangle = \sum_{n=-\infty}^{+\infty} \mathrm{e}^{i\kappa n} \sum_{\{s\}=1}^{d} \mathbf{v}_{\mathbf{L}}^{\dagger} \left[\prod_{m=-\infty}^{n-1} A^{s_m} \right] B^{s_n} \\
\times \left[\prod_{m=n+1}^{+\infty} A^{s_m} \right] \mathbf{v}_{\mathbf{R}} |\{s\}\rangle \quad (1)
\end{aligned}
$$

and can be understood as a localized disturbance of an essentially unchanged ground state. Because of its matrix product representation, this localized disturbance can spread out over a distance determined by the bond dimension D. As the variational subspace of excited states defined by (1) is linear, finding the best approximation for the lowest lying excited states is achieved by solving an eigenvalue problem.

Because of the locality of the ansatz (1), we can interpret the excitation as a particle and construct scattering states of two particlelike excitations. The variational ansatz for states with two elementary excitations with momenta κ_1 and κ_2 is taken to be ($\kappa = \kappa_1 + \kappa_2$)

$$|\Upsilon_{\kappa_1 \kappa_2}\rangle = |\chi_{\kappa_1 \kappa_2}(0)\rangle + \sum_{\alpha\beta} \sum_{n=1}^{+\infty} c_{\kappa_1 \kappa_2}^{\alpha\beta}(n) |\chi_{\alpha\beta,\kappa}(n)\rangle \quad (2)$$

with the states

$$|\chi_{\kappa_1 \kappa_2}(0)\rangle = \sum_{n=-\infty}^{+\infty} e^{i\kappa n} \sum_{\{s\}=1}^{d} \mathbf{v}_{\mathbf{L}}^{\dagger} \left[\prod_{m<n} A^{s_m}\right] C_{\kappa_1 \kappa_2}^{s_n} \left[\prod_{m>n} A^{s_m}\right] \mathbf{v}_{\mathbf{R}} |\{s\}\rangle, \quad (3)$$

$$|\chi_{\alpha\beta,\kappa}(n)\rangle = \sum_{n_1=-\infty}^{+\infty} e^{i\kappa n_1} \sum_{\{s\}=1}^{d} \mathbf{v}_{\mathbf{L}}^{\dagger} \left[\prod_{m<n_1} A^{s_m}\right] B_{\alpha}^{s_{n_1}} \left[\prod_{n_1<m<n_1+n} A^{s_m}\right] B_{\beta}^{s_{n_1+n}} \left[\prod_{m>n_1+n} A^{s_m}\right] \mathbf{v}_{\mathbf{R}} |\{s\}\rangle. \quad (4)$$

For the B_α and B_β in the states (4), we use the two B tensors that were found for the one-particle problems at momenta κ_1 and κ_2. This restriction is accurate when both particles are far away, but fails when the particles approach. The local term (3) should be able to correct for this, however, because of its ability to spread over some finite distance. For this reason, we keep all $D^2(d-1)$ variational parameters in $C_{\kappa_1 \kappa_2}^{s}$.

Finding eigenstates within this (linear) variational subspace requires solving the generalized eigenvalue problem $H_{\text{eff}}\bar{c} = \omega N_{\text{eff}}\bar{c}$ with $\bar{c} = \{C_{\kappa_1 \kappa_2}^{s}, c_{\kappa_1 \kappa_2}^{\alpha\beta}(n)\}$ containing all variational parameters, ω being the total energy of the excitation (with the ground state energy E_0 subtracted), and an effective Hamiltonian and norm matrix given by

$$H_{\text{eff}} = \langle\chi(n)|(\hat{H} - E_0)|\chi(n')\rangle,$$
$$N_{\text{eff}} = \langle\chi(n)|\chi(n')\rangle. \quad (5)$$

Finding solutions for this half-infinite eigenvalue problem with definite energy ω starts with an inspection of the asymptotic regime, i.e., the regime where the two particles are considered to be infinitely far apart. For $n', n \to \infty$ the effective norm matrix is diagonal and the effective Hamiltonian matrix is reduced to repeating rows of block matrices that decay exponentially away from the diagonal. These blocks can be considered to be zero if they are, say, $N+1$ sites from the diagonal and for every set (κ, ω), we obtain a recurrence relation for the coefficients $c^{\alpha\beta}(n)$. This recurrence relation typically has two solutions with modulus one, which correspond to the incoming and outgoing plane waves with total momentum κ and energy ω, a large number of solutions within the unit circle that correspond to decaying solutions as $n \to \infty$, and an equally large number of solutions with modulus larger than unity, which should

be discarded as they are non-normalizable (i.e., nonphysical) solutions to the eigenvalue problem.

We now construct solutions to the full eigenvalue problem that resemble these asymptotic solutions for $n \to \infty$. They are obtained by writing the coefficients $c^{\alpha\beta}(n)$ as $c = Qx$, where Q is a block diagonal of (i) a unit matrix of finite dimension, that leaves open the coefficients $c^{\alpha\beta}(n)$ for $n < N'$ and (ii) a matrix consisting of the asymptotic solutions, and x is a new vector of coefficients. We thus assume that the asymptotic regime is reached when the two particles are a finite distance N' apart; this implies that, when imposing $c = Qx$, the eigenvalue problem with energy ω is automatically fulfilled after N' rows. Consequently, we can truncate the infinite set of equations and solve the system to find the finite-dimensional vector x. When this whole procedure is done consistently, an exact solution to this slightly different scattering problem is guaranteed to exist and, when the approximations are negligible, should give an approximate stationary scattering state with total momentum κ and energy ω. More specifically, the coefficients $c^{\alpha\beta}(n)$ for this state converge asymptotically to the form

$$c_{\kappa_1 \kappa_2}^{\alpha\beta}(n) \overset{n\to\infty}{\to} u^\alpha(\kappa_1)u^\beta(\kappa_2)e^{i\kappa_2 n} - e^{i\phi}u^\alpha(\kappa_2)u^\beta(\kappa_1)e^{i\kappa_1 n},$$

where $u^\alpha(\kappa)$ and $u^\beta(\kappa)$ corresponds to the one-particle solution at momentum κ. This form allows for a direct calculation of the scattering phase ϕ [21].

Application.—The spin-1 Heisenberg antiferromagnet is defined by the Hamiltonian

$$\hat{H} = \sum_n \hat{S}_n^x \hat{S}_{n+1}^x + \hat{S}_n^y \hat{S}_{n+1}^y + \hat{S}_n^z \hat{S}_{n+1}^z. \quad (6)$$

Since Haldane's conjecture of the existence of a gap [22], the low-lying excitation spectrum has been studied

extensively [5,23]. The spectrum has an isolated, threefold degenerate one-particle (magnon) branch centered around momentum π. At momentum $\kappa \approx 0.22\pi$, this magnon triplet becomes unstable and a continuum of two-magnon scattering states emerges around momentum 0.

Magnon interactions have been studied in Ref. [15], where it was shown that the scattering of two magnons with individual momenta around π can be parametrized by one parameter, the scattering length a. Indeed, for small momenta ($\kappa_{1,2} \to \pi$) the phase shift behaves as $\phi(\kappa_1, \kappa_2) \approx -a(\kappa_1 - \kappa_2)$, hence, the definition of a. For the sector with total spin $S = 2$, this quantity can be determined from the finite size correction to the energy of the lowest lying state within this sector. DMRG simulations have given an approximate value of $a_2 \approx -2$ [15] and (more recently) a more precise value of $a_2 = -2.30(4)$ [24]. Through the identification of the Heisenberg chain with the nonlinear σ model (for which the full S matrix can be calculated exactly [25]), qualitative estimates of all three scattering lengths can be made (see Ref. [15]).

We now investigate the two-magnon scattering with our variational method. In Refs. [7] and [20] it was shown that the one-particle ansatz (1) is capable of describing the elementary magnon triplet with great precision. Now we can construct two-magnon states with every combination of individual momenta for which the magnon is stable (i.e., $|\kappa_{1,2}| > 0.22\pi$) and for every combination of individual spins. From the wave functions we can determine every phase shift and compute the full magnon-magnon S matrix. As the Hamiltonian (6) is $SU(2)$ invariant, we expect this S matrix to be diagonal in the coupled basis with the matrix elements equal within each sector of total spin.

In Fig. 1 we have plotted the scattering phases within each spin sector for different relative momenta (our method reproduces the block structure of the S matrix, so all information is contained in these three phases). We can clearly observe a linear regime where the relative momentum is small, with the slope giving us a direct measure of the scattering length in the different sectors. We find the following values for the scattering lengths [26]:

$$a_0 = 1.945, \qquad a_1 = -4.515, \qquad a_2 = -2.306.$$

The signs of these scattering lengths are in agreement with the predictions of the nonlinear sigma model. In the $S = 2$ sector we have excellent agreement with Ref. [24], while for the other sectors we have found no previous quantitative estimates.

When we go to larger relative momenta, the curve loses its linearity. In this regime, the low-energy description of the scattering process in terms of the scattering length is no longer valid and the S matrix can only be determined by solving the full microscopic scattering problem. Since the effective Hamiltonian (5) of the scattering problem indeed
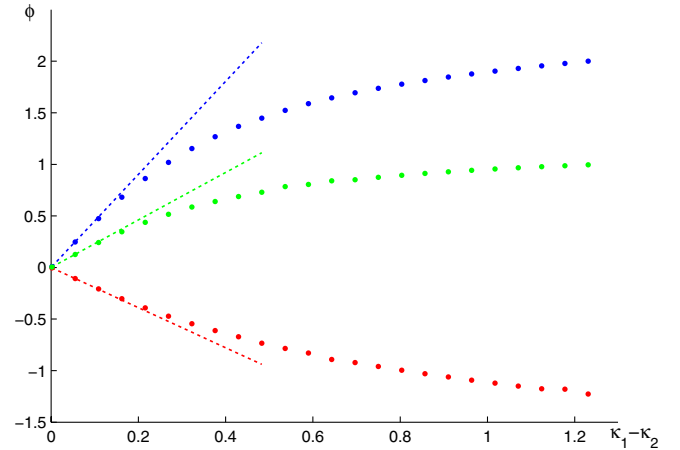

FIG. 1 (color online).   The angle of the S-matrix elements for the sectors of total spin $S = 2$ (green, middle curve), $S = 1$ (blue, upper curve), and $S = 0$ (red, lower curve) at total momentum $\kappa = 0$ and different relative momenta $\kappa_{\mathrm{rel}} = \kappa_1 - \kappa_2$. The linear regime for small relative momenta is clearly visible, as well as the deviations from that regime at higher relative momenta. Calculations were done with bond dimension $D = 64$.

captures the microscopic details of the magnon-magnon interaction, our method is able to study scattering in this nontrivial regime also.

Next we turn to the spectral function, defined as

$$S(\kappa, \omega) = \sum_{n=-\infty}^{+\infty} e^{-i\kappa n} \int_{-\infty}^{+\infty} dt\, e^{i\omega t} \langle \Psi_0 | S_n^y(t) S_0^y(0) | \Psi_0 \rangle.$$

Since we have constructed the wave function of all two-particle states explicitly, we can calculate their spectral weights and, consequently, the two-particle contribution to $S(\kappa, \omega)$. This contribution is expected to be dominant around momentum zero, as the two-particle states are the lowest lying excited states in that region [27]. In Fig. 2 we have plotted the spectral function at momentum $\kappa = (\pi/10)$. Comparing our results with Ref. [5], where the spectral function was calculated using DMRG techniques for real-time evolution and linear prediction, shows that we are able to capture the two-particle states perfectly.

We can get an idea of how well the full spectral function is reproduced by looking at its zeroth and first frequency moment, i.e., $s_0(\kappa) = \int (d\omega/2\pi) S(\kappa, \omega)$ and $s_1(\kappa) = \int (d\omega/2\pi) \omega S(\kappa, \omega)$. As the former is equal to the static structure factor and the latter can be written as the expectation value of a simple double commutator [28], both can be easily calculated with the MPS ground state. It appears that the two-particle contribution in Fig. 2 approaches the exact values up to 98.7% and 96.4%, showing indeed that the two-particle sector carries the dominant contribution of the spectral function at this momentum. Note that, as our method relies on the explicit wave function of the excitations directly in the
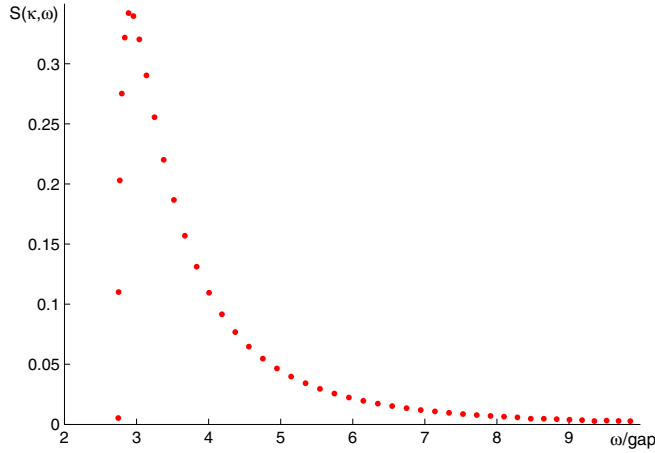
FIG. 2 (color online). The two-particle contribution for the spectral function $S(\kappa, \omega)$ at momentum $\kappa = (\pi/10)$. Calculations were done with bond dimension $D = 48$.
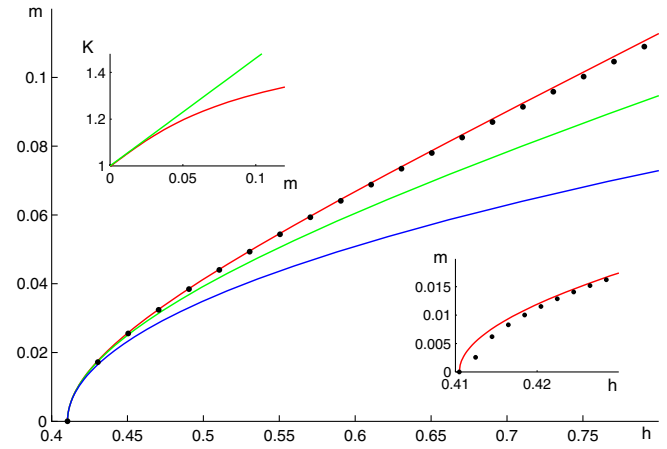

FIG. 3 (color online). The magnetization m versus applied magnetic field h for the spin-1 Heisenberg chain. Our results (red, upper curve) with bond dimension $D = 64$ are compared to the hard-core boson square-root dependence (blue, lower curve) [11] and first order corrections by the scattering length a_2 (green, middle curve) [15]. The direct MPS calculations (black dots) were done at the same bond dimension of $D = 64$. The bottom-right inset provides a close-up of the phase transition. The top-left inset provides our result for the LL parameter K in function of the magnetization m (red), compared to the linear relation based on the scattering length (green) [31].

thermodynamic limit, our results do not suffer from finite size effects nor statistical errors.

As another application, we use our variational results for the magnon dispersion and the magnon-magnon S matrix to study the magnetization of the Heisenberg chain when applying a critical magnetic field. In previous publications, the finite density of magnons has been described as a gas of interacting bosons [11] with quadratic dispersion, for which the scattering length gives a first-order correction to the hard-core boson description [15]. The magnetized chain has been characterized as a Luttinger liquid (LL) [29] with a LL parameter that varies with the magnetization [14,30,31].

As the present method provides complete information on two-magnon interactions, we can use this to approximately describe the finite density of magnons. Indeed, we can neglect three-particle interactions and write down the Bethe ansatz wave function [32] (with the variationally determined phase shifts) as an approximation of the true wave function of the magnon gas. Solving the corresponding Bethe equations (with our variationally determined dispersion relation) numerically [33], the magnetization curve as well as the LL parameter can be obtained (see Fig. 3). We expect this to be a good approximation at low magnon densities, where three-magnon interactions are negligible. A comparison with direct MPS calculations shows that our description is indeed very accurate in a broad regime and does not share the difficulties of traditional DMRG and MPS methods for capturing the onset of criticality.

Conclusions and outlook.—Starting from a successful particlelike ansatz for elementary excitations, we introduced a variational method for constructing two-particle states and determining their scattering phase shifts and spectral weights. This information was then used to determine the critical properties of a finite density of these excitations. We

believe that our methods open up new routes towards a better understanding of the low-lying dynamics of (quasi-) one-dimensional quantum spin systems.

Indeed, our methods can be straightforwardly applied to more interesting systems such as, e.g., spin ladders and dimerized chains beyond the strong-coupling limit [34]. Our formalism can be extended to topologically nontrivial excitations, so we can study, e.g., spinon interactions in half-integer spin chains, and bound states, which correspond to solutions of the scattering problem without any nondecaying asymptotic solutions. We might also study systems at finite temperature, using semiclassical approximations [17], the thermodynamic Bethe ansatz, and/or form-factor expansions [35].

Most importantly, as we have shown to give an accurate microscopic description of the interactions of elementary excitations, we are able to build an effective theory of interacting particlelike excitations for capturing the low-energy physics of generic spin chains. By gradually averaging out the microscopic details of the interactions, we can systematically make the connection to previous effective field theories based on phenomenological considerations and symmetries, globally determined parameters, and/or strong- or weak-coupling limits.

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