Non-classical correlations in a class of spin chains with long-range interactions and exactly solvable ground states

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Abstract
We introduce a class of spin models with long-range interactions—in the sense that they extend significantly beyond their nearest neighbors—whose ground states can be constructed analytically and that have a simple matrix product state representation. This enables the detailed study of ground state properties, such as correlation functions and entanglement, in the thermodynamic limit. The spin models presented here are closely related to lattice gases of strongly interacting polar molecules, or Rydberg atoms that feature an excluded volume or blockade interaction. While entanglement is only present between spins that are separated by no more than a blockade length, we show that non-classical correlations can extend much further, and we analyze them through quantum discord. We furthermore identify a set of seemingly critical points where the ground state approaches a crystalline state with a filling fraction that is given by the inverse of the blockade length. We analyze the scaling properties in the vicinity of this parameter region and show that the correlation length possesses a non-trivial dependence on the blockade length.

Keywords: spin systems, long-range interactions, quantum correlations
1. Introduction

Finding exact ground states of quantum many-body Hamiltonians with interactions that extend far beyond their nearest neighbors is typically a very challenging task in condensed matter physics. This is because exactly solvable cases (e.g., the Haldane–Shastry model [1]) are extremely rare, and the numerical treatment of long-range interactions is computationally demanding even with modern numerical tools such as the density matrix renormalization group [2, 3]. From the experimental side, ensembles of cold atoms, ions, and molecules offer a very promising route towards the controlled study of long-range interactions in quantum many-body systems. Very recent experimental approaches employ atoms in highly excited states—so-called Rydberg atoms—where they exhibit strong dipolar interactions. A characteristic feature of these systems is the presence of the dipole blockade, which prevents the excitation of an atom in the vicinity of an already-excited atom [4, 5]. In typical experimental setups, one can achieve situations in which a single excitation blocks tens or hundreds of atoms and can, in this sense, be regarded as long range. In the extreme case, the blockade can extend over an entire cloud, which leads to the formation of so-called ‘super atoms’—an entangled state of a single delocalized excitation [6]. Of particular interest is the more involved case in which the system size is larger than a blockade region. Clearly, the blockade leads to a strong anti-correlation of excitations at small distances, which has recently been observed experimentally in the statics [7] and dynamics [8] of Rydberg gases. However, the nature of the correlations at longer distances is, at present, not fully understood. A number of recent investigations suggest that the emerging states behave essentially classically, in the sense that their properties can be understood by drawing an analogy with arrangements of classical hard objects [8–14]. It is so far unclear to what extent quantum correlations that go beyond the aforementioned ‘super atom’ exist.

One purpose of this paper is to conduct a largely analytical study to shed some light on these questions. A second one is to introduce a class of long-range interacting one-dimensional spin models whose ground states, in some regime, can be solved exactly. The models, which are all of the Ising type, manifestly display the blockade effect due to an excluded volume interaction that encompasses $R$ spins. Moreover, they possess a potential tail which extends further than $R$, and therefore mimics to a good extent the typical features present in strongly interacting Rydberg gases. In the exactly solvable regime their ground states have the form of matrix product states, which permit the convenient calculation of the correlation properties in the thermodynamic limit. This unique property allows us to perform a scaling study of the correlation length, which is shown to exhibit a non-trivial power-law dependence on $R$. We find that the expectation values of classical observables can indeed be understood from analogous classical arrangements of hard objects, and that entanglement between two spins is only present when they are separated by, at most, one blockade length, $R$. When separated further, despite the absence of entanglement, non-classical correlations remain in the form of quantum discord [15, 16], which is regarded as a key resource for conducting quantum operations in the presence of noise, such as quantum illumination [17–19] and metrology with noisy probes [20, 21]. The fact that in the systems studied here quantum correlations extend over distances larger than $R$ also hints at the possibility of implementing non-classical operations between distant particles mediated by Rydberg interactions in experimental ensembles that are not fully blockaded.
The class of Hamiltonians we are considering is that of one-dimensional lattice spin-$\frac{1}{2}$ models with transverse and longitudinal magnetic fields and an Ising-type interaction potential:

$$H_0 = \sum_{k} \left( h_x \sigma_k^x + h_z \sigma_k^z + \sum_{m>k} V_{km} n_k n_m \right).$$

(1)

Here, $\sigma^x$ and $\sigma^z$ are Pauli matrices and $n = (1 + \sigma^x)/2$. The interaction energy, $V_{km}$, between spins positioned at sites $k$ and $m$ is given by the potential $V(k-m)$, with

$$V(r) = \begin{cases} 
\infty & \text{if } |r| \leq R, \\
V_0 \times [2R - (|r| - 1)] & \text{if } R < |r| \leq 2R, \\
0 & \text{if } |r| > 2R.
\end{cases}$$

(2)

It features a hard core interaction between up-spins up to a distance, $R$. Beyond that, the potential decays linearly until it reaches the distance $2R$, and from there onwards it is zero. With this potential, it is energetically forbidden to dynamically access configurations in which the separation between any two spins is smaller than $R$ sites.

Such potential can be linked to current studies of strongly interacting lattice gases of cold Rydberg atoms or polar molecules [10]. These systems can be described in terms of ensembles of interacting two-level systems whose excited state, $| e \rangle$, and ground state, $| g \rangle$, are coupled by a laser or microwave field of strength $\Omega$ and detuning $\Delta$. (b) Spins in the up-state interact with the interaction potential, $V(r)$, in (2), which can be regarded as an approximation of power-law potential of the form $V_0(r) = C_a/(a r)^\alpha$ where $a$ is the lattice spacing. For further explanation, see text.

2. Hamiltonian

The class of Hamiltonians we are considering is that of one-dimensional lattice spin-$\frac{1}{2}$ models with transverse and longitudinal magnetic fields and an Ising-type interaction potential:
power-law decay, the interaction potentials extend beyond $R_b$. These tails can be thought of as being mimicked by the linearly decaying part of $V(r)$, which is a more qualitative than quantitative statement. We approximately connect $V(r)$ to the power-law potentials $\alpha V(r)$ by setting $V(R + 1) = \alpha (R + 1)^{\alpha}$. A comparison of these potentials is shown in figure 1(b).

3. Exactly solvable parameter manifold

As $V(r)$ forbids the simultaneous excitation of spins at distances closer than or equal to $R$, the physically relevant subspace of the Hilbert space is spanned by all states, $\langle \nu |$, which obey $\langle \nu | n_k n_{k+1} | \nu \rangle = \langle \nu | n_k n_{k+2} | \nu \rangle = \ldots = \langle \nu | n_k n_{k+R} | \nu \rangle = 0$. Within this physical sector, it can be shown that the Hamiltonian (1) acquires a frustration-free or Rokhsar–Kivelson form [23], provided that the system parameters obey

$$h_z = \frac{1}{2} \left( \frac{h_x}{V_0} - V_0(2R + 1) \right).$$

(3)

Specifically, on this exactly solvable manifold, the Hamiltonian (1) can be brought into the form $H = E_0 + \sum_k H_k$ with

$$H_k = h_z \sum \sigma_k^x + \frac{h_x}{V_0} n_k + \frac{V_0}{h_x} P_k^R.$$

(4)

Here, we have abbreviated the string operators, $P_k^L = P_{k-1} P_{k-2} \ldots P_{k-R}$ and $P_k^R = P_{k+1} P_{k+2} \ldots P_{k+R}$, which are products of the projector, $P_k = 1 - n_k$, that projects on the spin-down state of the $k$-th spin. It is composed by local positive-semidefinite Hamiltonians, $H_k$, which in general do not commute. They all annihilate the ground state, $|z \rangle$ (see below for additional discussion); that is, $H_k |z \rangle = 0$, and hence the ground-state energy on the parameter manifold (3) is given by $E_0 = -N(h_z + V_0)$. This Hamiltonian is a generalization of the ones presented in [24–27] beyond $R = 1$. It is gapped for finite values of $V_0/h_z$, and therefore the properties of the ground state discussed in the following change smoothly when departing from the exactly solvable manifold (3).

4. Ground state wave function and correlations

The ground state wave function can be explicitly written as

$$|z \rangle = \prod_{k=1}^N e^{-z \sum \sigma_k^z} \frac{P_k^L P_k^R}{\sqrt{Z(z, N)}} |0\rangle,$$

(5)

where $|0\rangle = 1 \downarrow \downarrow \ldots \downarrow$ is the spin vacuum. The state $|z \rangle$ is a superposition of all classical spin configurations in which up-spins are at least separated by a distance, $R$. The relative weight of each configuration is given by $z^{2m}$, with the parameter $z = V_0/h_x$ (which we take to be positive in the following), and $m$ being the number of up-spins contained in the configuration. The state space is equivalent to that of hard $R + 1$-mers on a lattice, and hence the normalization constant, $Z(z, N)$, is given by the classical grand-canonical partition function of hard $R + 1$-mers with fugacity $z^2$. 


For a given $R$, the ground state (5) assumes an exact matrix product state (MPS) form [28, 29]; that is, $\psi\rangle = \sum_{i,i'\downarrow\uparrow} \psi_{ii'\downarrow\uparrow} |i\rangle \langle i'|$ with $\psi_{ii'\downarrow\uparrow} = \text{Tr}[X_i X_{i'} ... X_{i_N}]$. Here, $X_{i} = \delta_{i,R+1}$ and $X_{i} = \delta_{i,R} - z \delta_{R+1,R} + \sum_{m=1}^{R-1} \delta_{m+1,m}$ are $(R+1) \times (R+1)$-dimensional matrices. With the MPS representation, it is a relatively simple task to characterize the properties of the ground state (e.g., its correlation functions and entanglement properties in the thermodynamic limit) To this end, we define the transfer operator $E^O = \sum_{i,i'=1,1}^I X_i \otimes X_{i'} \langle i'| O | i\rangle$ such that the correlation functions can be brought into the form

$$\langle O_0 O'_\alpha \rangle = \sum_{\alpha=1} \lambda_{\alpha} e^{-\frac{\xi_{\alpha}}{2}} \left( \cos q_{\alpha} + i \sin q_{\alpha} \right),$$

where $c_{\alpha} = \langle l_\alpha | E^O | l_\alpha \rangle \langle l_\alpha | E^O | l_\alpha \rangle$, $l_\alpha$ and $l_\alpha$ form the left and right eigenbasis of the transfer operator, $E^1$, while $\xi_{\alpha}^{-1} = \log |\lambda_\alpha/\lambda_\alpha|$ and $q_{\alpha} = \text{arg}(\lambda_\alpha/\lambda_\alpha)$, where $|\lambda_\alpha| \geq |\lambda_{\alpha+1}|$ are the eigenvalues of $E^1$.

In figure 2, we display the density–density correlation function, $\langle n_0 n_{r} \rangle$, and the spatial coherence, $\langle \sigma_0^+ \sigma_r^- \rangle$. The density–density correlation function exhibits decaying oscillations at a length scale that is approximately given by $R$. With increasing $R$, and keeping $z$ fixed, the amplitude of the oscillations decreases. Keeping $R$ constant and varying $z$, we observe that the oscillations become increasingly pronounced with growing $z$. In the limit of $z \rightarrow \infty$, configurations that contain the highest possible number of excitations (compatible with the blockade) carry almost all the weight, and the ground state approaches a superposition of $R+1$ ‘crystalline’ states, $|c\rangle_m$, each of which contains a regularly ordered arrangement of up-spins with nearest-neighbor distance $R+1$ and the first up-spin located at site $m$: $|z \rightarrow \infty\rangle_R = |c\rangle_1 + ... + |c\rangle_{R+1}| \sqrt{R+1}$. The correlation length of $|z \rightarrow \infty\rangle_R$ is infinite, and in fact the two largest eigenvalues of the transfer operator, $E^3$ have the same magnitude when $z$ approaches infinity, which we will refer to as the critical limit from now on. The spatial coherence, $\langle \sigma_0^+ \sigma_r^- \rangle$, shows some qualitative analogies with the density–density correlation (see figure 2). It strongly decays with increasing spin separation, with an oscillatory pattern whose
contrast is more and more suppressed as $R$ increases. Opposite to the behavior of the density–density correlation function, the spatial coherence is more strongly suppressed the larger $z$ is, and vanishes at the critical point. These numerical results confirm the nature of the state $|z \to \infty \rangle_R$, for which one can show that the spatial coherence is identically zero for any pair of spins.

To conclude the discussion on the correlations, we consider the situation in which we keep the blockade length constant while decreasing the lattice spacing, $a$. In practice, this can be achieved experimentally in Rydberg (molecular) gases by increasing the density of atoms (molecules). This scenario is in fact interesting because recent studies of driven Rydberg gases \cite{11–13} suggest that spatial correlations can become enhanced by increasing the atomic density. To study whether this also applies here, we define the dimensionful blockade length, $\tilde{R} = a R$, and introduce a continuous set of coordinates, $x = k a$, with whose help we can express the ground state (5) as

$$|\tilde{z} \rangle = \frac{1}{\sqrt{\Xi(\tilde{z}, \tilde{R}, \tilde{L})}} \sum_{n=0}^{L/\tilde{R}} (-z)^n \frac{1}{n!} \int_0^L dx_1 \ldots dx_n \psi(x_1, \ldots, x_n) \phi^\dagger(x_1) \ldots \phi^\dagger(x_n) |0\rangle,$$

with $\psi(x_1, \ldots, x_n) = \theta(x_n - x_{n-1} - \tilde{R}) \ldots \theta(x_2 - x_1 - \tilde{R})$, $\psi^\dagger(x) = \sigma_z^+ \sqrt{\tilde{a}}$, and $\tilde{z} = z / \sqrt{\tilde{a}}$, $\theta(x)$ being the step function. The normalization is $\Xi(\tilde{z}, \tilde{R}, \tilde{L}) = \sum_n 0^{z n \tilde{z}^n} \xi(n, \tilde{R}, \tilde{L})$, where $\xi(n, \tilde{R}, \tilde{L})$ is the microcanonical partition function of a Tonks gas \cite{30} (i.e., of $n$ hard rods of length $\tilde{R}$ arranged in a system of length $\tilde{L} = a \tilde{L}$). The correlation length of the above state is controlled by the parameter $\tilde{z}$, which diverges as $a$ tends to zero. Hence, for fixed $z$ the density–density correlations become longer ranged when $a$ is decreased, (i.e. the density is increased). In order to define the state (8) with a finite $\tilde{R}$, we need to consider a diverging blockade length, $R$. In this limit, the bond dimension of $|z \rangle$ becomes infinite, such that (8) stands as an example of a continuous limit of an MPS, which is not expressible as a continuous matrix product state \cite{31, 32}.

5. Entanglement and non-classicality

Due to the structure of the ground state (5), the expectation value of classical observables, (e.g., the density–density correlation function) is equivalent to that of classical hard $R + 1$-mers with fugacity $z^2$ \cite{25}. However, as we have shown before, the ground state also exhibits quantum coherence.

We are therefore interested in whether it also features non-classical correlations, such as entanglement. To find an answer, we start by considering two figures of merit of entanglement: the block entropy and the concurrence \cite{33, 34}. The first captures the collective properties of the entanglement of a block of a certain number of contiguous spins, while the second quantifies the entanglement shared by a pair of spins. The block entropy, defined as $S_r = -\text{Tr} \rho \log_2 \rho$, depends on the reduced density matrix

$$\rho = \frac{1}{K^r} \text{Tr} \left[ \tilde{B} \prod_{j=1}^{r} E_{i_j, i'_j} \right] |i_1, i_2, \ldots, i_t \rangle \langle i'_1, i'_2, \ldots, i'_t|,$$

where $\tilde{B} = \lim_{L \to \infty} (E^2 / \lambda_1)^L$ and $E_{i_j, i'_j} = X_{i_j} \otimes X_{i'_j}$. The ground state (5) factorizes at the point $z = 0$ for any value of $R$, leading to zero entropy as a result, signaling an overall classical state.
In the limit \( z \to \infty \), on the other hand, the entropy approaches an asymptotic value which can be extracted from the state \( \lim_{z \to \infty} |z \rangle \rangle \). The state space is restricted to configurations with, at most, one up-spin, whereas as soon as \( R \leq r \), the number of accessible configurations grows fast, allowing for an entropy larger than the asymptotic value, \( S_r(R) \).

In [25] the single atom, entropy was considered in the case \( R = 1 \), and it was found to decrease monotonically with increasing \( z \). This is not true for general block sizes and blockade lengths \( R \), as shown in figure 3(a): if \( r \leq R \), the entropy is a monotonously increasing function in \( z \). However, as soon as the block size exceeds the blockade length, \( S_r \) exhibits a maximum in \( z \), whose precise location depends on \( R \) and \( r \). This qualitative change in the behavior is due to the fact that within the blockade length, the state space is restricted to configurations with, at most, one up-spin, whereas as soon as \( r > R \), the number of accessible configurations grows fast, allowing for an entropy larger than the asymptotic value, \( S_r(R) \).

To quantify the entanglement between pairs of spins separated by a distance, \( r \), we study the concurrence, which is defined as \( C(r) = \max \{ 2\lambda_1 - \text{Tr} B, 0 \} \), where \( \lambda_1 \) is the largest eigenvalue of the matrix \( B = \sqrt{\rho(r) \hat{\rho}(r) \rho(r)} \). Here, \( \rho(r) \) is the matrix expressed in the Bell basis [35]. The concurrence is plotted in figure 3(b) (cut for \( z = 0.3 \) and \( z = 2 \) at fixed \( R = 20 \)), as well as in the bottom panel of figure 3(c). Clearly there is no entanglement shared by two spins separated by a distance \( r > R \), since here \( C(r) \) is sharply to zero. Hence, the blockade length, \( R \), is equal to the range of entanglement. Linking back to the systems of interacting Rydberg atoms, this shows that entanglement indeed only extends over the size of a ‘super atom.’ Note that the sharp drop of the concurrence observed here is most certainly an effect of the potential (2). In Rydberg gases with power-law interaction we expect a sharp but smooth drop at the respective blockade radius.

However, entanglement does not represent all possible quantum correlations between two spins. They are instead captured by the quantum discord, which we study in the following. We use the local quantum uncertainty [21] as a measure of discord, defined as \( D(r) = 1 - \Lambda_{\text{max}} \), where \( \Lambda_{\text{max}} \) is the largest eigenvalue of the \( 3 \times 3 \) matrix of entries.
\( W_{ij} = \text{Tr}[\sqrt{\rho(r)} (\sigma^i \otimes \mathbb{1}) \sqrt{\rho(r)} (\sigma^j \otimes \mathbb{1})]. \) The discord is shown in figure 3(b) cut for \( z = 0.3 \) and \( z = 2 \) at fixed \( R = 20 \) and in the top panel of figure 3(c). Surprisingly, quantum correlations in the form of discord extend much further than entanglement. Note that this statement is only strictly valid on the exactly solvable parameter manifold (3). It might well be that away from this manifold, entanglement becomes longer ranged, which would need to be clarified numerically. This feature is analogous with the findings in [36], where discord was used to characterize quantum phase transitions. Furthermore, it is interesting to note that quantum discord shows an actual oscillatory behavior (figure 3(b)) as a function of \( r \).

6. Critical limit

As discussed previously, the limit \( z \to \infty \) can be thought of as a critical limit where, in fact, all ‘crystalline configurations,’ \( |c\rangle_m \), are valid ground states. Translational symmetry is broken as the states, \( |c\rangle_m \), are only invariant under translations by \( R \) sites. The formation and melting of such crystalline states realized in a lattice gas of interacting Rydberg atoms has been investigated in [37–39]. In [37], the authors identified a ‘devil’s staircase’ in the phase diagram formed by ‘crystals’ with different filling fractions. Linking to this study, we can now actually understand how, within our model, the correlation length, \( \xi \), diverges as \( z \) approaches infinity (i.e., when the crystal is formed). Interestingly, this does strongly depend on the value of \( R \). For all blockade lengths, \( \xi \) diverges with a characteristic power law, \( \xi_R \sim z^{\nu_R} \) as \( z \to \infty \), but with an \( R \)-dependent power, \( \nu_R \). In the cases \( R = 1, 2, 3 \), the characteristic polynomial of the transfer matrix is less than quintic, and we are able to extract this exponent analytically, finding \( \nu_1 = 1 \), \( \nu_2 = 2/3 \), and \( \nu_3 = 1/2 \). Numerical studies suggest that this power decreases monotonically with increasing \( R \).

7. Summary and outlook

We introduced and studied the ground states of a class of Hamiltonians with ‘blockade interaction.’ To do so, we defined a manifold in the parameter space where such Hamiltonians reduce to an exactly solvable model. We showed then, among other results, that entanglement is only present within the blockaded region, while non-classical correlations extend significantly further. One might speculate that this could find practical implications for the use of chains of Rydberg atoms or polar molecules as physical platforms for quantum information processing, communication, or metrology [40]. Finally, we gave a prediction on the critical exponent associated with the divergence of the correlation length as the system approaches crystalline states of different filling. These states are analogous to the ones studied analytically in [37], and those recently observed in experiments [7].

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