Dipoles on a Two-leg Ladder

Søren Gammelmark and Nikolaj Thomas Zinner

Department of Physics and Astronomy, Aarhus University, DK-8000 Aarhus C, Denmark

(Dated: May 11, 2014)

We study polar molecules with long-range dipole-dipole interactions confined to move on a two-leg ladder for different orientations of the molecular dipole moments with respect to the ladder. Matrix product states are employed to calculate the many-body ground state of the system as function of lattice filling fractions, perpendicular hopping between the legs, and dipole interaction strength. We show that the system exhibits zig-zag ordering when the dipolar interactions are predominantly repulsive. As a function of dipole moment orientation with respect to the ladder, we find that there is a critical angle at which ordering disappears. This angle is slightly larger than the angle at which the dipole moments are non-interacting along a single leg. This behavior should be observable using current experimental techniques.

I. INTRODUCTION

Cold and ultracold molecules have recently become experimentally accessible and such systems hold great promise for exploration of quantum systems with long-range and anisotropic interactions with applications to quantum simulation, quantum metrology, and quantum information and computation. However, strong dipolar interactions can induce collapse instabilities as well as strong chemical reaction losses. These problems can be overcome in low-dimensional geometries where the dipolar particles are confined to either two-dimensional (2D) planes or one-dimensional (1D) tubes with and without the presence of lattice potentials. A number of interesting predictions have been made for the phases of system with dipolar interactions, including exotic superfluids, Luttinger liquids, Mott insulators, interlayer pairing, non-trivial quantum critical points, modified confinement-induced resonances, roton modes and stripe instabilities, and crystallization, as well as formation of chain complexes.

In the present paper we consider dipolar particles confined to move in an optical lattice potential. The advantage of a lattice potential is the possibility of quenching the particle motion by tuning the hopping and thus vary the ratio of dipolar potential energy and motional kinetic energy in order to study transitions from quantum delocalized phases driven by kinetic motion towards the classical regime of large dipolar interaction. For dipolar particles in 1D with dipole moments perpendicular to the 1D tube, a transition from a linear configuration to a zig-zag phase has been predicted using both classical arguments and quantum Monte Carlo calculations and can be driven by tuning the transverse confining potential that keeps the particles in a 1D geometry. In a more recent paper, the same system was studied using Luttinger liquid techniques and the density matrix renormalization group (DMRG) and evidence for a non-local string ordering was presented that could give rise to edge states. In the DMRG this was done using a nearest-neighbour Hubbard-type model that was expected to show similar physics to the true system of dipolar particles.

Here we consider a Hubbard model that includes the dipole-dipole interaction for different orientations of the dipole moments of the particles with respect to the two-leg ladder geometry. By varying the hopping parameters and the dipole strength, we look for zig-zag ordering by using the string and Ising ordering parameters introduced in Ref obtained through the Matrix Product States (MPS) technique which is essentially equivalent to DMRG. This is done for different transverse hopping parameters and different strengths of the dipolar interaction. Our results demonstrate that there is a rich phase diagram in the system as function of the orientation of the dipole moment, and that the ordering changes character as the angle is varied. Surprisingly, we find that there is even a critical angle at which the system becomes completely disordered independently of the transverse hopping and dipolar strength. This critical angle occurs in the regime where two dipoles on the same leg of the ladder will repel each other. However, it is only a few degrees above the angle at which the interaction vanishes along the legs, indicating that it is the hopping along the legs that destroys ordering at the critical angle.

The paper is organized as follows. In Sec. III we introduce the formalism, the MPS technique we have employed, and the order parameters we study. Sec. IV contains our results discussing first the spatial and Fourier transforms of the ordering for different angles, then we present phase diagrams for different filling fractions, and finally we discuss the phase diagram for fixed filling fraction and dipolar strength as the orientation angle and transverse hopping parameter is varied. In Sec. V we discuss results and conclusion, as well as the experimental implementation of the system we study and detection schemes. In the appendix we elaborate on the numerical details, discuss finite size effects, and the truncation of the dipolar interaction and its influence on the order parameters.
II. FORMALISM

We study a two-leg ladder, i.e., a two parallel one-dimensional lattices that hold polar molecules which are allowed to hop both along the two legs (parallel hopping) and across the rung (perpendicular hopping). The setup is shown in Fig. 1. The lattice constant, $a$, is the same along the legs and across the rungs. The interaction of two polar molecules depends on their relative distance, $r$, through

$$V(r) = \frac{D^2}{r^3}(1 - 3\cos^2\alpha),$$

where $D^2 = d^2/4\pi\epsilon_0$ with $d$ the dipole moment and $\epsilon_0$ the vacuum permittivity. The angle $\alpha$ is defined through the distance and dipole moment vector, $d$, via $\cos \alpha = r \cdot d/rd$. Referring to Eq. (1) we parametrize $d$ by

$$d = d(\cos \theta \cos \phi, \cos \theta \sin \phi, \sin \theta).$$

The two-leg ladder is described by a tight-binding model with Hamiltonian

$$H = -\sum_{i,\sigma} \left( t_0 a_i^{\dagger,\sigma} a_{i-1,\sigma} + t_1 a_i^{\dagger,\sigma} a_{i,-\sigma} + \text{h.c.} \right) + \sum_{i,\sigma,k,\sigma'} V_{i,\sigma,k,\sigma'} n_i,\sigma n_k,\sigma',$$

where $a_i^{\dagger,\sigma}$ and $a_{i,\sigma}$ are bosonic operators that create and annihilate particles on the site with leg position $i$ (in units of the lattice constant $a$) and on the side of the rung indexed by $\sigma = \pm1$. The $\sum$ indicates that only nearest-neighbour hopping terms are included. The number operator is defined in the usual way, $n_{i,\sigma} = a_i^{\dagger,\sigma} a_{i,\sigma}$. The dipole-dipole interaction term may now be written

$$V_{i,\sigma,k,\sigma'} = D^2 \left[ \frac{1}{((i-k)^2 + \delta_{\sigma,-\sigma'})^{3/2}} ight.$$

$$\left. - 3 \cos^2 \theta \left( \cos \phi (i-k) + \sin \phi \delta_{\sigma,-\sigma'} \right) \right]/((i-k)^2 + \delta_{\sigma,-\sigma'})^{3/2},$$

where $\delta_{\sigma,-\sigma'}$ is zero for particles on the same leg and one for particles on opposite legs. In the numerical calculations we need to truncate the dipolar interaction which we will do at the next-next-nearest neighbour level (three sites removed). In appendix C we discuss the effects of truncation, and in particular the fact that previous studies that use truncation at nearest neighbour interactions (as in the so-called extended Bose-Hubbard models) may not be able to capture the full correlations induced by the long-range dipolar interactions. From now on we will use $t_0$ as the unit of energy. This means that $V_d = D^2/a^3/t_0$ is the dimensionless measure of the dipolar interaction strength, while $t_1/t_0$ measures the perpendicular hopping normalized to the parallel one.

We employ particle number-conserving matrix product states with each rung of the ladder as the site Hilbert spaces. In order to find the ground state of the Hamiltonian, we use repeated sweeps of local energy minimizations until the energy has converged to within a relative tolerance of $10^{-6}$. The Hamiltonian is represented by a matrix product operator whose bond-dimension depends linearly on the dipole-interaction truncation length. In order to keep the lattice site Hilbert space dimension small, we have assumed hard-core bosons, which can be achieved experimentally by tuning the on-site interaction $U n_{i,\sigma}(n_{i,\sigma} - 1)/2$ large using, e.g., a Feshbach resonance.

The Ising and string ordering that we compute is defined through the functions

$$C_I(r_i - r_j) = \langle \sigma_i \sigma_j \rangle,$$

$$C_{\text{string}}(r_i - r_j) = \langle \sigma_i \exp(i\pi \sum_{i<j} n_i) \sigma_j \rangle,$$

where $\sigma_i = n_{i,1} - n_{i,2}$. Here $n_{i,1}$ and $n_{i,2}$ are the density operators for site $i$ on legs 1 and 2 respectively. Notice that we have left out the factor $\cos(\pi\rho(r_i - r_j))$ in the Ising order as compared to Ref. 66, where $\rho$ is the density of particles. Using this definition we may then do a general Fourier transform of the Ising order (and string order as well) making it easier to identify periodicity even when it is not directly related to $\rho$. All Fourier transforms below are with respect to the basis function $\cos(\nu \pi (r_i - r_j))$ where $\nu$ has units of $1/a$. We denote the Fourier transform by a tilde, i.e., $\tilde{C}_I(\nu)$ and $\tilde{C}_{\text{string}}(\nu)$. A peak at $\nu = \rho$ therefore recovers the same ordering as
FIG. 2: Classical phase diagram \((t_0 = t_1 = 0)\) as function of density \(\rho\) and angle \(\theta\). The various classical configurations are illustrated at the top and right-hand side for \(\rho = 1/4\) and \(\rho = 1/3\). The latter case has frustration as shown in the drawings. This is generally true for \(\rho = 1/p\) with \(p\) an odd integer. Notice that below the solid horizontal line \((\theta_M = \cos^{-1}(1/\sqrt{3}))\) there is attraction along the legs and the particles will cluster on one side and increase the density. We consider hard-core bosons here so that we still have at most one particle per site.

The following subsections presents and discusses our results for selected parameters of interest. This includes different dipolar strengths, transverse hoppings, orientation angles, and filling fractions. For simplicity we have used \(\phi = 0\) throughout the paper, postponing a discussion of non-zero \(\phi\) to future studies.

A. Classical phase diagram

In Fig. 2 we show a classical phase diagram calculated by assuming that the hoppings are zero \((t_0 = t_1 = 0)\). As function of \(\rho\) and \(\theta\) we find three different regimes. A zig-zag phase is present for large \(\theta \gtrsim \pi/3\), while for \(\pi/3 \lesssim \theta > \theta_M = \cos^{-1}(1/\sqrt{3})\) an aligned phase occurs. The configurations of these phases are shown in Fig. 2 for the case of \(\rho = 1/3\) and \(\rho = 1/4\). In the case with \(\rho = 1/p\) where \(p\) is an odd integer, there is a frustrated configuration with an energy minimum that is degenerate as illustrated for \(p = 3\) in Fig. 2. The critical angle between the aligned and the zig-zag phases depends only weakly on \(\rho\). For \(\rho = 1/N\) and in the limit where \(N \to \infty\), one can show that the critical angle goes to \(\theta = \cos^{-1}(1/\sqrt{5})\) by comparing the energies of the two configurations. This is consistent with our numerical energy minimization. For \(\theta < \theta_M\), the interaction on a single leg is attractive and the minimum has all particles on the same leg and as close as possible, i.e. there will be a change of density at this point. Notice that we use hard-core bosons and thus can have at most one particle per site. In the numerical calculations with non-zero hopping below we will see that the zig-zag phase is associated with the string order, while the aligned phase is associated with the Ising order. The classical phase diagram is therefore very instructive in understanding the
behavior of the full quantum problem.

B. Perpendicular dipoles

We first focus on the case where the dipoles are perpendicular to the plane containing the two-leg ladder, i.e. $\theta = \pi/2$ and $\phi = 0$. This means that the dipole-dipole interactions are purely repulsive. This case was discussed recently in Ref. where numerical DMRG calculations are discussed for two choices of parameters in a model for the dipolar system including nearest neighbour interactions only and different interactions along the ladders as compared to along the rungs. Here we consider the full dipolar interaction given in Eq. (4) (with truncation at next-next-nearest neighbour for convergence, see Appendix B).

In Fig. 3 we show results of a calculations on a lattice of size $L = 48$ with filling $\rho = 1/3$ and dipolar interaction $V_d = 1.0$. The perpendicular hopping, $t_1$, is varied from 0.1 to 1.0 in four steps. For $t_1 = 0.1$ we clearly see the co-existence of both string and Ising orders, while for $t_1 \geq 0.2$ both orders show exponential decay. In the ordered regime, the string correlations are almost constant but with a small oscillatory component. Interestingly, this oscillatory behavior actually persists for other system sizes (see Appendix B with matching maxima and minima (except at the boundaries). While tempting, interpreting these oscillations as being due to finite-size seems not the case. In Fig. 3 we also see a clear boundary effect in the string order at the edge of the system as expected. As we discuss in Appendix B we expect only minute quantitative changes in our results for larger system sizes.

For larger values of $V_d$ we find that the orders persist to larger $t_1$ and the relevant parameter is $V_d/t_1$ (not shown here). This can be quantified by working out the phase diagram for the string and Ising orders as function of $V_d$ and $t_1$. In Fig. 4 we present the phase diagram which has been computed by using the largest Fourier component for each value of $V_d$ and $t_1$. The filling factor is $\rho = 1/3$. The order parameters are both non-zero for the larger part of the phase diagram. However, for low perpendicular hopping we see that the string order extends to smaller values of $V_d$, implying that Ising order vanishes slightly faster.

C. Transition to parallel dipoles

If the dipoles are instead oriented parallel to the legs of the ladder, we have purely attractive interactions on the legs, while the interaction across the rungs remain repulsive at short distance and then becomes attractive for larger distances between two sites. In Fig. 4 we show the profiles and Fourier transforms for parallel dipoles ($\theta = \phi = 0$) with all other parameters the same as in the perpendicular case in Fig. 3. The first observation is that the roles of Ising and string orders are reversed with respect to constant and oscillatory behaviors. This is consistent with the strong attraction along the legs making it favourable for the particles to cluster on one side of the system (which side is chosen is a matter of small breaking of symmetry in the initial condition of the calculation).
We also notice that the Ising order stays completely constant in the bulk region, avoiding the oscillatory component that is seen in the perpendicular case in Fig. 3 in the string ordered phase.

A striking difference to the perpendicular case is that the oscillation around zero in the string order is not around \( \nu = 1/3 \) but rather \( \nu = 1/2 \). This again is a result of the attraction on the legs which means that the cluster of particles is uniformly distributed along a leg, thus changing the sign of the string order for each site. For smaller \( V_d \) one can recover the peak at \( \nu = 1/3 \) but only for small \( V_d \sim 0.1 \) and for correspondingly small \( t_1 \) (in order to see ordering at all). This means that one can in principle choose a small \( t_1 \) value and then tune \( V_d \) to follow the transition from string ordering with two different characteristic periods. In contrast, for perpendicular dipoles the interactions are purely repulsive and the zig-zag phase with \( \nu = 1/3 \) will be generated for any \( V_d \) at sufficiently small \( t_1 \).

The above considerations begs the question as to what happens at some intermediate angle between the extreme case of perpendicular and parallel dipoles. In Fig. 5, we therefore show results for \( \theta = \pi/4 \) and \( \phi = 0 \) for the string order at different values of \( V_d \). In this case the attraction along the legs is present but much smaller than for parallel dipoles, while the repulsion across the rung is the same as both parallel and perpendicular orientations. The figure demonstrates a transition from \( \nu = 1/3 \) to \( \nu = 1/2 \) as \( V_d \) increases as one goes from a zig-zag configuration driven by repulsion to a clusterization on one leg driven by the attraction. This is consistent with the classical behavior discussed above. The Fourier coefficients spread out and their magnitudes decrease (note the different vertical scales in Fig. 5) as we transition to the cluster state at large \( V_d \). In our numerical calculations the cluster state is only stabilized by the hard-core nature of the bosons. If this condition is removed the system will have a negative compressibility. This also suggests that the transition to the clustered state could be first order transition since the density changes as we cross the critical angle towards the attractive regime at small \( \theta \). This is an example of the competition between different signs of the dipolar interaction and its influence on the non-local string order. This should have a clear signal in experimental setups that seeks to measure string correlations.

### D. Phase diagrams

We now consider the different phase diagrams that are possible to explore through a change of \( V_d \), \( t_1 \), \( \theta \), and the filling fraction. Note that the phase diagrams that we plot here show the strength (absolute value of largest Fourier component) of the Ising and string order (given by the correlation functions in Eqs. (5) and (6)). As the two orders tend to be non-vanishing at the same time (but of different magnitude), we plot the two in separate graphs. The more traditional approach would be to plot where each are non-zero or vanishing in a single plot, but we feel that the present form contains more information.

The first case is perpendicular dipoles which is shown in Fig. 6 for \( \rho = 1/3 \). The left side gives the Ising while the right side shows the string order (color coding on the far right). Note that we have normalized the order parameters so that their largest value in the whole phase diagram is one. As \( t_1 \) increases, both orders eventually go to zero as expected. What is more interesting is that they tend to be pinned to each other and disappear along
roughly the same line in the phase diagram. In the ordered phase, however, the string order tends to have a larger (relative) magnitude than the Ising order. This should be compared to the results presented in Ref. 66 where phases of vanishing Ising but non-vanishing string was obtained. The model in Ref. 66 has large repulsion along the rungs, uses only nearest neighbour interactions, and is thus different from the more realistic dipole-dipole interaction that we consider here.

For lower filling fractions the orders are expected to be less robust as the transverse hopping is increased since correlations vanish faster at lower filling. This can be seen in Fig. 4 which is also for the case of perpendicular dipoloes, but this time with filling \( \rho = 1/4 \). The picture is similar to that in Fig. 4 but with a severely shrink ordered region. This is generally the case for small \( \rho \). The string and Ising orders are still pinned to each other, with the string slightly stronger in the ordered region. For larger filling fractions (not shown here), we find larger ordered regions as expected.

We now consider the phase diagram as a function of \( \theta \) which is shown in Fig. 5. Our calculations show that a critical angle \( \theta_0 \sim \pi/3 \) exists at which the system has neither Ising nor string order for any value of \( t_1 \). This critical angle seems to be independent of \( \rho \) and \( V_d \) according to numerical results. This is supported by the classical calculations shown in Fig. 2. If we consider small transverse hopping, \( t_1 \ll 1 \), then \( \theta_0 \) is the point at which the system changes character from being Ising ordered at \( \nu = 0 \) due to clustering on one leg for \( \theta < \theta_0 \) to being string ordered due to the repulsively induced zig-zag behavior at \( \nu = 1/3 \) for \( \theta > \theta_0 \). For smaller values of \( V_d \) the maximum Fourier component will change its frequency \( \nu \) (as seen in Fig. 5) but the behavior is the same with a critical \( \theta_0 \) at which the order parameters vanish. It is interesting to compare the angle \( \theta_0 \) to the so-called magic angle, \( \theta_M = \arccos(\frac{1}{\sqrt{3}}) \approx 0.955 \approx 55^\circ \), at which two dipoles with this orientation will be non-interacting. This is about 5 degrees smaller than \( \theta_0 \). Since \( \theta_0 > \theta_M \) we see that it takes a finite amount of repulsive strength along the legs of the ladder to go from Ising order to string ordering at very small \( t_1 \). This is in spite of the fact that \( V_d \) is large compared to the hopping along the legs in the phase diagram in Fig. 5. The dipolar interactions also act along the diagonals of the ladder (also up to third removed neighbour site) and diminishes the repulsion from the longer ranges (although it never switches sign). The local repulsion from the site directly across on the other leg, however, appears to be insufficient for ordering for any \( t_1 \). Below angles of \( \theta \sim 50^\circ \) both order parameters become frustrated as the interactions become dominantly attractive, as seen also in the classical phase diagram. Note that the quantum delocalization moves the critical angle to 50 degrees which is slightly below the classical value of \( \theta_M = 54.7 \) degrees. For small angles both order parameters settle on a (small) non-zero value. However, in this part of the phase diagram, the system is effectively attractive and will be unstable as discussed above.

The diagram in Fig. 5 was obtained using a large value \( V_d = 10 \). Smaller values of \( V_d \) give qualitatively the same behavior and the only significant difference is a shrinking of the ordered region to smaller values of \( t_1 \). This is consistent with the fact that the classical transition from zig-zag to aligned does not depend on the size of \( V_d \). Also, we have used a filling of \( \rho = 1/3 \). Smaller fillings will shrink the ordered region, while at \( \rho = 1/2 \) the region of order is maximized such that the magnitude of the order is larger everywhere expect for the wedge termination at the critical angle \( \theta_0 \) that is still the same as for \( \rho = 1/3 \) from Fig. 5.

An interesting question beyond the scope of the current paper concerns the low-energy theory around the critical angle where both orders vanish. Similar geometries without the in-tube lattice have been studied using Luttinger liquid theory. In particular, Ref. 24 has presented a phase diagram using a Luttinger approach for \( \phi = 0 \) and \( \theta \) around our critical value for the zig-zag to aligned transition, although with no intertube hopping term and using fermionic dipolar particles. Since we use hard-core bosons, this should nevertheless be comparable. For large angles close to \( \theta = \pi/2 \), a density-wave state is found which is consistent with our findings. Around the critical angle, there could be other phases appearing, and with a lattice in the tube a number of crystalline phases have been discussed. It would be interesting to combine bosonization and mean-field theory as described in Ref. 17 with the in-tube lattice of the present setup (possibly along the lines of Ref. 24).

\section*{IV. CONCLUSIONS}

We studied a two-leg ladder containing dipolar particles as function of interaction strength, transverse hopping, and orientation angle of the dipole moments

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure7}
\caption{Phase diagrams for the Ising (left) and string (right) orders as a function of \( V_d \) and \( t_1 \) for filling factor \( \rho = 1/4 \) and perpendicular dipoles, \( \theta = \pi/2 \).}
\end{figure}
with respect to the ladder plane in order to investigate the presence of the quantum zig-zag phase. Within a Hubbard-type model with long-range dipole-dipole interaction, we computed Ising and string correlation that display ordered phases for repulsive dipolar interactions and low transverse hopping. Two different kinds of string ordering was obtained for filling fraction of one-third with different characteristic frequencies and a transition between these takes place as the orientation of the dipoles is changed from being parallel to perpendicular to the ladder plane. Furthermore, we find that there is a critical angle of about 60 degrees at which neither Ising nor string ordering survives at finite transverse hopping. Our numerical calculations indicate that this critical angle is insensitive to filling fraction and dipolar strength.

An interesting question concerns the order of the transitions in our phase diagrams as function of dipolar strength for fixed angle or vice versa, and for different values of the transverse hopping. We have seen in Fig. 8 that as the angle is varied the Fourier components will diminish, flatten out, and re-emerge with a peak at a different frequency as we tune across the transition of the different kinds of string order. This seems to be a smooth behavior and not a first order transition. However, as we have discussed above this is driven by attractive interactions and there may thus indeed be a change in density once the interaction is strong enough to compensate the kinetic energy in the hopping terms. This would be a sudden change in density and could indeed be a first order transition taking place for a sufficiently small and fixed $\theta$ as function of $V_d/t_1$. The phases for fixed dipolar strength, $V_d$, as function of the angle, $\theta$, in Fig. 8 have a rather abrupt behavior around the critical angle where the both Ising and string orders vanish. This is reminiscent of the density-wave state discussed recently in Ref. 69. This could indicate a first order transition. On the other hand, as we saw in the classical phase diagram the zig-zag to aligned transition will not change the total density of the system but merely the density on individual legs of the ladder. This would suggest that the transition could be smooth both for vanishing and finite transverse hopping, $t_1$. This would imply that string and Ising orders do not compete in the effectively repulsive regime, $\theta > \theta_M = \cos^{-1}(1/\sqrt{3})$. Further investigation seems necessary to settle these issues.

In order to implement the model we have studied here experimentally, one can use heteronuclear molecules with dipolar moments that can be controlled by externally applied fields. Alternatively, one can also use neutral atoms with sizable magnetic dipole moments.
or Rydberg atoms\textsuperscript{75–77}. Measuring the bulk ordering such as Ising and string orders seems very realistic given current experimental developments using single-site addressing\textsuperscript{78,79}. In particular, string order in Mott insulators have been probed in one dimension\textsuperscript{80} and crystal structure has been probed in a Rydberg gas in two dimensions\textsuperscript{81}. Even dynamics has been accessible in recent experiments\textsuperscript{82}. The two-leg ladder geometry can be realized using a superlattice in the transverse confinement direction which should be compatible with the observation techniques.

Acknowledgments

We thank Erez Berg for illuminating discussions and Klaus Mølmer for his continuous encouragement and support. N.T.Z. is supported by the Danish Council for Independent Research - Natural Sciences, while S.G. acknowledges support from the Villum Kann Rasmussen foundation.

Appendix A: Numerical details

The numerical method used here is well-documented and compared to other methods in wide use (such as the density matrix renormalization group method) in the papers by Verstreate \textit{et al.}\textsuperscript{83} and by Crosswhite and Bacon\textsuperscript{84}. We will therefore not enter a discussion of the full numerical details but only sketch a few of the essential ideas. The long-range Hamiltonian is represented by a single matrix product operator (MPO) in our calculations. A simple way of constructing the matrices of the MPO is to utilize the connection with finite automata or hidden Markov models\textsuperscript{68,83}, where the matrices represent the action of a finite automaton or the transition rules of a hidden Markov model where the emitted symbols are exactly the strings of operators whose tensor product occurs in the Hamiltonian Eq. (3). A hidden Markov model for a single leg of dipoles with long-range interactions is illustrated in Fig. [9] and the generalization to multiple legs is straight forward. By using an MPO formulation of the Hamiltonian it is straightforward to evaluate the variance of the energy of the calculated state which provides an independent bound on the accuracy of the ground-state energy.

Appendix B: Finite size effects

To investigate potential effects of the finite system sizes that we work with, we have checked that our results are insensitive to increases in system size while keeping the filling fraction, $\rho$, the same. In Fig. [10] panels a) and b) we show an example of the behavior of the string correlation order parameter as the size is increased from $L = 24$ (dashed lines) to $N = 48$ (solid lines) while keeping $\rho = 1/3$. The results shown have $V_d = 4.0$, $\phi = 0$, and $\theta = \pi/2$, i.e. perpendicular dipoles. In Fig. [10]b) the upper curves that oscillate around a finite value are for $t_1 = 0.1$ while the decaying profiles in the lower part have $t_1 = 1.0$. The former are in the string ordered phase while the latter are in the string disordered phase. The curves show a very good resemblance of profiles for both the average values and the oscillatory peaks irrespective of system size. This shows that our results do not suffer from sizable finite size effects. For comparison, we show in Fig. [11]b) the Fourier transform of the profiles in Fig. [10]b). Here we do see some differences at larger frequency values for the $t_1 = 0.1$ case, but only of subleading nature in comparison to the main peak at zero frequency which is properly reproduced.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig9}
\caption{Illustration of a long-range interaction MPO for a single leg.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig10}
\caption{Exploration of finite size and dipolar interaction range truncation effects on the string order for $\phi = 0$ and $\rho = 1/3$. a) String order parameter profile for $V_d = 4.0$ and $\theta = \pi/2$ with $L = 48$ ($N = 32$) as solid line and $L = 24$ ($N = 16$) as the dashed line. The upper curves have $t_1 = 0.1$ and the lower ones have $t_1 = 1.0$. b) Fourier transform of the profiles in a). c) $V_d = 10$ and $\theta = 0.96$ (55 degrees) for truncation of the dipolar interaction at nearest (dotted line), next-nearest (dashed line), and next-next-nearest neighbour (solid line). Profiles for $t_1 = 0.05$ and $t_1 = 0.5$ are shown. d) Same as in c) for $\theta = 1.22$ (70 degrees).}
\end{figure}
Appendix C: Dipolar interaction range

Another issue with the implementation of dipolar interactions in the matrix product state procedure is the necessary truncation at some finite neighbour distance. In order to gauge whether this truncation posed can potentially change any of the results presented in this paper, we have studied the behavior of the system as the number of neighbour sites over which the dipolar force acts is varied. In Fig. (10) and (d), we show the string order parameter for \( L = 48, \rho = 1/3, V_d = 10 \), and for two different values of \( t_1 = 0.05 \) (thick lines) and \( t_1 = 0.5 \) (thin lines). The angles are \( \phi = 0 \) and \( \theta = 0.96 \) (55 degrees) which is in the string disordered phase (thus the oscillatory pattern around zero). The truncation has been done at nearest (dotted), next-nearest (dashed), and next-next-nearest (solid) neighbour sites. For the lower \( t_1 = 0.05 \) the three curves are virtually the same and no truncation effects can be seen. However, as we increase to \( t_1 = 0.5 \), we see that the nearest neighbour truncation differs from the others, while next and next-next values are very close. This shows that truncation at next-nearest neighbour is adequate for our purposes, while using only nearest neighbour dipolar interactions would miss some long-range correlations in the system as we see by the faster decay in that case in Fig. (11). The same story plays out in Fig. (12) where we have used \( \theta = 1.22 \) (70 degrees) and are thus in the string ordered regime of the phase diagram. Again we see that truncation at only nearest neighbour tends to miss correlations at longer range for larger \( t_1 \). The results presented in the main text have all be computed using the next-next-nearest neighbour truncation.

---

1. S. Ospelkaus, A. Pe’er, K.-K. Ni, J. J. Zirbel, B. Neyenhuis, S. Kotochigova, P. S. Julienne, J. Ye, and D. S. Jin, Nature Phys. 4, 622 (2008).
2. K.-K. Ni, S. Ospelkaus, M. H. G. de Miranda, A. Pe’er, B. Neyenhuis, J. J. Zirbel, S. Kotochigova, P. S. Julienne, D. S. Jin, and J. Ye, Science 322, 231 (2008).
3. J. Deiglmayr, A. Crochola, M. Repp, K. Möttölä, C. Glück, J. Lange, O. Dulieu, R. Wester, and M. Weidmüller, Phys. Rev. Lett. 101, 133004 (2008).
4. F. Lang, K. Winkler, C. Strauss, R. Grimm, and J. Hecker Denschlag, Phys. Rev. Lett. 101, 133005 (2008).
5. S. Ospelkaus, K.-K. Ni, D. Wang, M. H. G. de Miranda, B. Neyenhuis, G. Quémener, P. S. Julienne, J. L. Bohn, D. S. Jin, and J. Ye, Science 101, 853 (2010).
6. K.-K. Ni, S. Ospelkaus, D. Wang, G. Quémener, B. Neyenhuis, M. H. G. de Miranda, J. L. Bohn, J. Ye, and D. S. Jin, Nature (London) 464, 1324 (2010).
7. E. S. Shuman, J. F. Berry, and D. DeMille, Nature (London) 467, 820 (2010).
8. M. H. G. de Miranda, A. Chotia, B. Neyenhuis, D. Wang, G. Quehen, S. Ospelkaus, J. L. Bohn, J. Ye, and D. S. Jin, Nature Phys. 7, 502 (2011).
9. A. Chotia, B. Neyenhuis, S. A. Moses, B. Yan, J. P. Covey, M. Foss-Feig, A. M. Rey, D. S. Jin, and J. Ye, Phys. Rev. Lett. 108, 080405 (2012).
10. M. A. Baranov, Phys. Rep. 464, 71 (2008).
11. T. Lahaye, C. Menotti, L. Santos, M. Lewenstein, and T. Pfau, Rep. Prog. Phys. 72, 126401 (2009).
12. L. D. Carr, D. DeMille, R. V. Krems, and J. Ye, New J. Phys. 11, 055049 (2009).
13. M. A. Baranov, M. Dalmonte, G. Pupillo, and P. Zoller, Chem. Rev. 112, 5012 (2012).
14. P. M. Lushnikov, Phys. Rev. A 66, 051601 (2002).
15. G. M. Bruun and E. Taylor, Phys. Rev. Lett. 101, 245301 (2008).
16. N. R. Cooper and G. V. Shlyapnikov, Phys. Rev. Lett. 103, 155302 (2009).
17. J. M. Fellows and S. T. Carr, Phys. Rev. A 84, 051602(R) (2011).
18. B. Capogrosso-Sansone and A. Kuklov, J. Low Temp. Phys. 165, 213 (2011).
19. T. N. De Silva, Phys. Lett. A 377, 871 (2013).
20. R. Citro, E. Orignac, S. De Pala, and M. L. Chiofalo, Phys. Rev. A 75, 051602(R) (2007).
21. R. Citro, S. De Pala, E. Orignac, P. Pedri, and M. L. Chiofalo, New J. Phys. 10, 045011 (2008).
22. C.-M. Chang, W.-C. Shen, C.-Y. Lai, P. Chen, and D.-W. Wang, Phys. Rev. A 79, 053630 (2009).
23. Y.-P. Huang and D.-W. Wang, Phys. Rev. A 80, 053610 (2009).
24. M. Dalmonte, G. Pupillo, and P. Zoller, Phys. Rev. Lett. 105, 140401 (2010).
25. C. Kollath, J. S. Meyer, and T. Giamarchi, Phys. Rev. Lett. 100, 130403 (2008).
26. A. Argüelles and L. Santos, Phys. Rev. A 75, 053613 (2007).
27. M. Bauer and M. M. Parish, Phys. Rev. Lett. 108, 255302 (2012).
28. D.-W. Wang, Phys. Rev. Lett. 98, 060403 (2007).
29. A. Pikovski, M. Klawunn, G. V. Shlyapnikov, and L. Santos, Phys. Rev. Lett. 105, 215302 (2010).
30. A. C. Potter, E. Berg, D.-W. Wang, B. I. Halperin, and E. Demler, Phys. Rev. Lett. 105, 220406 (2010).
31. N. T. Zinner, B. Wunsch, D. Pekker, and D.-W. Wang, Phys. Rev. A 85, 013603 (2012).
32. P. Lecheminant and H. Nonne, Phys. Rev. B 85, 195121 (2012).
33. A. M. Tsvelik and A. Kuklov, New J. Phys. 14, 115033 (2012).
34. S. Sinha and L. Santos, Phys. Rev. Lett. 99, 140406 (2007).
35. M. Bortolozzo, D. J. Papoular, L. Barbiero, C. Menotti, and A. R. Zinner, Phys. Rev. A 88, 023603 (2013).
36. F. Deuretzbacher, G. M. Bruun, C. J. Pethick, M. Jona-Lasinio, S. M. Reimann, and L. Santos, Phys. Rev. A 88, 033611 (2013).
37. L. Guan, X. Cui, R. Qi, and H. Zhai, arXiv:1307.0899 (2013).
38. Y. Yamaguchi, T. Sogo, T. Ito, and T. Miyakawa, Phys. Rev. A 82, 013643 (2010).
39. K. Sun, C. Wu, and S. Das Sarma, Phys. Rev. B 82, 075105 (2010).
40. N. T. Zinner and G. M. Bruun, Eur. Phys. J D 65, 133
