Quantum spin chains is the fertile ground to study strongly correlated quantum many body systems. One of the most studied models is the quantum Heisenberg model. For antiferromagnetic coupling ($J_1 > 0$) the spin correlation of its ground state decays as $1/r$ up to a logarithm correction, displaying quasi-long range order (QLRO). The model with a next-nearest neighbour added is known as the $J_1 - J_2$ or zigzag spin chain. It is frustrated when $J_2 > 0$. A dimerization transition occurs at $J_2/J_1 \approx 0.2411$ after which it has a valence-bond-solid (VBS) order and incommensurate spiral spin correlation emerges after the Majudar-Ghosh (MG) point at $J_2/J_1 = 0.5^{2,5}$. Beyond the next-nearest terms, the system can be build up with even long-range interactions (LRI). The models with power law decay of LRI coupling $J_r \sim (-1)^{r-1} r^{-\alpha}$ have attracted many attentions, even though it has been strictly ruled out from 1D short-range rotation invariant models at even zero temperature. Recently, Sandvik proposed the combination of the $J_1-J_2$ model and the long-range nonfrustrated terms for studying the interplay between them, the Hamiltonian being

$$H = \sum_{i=1}^{N} \sum_{j=i+1}^{N} J_{|j-i|} \vec{S}_i \cdot \vec{S}_j \tag{1}$$

$$J_2 = g, \quad J_r \neq 2 = (-1)^{r-1} r^{-\alpha} / n(N, \alpha),$$

where the normalization factor $n(N, \alpha) \equiv 1 + \sum_{r=3}^{N/2} r^{-\alpha}$ ensures finite energy per site for infinite $N$ when $\alpha \leq 1$.

In the last decade quantum entanglement in the quantum many body systems have been extensively studied, among which, a central notion formed is the area law. For a short-range and gapless system divided into subsystems $A$ and $B$, the entanglement entropy $S_A = -\text{Tr}(\rho_A \ln \rho_A)$ for the ground state $|\psi\rangle$ is proportional to the boundary area of $A$, where $\rho_A = \text{Tr}_B (|\psi\rangle \langle \psi|)$ is the reduced density matrix. This is remarkable, as it means that physical ground states are “slightly” entangled. In particular for 1D systems it have been proved rigorously for gapped Hamiltonian, and is shown to be violated mildly by logarithmic divergence for gapless systems. Whereas it is still not very clear up to now the behaviour of entanglement in systems with LRI, especially that should then the area law be severely violated? Recently Koffel et. al made an achievement in this direction, showing interestingly that in the LRI transverse Ising model a gapped phase can even have logarithmic scaling of entanglement.

The model studied in Ref. is polarized, if the system is rotation invariant, stronger quantum fluctuation and entanglement will present, which to our knowledge has not been considered so far. In this paper, we study the rotation invariant, frustrated and long-range interacted model Eq.1 using the matrix product state (MPS) approach for both the ground state entanglement and phase diagram properties. We find that the distribution of entanglement in the parameter plane can determine several phase boundaries. In particular a line segment in the plane with minimum entanglement marks the development of the Majudar-Ghosh point. The largest amount of entanglement is found in the long range ordered AFM phase in the deep LRI and low frustration regime, but remarkably, the scaling of entanglement can be still fitted with logarithm functions. This indicates that, in contrary to one might expected, the area law is not severely violated in this system. The large entanglement in this regime causes some difficulties for the method, that we will also discuss in depth. In contrast the regime with moderate frustration $g$ is less entangled and relatively easier to simulate. It should be related to the spiral state in the ab initio study of realistic metallic chains. We determine approximately the transition from the incommensurate VBS phase to a decoupled phase in this regime, which improves significantly over previous exact diagonalization (ED) studies. In the end we argue that the model is illustrative enough to show that the entanglement in the long range ordered AFM phase should be an upper bound for all power law decay and two body interaction spin models.

It is conventionally difficult to simulate systems with LRI using density matrix renormalization group
Further more, the phase boundary between the decoupled phase is the same as Kumar and Soos\cite{16}, but differs with the name VBS-QLRO\cite{17} used by Sandvik.

The variational MPS (VMPS) algorithm\cite{21} to simulate the ground states for finite open chains with $N$ ranging from 16 to 100 and truncation dimension $D$ up to 520. It is implemented with the 1-site algorithm and density matrix correction\cite{22} that reduces the chance being stuck. The quality of the variational ground state is gauged by the average variance $v = \langle (H^2) - \langle H \rangle^2 \rangle / N$, kept smaller than 1e-4 for the hardest case. The infinite-system DMRG (iDMRG)\cite{23} algorithm is used to study infinite systems. This method exploits the translation invariance, such that the computation effort is reduced and boundary effect is avoided. It is implemented with a 4-site unit cell, from which an infinite MPS representation can be reconstructed after convergence\cite{24} for measuring physical observables. The maximal $D$ used is 1000 for generating a well converged fixed point with truncation error restricted to smaller than 1e-6, while at some point we also use iDMRG to generate a finite open chain with even larger $D$.

We re-plot the ground state phase diagram in Fig. 1 and show the distribution of entanglement on the parameter plane in Fig. 2. The entanglement is generally higher as $\alpha$ reduces; rather high in the top left corner while low in the bottom center. These already give a rough profile of several of the phase boundaries. The name of the dimerized phase is the same as Kumar and Soos\cite{16}, but differs with the name VBS-QLRO(\pi/2) used by Sandvik. Further more, the phase boundary between the decoupled phase and the dimerized incommensurate phase is qualitatively different from both previous works. We will prove this later. For the time being, let us discuss the development of the dimerized and commensurate phase of the $J_1-J_2$ model under the influence of LRI. Sandvik shows by excitation state level crossing that the dimerization critical point develops to (1.7, 0.41) as $\alpha$ reduces and then to a first order transition\cite{7}. Below, we determine the development of the Majudar-Ghosh point as well, but from an entanglement perspective.

Fig. 2 shows in particular dependence of entanglement $S$ on $g$ for several values of $\alpha$ with $N = 100$. Inset displays in great detail of the lines around $g = 0.4$ for $\alpha = 1.8, 1.7$ and 1.6.
The fitting line is \( g_N \) from iDMRG or random state; open square: VMPS with \( N \) from different algorithms. Open triangle: VMPS initiated with tanglement as a function of iDMRG steps at \( \alpha \) extrapolation with \( D \) larger than 1e-4 for the maximal length \( \alpha \) in average variance and entanglement on these difficulties. Fig.4(a) shows dependence of both with entanglement since the computational effort for it scales exponentially phase poses considerable difficulties to the MPS method, decoupled phase first order phase transition from the AFM phase to the multi-critical point, entanglement becomes discontinuous and incommensurate correlation on either side. After the a disorder-line appears as a valley in Fig.2, where it should also have minimum correlation length, and thus can be thought of as the maximum correlation length, and thus can be thought of as an effective central charge \( c \), \( r \) being stuck, but soon become unpractical. A two-site algorithm with density matrix correction won’t solve it either. It turns out a nice solution is to provide a better initial state, e.g., use the state of a smaller \( g \) as the input of larger \( g \) close to the right of the boundary (see [27] for alternative ways such as adding a pinning term for fixing this). In this way, the peaks for each lengths are unambiguously determined and the extrapolated value of the transition point is \( g_c = 0.339 \) (see inset of Fig.4(b)). As for the infinite algorithm, the metastable issue is more severe. It is stuck in a wider range, which, we however haven’t found a way to avoid. For \( g \) close to 0 the energy still deviates with VMPS. This is not because of getting stuck but is a convergence problem due to too fast growing of entanglement and at the same time relatively slow convergence of energy. As shown in Fig.4(c), entanglement suddenly drops after around 30 iteration steps (120 chain length) if \( D = 1000 \) is kept not increased and eventually converged to a wrong fixed point. One could stop iteration before the drop (this is where the data points of energy we adopted), but energy and other quantity are far from convergence. In all we find good convergence of VMPS for the parameter range studied, while iDMRG has either metastable state or convergence problems in the AFM phase.

Then the question follows is to what extent the entanglement in the strong LRI regime violates the area law, given that the Heisenberg point has already logarithmic scaling of entanglement. To this end we study the scaling of entanglement on sub-system lengths. To address larger system sizes, we use iDMRG to generate a finite MPS of \( N = 200 \) for measuring the bipartite entanglement at each sub-system length \( L \le N/2 \), during which truncation error is kept smaller than 1e-8 and \( D \) is needed up to 2000. The result is shown in Fig.4(a) and inset of Fig.4(b). One can see that, remarkably, \( S(L) \) for \( L \) not too close to the chain center can be well fitted with the logarithmic function. We extract an effective central charge \( c \) according to the formula \( S = \frac{c}{2} \ln(L) + \text{const} \), as shown in Fig.4(b). It is difficult to determine \( c \) very accurately in this way, as there is oscillation on odd and even bond for open antiferromagnet chains, and entanglement on only odd bonds are shown in Fig.5. One can see that \( c \) is near to 1.0 (the exact value for QLRO phase) for \( \alpha \le 2.5 \), after which, \( c \) increase quickly with \( \alpha \) and can go larger than 3.0 at \( \alpha = 1.0 \). This behaviour is in overall agreement with the transition point determined by ED as at \( \alpha_c = 2.22 \) between the QLRO and AFM phases.

We next turn to the right part of the phase diagram. Focusing on one line \( g = 0.7 \), we measure the spin correlation

\[
C(r) = \langle S_i^z S_{i+r}^z \rangle
\]  

and see how it changes as \( \alpha \) reduces. Here the spin chain is considered to be divided into odd and even sublattices, as is usually did for the \( J_1 - J_2 \) model. The upper panel of Fig.4 shows only the intra-sublattice (even \( r \) correla-
FIG. 5. (a) Bipartite entanglement entropy as a function of sub-system length $L$ for each $\alpha$ with $g = 0.0$. Only bipartition on odd bonds (odd $L$) are drawn. Data points are obtained by measuring finite MPS with $N = 200$ generated from iDMRG for $D$ up to 2000. Solid lines are fitting to $S = \frac{c}{2} \ln(L) + \text{const}$ for $1 \leq L \leq 80$. A log-linear scale plot of the same graph is shown in the inset of (b). (b) Effective central charge as a function of $\alpha$. 

One can see that for large $\alpha$ values $C(r)$ decreases exponentially with jumps in the curve. The jumps signify the incommensurate behaviour: Following the treatment of White and Affleck of the $J_1 - J_2$ model, we multiplying $C(r)$ e.g. at $\alpha = 1.4$ and $g = 0.7$ by $\sqrt{\gamma} \xi$ $r$, then the sinusoidal modulation is clearly seen in the inset of the graph, where the correlation length $\xi = 44.7$ is chosen such that the waves of the amplitude are as flat as possible. By evaluating $C(r)$ for $r$ up to 1000, we only find jumps for $\alpha > 1.2$. For $\alpha \leq 1.2$, $C(r)$ displays algebraic decay (for reference $C(r) \sim 1/r^\gamma$ with $\gamma = 1.18$ at $\alpha = 1.0$). This indicates a possible critical value $\alpha_c$ of a continuous phase transition at roughly 1.2. The transition point for other $\alpha$ can be determined likewise and this gives a approximate phase boundary. We find that $\alpha_c$ increases with $g$ and it should that $\alpha_c \rightarrow \infty$ as $g \rightarrow \infty$.

For further understanding the nature of the transition, we plot the inter sublattice correlation for $r = 1$ and the dimerization order parameter $d = \langle S^z_i S^z_{i+1} \rangle - \langle S^z_i S^z_{i+1} \rangle$ as a function of $D$ in the lower panel of Fig. [4(b)]. One can see that, while for $\alpha = 2.0 > \alpha_c$ the inter chain correlation and dimerization are clearly nonzero, for $\alpha = 1.0 < \alpha_c$ $C(1)$ and $d$ are very small and appear to vanish as $D$ increases. These altogether show that the transition should be from a dimerized and incommensurate phase to a phase decoupled into odd and even sublattice — either sublattice can be think of as the Heisenberg model with nearest neighbour coupling $g$ and with long range ferromagnetic coupling as perturbations. Note that for the $J_1 - J_2$ model, White and Affleck used field theory to predict that there is exponential small gap and dimerization for arbitrary large $g$, except for $g = \infty$ where it decouples exactly into two Heisenberg chain, and supported it by DMRG. While our arguments above essentially states that, the spin chain can be decoupled for modest $g$ at small $\alpha$. Nevertheless, the decay of $C(1)$ and $d$ with $D$ is somewhat slow, so we are still not completely sure whether the incommensurability and dimerization (and also spin gap) should be exponentially small but nonzero even as $\alpha$ approaches 0, which is very difficult to confirm numerically. A field theory study for small $\alpha$ may be desirable as well as that for the $J_1 - J_2$ model at large $g$.

In summary, we studied the frustrated spin chain with long range interactions using the matrix product state approaches. We find that it is most entangled in the rotation invariant long range ordered AFM phase in the deep LRI and low frustration regime, where the entanglement
scales at most logarithmically. We also studied correlation and dimerization for moderate frustration and determined an approximate boundary for the transition from the dimerized and incommensurate phase of the $J_1 - J_2$ model to a decoupled phase.

The entanglement in the AFM phase should be a upper bound for all 1D spin chains models with arbitrary power law decay long range and two body interaction. Because, first, models with rotation invariance is generally more entangled than polarized ones; Second, the rotation invariant model with a frustration term is illustrative enough to show that any change in the Hamiltonian that breaks the perfect long range order should only reduce entanglement. So it is reasonable to conjecture that all such type of systems should have at most logarithmic divergence of entanglement, and is in this sense not severely breaking the area law.

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