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Exotic phases of matter in quantum magnets

A tensor networks tale

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Publication date

2018

Document Version

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Citation for published version (APA):

Niesen, I. A. (2018). *Exotic phases of matter in quantum magnets: A tensor networks tale*.

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Competing plaquette states in the Shastry-Sutherland model

By means of infinite projected entangled pair states (iPEPS), the competition between the so-called empty and full plaquette phases of the Shastry-Sutherland (SSL) model is investigated. A recent study by Zayed et al. [54] based on pressure measurements of $\text{SrCu}_2(\text{BO}_3)_2$, the material for which the SSL model provides an effective description, suggested that the phase separating the dimer and antiferromagnetic phases of the SSL model is the full plaquette phase. However, our simulations in the intermediate plaquette phase show that the empty plaquette states are lower in energy than the full plaquette states, seemingly contradicting Zayed et al.'s result. Nevertheless, we do find that, by adding an artificial bias of only a few percent, the full plaquette state become favorable in energy, suggesting that the ground state of the SSL model is susceptible to lattice anisotropies. Possibly, the pressure applied to $\text{SrCu}_2(\text{BO}_3)_2$ distorts the lattice in such a way as to favor the full plaquette phase, which would explain the apparent discrepancy between our result and that of Zayed et al.

This chapter is based on the iPEPS part of Ref. [4].

5.1 Introduction

The Shastry-Sutherland (SSL) model, also known as the orthogonal dimer model [194], was introduced by Shastry and Sutherland in 1981 [195]. It consists of a lattice (Fig. 5.1) with spin-1/2 particles on each vertex, interacting with their nearest and next-nearest neighbors through the Hamiltonian defined by

$$H = J' \sum_{\langle i,j \rangle_s} \mathbf{S}_i \cdot \mathbf{S}_j + J \sum_{\langle\langle i,j \rangle\rangle_a} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (5.1)$$

In the equation above, the first sum runs over all nearest-neighbor bonds that form the square lattice (solid lines in Fig. 5.1), the second sum runs over all next-nearest-neighbor dimer bonds (dashed lines in Fig. 5.1), and $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ is the vector of spin matrices¹ for the spin-1/2 particle at site i :

$$S_i^x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_i^y = \frac{i}{2} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \text{and,} \quad S_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The SSL model was constructed in such a way that it admits an exact ground state made up of a product of singlet dimers, making it one of the few two-dimensional antiferromagnetic models for which an exact ground state is known².

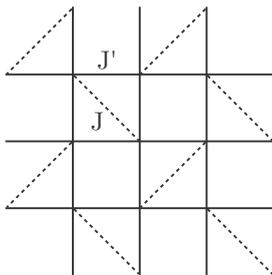


Figure 5.1: The SSL model has ordinary Heisenberg two-body interaction terms along every bond, with corresponding interaction strengths given by J' for bonds that are part of the square lattice (solid lines), and J for diagonally oriented bonds (dashed lines).

Because the SSL model is frustrated, it is for the most part inaccessible to quantum Monte Carlo simulations due to the negative sign problem [44]. In this chapter, we shall focus on the parameter regime of the SSL model wherein all coupling parameters are non-negative.

¹Setting $\hbar = 1$.

²The construction of the SSL model was inspired by the Majumdar-Ghosh chain and the exact ground state thereof [196].

The SSL model attracted attention when it became clear that it provides an effective description of the magnetic properties of $\text{SrCu}_2(\text{BO}_3)_2$ [194, 197, 198]. The parameter values of the SSL model that describe $\text{SrCu}_2(\text{BO}_3)_2$ are estimated to lie in the interval around $J'/J = 0.60 - 0.64$ for typical values of $J = 71 - 85K$ [72, 199–201].

For $J = 0$, the SSL model reduces to a square lattice Heisenberg antiferromagnet (AFM), which is gapless and has a Néel ordered ground state. In the opposite limit $J' = 0$, the system is gapped, and the above-mentioned dimer state is the exact ground state. Remarkably, this particular dimer state actually remains an eigenstate of the Hamiltonian—not necessarily the one with lowest energy—even when $J' > 0$ [195]. However, what exactly happens in the region between the dimer and AFM phases has been the subject of a longstanding debate.

A Schwinger boson mean-field theory study by Albrecht et al. [202] predicted the occurrence of a helical phase in between dimer and the AFM phases. Somewhat in line with this result is the work in Ref. [199], that suggests the existence of an intermediate phase, the nature of which the authors do not manage to identify. To the contrary of the above, there also appeared several studies that predicted a direct transition between the dimer and AFM phases [194, 198, 203, 204]. Furthermore, a series expansion study by Koga and Kawakami [205], found that the dimer and AFM phases are separated by an intermediate plaquette phase that is shown to be gapped, with a first order transition from the dimer to the plaquette phase, and a second order transition from the plaquette to the AFM phase. The plaquette phase, while not being magnetized, does break translational symmetry due to bond energy differences, in the sense that the energies on the thick bonds are lower than those on the thin bonds (Fig. 5.2 *left*).

The existence of the plaquette phase has also been confirmed by other studies, such as the series expansion study in Ref. [206], which shows that the plaquette phase is adiabatically connected to the ground state of the 1/5-depleted square lattice Heisenberg model, and the dimer/quadrumer boson and exact diagonalization study in Ref. [207]. Furthermore, Ref. [208] finds several short and long range ordered phases—such as dimer, plaquette and helically ordered phases—in the large N limit when increasing the symmetry of H to $\text{Sp}(2N)$. However, a series expansion study [209] challenged the existence of the plaquette phase, and suggested instead that the intermediate phase could have columnar-dimer order instead.

In 2012, Corboz et al. [70] investigated the competition between plaquette and columnar-dimer order by means of iPEPS, and demonstrated that ground state has plaquette order. Moreover, the dimer to plaquette and plaquette to AFM transitions were estimated to be located at $J'_{\text{dim-plaq}} = 0.675(2)$ and $J'_{\text{plaq-afm}} = 0.765(15)$ respectively (setting $J = 1$), and both transitions were determined to be first order. By trying different types of iPEPS setups, the column-dimer order was shown to be stable only for low bond dimension D , but as D increases the

column-dimer order gets destroyed. The plaquette phase, on the other hand, only becomes competitive for higher values of D , and is therefore absent from a $D = 2$ study presented in Ref. [210]. Another tensor network study using MERA—also conducted in 2012—finds the same intermediate plaquette phase [211], with a slightly larger estimate for $J'_{\text{dim-plaq}}$ that lies in between the $D = 3$ and $D = 4$ iPEPS estimates for $J'_{\text{dim-plaq}}$.

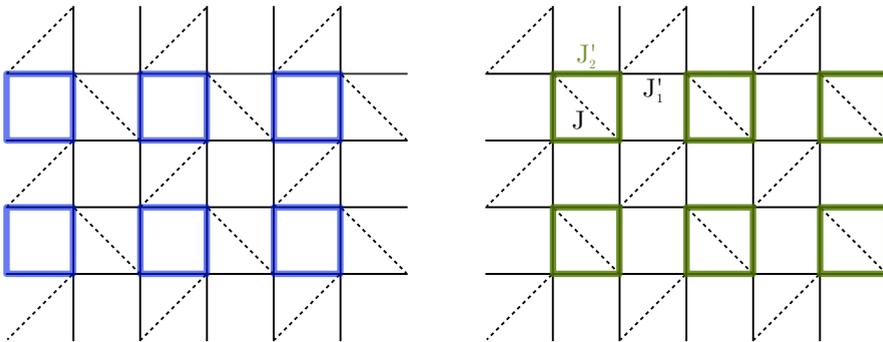


Figure 5.2: The plaquettes phases of the SSL model. Thicker bonds signify a lower bond energy. Left: the *empty plaquette phase*, with plaquettes centered at empty squares. Right: the *full plaquette phase*, with plaquettes centered around a square containing a diagonal interaction. The coupling parameters of the biased SSL Hamiltonian in Eq. (5.2) are displayed in the right figure showing the full plaquette phase.

More recently, Zayed et al. [54] conducted an experimental study of $\text{SrCu}_2(\text{BO}_3)_2$ by exposing it to different pressures, effectively changing the coupling parameters in the SSL-description of $\text{SrCu}_2(\text{BO}_3)_2$. By fitting the measured magnetic susceptibility as a function of temperature for different pressures (using 20-site exact diagonalization for the fit), Zayed et al. computed how the coupling parameters J and J' change with pressure, which allowed them to experimentally model the SSL model for several values of J and J' . Zayed et al. also encountered an intermediate plaquette phase—of which they also confirm that it is gapped—in between the dimer and AFM phases. However, the plaquette phase found by Zayed et al. has the plaquettes centered around a diagonal bond, hereafter referred to as the *full plaquette phase*³, see Fig. 5.2 *right*. This surprising result contradicts Refs. [70, 205, 207, 211], who instead claimed that the plaquette phase has the plaquettes centered at empty squares, from hereon referred to as the *empty plaquette phase*, displayed in Fig. 5.2 *left*.

In this chapter, we present a comparison of the two competing plaquette phases. To do so, we investigate the SSL model with a bias towards the full plaquette

³Note that the full plaquette phase had previously been investigated by Ref. [206], who demonstrated that it is adiabatically connected to the orthogonal dimer chain [212].

states, given by the Hamiltonian

$$H = J'_1 \sum_{\langle i,j \rangle_t} \mathbf{S}_i \cdot \mathbf{S}_j + J'_2 \sum_{\langle i,j \rangle_p} \mathbf{S}_i \cdot \mathbf{S}_j + J \sum_{\langle\langle i,j \rangle\rangle_d} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (5.2)$$

where J'_1 corresponds to the thin bonds on the square lattice, J'_2 corresponds to the plaquettes (thick bonds), and J —as before—signifies the dimer coupling strength; see Fig. 5.2 *right*. For the remainder of this chapter we set the dimer interaction strength to one: $J = 1$, and investigate the model as a function of J'_1 and the bias towards the full plaquette phase, which is given by $c := J'_2/J'_1$. We simulate states in both plaquette phases using iPEPS for several values of J'_1 and c , and compare their energies to determine the extent of the two plaquette phases.

After a brief discussion on the simulation setup in Section 5.2, we present our results in Section 5.3, and show that for $J'_1 = 0.7$ and $c = 1$ (no bias) the empty plaquette state is slightly lower in energy than the full plaquette state. We then proceed to run simulations for several values of $c > 1$, still at $J'_1 = 0.7$, and determine that the empty plaquette state remains the ground state up to the critical $c_{\text{empty-full}} = 1.060(8)$, whereafter the full plaquette state becomes the ground state of biased SSL model. Finally, we conclude our study by providing an approximate plot of the complete phase boundary separating both plaquette phases using fixed $D = 10$ full update simulations, and discuss how our findings compare to those of Zayed et al. [54] in Section 5.4.

5.2 Simulation details

There are several ways to simulate the SSL model with iPEPS. It is possible to have a single tensor represent either a single site, or more than one; and in the latter case, a choice must be made regarding to which sites are combined into a single tensor. Each of those choices we refer to as an iPEPS setup. It should be noted that, for lower (fixed) values of the bond dimension D , depending on the setup, one type of iPEPS might exhibit a lower energy than another. But, in the high D limit, after minimizing the energy, the same lowest energy state—the actual ground state of the system—should be obtained regardless of the iPEPS setup chosen.

In Ref. [70], four such setups have been examined, and it was shown that independent of the choice of setup, the final results are the same provided D is large enough⁴. However, it turns out that, in order to investigate the plaquette phase, the dimer-setup (Fig. 5.3) is the most suitable, because it gives the lowest fixed- D energies for the plaquette and AFM phases, and it is able to reproduce the dimer

⁴The setups examined are the original (o), the dimer (d), the plaquette (p) and the columnar setups (c), see Ref. [70] for details.

phase with bond dimension as low as⁵ $D = 1$. Therefore, we have opted to use the dimer setup for the investigation presented in this chapter. The added advantage of the dimer setup, is that the SSL Hamiltonian becomes a square lattice nearest-neighbor Hamiltonian when two sites connected by a diagonal bond are combined into one, allowing us to use the more efficient nearest-neighbor square lattice iPEPS algorithms for the investigation of the biased SSL model.

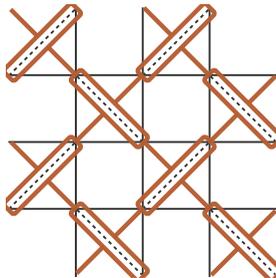


Figure 5.3: The iPEPS setup used for the simulations discussed in this chapter combines two physical sites connected by a dimer bond into a single local tensor. The resulting network structure is that of a square lattice iPEPS.

We obtain initial states in the full or empty plaquette phase by evolving randomly initialized states in imaginary time with a Hamiltonian that is strongly biased towards either the full or the empty plaquette phase⁶. Now, the extent of the full and empty plaquette phases in the phase diagram of the biased SSL model, defined by Eq. (5.2), is determined as follows. By initializing simulations from any of the two the initial states defined above, and thereafter minimizing the energies through imaginary time evolution or variational optimization using the Hamiltonian from Eq. (5.2) for several values of J'_1 and c , we obtain energies per site of the full and empty plaquette phases for (parts of) the phase diagram of the biased SSL model. Close to the transitions between the empty and the full plaquette phases, states in both phases are metastable and can both be simulated. Comparing their energies per site then allows us to estimate the phase boundary between the full and empty plaquette phases.

5.3 iPEPS results

We first investigate the ground state of the regular (unbiased) SSL model, by comparing the two competing plaquette states at a point in the middle of the

⁵Since two sites connected by a dimer bond are combined into a single local tensor.

⁶Meaning that the initial states are ground states of the biased Hamiltonian for values of the coupling parameters such that the corresponding points in parameter space lie deep within the phases the initial states represent.

plaquette phase of the unbiased SSL model, given by $J'_1 = 0.7$ and $c = 1$. The left

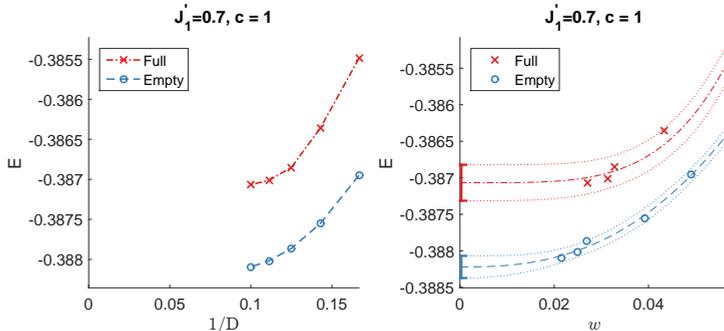


Figure 5.4: Energy per site of the empty and full plaquette states for $J'_1 = 0.7$ in the middle of the plaquette phase of the unbiased ($c = 1$) SSL model as a function of one over the bond dimension $1/D$ (left) or truncation error w (right). The right plot is fitted with a power-law function.

plot in Fig. 5.4 shows the energy per site for states initialized from within the full and the empty plaquette phase as a function of $1/D$, and the right plot displays the same energies as a function of truncation error [132]. The fitting graphs in the right plot of Fig. 5.4 are obtained by fitting a power-law function $f(w) = a + bw^c$ to the data points, with $b, c > 0$. The error bars signify one σ confidence bounds on the coefficients b and c .

We extrapolate $D \rightarrow \infty$, or equivalently $w \rightarrow 0$, to obtain energy estimates of the true low energy plaquette states of which the fixed D iPEPS are less-entangled approximations. Clearly, as can be seen by both the $1/D$ and truncation error plots, the empty plaquette state has a lower energy than the full plaquette state in the $D \rightarrow \infty$ limit. The above confirms that, in agreement with the earlier iPEPS study of Ref. [70], the empty plaquette state is the ground state of the SSL model at zero bias for $J'_1 = 0.7$. However, from Fig. 5.4, we do observe that the full plaquette state is close in energy to the empty plaquette state.

We next study the SSL model biased towards the full plaquette phase, defined by Eq. (5.2), and investigate for what value of the bias the full plaquette state becomes lower in energy than the empty plaquette state. In order to do so, we keep $J'_1 = 0.7$, run simulations for several values of $c > 1$ and compare the energies of the full and empty plaquette simulations.

It turns out that the energies of the full and empty plaquette iPEPS become comparable around $c = 1.06$. Zooming in on this particular value of the bias, Fig. 5.5 shows the energies per site of full and empty plaquette simulations plotted as a function of truncation error for $c = 1.05 - 1.07$. After linearly interpolating the energies (in c) and taking the error bars into account, we conclude that, for

$J'_1 = 0.7$, the transition from the empty to the full plaquette phase occurs at $c_{\text{empty-full}} = 1.060 \pm 0.008$, which corresponds to $J'_2 = 0.7420 \pm 0.0056$.

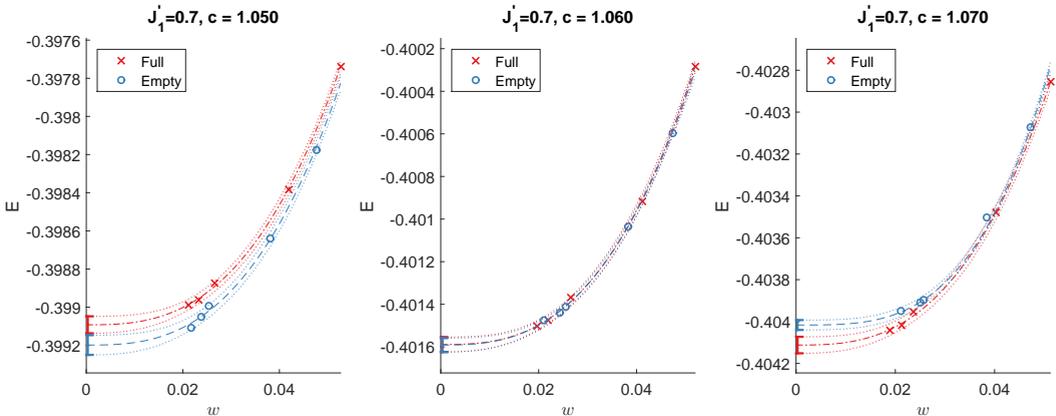


Figure 5.5: Energy per site of the empty and full plaquette states for $J'_1 = 0.7$ as a function of truncation error w for different values $c = 1.05 - 1.07$ of the bias, fitted with power-law functions.

Next, we map the entire phase boundary between the full and empty plaquette phases. From Figs. 5.4 and 5.5 we observe that the $D = 10$ simulations already provide very good estimates of the $D \rightarrow \infty$ extrapolated energies. Therefore, we shall execute several $D = 10$ full update simulations in both plaquette phases, and estimate the phase boundary by computing the points where the linearly interpolated energies intersect. Similarly, we obtain an estimate of the dimer-to-plaquette phase boundary by comparing the energies of fixed $D = 10$ plaquette simulations to the exact dimer energy per site of -0.375 . Doing so yields the approximate⁷ phase diagram displayed in Fig. 5.6.

We would like to add that the dotted lines in Fig. 5.6 are merely meant as a guide to the eye. For the transition between the empty and the full plaquette phases, they are obtained by superimposing the error bar of Fig. 5.5 onto the phase boundary. For the dimer to empty plaquette transition, the width of the dotted lines is based on the error bar for the dimer-to-plaquette phase boundary, obtained from the iPEPS study of the unbiased SSL model by Corboz et al. [70]. Note that the dimer-to-empty plaquette phase boundary can only move towards the dimer phase as D increases, because dimer energy is independent of D . Consequently, the dotted line is only shown on the dimer side of the transition.

⁷In order to obtain the exact phase boundaries, in principle a truncation error or $1/D$ extrapolation should be done at several points along the boundaries. However, this procedure is computationally more expensive, and the accuracy obtained by the fixed $D = 10$ simulations is sufficient for our current purpose.

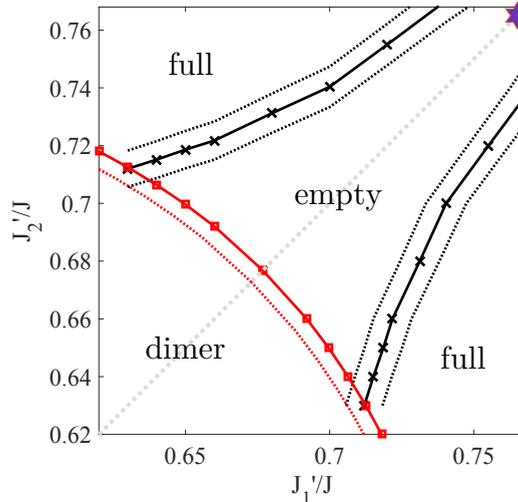


Figure 5.6: The $D = 10$ full update phase diagram. The error bars, which are only meant to be a guide to the eye, are based on the error bar obtained from Fig 5.5 for the full-to-empty plaquette transition, and on Ref. [70] for the empty plaquette to dimer phase transition. The star indicates the empty plaquette to AFM phase transition, also from Ref. [70].

Fig. 5.6 shows that the ground state phase diagram of the biased SSL model is symmetric with respect to the $J'_1 = J'_2$ line. This can be understood as follows. Instead of varying J'_2 while keeping J'_1 fixed, we can also vary J'_1 while keeping J'_2 fixed. As can be seen in Fig. 5.2 *right*, the effect of the latter is that we bias towards another full plaquette state, the one for which the diagonal bonds contained within the plaquettes connect the upper-right to the lower-left corner, rather than the upper-left to the lower-right corner. Both full plaquette states are equivalent, as they are related by a symmetry transformation, and therefore the phase diagram is symmetric.

To summarize, our simulations show that (i) the empty plaquette state is the ground state of the unbiased SSL model, and (ii) the full plaquette phase is separated from the unbiased SSL model ($c = 1$, diagonal $J'_1 = J'_2$ line in Fig. 5.6) by a non-negligible region in parameter space.

5.4 Conclusion

Motivated by the prediction by Zayed et al. [54] that the intermediate plaquette phase of the SSL model is the full plaquette phase, we have investigated the ground

state of the SSL model with artificial bias $c = J'_2/J'_1$ towards the full plaquette phase. By directly comparing the energies of iPEPS simulations initialized from full and empty plaquette states respectively, we showed that in the middle of the intermediate plaquette phase ($J'_1 = 0.7$) of the SSL model, the ground state lies in the *empty* plaquette phase rather than the full plaquette phase, and remains so up to a critical value of the bias of $c_{\text{empty-full}} = 1.060(8)$, after which the full plaquette phase takes over. Given that $J'_1 = 0.7$, this critical value of the bias corresponds to $J'_2 = 0.7420(56)$. Having thoroughly investigated the cut at $J'_1 = 0.7$, we then expanded our study to a larger parameter regime in the $J'_1 - J'_2$ plane and determined the entire empty-to-full plaquette phase boundary using fixed $D = 10$ full update simulations. The resulting phase diagram, shown in Fig. 5.6, clearly shows that the empty plaquette phase takes up a significant portion of the ground state phase diagram of the SSL model, even in the presence of an artificial bias towards the full plaquette phase.

At first sight, there seems to be a discrepancy between our results and those of the experimental study by Zayed et al. [54], who demonstrated that the full plaquette state is realized in $\text{SrCu}_2(\text{BO}_3)_2$ under pressure. However, it is conceivable that the pressure distorts the lattice in a such way that it breaks the C4-rotational symmetry around the empty plaquettes, changing the effective coupling parameters J'_1 and J'_2 relative to one another. Given that we find that the bias required to make the full plaquette phase favorable over the empty plaquette phase is of the order of only a few percent, it is not at all unlikely that the pressure applied to $\text{SrCu}_2(\text{BO}_3)_2$ causes the effective SSL coupling parameters to detune to a point in parameter space where the full plaquette state is the ground state.

Interestingly, the effect of a typical lattice distortion of the SSL model has previously been investigated by Moliner et al. [213]. According to the authors, subjecting $\text{SrCu}_2(\text{BO}_3)_2$ to high hydrostatic pressure naturally leads to a difference in intra-dimer coupling strengths. Moreover, in the regime of significant distortion, the ground state lies in an effective one-dimensional Haldane phase of nearly decoupled two-leg ladders. The full plaquette phase, on the other hand, is adiabatically connected to the plaquette phase of decoupled one-dimensional orthogonal dimer chains [206]. For a future work, it would be interesting to see if there is a relationship between these two phases.