Exotic phases of matter in quantum magnets
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CHAPTER 6

The sign problem in an extended Shastry-Sutherland model

The quantum Monte Carlo sign problem in the extended Shastry-Sutherland (SSL) model that interpolates between the original SSL and the fully-frustrated bilayer models, completely disappears at low temperature when the Hamiltonian is expressed in the dimer basis. The disappearance of the minus sign is a consequence of the fact that the product of dimer singlets is the exact ground state not only of the extended SSL model, but also of the minus sign-free model obtained by changing the sign of the positive off-diagonal matrix elements in the dimer basis. Comparing to our infinite projected entangled pair states (iPEPS) study of the same model, we observe that, indeed, the region wherein the sign problem disappears is completely contained within the dimer phase. This absence of the sign problem allows us to calculate the temperature dependence of the susceptibility and the specific heat of the Shastry-Sutherland model with high accuracy up to intermediate inter-dimer coupling on large systems and down to zero temperature.

This chapter is based on Ref. [5], with a larger emphasis on the iPEPS part.

6.1 Introduction

Frustrated quantum magnets in which local exchange processes are in competition are believed to host extremely rich physics, ranging from various kinds of valence
bond solids to quantum spin liquids [214–217]. The investigation of these models, however, is a real challenge because in general there is no unbiased method to study their properties on large enough lattices and at low enough temperature. In two dimensions, the method of choice to study the thermal properties of unfrustrated systems, Quantum Monte Carlo (QMC), suffers from a very severe minus sign problem when applied to frustrated systems in the standard basis of spin configurations. This makes it difficult to get accurate results for temperatures far below the typical coupling constants; the interesting regime unfortunately when looking for exotic quantum physics.

The Shastry-Sutherland (SSL) model—introduced in Chapter 5—with its remarkable and still debated series of magnetization plateaus [72,75,197,218–224]—is one of the paradigmatic two-dimensional spin-1/2 frustrated models with experimental realization. Because it has triangles as building blocks, the SSL model has a severe minus sign problem [44]. Nevertheless, the ground state of the Shastry-Sutherland model been known for nearly forty years1 [195, 198]. It seems logical to expect that knowledge of the ground state should help to investigate the low-temperature thermodynamics, but this is not the case. The interpretation of the temperature dependence of the susceptibility [197] and of the specific heat of SrCu$_2$(BO$_3$)$_2$ [225], the nearly exact experimental realization of the Shastry-Sutherland model, relies mainly on exact diagonalization results on small lattices up to 20 sites2 [194,198,226].

In this chapter, we show that the knowledge of the exact ground state of the Shastry-Sutherland model indeed provides a considerable advantage if the QMC simulations are formulated in the dimer basis [227–231] rather than the configuration basis. Unlike a number of fully frustrated models studied recently, in which the minus sign disappears altogether in the dimer basis, the minus sign problem is still present for the Shastry-Sutherland model. However, it turns out that the minus sign decreases at low temperature and disappears completely at zero temperature, as long as the singlet dimer ground state is not only the ground state of the model itself, but also of the model obtained by changing the sign of the positive off-diagonal matrix elements in the dimer basis. In order to obtain a better understanding of where and why the sign problem disappears, we employ iPEPS to map the complete ground state phase diagram. Our iPEPS data confirm that, as expected, the region wherein the minus sign disappears is completely contained in the dimer phase. The above result shows that, provided the ground state is known exactly, there is a possibility that QMC can be used to study the low temperature thermodynamics of frustrated models.

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1That is, for relatively strong intra-dimer coupling. As mentioned in the introduction of Chapter 5, by construction, the SSL model has an exact ground state made up of a product of singlet dimers.

2The magnetic susceptibility $\chi$ has also been analyzed by series expansions [198, 203], but these are accurate only for temperatures above the maximum of $\chi$. 

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This chapter is organized as follows. In Section 6.2 we introduce an extension of the SSL model that interpolates between the original SSL model and the fully-frustrated bilayer model. We then proceed with our iPEPS study of the extended SSL model, and map the entire ground state phase diagram in Section 6.3. Next, we devote Section 6.4 to the sign problem in QMC, providing a brief introduction into the basic concepts involved, after which we proceed with a construction of a sign-free Hamiltonian that shares the dimer ground state with the extended SSL model, and discuss the disappearance of the sign problem in a large portion of the dimer phase of the latter. Finally, in Section 6.5, we build on the absence of the sign problem in a large part of the phase diagram to derive the low-temperature susceptibility and specific heat of the SSL model up to a relative inter-dimer coupling of $J/J_D = 0.526(1)$, after which we conclude in Section 6.6.

6.2 The model

In this chapter, we study the Shastry-Sutherland (SSL) model [195] extended with another inter-dimer coupling $J_2$ [203,204], defined by the Hamiltonian

$$H_{\text{ext}} = J_D \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} \vec{S}_i \cdot \vec{S}_j. \quad (6.1)$$

Here, $J_D$ and $J$ are the intra and inter-dimer couplings of the original SSL model (see Fig. 6.1, left), and $J_2$ allows for continuous interpolation between the original SSL model ($J_2 = 0$) and the fully-frustrated bilayer model ($J_2 = J$) [228,229,231–236]. The SSL lattice can be interpreted as a square lattice with some diagonal couplings, or as a square lattice of coupled dimers\(^3\). The equivalence of the extended SSL model for $J_2 = J$ and the fully-frustrated bilayer model becomes visible when rotating all dimers by $\pi/2$ to make them perpendicular to the plane (see Fig. 6.1 right). For the remainder of this chapter, we shall study the extended SSL model in the challenging and experimentally relevant [194,197,198] parameter regime of non-negative coupling constants $J, J_D, J_2 \geq 0$.

As we shall see later in this chapter, the extended SSL model from Eq. (6.1) can be studied by QMC as long as both inter-dimer couplings $J$ and $J_2$ are not too large. However, before delving into the QMC simulations and the related sign problem, it will prove insightful to first obtain the zero-temperature phase diagram. To do so, we have modeled the extended SSL model with iPEPS, shown previously to lead to very accurate results for the original Shastry-Sutherland model [70].

\(^3\)Note that, for $J_2 = 0$, the lattice in Fig. 6.1 is equivalent to the one shown in Fig. 5.1. Depending on which representation of the lattice is chosen, either two sites connected by a dimer bond are considered nearest neighbors, as in Fig.6.1, or next-nearest neighbors, as in Fig. 5.1. Regardless of the apparent discrepancy, the Hamiltonian in Eq. (6.1) with $J_2 = 0$ is equivalent to that of and Eq. (5.1) provided we associate $(J_D, J)$ with $(J, J')$. 
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Figure 6.1: Sketch of the Shastry-Sutherland model and of its interpolation to the fully frustrated bilayer (left). The right panel shows a topologically equivalent representation as a frustrated bilayer square lattice.

6.3 iPEPS phase diagram

6.3.1 Simulation details

In order to study the SSL model using iPEPS, we use the same setup as the one used in Chapter 5. That is, each local tensor has one physical leg which represents two physical sites on a dimer, and four auxiliary legs that connect to neighboring local tensors forming a square lattice pattern in accordance with the lattice structure in Fig. 6.1 (right). All phases\(^4\) in the phase diagram of the extended SSL model (Fig. 6.2) can be represented by an iPEPS with a 2-sublattice unit cell consisting of two local tensors (four physical sites).

To construct the phase diagram, we have employed fixed \(D = 10\) simple update simulations which already provide a good estimate of the phase boundaries in the exact infinite \(D\) limit as we show below. We have computed transition points along several horizontal (and vertical) cuts in the phase diagram. Along each cut (e.g. a fixed value of \(J_2/J\) for a horizontal cut) the critical coupling \(J_c/D\) is determined by locating the intersection point where the linearly-interpolated energies of the states initialized in the two adjacent phases intersect (making use of hysteresis in the vicinity of a first-order phase transition).

6.3.2 iPEPS results

The iPEPS phase diagram is shown in Fig. 6.2 for\(^5\) \(J \leq J_D\). It consists of three phases: a the dimer singlet phase at small inter-dimer coupling, an antiferromag-

\(^4\)Note that we have looked for phases other than the three shown in Fig. 6.2 by executing randomly initialized iPEPS simulations scattered throughout the phase diagram, but all of these simulations converged to states that lie in one of the three phases displayed in the figure.

\(^5\)For \(J > J_D\), the ground state shows the same antiferromagnetic order as that of the rightmost phase displayed in Fig. 6.2.
6.3. iPEPS phase diagram

Figure 6.2: $D = 10$ simple update phase diagram of the generalized SSL model that interpolates between the original SSL ($J_2 = 0$) and the fully-frustrated bilayer ($J_2 = J$) models. The star indicates an accurate series expansion result [203, 204] for the dimer to AFM phase transition for $J_2 = J$, located at $J/J_D = 0.42957(2)$.

Nematic phase at large inter-dimer coupling, and a small intermediate plaquette phase at small third-neighbor coupling. All phase transitions are first order. Note that the Hamiltonian is symmetric under exchange of $J \leftrightarrow J_2$ while simultaneously interchanging all particles connected by a dimer bond, as can be seen from the lattice structure in Fig. 6.1 right. For this reason, we have only mapped the region for which $J_2 \leq J$. We remark that a previous investigation [204] came to a very similar phase diagram except that it missed the intermediate plaquette phase.

To determine the accuracy of the fixed $D$ simple update phase diagram, we have executed additional full and variational update simulations followed by $D \to \infty$ extrapolations along several cuts in parameter space. The extrapolations were done using the so-called truncation error, see Ref. [132]. Comparing with the $D = 10$ simple update phase boundaries along four horizontal cuts at $J_2/J = 0.25$, 0.50, 0.75 and 1.00, we observe that the dimer to AFM boundary displayed in Fig. 6.2 agrees with the variational update $D \to \infty$ phase boundary up to the first four digits. The above results also agree up to the same precision with the $J_2/J = 1$ series expansion result [203,204] marked by the star in Fig. 6.2.

The uncertainty of the phase boundaries of the plaquette phase is shown by the error bars in Fig. 6.3. The horizontal error bars are those from the previous full
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update iPEPS study by Corboz et al. [70]. The vertical error bar is based on an energy per site comparison of plaquette and AFM initialized states shown in Figs. 6.9 and 6.10 in Appendix 6.A. Note that the error bars for the plaquette to AFM and plaquette to dimer phase transitions are wider than those corresponding to the dimer to AFM transition, from which we conclude that in particular the plaquette to AFM transition seems to be only weak first order. Accordingly, the phase boundaries displayed in Fig. 6.2 have been thickened in to represent the uncertainty coming from the error bars shown in Fig. 6.3 (the effect of which, especially for larger values of \(J_2\), is too small to be noticeable in Fig. 6.2).

Having established the ground state phase diagram by means of iPEPS, we shall next turn our attention to the sign problem of the extended SSL model.

6.4 The minus sign problem

6.4.1 A quick introduction to QMC

The main idea behind QMC is to first map a given quantum system to a classical system, and then perform classical Monte Carlo on the resulting classical system [43,237]. One way to design such a mapping is by taking Feynman’s path integral approach. For example, in order to compute the main quantity of interest in a thermodynamic system: the partition function \(Z = \text{Tr}[\exp(-\beta H)]\) (and derivatives thereof), we proceed as follows. Let \(\mathcal{H}\) be the Hilbert space on which
6.4. The minus sign problem

$H$ acts, and let $\{|i\rangle\}$ be some orthonormal basis of $\mathcal{H}$. Defining $\tau = \beta/M$ for some (soon to be large) number $M$, we can approximate the partition function by inserting resolutions of the identity $I = \sum_i |i\rangle\langle i|$, as shown below:

$$Z = \text{Tr}[\exp(-\beta H)] = \text{Tr}[\exp(-\tau H)^M]$$
$$= \text{Tr}\left[(U + \mathcal{O}(\tau^2))^M\right] = \text{Tr}[U^M + \mathcal{O}(\tau)]$$
$$= \sum_{i_1,\ldots,i_M} \langle i_1|U|i_2\rangle \langle i_2|U|i_3\rangle \cdots \langle i_{M-1}|U|i_M\rangle + \mathcal{O}(\tau),$$

where $U := 1 - \tau H$. In the large $M$ limit, the $\mathcal{O}(\tau)$ term becomes negligibly small, and what remains is

$$Z \approx \sum_{i_1,\ldots,i_M} \langle i_1|U|i_2\rangle \cdots \langle i_{M-1}|U|i_M\rangle = \sum_{i_1,\ldots,i_M} W_{i_1,\ldots,i_M} \quad (6.2)$$

By interpreting each $\langle i_k|U|i_{k+1}\rangle$ as a weight, the expression in Eq. (6.2) can be thought of as a probability distribution on the classical configuration space $\mathcal{C}^M$—where $\mathcal{C} = \{|i\rangle\}$ is the classical configuration space of all basis states of $\mathcal{H}$—that we can sample from using classical Monte Carlo.

Another common approach to QMC is the *stochastic series expansion*, or SSE for short [238, 239]. The main idea behind SSE is to directly Taylor expand the exponential in the partition function:

$$Z = \text{Tr}\exp(-\beta H) = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \text{Tr}(-H)^n$$
$$= 1 + \sum_{n=1}^{\infty} \frac{\beta^n}{n!} \sum_{i_1,\ldots,i_n} \langle i_1|-H|i_2\rangle \langle i_2|-H|i_3\rangle \cdots \langle i_{n-1}| - H|i_n\rangle,$$

and interpret the final summand as a product of weights that generates a distribution that can be sampled from. For finite systems (of $N_s$ sites) at non-zero temperature ($\beta$), the sum over $n$ peaks at the saddle point $n \approx N_s \beta$, and can be safely truncated at a cutoff\(^6\) $\Lambda \propto N_s \beta$ without introducing systematic errors.

The QMC part of this chapter makes use of SSE. Also, in the remainder of this chapter, we shall combine all indices $i_1,\ldots,i_M$ into a single multi-index, which for convenience will simply be labeled $i$.

The problem that can arise is that the above-mentioned weights are in general not guaranteed to be non-negative. Systems for which not all weights are non-negative, as said to suffer from the *sign problem* [44]. Note that the sign of the weights is basis dependent, and so systems that suffer from the sign problem in one basis may turn out to actually be sign-free in some other basis. For this reason, a

\(^6\)Determined during the equilibration part of the simulation.
large amount of effort is put into designing methods that circumvent it. However, this is in general not an easy task, as it has been shown that a generic solution of the sign problem is NP-hard [240].

6.4.2 The sign-free Hamiltonian

It is always possible to simulate a model with QMC using the weights of the minus-sign free model obtained by changing the sign of some off-diagonal matrix elements of $H$ in a given basis in to make all off-diagonal elements non-positive (in which case both $U = 1 - \tau H$ and $-H$ become non-negative; to the latter we can add an additive constant to make all diagonal elements non-negative). Let us denote the minus-sign free Hamiltonian\(^7\) obtained this way from $H_{\text{ext}}$ in the dimer basis by $\tilde{H}$. Since this Hamiltonian has no minus sign by construction, it can be studied down to very low temperatures by QMC. The resulting ground state energy of the sign-free model derived from the original Shastry-Sutherland model—i.e. $\tilde{H}$ for $J_2 = 0$—is shown in Fig. 6.4. Quite interestingly, the ground state is still the product of singlets up to an inter-dimer coupling of $J \approx 0.526(1)J_D$, with of course the same energy as the Shastry-Sutherland model ($-3J/4$ per dimer) since the diagonal term is the same. At that coupling constant, a level crossing takes place, signaling a first-order transition to another phase\(^8\).

It is actually simple to see that, at small inter-dimer coupling, the ground state of the minus-sign free Hamiltonian must be the same as that of the Shastry-Sutherland model. Let us take $\{ |S\rangle, |\tilde{S}\rangle, |0\rangle, |+\rangle \}$, where $|S\rangle$ is the singlet state, and the other three are the triplet states, as a local basis for a single dimer. Since $H_{\text{ext}}$ is only a nearest-neighbor Hamiltonian in terms of dimers, it can be written as a sum over all dimers in the lattice

$$H_{\text{ext}} = \sum_{\langle d,d' \rangle} H_{dd'},$$

where $H_{dd'}$ is a $16 \times 16$ matrix that measures the energy of a single dimer bond connecting dimer $d$ and $d'$. The fact that the product of dimers is an eigenstate of $H_{\text{ext}}$, implies that, after choosing a labeling the two-dimer basis such that the first vector corresponds to the product of singlets $|S_d, S_{d'}\rangle$, $H_{dd'}$ takes the form

$$H_{dd'} = \begin{pmatrix} -3J_D/4 & 0 \\ 0 & * \end{pmatrix}$$

\(^7\) More details on the construction of $\tilde{H}$ can be found in Appendix 6.A.2.

\(^8\) Since $\tilde{H}$ is not physical, but only useful to discuss QMC simulations of the Shastry-Sutherland model, we have not tried to understand the precise nature of this other phase. We would only like to point out that the dimer phase extends up to relatively large coupling without any sign of an intermediate phase. Given the very complicated form of the model, it is not clear what the physics will be beyond the dimer phase.
6.4. The minus sign problem

Figure 6.4: Ground state energy of the minus-sign-free model $\tilde{H}$ at $J_2 = 0$ as extracted from QMC simulations with a kink displayed near $J/J_D = 0.526(1)$.

where “*” indicates a $15 \times 15$ matrix, and “0” a row or column of 15 zeros. Since $\tilde{H}$ is obtained from $H_{\text{ext}}$ by changing signs of some of the off-diagonal coefficients, $\tilde{H}_{dd'}$ has exactly the same form as $H_{dd'}$ (except that * has some signs flipped). Consequently, the product of dimers is also an eigenstate of $\tilde{H}$, and its energy is given by $-3J_D/4$. Moreover, the dimer state is clearly the ground state of $\tilde{H}$ with vanishing off-diagonal matrix elements—i.e. at $J = 0$—and it is separated from the first excited state by an energy equal to the intra-dimer coupling $J_D$. Therefore, a simple perturbative argument implies that the dimer state has to remain the ground state as long as the off-diagonal matrix elements are small compared to the intra-dimer coupling $J_D$.

Computing averages for a system with a sign problem using the corresponding sign-free Hamiltonian works as follows. The average of any observable $A$ is given by the ratio of the averages of the observable and of the sign calculated for the minus-sign free model [44,237,240]:

$$
\langle A \rangle = \frac{\sum_i W_i A_i}{\sum_i W_i} = \frac{\sum_i \text{sign}(W_i)|W_i|A_i}{\sum_i \text{sign}(W_i)|W_i|} = \frac{\langle \text{sign } A \rangle}{\langle \text{sign } \rangle} \langle | \rangle
$$

In this expression, $\langle \cdot \rangle$ denotes the average with respect to the minus-sign free Hamiltonian. In general, the average in Eq. (6.3) is useless when the temperature is low as compared to typical couplings because the average sign in the denominator of Eq. (6.3) essentially vanishes, inducing error bars bigger than the signal.
6.4.3 The minus sign in the extended SSL model

The central result of the present chapter, reported in Fig. 6.5, is that, in the dimer basis, the minus sign indeed gets very small when the temperature gets below typical couplings, however, provided the ground state of the minus-sign free model is the product of singlets, it starts increasing again at low temperatures and even reaches the value 1 at zero temperature. This is true up to a ratio of $J/J_D \approx 0.526(1)$ for the Shastry-Sutherland model (see Fig. 6.4). Above that value, the behavior is typical of any model with a minus sign: the average sign gets very small and never increases again [237,240].

![Figure 6.5: Temperature dependence of $\langle \text{sign} \rangle ||$ for the SSL model ($J_2 = 0$) for different values of the intra-dimer interaction.](image)

The fact that the average sign goes rigorously to 1 at zero temperature is a simple consequence of the fact that the Shastry-Sutherland model and its minus-sign free counterpart have the same ground state. Consequently, the average of any quantity has to be equal to the numerator of Eq. (6.3), and the denominator has to be strictly equal to 1. This should be contrasted to the case of the fully-frustrated ladder in which periodic boundary conditions introduce a minus sign [230]: in that case, the average sign increases again at low temperature and goes back to a value close to 1, but not exactly to 1.

The calculation of the average sign can also be performed for the extended model $H_{\text{ext}}$. The value of the average sign at a temperature of $T = 0.1J_D$ is shown in Fig. 6.6. The sign is essentially equal to 1 in a large portion of the dimer phase. The border of the sign-free region is almost vertical at small third-neighbor coupling $J_2$, as a consequence of a phase transition in the (unphysical) minus-sign free model $H$. By contrast, comparing to the phase boundaries in Fig. 6.2...
6.5. QMC results

In the regime $J \lesssim 0.5J_D$, we obtain very accurate results for the magnetic susceptibility $\chi$ (Fig. 6.7) and the specific heat $C$ (Fig. 6.8) on large lattices. Figs. 6.7 and 6.8 show results for $10 \times 10$ dimers, corresponding to a system containing 200 spin-1/2 particles. In this regime, finite-size effects are so small that these results can be considered representative of the thermodynamic limit (see Appendix 6.A.3).

In the limit $J = 0$, we recover decoupled dimers for which the corresponding results are analytically known and shown by the dashed curves [227, 241–243]. Upon increasing $J$, the magnetic susceptibility $\chi$ (Fig. 6.7) shows a flattening of its maximum, accompanied by a down-shift of its low-temperature flank, signaling a decreasing spin gap. The specific heat $C$ exhibits similar features, see...
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Figure 6.7: Temperature dependence of the susceptibility of the SSL model \((J_2 = 0)\) for different values of the intra-dimer interaction and different sizes.

Fig. 6.8, except that for \(J/J_D \to 0.5\), a distinct low-temperature maximum starts to emerge.

Figure 6.8: Temperature dependence of the specific heat of the SSL model \((J_2 = 0)\) for different values of the intra-dimer interaction and different sizes.

Fig. 6.11 in Appendix 6.A.3 provides a closer look at three larger values of \(J/J_D\). Beyond the QMC results, Fig. 6.11 also contains exact diagonalization (ED) results.
6.6 Conclusion

We have shown that, even if quantum Monte Carlo (QMC) simulations suffer from a minus sign, it can be possible to get extremely accurate results for the low-temperature thermodynamics. A sufficient condition for obtaining accurate QMC results in the presence of a sign problem is that the ground states of the physical model in question and the corresponding minus-sign free model with non-positive off-diagonal matrix elements are the same. In particular, we demonstrated that the above condition holds for a large part of the parameter regime of the extended Shastry-Sutherland (SSL) model, which has allowed us to get numerically exact results for the temperature susceptibility and specific heat of the SSL model whenever the ratio of the inter to intra-dimer couplings is at most equal to $J/J_D = 0.526(1)$. A comparison to our iPEPS study of the ground state phase diagram of the extended SSL model confirmed that, as expected, the region for which the sign problem disappears at low temperatures is completely contained within the dimer ground state phase of the extended SSL model. It is of course unfortunate that the ratio of 0.526(1) is smaller than that realized in SrCu$_2$(BO$_3$)$_2$ [197], which is believed to be around 0.63 [194].

Beyond the Shastry-Sutherland model, we believe that this method should apply to any model whose ground state is exactly known, provided that the Hamiltonian can be expressed in a basis that contains this exact ground state as one of its basis vectors.
6. Appendix

6.A.1 Additional iPEPS data

In order to investigate the accuracy of the $D = 10$ plaquette to AFM phase boundary displayed in Fig. 6.2, we have executed variational update simulations up to $D = 10$ close to the phase boundary along the vertical cut given by $J / J_D = 0.7$.

![Figure 6.9: Energy per site of states in the plaquette and AFM phases—in blue and dark red respectively (color online)—as a function of truncation error for $J / J_D = 0.7$ and $J_2 / J = 0.03 - 0.07$. The simulations were obtained by the variational update algorithm.](image-url)

By initializing the variational update simulations in the plaquette and AFM phases respectively, due to hysteresis across a first order transition, we obtain states in
both phases for several values of $J_2/J$ in the vicinity of the transition. The energies per site of the corresponding simulations are displayed in Fig. 6.9 as a function of the truncation error.

We extrapolate truncation error—which signifies how far the state is from convergence in $D$—to zero [132] to obtain the $D \to \infty$ extrapolated energies. The error bars are centered at the value of the fitting function at zero truncation error, and have a width that is half the distance between the lowest obtained ($D = 10$) energy and the energy of the fit at zero truncation error. This measure of the error has the expected behavior that it decreases when the highest $D$ simulation is closer to convergence and the energy as a function of truncation error flattens out.

Focusing on the AFM simulations, we see that the width of the error bar decreases as we move deeper into the AFM phase, reflecting the fact that the AFM simulations converge faster in $D$ when the ground state is actually antiferromagnetically ordered.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6_10}
\caption{Extrapolated energies per site of states in the plaquette and AFM phases—in blue and dark red respectively (color online)—at $J/J_D = 0.7$ as a function of $J_2/J$ for $J_2/J = 0.03 - 0.07$. Shown are the upper and lower bounds of the error bars from Fig. 6.9. “U-bnd” and “L-bnd” signify the points where the energy bands separate.}
\end{figure}

Next, the tops and bottoms of the error bars of the energies per site from Fig. 6.9 are linearly interpolated as a function of $J_2/J$, the result of which can be found in Fig. 6.10. The estimated location of the phase transition at $J_2/J = 0.0534$, marked by ”Est.”, sits at the point where the centers of the energy bands intersect; the vertical lines marked with ”L-bnd.” and ”U-bnd.”, located at $J_2/J = 0.0448$ and $J_2/J = 0.0584$ respectively, mark the points where the energy bands separate and thus provide an error bar for the estimated transition point. The $D = 10$ simple
update transition point at $J/J_D = 0.7$ in Fig. 6.3 is consistent with the variational
update result, as it lies within the $D \to \infty$ extrapolated variational update error bar—displayed in Fig 6.3 by the vertical red line at $J/J_D = 0.7$.

6.A.2 Details on the sign-free Hamiltonian

It is possible to construct a minus-sign free Hamiltonian from the extended SSL
model by changing the sign of all off-diagonal matrix elements in the dimer basis
in such a way that they are all non-positive.

In order to construct this sign-free Hamiltonian, we first introduce the total spin
operator $\vec{T}^d = \vec{S}^d_1 + \vec{S}^d_2$ as well as the spin difference operator $\vec{D}^d = \vec{S}^d_1 - \vec{S}^d_2$
for a given $J_D$-dimer bond $d$ in terms of the two spins $\vec{S}^d_1$ and $\vec{S}^d_2$ that form
this dimer. In defining $\vec{D}^d$, we have to fix a convention regarding the assignment
of the integer labels 1 and 2 to the corresponding spins. Here, we denote the left
(lower) spin on a horizontal (vertical) dimer in the left panel of Fig. 6.1 by $\vec{S}^d_1$.

For a given dimer $d$, we then consider the local singlet and triplet states,
$|S\rangle_d = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle_d - |\downarrow\uparrow\rangle_d)$,
$|0\rangle_d = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle_d + |\downarrow\uparrow\rangle_d)$,
$|+\rangle_d = |\uparrow\uparrow\rangle_d$,
$|-\rangle_d = |\downarrow\downarrow\rangle_d$.

on which the total spin and spin difference operators act as shown in Tab. 6.1,
where $T^\pm_d = T^x_d \pm iT^y_d$ and $D^\pm_d = D^x_d \pm iD^y_d$ have been defined in the usual way.

| $|S\rangle_d$ | $|0\rangle_d$ | $|+\rangle_d$ | $|-\rangle_d$ |
| $T^2_d$ | $T^x_d$ | $T^y_d$ | $T^z_d$ |
| $D^\pm_d$ | $D^\mp_d$ | $D^\pm_d$ |
| $|S\rangle_d$ | 0 | 0 | 0 | 0 | 0 | 0 |
| $|0\rangle_d$ | 2 | 0 | $\sqrt{2} |+\rangle_d$ | $\sqrt{2} |-\rangle_d$ | $|S\rangle_d$ | 0 | 0 |
| $|+\rangle_d$ | 2 | 1 | $\sqrt{2} |0\rangle_d$ | $\sqrt{2} |0\rangle_d$ | 0 | 0 | 0 |
| $|-\rangle_d$ | 2 | -1 | $\sqrt{2} |0\rangle_d$ | 0 | 0 | $\sqrt{2} |S\rangle_d$ | 0 |

Table 6.1: Action of local total-spin and spin-difference operators on the local spin-dimer basis states. Because $T^2_d$ and $T^x_d$ are diagonal in this basis, we give only the eigenvalues for these operators. Note that in this basis, $D^2_d$ is not diagonal.

The Hamiltonian $H_{ext}$ consists of (i) a sum of local terms $H_d$ acting on each
individual dimer $d$ and (ii) the inter-dimer terms with couplings $J$ and $J_2$ that
couple two neighboring dimers $d$ and $d'$. In terms of the total spin operators, the
local contribution is given by

$$H_d = \frac{1}{2} T^2_d - \frac{3}{4}. \quad (6.4)$$

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The inter-dimer Hamiltonian term coupling two neighboring dimers \( d \) and \( d' \) reads

\[
H_{d-d'} = \frac{J + J_2}{2} \mathbf{T}_d \cdot \mathbf{T}_{d'} - \frac{J - J_2}{2} \mathbf{T}_d \cdot \mathbf{D}_{d'}
\]  

(6.5)

when expressed in terms of the total spin and spin difference operators. It follows that for the special case of \( J_2 = J \), the second, TD-coupling terms vanishes, and in this limit of the fully frustrated bilayer model QMC simulations can be performed sign-problem free if formulated in the spin-dimer basis. On the other hand, for \( J_2 \neq J \), and in particular for the original Shastry-Sutherland model \( (J_2 = 0) \), a non-zero TD-term is present in addition to the TT-terms. This leads to the unfortunate reappearance of a minus signs.

Next, we construct a sign-problem free Hamiltonian \( \tilde{H} \) starting from \( H_{\text{ext}} \) by changing the sign of all its off-diagonal matrix elements in the dimer basis in such a way that they are all non-positive. The resulting inter-dimer exchange terms can be expressed more explicitly using transfer operators within the basis of the two-dimer states. For example, the contributions of the TD-terms to the off-diagonal parts of \( \tilde{H} \) are given by

\[
\tilde{H}_{d-d'}^{\text{TD,off}} = -\frac{|J - J_2|}{2} \left[ |+S\rangle \langle +0| + |+0\rangle \langle +S| + 2 |+-\rangle \langle 0S| + 2 |+-\rangle \langle -S| + 2 |+S\rangle \langle 0+| + 2 |+S\rangle \langle -+| + (\leftrightarrow) \right].
\]

Here, \(|S+\rangle = |S\rangle_d \otimes |+\rangle_{d'}\), etc., and the above form is readily obtained with the help of Tab. 6.1. The full minus-sign free Hamiltonian \( \tilde{H} \) is the sum of the diagonal part of the extended Shastry-Sutherland model of Eq.(6.1) in the dimer basis, and the contributions from all such off-diagonal inter-dimer terms.

6.A.3  More QMC results

Fig. 6.11 shows the specific heat and magnetic susceptibilities for different values of \( J/J_D \) and different system sizes. Note that the \( N = 200 \) data has already been shown in Figs. 6.8 and 6.7. From the fact that deviations between \( N = 32 \) and 200 are negligible for \( J/J_D = 0.5 \), we conclude that the latter can indeed be considered representative of the thermodynamic limit. On the other hand, deviations from the exact diagonalization (ED) data for \( N = 20 \) start to be visible in particular around the maximum of the specific heat (see top left panel of 6.11). This indicates that finite-size effects in \( N \leq 20 \) ED results start to be relevant for \( J \geq 0.5 J_D \).
Figure 6.11: Temperature dependence of the specific heat (left column) and magnetic susceptibility (right column) of the SSL model ($J_2 = 0$) for different values of the intra-dimer interaction and different sizes.