Stochastic series expansion algorithm
for the $S = 1/2$ XY model with four-site ring exchange

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We describe a stochastic series expansion (SSE) quantum Monte Carlo method for a two-dimensional $S = 1/2$ XY-model (or, equivalently, hard-core bosons at half-filling) which in addition to the standard pair interaction $J$ includes a four-particle term $K$ that flips spins on a square plaquette. The model has three ordered ground state phases; for $K/J \lesssim 8$ it has long-range $xy$ spin order (superfluid bosons), for $K/J \gtrsim 15$ it has staggered spin order in the $z$ direction (charge-density-wave), and between these phases it is in a state with columnar order in the bond and plaquette energy densities. We discuss an implementation of directed-loop updates for the SSE simulations of this model and also introduce a “multi-branch” cluster update which significantly reduces the autocorrelation times for large $K/J$. In addition to the pure J-K model, which in the $z$ basis has only off-diagonal terms, we also discuss modifications of the algorithm needed when various diagonal interactions are included.

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I. INTRODUCTION

In the ongoing quest to explore possible ground states and quantum phase transitions in quantum condensed matter systems (fermions, bosons, or quantum spins), numerical studies are important for establishing the true nature of the phases and transitions of relevant model Hamiltonians. In particular, recent interest in “exotic” phenomena has focused attention on models with frustrated or competing interactions, in which interplay between adjacent ordered phases often gives rise to interesting effects. For classical models, Monte Carlo simulations in combination with finite-size scaling can be used very successfully in studies of a wide range of systems with and without frustration. However, only a limited class of quantum models are amenable to such studies, as the infamous sign problem prohibits large-scale quantum Monte Carlo (QMC) studies of frustrated antiferromagnetic spin systems and fermions in more than one dimension. It is therefore important to search for non-sign-problematic quantum models, possibly with competing interactions, that display complex ground state phase diagrams and can be efficiently studied using Monte Carlo simulations. Although not all possible types of ground states and quantum phase transitions may be realizable within this class of Hamiltonians, it is likely that many insights into the low-temperature physics of quantum matter can still be gained in this way. Constructing optimized and efficient quantum Monte Carlo algorithms for such candidate Hamiltonians is hence an important task.

In this paper, we present the details of a stochastic series expansion (SSE) algorithm that we have developed for large-scale QMC studies of a two-dimensional (2D) $S = 1/2$ XY model with an added four-site ring-exchange term (the method can be easily generalized for three-dimensional systems). Defining the following bond and plaquette operators;

$$B_{ij} = S_i^+ S_j^- + S_i^- S_j^+ = 2(S_i^+ S_j^+ + S_i^- S_j^-),$$

$$P_{ijkl} = S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+,$$

the J-K Hamiltonian is given by

$$H = -J \sum_{\langle ij \rangle} B_{ij} - K \sum_{\langle ijkl \rangle} P_{ijkl},$$

where $\langle ij \rangle$ denotes a pair of nearest-neighbor sites on a 2D square lattice and $\langle ijkl \rangle$ are sites on the corners of a plaquette, as illustrated in Fig. 1(a). The plaquette-flip $P_{ijkl}$ is only a subset of all the possible cyclic exchanges among four spins and corresponds to retaining only the purely $x$- and $y$-terms; it has a non-vanishing matrix element only between the two spin states with alternating (staggered) spins on the corners of the plaquette, as illustrated in Fig. 1(b). In the standard way, the J-K Hamiltonian can also be considered as a half-filled hard-core boson model, where up and down spins correspond to filled and empty sites and $J$ is the nearest-neighbor hopping. We will frequently use terminology referring to this boson representation. With the negative sign in front of the plaquette-term ($K > 0$), the J-K model can be studied using QMC methods without a sign problem (the sign of the $J$-term is actually irrelevant in this regard). In this model, there is no frustration in the conventional sense, i.e., antiferromagnetic interactions on lattice loops with an odd number of links (which leads to sign problems). However, the $J$- and $K$-terms individually favor different types of ground states, which leads to interesting competition effects at intermediate $K/J$.

The J-K model was recently found to exhibit three different ordered ground states as a function of the ratio $K/J$ of the four-site ($K$) and two-site ($J$) terms. It was argued that the transition between the magnetically
ordered state for $K/J \lesssim 8$ and a striped (or valence-bond-solid, VBS) phase at higher $K/J$ is a continuous quantum phase transition, contrary to general expectations for an order-order transition. Subsequently, this transition was proposed to possibly be a realization of a “deconfined” quantum-critical point. We have used the SSE algorithms to further study the quantum-critical scaling and finite-$T$ transitions in this model. However, in this paper we only briefly summarize the results and focus on the algorithmic issues. A full account of the results will be presented elsewhere.

For $K = 0$, the J-K model reduces to the standard XY-model, which undergoes a Kosterlitz-Thouless transition at $T_{KT}/J \approx 0.69$. In the boson language, the system is a superfluid below $T_{KT}$. The main features of the $T = 0$ phase diagram for $K/J > 0$ were presented in Ref. [6]. Our most recent simulations show that the superfluid density vanishes at $K/J \approx 7.91$. At the same point, within the accuracy of our calculations, the ground state develops a stripe order, where the bond and plaquette strengths $\langle B_{ij} \rangle$ and $\langle P_{ijkl} \rangle$ are modulated at wavevector $\mathbf{q} = (\pi, 0)$ or $(0, \pi)$. This state can also be considered a columnar VBS, since not all the bonds within the “ladders” of strong bonds are equal—the strongest ones are those on the rungs of the ladders. The VBS order vanishes at $K/J \approx 14.5$, in a first-order transition to an Ising-type antiferromagnetic state (a charge-density-wave, CDW, at $\mathbf{q} = (\pi, \pi)$ in the boson picture). We have not observed any signs of first-order behavior at the superfluid-VBS transition, nor any region of coexistence of the two phases. Numerically we can of course never exclude an extremely weakly first-order transition or a very narrow coexistence region. At the transition, we do observe power-law scaling with nontrivial exponents for the superfluid density as well as for the order parameter corresponding to the VBS phase. We have also recently studied the evolution of the VBS phase boundaries when the system is coupled to an external magnetic field.

The outline of the rest of this paper is the following: In Sec. II we describe the SSE algorithm for the J-K Hamiltonian. Implementations of the SSE scheme for various spin and 1D fermion models have been discussed at length in several recent papers, but since the four-particle term necessitates a more complex sampling scheme, with some important new features, we describe our algorithm in detail here. We have constructed two types of cluster updates for sampling the SSE configurations; a directed-loop update as well as a “multi-branch” cluster update. The latter significantly reduces the autocorrelation times for large $K/J$. In Sec. II we also discuss estimators for several important physical quantities. We discuss autocorrelation functions in the different ordered phases in Sec. III. In Sec. IV we discuss modifications of the algorithm when different types of potential-energy terms are included in addition to the $J$ and $K$ terms. We conclude with a brief discussion in Sec. V.

II. STOCHASTIC SERIES EXPANSION

The SSE method is an efficient and widely applicable generalization of Handscomb’s power-series method for the $S = 1/2$ Heisenberg model. It has previously been used for several models with two-body interactions, including the pure XY-model $[K = 0$ in Eq. (3)] and in world-line Monte Carlo loop-cluster algorithms. Recently, a framework was devised for constructing and optimizing loop-type algorithms under very general conditions. Here we will apply this directed loop scheme to SSE simulations including the four-spin term. A loop-type algorithm cannot be constructed for the pure K-model $[J = 0$ in Eq. (3)], however, and the loops are also inefficient when $J/K \ll 1$. We therefore also develop a new type of multi-branch cluster update, that can be used in combination with the directed loops, and enables efficient simulations for any $J/K$. The multi-branch update bears some resemblance to, but is more complex than, a “quantum-cluster” update recently developed for the transverse Ising model.

Below, we give a brief general summary of the SSE method. We then develop the directed loop and multi-branch cluster updates for the J-K Hamiltonian and discuss the SSE estimators of several important physical quantities. We present some illustrative results for autocorrelation functions obtained with and without the multi-branch cluster update before concluding with a discussion of the directed-loop equations for the Hamiltonian with various diagonal interaction included.

A. General SSE formalism

To construct the SSE representation of a quantum mechanical expectation value at temperature $T = 1/\beta$:

$$\langle A \rangle = \frac{1}{Z} \text{Tr} \{ A e^{-\beta H} \}, \quad Z = \text{Tr} \{ e^{-\beta H} \},$$

the Hamiltonian is first written as a sum of elementary interactions

$$H = - \sum_t \sum_a H_{t,a},$$
where in a chosen basis \( \{|\alpha\rangle\} \) the operators satisfy
\[
H_{t,a} |\alpha\rangle \sim |\alpha'\rangle,
\]
where \( |\alpha\rangle \) and \( |\alpha'\rangle \) are both basis states. The indices \( t \) and \( a \) refer to the operator types (various kinetic and potential terms) and the lattice units over which the interactions are summed (bonds, plaquettes, etc.). A unit operator \( H_{0,0} \equiv 1 \) is also defined. Using the Taylor expansion of \( e^{-\beta H} \) truncated at order \( M \), the partition function can then be written as
\[
Z = \sum_{\alpha} \sum_{S_M} \frac{\beta^n (M - n)!}{M^n} \left\langle \alpha | \prod_{i=1}^{M} H_{t_i,a_i} |\alpha\rangle \right\rangle,
\]
where \( S_M \) denotes a sequence of operator-indices,
\[
S_M = [t_1, a_1], [t_2, a_2], \ldots, [t_M, a_M],
\]
and \( n \) denotes the number of non-\([0,0]\) elements in \( S_M \) (i.e., the actual expansion-order of the terms). The finite truncation \( M \) and the use of a fill-in operator \( H_{0,0} \) are not strictly necessary but simplify some aspects of the algorithm. \( M \) can be adjusted during the equilibration of the simulation, so that it always exceeds the highest power \( n \) reached; \( M = AR_{\max} \), where a suitable value for the factor is \( A \approx 1.25 \). This leads to \( M \sim \beta N \), where \( N \) is the system volume, and the remaining truncation error is completely negligible. The adjustment of \( M \) has been discussed in more detail in Ref. [13].

Defining a normalized state \( |\alpha(p)\rangle \) obtained by acting on \( |\alpha\rangle = |\alpha(0)\rangle \) with the first \( p \) operators in the product in Eq. (7),
\[
|\alpha(p)\rangle \sim \prod_{i=1}^{p} H_{t_i,a_i} |\alpha\rangle,
\]
the requirement for a non-zero contribution to \( Z \) is the propagation periodicity \( |\alpha(M)\rangle = |\alpha(0)\rangle \). This implies considerable constraints on the off-diagonal operators in the product, and clearly the vast majority of the terms are zero. In an efficient SSE method, transitions \((\alpha, S_M) \rightarrow (\alpha', S'_M)\) satisfying detailed balance should be attempted only within the subset of contributing configurations. Although the details of such sampling procedures to some extent depend on the model under study, three different classes of updates are typically used. We here summarize these in general terms, before turning to the implementation for the J-K model:

(i) The expansion order \( n \) is changed in diagonal updates, where a fill-in unit operator is replaced by a diagonal operator from the sum [6], and vice versa, i.e., \( H_{0,0} \leftrightarrow H_{d,a} \), where the type-index \( d \) corresponds to a diagonal operator in the basis used.

(ii) Off-diagonal operators cannot be added and removed one-by-one with the periodicity constraint \( |\alpha(M)\rangle = |\alpha(0)\rangle \) maintained. Local updates involving two simultaneously replaced operators can be used for this purpose [15]. However, much more efficient cluster-type updates, which may involve a large number of operators, can also be constructed [15,15]. Here the general strategy is to find a set of operators \( \{t_i,a_i\}_i \), such that a new valid configuration can be obtained by changing only the type-indices \( t_i \). For the J-K Hamiltonian, we will discuss two such updates: directed loops and multi-branch clusters.

(iii) A third type of update is one that affects only the state \( |\alpha\rangle \). This state, which is just one out of the whole cycle of propagated states \( |\alpha(p)\rangle \), can change also in the updates (ii) involving off-diagonal operators. However, at high temperatures many sites will frequently have no operators acting on them. The local states at these sites will then not be affected by the off-diagonal updates. They can instead be randomly modified as they do not affect the weight. Such state updates can improve the statistics at high temperatures but are often not required for the sampling to be ergodic.

B. Plaquette operators

Turning now to the J-K model, we use the standard \( z \)-component basis
\[
|\alpha\rangle = |\sigma_i^z, \ldots, \sigma_N^z\rangle, \quad \sigma_i^z = \pm 1
\]
where \( S_i^z = 1/2\sigma_i^z \), on lattices with \( N = L_x \times L_y \) sites (or \( N \) plaquettes). Typically we consider square lattices, \( L_x = L_y \), but some results for rectangular, \( L_x \neq L_y \), systems have also been discussed [15]. It is convenient to express all interactions in the Hamiltonian [4] in terms of plaquette operators,
\[
H_{1,a} = CI_{ijkl}, \quad H_{2,a} = (J/2)B_{ij}I_{kl}, \quad H_{3,a} = (J/2)B_{jk}I_{il},
\]
\[
H_{4,a} = (J/2)B_{kl}I_{ij}, \quad H_{5,a} = (J/2)B_{il}I_{jk}, \quad H_{6,a} = K P_{ijk},
\]
where \( I_{ij} \) and \( I_{ijkl} \) are unit operators associated with bonds and plaquettes, respectively, and the indexing is defined in Fig. [11]. Up to a constant \( NC \), the Hamiltonian is then given by a sum [4], where the type index \( t = 1, \ldots, 6 \), and \( a \) is the plaquette index; \( a = 1, \ldots, N \). As explained above, there is also a unit operator \( H_{0,0} \equiv 1 \), which is not part of the Hamiltonian but has been introduced only as a fill-in element for augmenting the operator-index sequences of length \( n < M \) in the truncated partition function (Eq. (7)) to \( M \).

C. Diagonal update

Because there are no diagonal operators in the original Hamiltonian [4], the constant operators \( H_{1,a} \) have been added in order to enable diagonal updates of the form \([0,0] \leftrightarrow [1,a]\) in \( S_M \). For all elements \([a_p,t_p]\) with \( t_p =
0, 1, such substitutions can be carried out sequentially for $p = 1, \ldots, M$. In the $\rightarrow$ direction, the plaquette index $a$ is chosen randomly among 1, \ldots, $N$. The Metropolis acceptance probabilities are then

$$P([0,0] \rightarrow [1,a]) = \frac{NC\beta}{M-n},$$

(12)

$$P([1,a] \rightarrow [0,0]) = \frac{M-n+1}{NC\beta},$$

(13)

where $P > 1$ should be interpreted as probability one. If an attempt to remove a plaquette operator, i.e., $[1,a] \rightarrow [0,0]$, is not accepted, a new plaquette index $a$ can be generated at random. Note that for this model, where the only diagonal operators are the added constants $H_{1,a}$, it is not necessary to keep track of the propagated states during the diagonal update. In general, e.g., if a diagonal interaction is added to the Hamiltonian (3), the constant $C$ in Eqs. (12) and (13) should be replaced by the matrix element $\langle \alpha(p)|H_{1,a}|\alpha(p-1)\rangle = \langle \alpha(p)|H_{1,a}|\alpha(p)\rangle$ of the diagonal operator in the propagated state at which the replacement is done.

D. Linked vertices

In the directed loop and multi-branch cluster updates, which we will discuss below, it is useful to represent the matrix elements in Eq. (7) as a linked lists of “vertices” \[P\] The weight of a configuration $(\alpha, S_M)$ can be written as

$$W(\alpha, S_M) = \frac{\beta^n(M-n)!}{M!} \prod_{p=1}^{M} W(p),$$

(14)

where $W(p)$ is a vertex weight, which is simply the matrix element of the corresponding plaquette operator at position $p$ in $S_M$:

$$W(p) = \langle \alpha(p)|H_{p,a_p}|\alpha(p-1)\rangle,$$

(15)

which with the operators \[P\] can take the values C, J/2, or K. Since the loop and cluster updates are carried out within sectors of fixed $n$ (only the diagonal update changes $n$), the fill-in operators $H_{0,0}$ are not needed in the linked-vertex representation. A vertex represents the local four-spin states on plaquette $a_p$ in the matrix element (15) before and after the plaquette operator has acted. These eight spin states constitute the legs of the vertex. For the J-K model, there are three classes of vertices, as illustrated in Fig. 2. The constant operators $H_{1,a}$ correspond to C-vertices (with weight C), the bond-flip operators $H_{2,a}$ to J-vertices (with weight J/2) and the plaquette-flip operators $H_{6,a}$ to K-vertices (with weight K). An example of a linked-vertex representation of a term with three plaquette operators is shown in Fig. 2. The links connect vertex-legs on the same site, so that from each leg of each vertex, one can reach the next or previous vertex-leg on the same site (i.e., the links are bidirectional). In cases where there is only one operator acting on a given site, the corresponding “before” and “after” legs of the same vertex are linked to each other (as is the case with the legs on sites 1 and 2 in Fig. 3).

During the simulation, the spin state $|\alpha\rangle$ and the operator list $S_M$ are stored at all times. The linked-vertex representation is created after each full sweep of diagonal updates. After the directed loop and multi-branch cluster updates have been carried out, the changes are mapped back into a new $|\alpha\rangle$ and $S_M$. We will not discuss here how these data structures are implemented and used in practice in a computer program. The procedures are completely analogous to simulations with two-body interactions, for which an implementation was described in detail in Ref. 12.

E. Directed loops

In the original QMC loop algorithm, spins are flipped along a one-dimensional closed path (the loop) on the space-time lattice of the discretized

\[P\]
(Trotter-decomposed) or continuous\(^{23}\) path-integral representation. The path is self-avoiding, and a configuration can be subdivided into loops that may be flipped independently of each other. Allowing the path to self-intersect and backtrack, one can construct valid algorithms for a much larger class of models. Such general loop-type algorithms have been constructed both for continuous-time world-lines (the worm algorithm\(^{24}\)) and for SSE (the operator-loop algorithm\(^{18}\)) \footnote{In an SSE operator-loop algorithm, where the loops constitute connected strings of operators (or vertices in the linked-vertex representation)\(^{18}\) the building of a loop consists of a series of steps, in each of which a vertex is entered at one leg (the entrance leg) and an exit leg is chosen according to probabilities that depend on the entrance leg and the spin states at all the legs. The entrance to the following vertex is given by the link from the chosen exit leg. The spins at all vertex-legs visited are flipped during the loop building.}

The detailed balance equations—the directed loop equations—that must be satisfied when constructing general self-intersecting and back-tracking loops were recently derived within the SSE framework, and a generalization to the path integral representation was also shown\(^{18}\). Here we will implement the directed-loop scheme for SSE sampling of the \(J\) and \(K\) terms.

In an SSE operator-loop algorithm, where the loops constitute connected strings of operators (or vertices in the linked-vertex representation)\(^{18}\) the building of a loop consists of a series of steps, in each of which a vertex is entered at one leg (the entrance leg) and an exit leg is chosen according to probabilities that depend on the entrance leg and the spin states at all the legs. The entrance to the following vertex is given by the link from the chosen exit leg. The spins at all vertex-legs visited are flipped during the loop building.

The original starting point of the loop is chosen at random. Two link-discontinuities are created when the first pair of entrance and exit spins is flipped, i.e., the legs to which these are linked will be in different spin states (this is analogous to introducing the two sources in the worm algorithm\(^{24}\)). Configurations contributing to \(Z\) only contain links between legs in the same spin states. One of the discontinuities will be propagated during the loop-building, whereas the other one will remain at the original starting point. The loop closes when the propagating discontinuity reaches the stationary one, so that they annihilate each other. A new contributing configuration has then been generated. If the path is self-intersecting (which is not always the case\(^{18}\)), the changes in the configuration may in effect correspond to several disconnected loops.

When a vertex has been entered at a given leg, the probabilities for choosing one out of the possible exit legs have to be chosen so that detailed balance is satisfied. In general, these probabilities are not unique, and in most cases the most evident ones involve high probabilities for bounces, where the exit and entrance legs are the same and the loop building hence backtracks one step\(^{23}\). It is normally desirable to minimize the probability of bounces. The directed loop scheme\(^{18}\) systematizes the search for valid sets of exit probabilities and enables a minimization of the bounce probability. To construct the directed loop equations for the exit probabilities, weights are first assigned to all possible paths through a vertex from a given entrance leg. The sum of all these path weights must equal the bare vertex weight\(^{15}\), i.e., the matrix element before the entrance and exits spins have been flipped. The actual normalized exit probability is the path weight divided by the bare vertex weight. The key element of the scheme is that weights for vertex-paths that constitute each other’s reverses have to be equal in order for detailed balance to be fulfilled (a generalized scheme where this is not necessarily the case has also been discussed recently\(^{18}\)). Examples of such related vertex-paths in the J-K model are shown in Fig.\(^4\). The directed loop equations written down on the basis of these simple rules often form several different closed sets that can be solved for the path weights independently of each other. Because of symmetries, many of the equation sets can also be also identical. In general, the directed loop equations have an infinite number of solutions, which can be significantly restricted by minimizing the bounce probabilities. In some cases there is a unique minimum-bounce solution (sometimes with zero bounce probability), but often there is still a high degree of freedom left\(^{12,26,27}\).

For the J-K model, a one dimensional path segment can in one step transform a C-vertex into a J-vertex, and vice versa, an example of which is shown in Fig.\(^4\)(a). A J-vertex can be transformed into a K-vertex, and vice versa, as shown in Fig.\(^4\)(b). C- and K-vertices cannot be directly transformed into each other, however. As a consequence, the closed sets of vertex-paths that contain C→J transformations are independent from those containing J→K transformations.

The closed sets containing C→J transformations are similar to those for the XY-model\(^{12}\), although the sets

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig4.png}
\caption{(a) A process, and its reverse, where a C-vertex is transformed into a J-vertex. (b) Two related J↔K transformations. In the loop construction the spin states at the entrance and exit legs are flipped. The spin states shown in the vertices here are those before the flips have been carried out.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5.png}
\caption{A closed set of C and J vertex-paths, with their corresponding weights \(a_{ij}\) that have to satisfy the directed loop equations.}
\end{figure}
are larger because a C-vertex can be transformed into two different J-vertices. As in the XY-model, no bounces
are required for detailed balance in this case, until we
discuss the inclusion of additional diagonal interactions
in Sec. IV. One closed set with C→J transformations is
shown in Fig. 5. To construct such a set, one first selects a
“reference” vertex (any vertex) and an entrance leg, and
then finds all paths that lead to new valid vertices, sampling all allowed exit legs. This corresponds to the
first row of Fig. 5 where the bounce process has not been
included since, as will be shown below, its weight can be
set to zero in this case. Each of the resulting vertices (i.e.,
when the entrance and exit spins have been flipped) are
then considered in turn, using as the entrance legs the
exit legs from the previous step. This leads to rows two
to four in Fig. 5. The procedure is repeated for each
new combination of vertex and exit leg that is created.
This systematically generates all pairs of vertex-paths
that constitute each other’s reverses, i.e., those that must
have equal weights for detailed balance to be satisfied. In
the case considered here, no new vertex-paths are created
after row four, as the reverse of each path has then already
been generated. The set is hence closed. Other
closed sets are constructed by picking a starting vertex and entrance leg combination that has not yet appeared
within the sets already completed. This is repeated until
all vertices and entrance legs combinations have been
exhausted.

The directed loop equations corresponding to the
closed set shown in Fig. 5 are

\[
\begin{align*}
a_{11} + a_{12} + a_{13} &= W_1 = C, \\
a_{21} + a_{22} + a_{23} &= W_2 = C, \\
a_{31} + a_{32} + a_{33} &= W_3 = J/2, \\
a_{41} + a_{42} + a_{43} &= W_4 = J/2,
\end{align*}
\]

where the weights \(a_{ij}\) are identified with the paths in
the figure and \(W_i\) are the bare vertex weights before the
entrance and exit spins have been flipped. Detailed balance
requires that the weights corresponding to opposite
vertex-paths are equal, i.e.,

\[
\begin{align*}
a_{21} &= a_{11}, \\
a_{31} &= a_{12}, \\
a_{32} &= a_{22}, \\
a_{41} &= a_{13}, \\
a_{42} &= a_{23}, \\
a_{43} &= a_{33}.
\end{align*}
\]

The weights also have to be positive definite, since they
are related to probabilities by dividing with the positive
matrix elements \(W_i\). Even with these constraints, the
solution is not unique. One can reasonably assume that
the most efficient solution also has equal weights for paths
that are related by symmetries, e.g., \(a_{12} = a_{13}\). Using all
such symmetries, the solution is still not unique, however.

It can be expected that it is efficient to maximize the
weights of the paths that transform a C-vertex into a
J-vertex, which is equivalent to minimizing the weights of
the continue-straight paths that transform a C-vertex
into another C-vertex. We have no proof of our assertion
that this is a good strategy, but as it is a quite challenging
task to investigate all possible valid solutions, we will
use it and leave other possibilities for future studies (this
issue has in fact recently been addressed in the context
of other models\(^{28}\)). In Fig. 6 there are only two C→C
paths; the pair with weights \(a_{11}, a_{21}\). The minimum
value of these is \(a_{11} = a_{21} = C - J/2\), which also implies
\(C \geq J/2\). There are now enough conditions to render a
unique solution to this set of directed loop equations;

\[
\begin{align*}
a_{11} &= C - J/2, \\
a_{21} &= C - J/2, \\
a_{31} &= J/4, \\
a_{32} &= J/4, \\
a_{33} &= 0, \\
a_{41} &= J/4, \\
a_{42} &= J/4, \\
a_{43} &= 0.
\end{align*}
\]

The actual exit probabilities \(P_{ij}^a = a_{ij}/W_i\) are

\[
\begin{align*}
P_{11} &= 1 - J/2C, \\
P_{12} &= J/4C, \\
P_{13} &= J/4C, \\
P_{21} &= 1 - J/2C, \\
P_{22} &= J/4C, \\
P_{23} &= J/4C, \\
P_{31} &= 1/2, \\
P_{32} &= 1/2, \\
P_{33} &= 0, \\
P_{41} &= 1/2, \\
P_{42} &= 1/2, \\
P_{43} &= 0,
\end{align*}
\]

where the superscript \(a\) is used as a reminder that these
probabilities correspond to the paths shown in Fig. 5. Note
that the probabilities here depend only on the type of
vertex transformation, C→C \((P = 1 - J/2C)\), C→J
\((P = J/2C)\), J→J \((P = 0)\), or J→C \((P = 1/2)\), which
can aid the implementation of the probability tables in
the code. All other sets with C→J transformations are ei-
ther related by trivial symmetries to that shown in Fig. 5
or are very similar to it. The exit probabilities are given
simply by the type of the corresponding vertex transfor-
mation exactly as above.

The directed loop equations for the closed sets of
paths that involve J+K transformations sometimes re-
quire non-zero bounce probabilities. A closed set of paths
is shown in Fig. 6. The corresponding equations for the
path weights \(b_{ij}\) are

\[
\begin{align*}
b_{11} + b_{12} + b_{13} + b_{14} + b_{15} &= J/2, \\
b_{21} + b_{22} + b_{23} + b_{24} + b_{25} &= J/2, \\
b_{31} + b_{32} + b_{33} + b_{34} + b_{35} &= K, \\
b_{41} + b_{42} + b_{43} + b_{44} + b_{45} &= J/2, \\
b_{51} + b_{52} + b_{53} + b_{54} + b_{55} &= J/2.
\end{align*}
\]

Again, it is in general advantageous to minimize the
bounce probabilities, i.e., the bounce weights \(b_{ij}\) above.
For \(K \leq 2J\) all the bounce weights can in fact be zero.
The weight of the continue-straight paths (e.g., \(b_{11}\)),
which here transform a J-vertex into a J-vertex with the
same spin flips (i.e., the same plaquette operator), can
be set to zero. A symmetric \(K \leq 2J\) solution is then:
For $K > 2J$, the bounce weight $b_{35}$ has to be non-zero for a positive-definite solution. Minimizing this weight one obtains the following solution:

\begin{align}
  b_{11} &= 0, & b_{12} &= J/2, & b_{13} &= 0, & b_{14} &= 0, & b_{15} &= 0, \\
  b_{21} &= 0, & b_{22} &= J/2, & b_{23} &= 0, & b_{24} &= 0, & b_{25} &= 0, \\
  b_{31} &= J/2, & b_{32} &= J/2, & b_{33} &= J/2, & b_{34} &= J/2, & b_{35} &= K - 2J, \\
  b_{41} &= 0, & b_{42} &= 0, & b_{43} &= 0, & b_{44} &= J/2, & b_{45} &= 0, \\
  b_{51} &= 0, & b_{52} &= 0, & b_{53} &= J/2, & b_{54} &= 0, & b_{55} &= 0.
\end{align}

The exit probabilities are hence, for $K \leq 2J$:

\begin{align}
  P_{11}^b &= 0, & P_{12}^b &= K/2J, & P_{13}^b &= 1/2 - K/4J, & P_{14}^b &= 1/2 - K/4J, & P_{15}^b &= 0, \\
  P_{21}^b &= 0, & P_{22}^b &= K/2J, & P_{23}^b &= 1/2 - K/4J, & P_{24}^b &= 1/2 - K/4J, & P_{25}^b &= 0, \\
  P_{31}^b &= 1/4, & P_{32}^b &= 1/4, & P_{33}^b &= 1/4, & P_{34}^b &= 1/4, & P_{35}^b &= 0, \\
  P_{41}^b &= 1/2 - K/4J, & P_{42}^b &= 0, & P_{43}^b &= 1/2 - K/4J, & P_{44}^b &= K/2J, & P_{45}^b &= 0, \\
  P_{51}^b &= 1/2 - K/4J, & P_{52}^b &= 0, & P_{53}^b &= K/2J, & P_{54}^b &= 1/2 - K/4J, & P_{55}^b &= 0,
\end{align}

and for $K > 2J$:

\begin{align}
  P_{11}^b &= 0, & P_{12}^b &= 1, & P_{13}^b &= 0, & P_{14}^b &= 0, & P_{15}^b &= 0, \\
  P_{21}^b &= 0, & P_{22}^b &= 1, & P_{23}^b &= 0, & P_{24}^b &= 0, & P_{25}^b &= 0, \\
  P_{31}^b &= J/2K, & P_{32}^b &= J/2K, & P_{33}^b &= J/2K, & P_{34}^b &= J/2K, & P_{35}^b &= 1 - 2J/K, \\
  P_{41}^b &= 0, & P_{42}^b &= 0, & P_{43}^b &= 0, & P_{44}^b &= 1, & P_{45}^b &= 0, \\
  P_{51}^b &= 0, & P_{52}^b &= 0, & P_{53}^b &= 1, & P_{54}^b &= 0, & P_{55}^b &= 0.
\end{align}

Note that the solution is continuous across $K = 2J$.

Also in this case the probabilities are seen to depend only on the type of vertex class transformation, $J \rightarrow J'$, $J \rightarrow K$, $K \rightarrow J$, or $K \rightarrow K$ (bounce). Here one has to distinguish between a continue-straight $J \rightarrow J$ transformation where the spin-flip remains on the same bond (e.g., $b_{11}$), and a $J \rightarrow J'$ transformations where the spin-flip moves to a neighboring bond on the plaquette (e.g., $b_{13}$).

There is one more type of closed set of vertex-paths, an example of which is shown in Fig. 6. In this case, neither a valid $K$-vertex nor a $J$-vertex with the flip moved to a different nearest-neighbor pair can be reached from the
generating the exit leg. These probabilities can be stored the exit probabilities in Table I should be applied when all the spin states on the vertex determine which one of first chosen at random. This entrance leg together with summarized in Table I.

Eq. (3), the exit probabilities for the J-K model are sum-
tions become more complicated, however the directed-
the Hamiltonian. In that case the solutions to the equa-
consider inclusions of additional diagonal interactions in
properties will be discussed further in Sec. IV, where we shown in Figs. 5, 6, and 7, and in all cases the proba-
J-vertex and the chosen entrance leg. As the two vertices
have the same bare energies, no bounce processes have to be included and the exit is unique:

\[
P_1^c = 1, \quad P_2^c = 1. \quad (25)
\]

All closed sets of vertex-paths can be related to those shown in Figs. 5, 6, and 7 and in all cases the probabil-
dependencies depend only on how the paths transform the vertices between the classes C, J, and K. This simplifying property will be discussed further in Sec. IV, where we consider inclusions of additional diagonal interactions in the Hamiltonian. In that case the solutions to the equations become more complicated, however the directed-loop framework is still required in order to develop effi-
codes. For the case of zero diagonal interactions, Eq. (3), the exit probabilities for the J-K model are summarized in Table I.

To carry out a directed loop update, a vertex-leg is first chosen at random. This entrance leg together with all the spin states on the vertex determine which one of the exit probabilities in Table I should be applied when generating the exit leg. These probabilities can be stored in a pre-generated table. When the exit has been selected, the link from it is used to enter another vertex, from which an exit is again chosen, etc., until the loop closes. The number of loops to be generated during each Monte Carlo step is adjusted such that the total number of vertices visited is, on average, of the same order as (e.g., equal to or twice) the number of vertex-legs \(8n\), e.g., \(4(n)\) or \(4M\).

In some cases, a loop can become very long before it closes. In order to avoid problems with loops that do not close within a reasonable time, one can impose a maximum loop length. If this limit is exceeded, the loop building is terminated and the changes in the vertices are disregarded. This does not introduce any bias in quantities measured in the \((\alpha, S_M)\) representation. In practice, the termination can easily be accomplished by simply exiting the loop-update routine without mapping the linked-vertex representation back into a state \(|\alpha\rangle\) and an operator list \(S_M\); in order to discard only the loop currently under construction, its history would have to be stored. Hence, not only the terminated loop itself is discarded, but also all other loops constructed since the previous diagonal update. This is not a problem as long termination does not occur frequently. We typically set the maximum loop length to \(\approx 100/n\), and the fraction of terminated loops is then very small.

**F. Multi-branch clusters**

Since a K-vertex cannot be generated directly out of a C-vertex, but requires the presence of J-vertices, the directed loop update cannot be used when \(J = 0\). As will be demonstrated in Sec. III it is also inefficient for large \(K/J\). This can be understood from Table I where the bounce probability off a K-vertex is seen to approach 1 as \(K \to \infty\). In principle the directed-loop update, in combination with the diagonal update, is ergodic for any finite \(K/J\), but for \(K/J \gtrsim 12\) it becomes difficult to obtain good results this way. In order to improve the performance for large \(K/J\), a type of multi-branch cluster update is developed here. It is similar to a quantum-cluster update recently developed for the transverse Ising model where it can be considered a direct generalization of the classical Swendsen-Wang algorithm. The multi-branch cluster update for the J-K model is more complex, due to the larger number of different interaction vertices and the multitude of possible transformations among them.

In order to transform a C-vertex directly into a K-vertex, spins at four legs have to be flipped. If this is done, spins also have to be flipped at all the legs to which these four legs are linked. This will in turn force additional spin flips in the vertices to which they are linked, etc. Clearly, such a process can branch out very quickly to a large number of vertices. Even if a scheme can be found where detailed balance is maintained, there is in general nothing that guarantees that the process ever ter-
FIG. 8: Vertex transformations in the multi-branch cluster update. The entrance leg is denoted by an arrow pointing into the vertices on the left. In the updated vertices to the right, the spins at the outgoing arrows have been flipped. The branching for all entrance legs and vertices not shown here are obtained by applying trivial symmetries to one of the cases shown in (a)-(i).

FIG. 9: Multi-branch cluster update in which two C-vertices are transformed into two K-vertices. The initial entrance leg is at the inward pointing arrow in the linked-vertex representation to the left. The resulting vertices with their arrows indicating legs visited are shown to the right.

To start a cluster, a vertex-leg which does not belong to a cluster already constructed is first chosen at random, and the branching is assigned according to the rules defined in Fig. 8. Flags are set on all the exit legs, to indicate that they have been visited (corresponding to the outgoing arrows Fig. 8). Note that the entrance also becomes an exit leg with an outgoing arrow. If the cluster is to be flipped (which it should with probability 1/2), the spins at all the exit legs are flipped. All exit legs are put on a stack. They are subsequently picked one-by-one from the stack, and the legs to which they are linked are used as entrance legs to other vertices if they have not yet been visited, i.e., these legs are flipped and put on the stack only if they have not been visited before. In the graphical representation, a cluster-branch ends when an arrow is encountered. The whole cluster is completed when all arrows point to other arrows; the stack with unprocessed entrance legs is then empty. A completed cluster with only two vertices is illustrated in Fig. 9.

Although the autocorrelation measurements discussed in Sec. III provide a quantification of the “effectiveness” of the multi-branch cluster updates, we pause here to simply illustrate the cluster characteristics as implemented.
any case the multi-branch update does significantly im-

prove our J-K model. A histogram of cluster sizes gener-

ated at large $K/J$ is shown in Fig. 10. Clearly, the vast

majority of clusters built in this case are small eight-

leg clusters (an example of which is illustrated in Fig. 9),

while data in the lower figure was re-binned to 100 legs per

vertex legs). Data in the upper figure is for the smaller bins,

with significant occupation in the smaller bins up to clus-

ters of size 128. A second peak occurs in the histogram

with an MCS defined as a sweep of diagonal updates, fol-

lowed by construction of the linked vertex list, in which

a fixed number of loop updates are carried out. In the

same linked list, all multi-branch clusters are constructed

and flipped with probability 1/2. After this, the updated

vertex list is mapped back into a new state $|\alpha\rangle$ and an

operator list $S_M$. This is the representation used for the

measurements. The fill-in elements $H_{0,0}$ in $S_M$ are re-

levant at this stage, and we therefore now consider the

reduced list $S_n$ without these operators. There are hence

$n + 1$ propagated states $|\alpha(p)\rangle = |\sigma_1^z(p), \ldots, \sigma_5^z(p)\rangle$, which are obtained one-by-one when operating with the

first $p$ operators, $p = 0, \ldots, n$, on the initially stored state

$|\alpha(0)\rangle = |\alpha(n)\rangle$. Although measurements can involve all

the states, at any given time only a single $|\alpha(p)\rangle$ has to be stored.

The $z$-component of the spin-spin correlation function can be easily obtained, as it is diagonal in the representa-
tion used. Equal-time correlations can be averaged over

the propagated states, i.e.,

$$
\langle S_k^z S_l^z \rangle = \frac{1}{4} \left\langle \sum_{p=0}^{n-1} \sigma_k^z(p) \sigma_l^z(p) \right\rangle,
$$

where in the special case $n = 0$, which occurs in practice

only for small $N$ at very high temperatures, the averaged

sum should be replaced by $\sigma_k^z(0) \sigma_l^z(0)$. Since states

$p$ and $p + 1$ differ only by two or four flipped spins, the

sum in (26) can be replaced by a sum where only, e.g., ev-

every $N$th state is included. We often consider the Fourier

transform of the correlation function, i.e., the static spin

structure factor

$$
S_s(q_x, q_y) = \frac{1}{N} \sum_{k,l} e^{i(r_k - r_l) \cdot q} \langle S_k^z S_l^z \rangle,
$$

where $r_i = (x_i, y_i)$ is the lattice coordinate (with lattice

spacing 1) and $q = (q_x, q_y)$ is the wave-vector. We also

study the corresponding static susceptibility,

$$
\chi_s(q_x, q_y) = \frac{1}{N} \sum_{k,l} e^{i(r_k - r_l) \cdot q} \int_0^\beta \langle S_k^z(\tau) S_l^z(0) \rangle.
$$

It has been shown that the SSE estimator for the Kubo

integral is

$$
\int_0^\beta d\tau \langle S_k^z(\tau) S_l^z(0) \rangle = \frac{\beta}{4} \left\langle \sum_{p=0}^{n-1} \sigma_k^z(p) \langle \sum_{p=0}^{n-1} \sigma_l^z(p) \rangle + \sum_{p=0}^{n-1} \sigma_k^z(p) \sigma_l^z(p) \right\rangle.
$$

G. Physical observables

In this section we summarize the physical observables relevant to studies of the J-K model and present the estimators used to evaluate them in the SSE method. The general forms of the estimators have been derived in

previous papers. Here we only apply those derived forms to the particular quantities of interest for the J-K model.

We typically carry out measurements on the configurations generated after every Monte Carlo step (MCS), with an MCS defined as a sweep of diagonal updates, followed by construction of the linked vertex list, in which a fixed number of loop updates are carried out. In the same linked list, all multi-branch clusters are constructed and flipped with probability 1/2. After this, the updated vertex list is mapped back into a new state $|\alpha\rangle$ and an operator list $S_M$. This is the representation used for the measurements. The fill-in elements $H_{0,0}$ in $S_M$ are irrelevant at this stage, and we therefore now consider the reduced list $S_n$ without these operators. There are hence $n + 1$ propagated states $|\alpha(p)\rangle = |\sigma_1^z(p), \ldots, \sigma_5^z(p)\rangle$, which are obtained one-by-one when operating with the first $p$ operators, $p = 0, \ldots, n$, on the initially stored state $|\alpha(0)\rangle = |\alpha(n)\rangle$. Although measurements can involve all the states, at any given time only a single $|\alpha(p)\rangle$ has to be stored.

The $z$-component of the spin-spin correlation function can be easily obtained, as it is diagonal in the representation used. Equal-time correlations can be averaged over the propagated states, i.e.,

$$
\langle S_k^z S_l^z \rangle = \frac{1}{4} \left\langle \sum_{p=0}^{n-1} \sigma_k^z(p) \sigma_l^z(p) \right\rangle,
$$

where in the special case $n = 0$, which occurs in practice only for small $N$ at very high temperatures, the averaged sum should be replaced by $\sigma_k^z(0) \sigma_l^z(0)$. Since states $p$ and $p + 1$ differ only by two or four flipped spins, the sum in (26) can be replaced by a sum where only, e.g., every $N$th state is included. We often consider the Fourier transform of the correlation function, i.e., the static spin structure factor

$$
S_s(q_x, q_y) = \frac{1}{N} \sum_{k,l} e^{i(r_k - r_l) \cdot q} \langle S_k^z S_l^z \rangle,
$$

where $r_i = (x_i, y_i)$ is the lattice coordinate (with lattice spacing 1) and $q = (q_x, q_y)$ is the wave-vector. We also study the corresponding static susceptibility,

$$
\chi_s(q_x, q_y) = \frac{1}{N} \sum_{k,l} e^{i(r_k - r_l) \cdot q} \int_0^\beta \langle S_k^z(\tau) S_l^z(0) \rangle.
$$

It has been shown that the SSE estimator for the Kubo integral is

$$
\int_0^\beta d\tau \langle S_k^z(\tau) S_l^z(0) \rangle = \frac{\beta}{4} \left\langle \sum_{p=0}^{n-1} \sigma_k^z(p) \langle \sum_{p=0}^{n-1} \sigma_l^z(p) \rangle + \sum_{p=0}^{n-1} \sigma_k^z(p) \sigma_l^z(p) \right\rangle.
$$
Here the first term typically dominates; it is obtained by first summing the spins at \( k \) and \( l \) over the propagated states, and then multiplying the sums. The full sums must clearly be calculated here, but one can still take advantage of the fact that only two or four out of the \( N \) spins \( \sigma_k^\pm(p) \) change at every propagation \( p \rightarrow p + 1 \). One can thus evaluate the sums for all sites \( k \) in \( n \sim N/\beta \) steps. The second term in \( \langle H \rangle \) vanishes as \( N \rightarrow \infty \), but typically it gives a non-negligible relative contribution for small \( N \) calculations and should always be kept. This sum is the same as in the equal-time correlation \( \langle B_{ij} \rangle \) and can again be replaced by a partial summation without introducing a bias. In the case \( n = 0 \), the whole expression within \( \langle \rangle \) in Eq. \( \langle \rangle \) should be replaced by \( \sigma_k^+(0)\sigma_k^-(p) \).

We are also interested in the spin stiffness, or the superfluid density in the boson representation, which at \( T = 0 \) is defined by

\[
\rho_s = \frac{\partial^2 E(\phi)}{\partial \phi^2},
\]

where \( E(\phi) = \langle H(\phi) \rangle /L^2 \) is the ground state energy per site and \( \phi \) is a twist which is imposed on all bonds \( (i,j) \) in either the \( x \) or \( y \) lattice direction, so that the corresponding bond operators \( B_{ij} \) become

\[
B_{ij}(\phi) = \cos(\phi)(S_i^x S_j^x + S_i^y S_j^y) + \sin(\phi)(S_i^x S_j^y - S_i^y S_j^x).
\]

This leads to a shift in the ground state energy \( E \) to second order in \( \phi \). With the plaquette operator \( P_{ijkl}(\phi) \), the leading-order energy shift is \( \propto \phi^4 \), and hence it will not appear in the estimator for the stiffness. The derivative at \( \phi = 0 \) in Eq. \( \langle \rangle \) can therefore be directly estimated using the winding number fluctuations in the SSE simulations\(^\text{22}\) in a way very similar to the way it is done in path integral methods\(^\text{23}\). Defining the winding numbers \( w_x \) and \( w_y \) as

\[
w_\alpha = (N^\alpha_+ - N^\alpha_-)/2L,
\]

where \( N^\alpha_+ \) denote the number of operators in \( S_\alpha \) which transport a boson (or spin-\( \uparrow \)) \( \pm 1 \) lattice steps in the \( \alpha \)-direction. In the J-K model, only the bond operators \( B_{ij} \) can transfer a net number of particles; in terms of the corresponding plaquette operators \( P_{ijkl} \), the pairs \( H_{2,a}, H_{4,a}, H_{4,a} \), and \( H_{5,a} \) transfer particles along the \( x \)- and \( y \)-axis, respectively. By operating successively with all operators in \( S_\alpha \) on the state \( |\alpha\rangle \) one can determine all the numbers \( N^\alpha_+ \) needed to obtain the winding numbers. The stiffness is then given by

\[
\rho_s = \frac{1}{2\beta} (w_x^2 + w_y^2).
\]

At finite \( T \), the ground state energy \( E(\phi) \) in Eq. \( \langle \rangle \) should be replaced by the free energy \( F(\phi) \). It turns out that this leads to exactly the same estimator, Eq. \( \langle \rangle \). A detailed derivation of this well known result\(\text{24}\) for lattice models has been presented in Ref. \(\text{22}\).

In order to detect the modulations of the bond and plaquette expectation values \( \langle B_{ij} \rangle \) and \( \langle P_{ijkl} \rangle \) in the striped phase, one can use open boundary conditions in order to break the translational symmetry. In order to break the 90° rotational symmetry, rectangular lattices can be used. On these lattices one can observe a unique bond/plaquette pattern\(\text{25}\). However, for careful finite-size scaling studies it is preferable to consider periodic \( L \times L \) lattices, on which all bond and plaquette expectations average to uniform values. We hence instead consider the corresponding correlation functions, and also calculate the associated susceptibilities. The static plaquette structure factor is defined as

\[
S_p(q_x, q_y) = \frac{1}{N} \sum_{a,b} e^{i(q_x r_a-r_b)} \langle P_a P_b \rangle,
\]

where \( P_a \) is the plaquette operator \( \text{2} \) with the plaquette subscript \( a \) defined in Fig. 1. The corresponding susceptibility is completely analogous to Eq. \( \langle \rangle \),

\[
\chi_p(q_x, q_y) = \frac{1}{N} \sum_{a,b} e^{i(q_x r_a-r_b)} \int_0^\beta d\tau \langle P_a(\tau) P_b(0) \rangle.
\]

Bond structure factors and susceptibilities are defined in the same way; we here consider those corresponding to correlations between bonds in the same lattice direction. Hence, defining \( x_k \) and \( y_k \) as the nearest-neighbor sites of site \( k \) in the \( x \)- and \( y \)-directions, the bond structure factors \( S_{b,x} \) and \( S_{b,y} \)

\[
S_{b,x}(q_x, q_y) = \frac{1}{N} \sum_{a,b} e^{i(q_x r_a-r_b)} \langle B_{a,b} B_{b,a} \rangle,
\]

and clearly \( S_{b,x}(q_x, q_y) = S_{b,y}(q_y, q_x) \). The corresponding susceptibilities are again defined as in Eq. \( \langle \rangle \).

For expectation values involving products of operators that also appear as terms in the Hamiltonian, such as the above plaquette and bond structure factors and susceptibilities, the SSE estimators are remarkably simple expressions involving only numbers of operators or operator combinations in the list \( S \). The simplest case is the expectation value of a single operator,

\[
\langle H_{t,a} \rangle = \frac{\langle n([a,b]) \rangle}{\beta},
\]

where \( \langle n([a,b]) \rangle \) is the number of elements \( [a,b] \) in the list \( S \). This gives the internal energy

\[
E = -\frac{\langle n \rangle}{\beta},
\]

which is identical to the expression obtained by Handscomb\(\text{26}\). An equal-time correlation function of two operators appearing in the Hamiltonian is given by

\[
\langle H_{t,a} H_{t,b} \rangle = \frac{1}{\beta^2} \langle n-1 \rangle N([s,a]|t,b)\rangle,
\]

where

\[
\langle n \rangle = \frac{1}{\beta} \sum_{t,b} \langle H^{(t,b)}_{s,a} \rangle = \frac{1}{\beta} \sum_{t,b} \langle H^{(t,b)}_{s,b} \rangle.
\]
where \( N([s, a][t, b]) \) denotes the number of occurrences of the operators \([s, a]\) and \([t, b]\) next to each other, in the given order, in \( S_n \) (with the periodicity of \( S_n \) taken into account). The corresponding Kubo integral is \( \int d\tau \langle H_{s,a}(\tau)H_{t,b}(0) \rangle = \frac{1}{\beta} \langle N([s, a])N([t, b]) - \delta_{st}\delta_{ab}N([s, a]) \rangle \),

where \( N([s, a]) \) is the number of operators \([s, a]\). Using Eqs. (39) and (41), the estimators for (34)-(36) can be easily obtained.

### III. AUTOCORRELATIONS

We here show some results illustrating the performance of the algorithm, focusing in particular on the efficiency boost achieved with the multi-branch update. It would clearly be interesting to extract the dynamic exponent of the simulations at the various phase transitions, but we will not attempt this here. Instead, we will focus on the simulation dynamics inside the ordered phases. Particularly in the striped and staggered phases, which break spatial symmetries, we expect slow modes corresponding to transitions between the different degenerate states. One might also expect potential problems related to long-lived defects forming in these states.

For a quantity \( Q \), the normalized autocorrelation function is defined in the standard way as

\[
A_Q(t) = \frac{\langle Q(i+t)Q(i) \rangle - \langle Q(i) \rangle^2}{\langle Q(i)^2 \rangle}.
\]

where the averages are over the Monte Carlo time (steps) \( i \). We will compare autocorrelation functions in the three different ordered phases, obtained in simulations with and without multi-branch cluster updates. A Monte Carlo step is defined as a full sweep of diagonal updates, followed by a number of directed-loop updates, and, if multi-branch updates are carried out, decomposition of the configuration into clusters, each of which is flipped with probability \( 1/2 \). In these simulations the number of directed-loop updates per step was chosen so that, on average, the total number of vertices visited is \( 4M \), with the truncation \( M \) of the index sequence chosen equal to 1.25 times the maximum expansion order \( n \) reached during equilibration (the dependence of \( M \) on the length of the equilibration is in practice very small and introduces

FIG. 11: Autocorrelation function for the spin stiffness (upper panel) and the plaquette-stripe order parameter (lower panel) in simulations of \( L = 16 \) systems at \( K/J = 4 \) and 7, both at inverse temperature \( K/T = 16 \). Results of simulations both with and without the multi-branch cluster update are shown.

FIG. 12: Autocorrelation function for the plaquette-stripe order parameter at \( K/J = 12 \) and inverse temperature \( K/T = 32 \). Results with (solid curves) and without (dashed curves) multi-branch clusters are compared for three different system sizes.
only a negligible ambiguity in the definition of the Monte Carlo time).

Fig. 13 shows autocorrelation results for the superfluid density $\rho_s$ and the squared stripe-order-parameter $M^2_P$ inside the superfluid phase for a $16 \times 16$ lattice at $K/T = 16$. At $K/J = 4$, the $\rho_s$ autocorrelations drop very rapidly (the integrated autocorrelation time is less than 1), and there are no discernible effects of including multi-branch updates. The autocorrelation time for $M^2_P$ is also very short, but here there are clear improvements with the multi-branch updates. However, considering that the CPU time is almost doubled when including multi-branch updates, including them at $K/J = 4$ is not advantageous. At $K/J = 7$, which is approaching the transition point to the striped phase at $K/J \approx 7.9$, the autocorrelations decay much slower, and although there are visible favorable effects of the multi-branch updates in both quantities, the gain is hardly worth the additional CPU time cost. In Fig. 13 results are shown for the stripe order parameter at $K/J = 12$, well inside the striped phase, for three different system sizes at inverse temperature $K/T = 32$. The multi-branch updates have clear favorable effects on the autocorrelations, but although the initial drop is considerably faster, the asymptotic autocorrelation time, i.e., the long-time linear decay seen on the linear-log scale used in the figures, changes very little. In this case the reduction of the integrated autocorrelation time may (depending on the exact value of $K/J$, and the system size) motivate the additional computational effort of the multi-branch update.

The multi-branch cluster update improves the simulation efficiency considerably inside the CDW phase, as illustrated in Fig. 13 for three different system sizes with $K/J = 32$ at a low temperature. Here the improvement in the simulation efficiency for the squared staggered order parameter $M^2_S$ is clearly significant enough to motivate the cost of the multi-branch clusters, especially for large system sizes. An interesting feature to note here is that when the multi-branch clusters are included, the asymptotic autocorrelation time actually decreases for $L = 32$ relative to $L = 16$, and $L = 16$ and $L = 8$ show almost identical autocorrelation functions. This surprising trend for increasing $L$ can probably be traced to the fluctuations in the CDW order parameter for a given SSE configuration. Fig. 14 shows the dependence of the staggered order parameter on the propagation number $p$ [re-
ferring to the propagated states, Eq. (9) divided by the total number of operators \( n \) for an equilibrated configuration. The fraction \( \frac{p}{n} \) corresponds roughly to the normalized imaginary-time \( \tau/\beta \) in the standard Euclidean path integral formalism. For a small system, exemplified by \( L = 8 \) in the figure, the order parameter fluctuates between positive and negative values, whereas for a large system, exemplified here by \( L = 32 \), fluctuations sufficiently large to “tunnel” the system between positive and negative order parameters are very rare. Clearly, as \( T \to 0 \), there would be such tunneling events also in a large system, but if \( T \) is not low compared to the gap between the symmetric and antisymmetric linear combinations of the two different real-space ordered states (which decreases exponentially fast with increasing \( L \)), such events are not present in typical configurations. The shorter autocorrelation time for \( L = 32 \) than for \( L = 16 \) (when multi-branch updates are included) in Fig. 13 may hence be related to the larger fluctuations in \( M_s \) for the smaller system size, which can lead to various tunneling events that are not so easily added or removed from the configurations. For the larger system size, there are in practice no tunneling events at the temperature used here, and the difficulties in adding/removing them in this case would only show up at very long times as an unde-
Note the clear anti-correlations between the stripe order and superfluid density in Fig. 16. These do not, however, give an indication of the order of the phase transition between the two phases, as anti-correlations are expected at both continuous and first-order transitions.

IV. DIAGONAL PLAQUETTE INTERACTIONS

In general, diagonal terms can be added to the Hamiltonian Eq. (1) without the development of a new directed-loop algorithm; only the exit probability tables change, due to the modified weights of the relevant diagonal (C) vertices illustrated in Fig. 3 (and symmetry related sets). We here consider three different diagonal terms: (i) one which enhances or suppresses staggered (“flippable” by the K-term) plaquettes, (ii) a uniform external magnetic (Zeeman) field, and (iii) a staggered field.

A. Flippable-plaquette interaction

The full spin Hamiltonian including the flippable-plaquette interaction is

\[ H = -J \sum_{\langle ij \rangle} B_{ij} - K \sum_{ijkl} P_{ijkl} - V \sum_{ijkl} Q_{ijkl}, \]

where the bond \( B_{ij} \) and plaquette \( P_{ijkl} \) operators are defined in Eqs. (1) and (2) and symmetry arguments as previously to constrain the equations and produce a unique solution. Our choice of symmetry conditions here correspond to

\[ v_{12} = v_{13}, \]
\[ v_{22} = v_{23}, \]
\[ v_{34} = v_{44}. \]

Two forms of the solutions are needed in order to ensure positive-definite vertex weights for all choices of parameters. The first solution is valid for small couplings, \( |V| \leq J \), and can be formulated without the undesirable bounce processes (the right-hand column):

\[
\begin{align*}
  v_{11} &= C - J/2 + V/2, \quad v_{12} = J/4 - V/4, \quad v_{13} = J/4 - V/4, \quad v_{14} = 0, \\
  v_{21} &= C - J/2 + V/2, \quad v_{22} = J/4 + V/4, \quad v_{23} = J/4 + V/4, \quad v_{24} = 0, \\
  v_{31} &= J/4 - V/4, \quad v_{32} = J/4 + V/4, \quad a_{33} = 0, \quad v_{34} = 0, \\
  v_{41} &= J/4 - V/4, \quad v_{42} = J/4 + V/4, \quad a_{43} = 0, \quad v_{44} = 0.
\end{align*}
\]

where we see that the constant \( C \) must be greater than \( J/2 - V/2 \) to ensure that \( v_{11} \) remains positive. However, in order to satisfy the requirement that \( a_{11} \) is positive for vertex-path sets not affected by the V term, one should set \( C > J/2 \) for the case \( V > 0 \). For \( V < 0 \), one must in addition ensure that the weight \( W^V \) in Eq. (42) remains positive, requiring a constant \( C > J/2 + |V|/2 \). Note that in the limit \( V \to 0 \), this equation set is equal to the
This last equation set imposes the requirement that $C > 2|V| - J$. In Eqs. (46) to (48), the actual exit probabilities for the directed-loop algorithm are obtained in the usual way by dividing the matrix elements by the vertex weights: $P_{ij}^e = v_{ij}/W_i$, where $W_i$ is the relevant matrix element.

Note again that when implementing a diagonal interaction such as the $V$ term, only the change required in the simulation code, relative to the pure J-K model, is the probability weights of only the specific relevant vertex-paths affected. In the case above for the plaquette $V$ term, only the vertex set shown in Fig. 17, and the related set with the other staggered vertex, will use the solutions outlined in Eqs. (46), (47) and (48). All other C to J vertex sets which do not contain fully-staggered diagonal vertices will use the original solution, Eq. (18).

\[ v_{11} = C, \quad v_{12} = 0, \quad v_{13} = 0, \quad v_{14} = 0, \]
\[ v_{21} = C, \quad v_{22} = J/2, \quad v_{23} = J/2, \quad v_{24} = V - J, \]
\[ v_{31} = J/2, \quad v_{32} = 0, \quad v_{33} = 0, \quad v_{34} = 0, \]
\[ v_{41} = J/2, \quad v_{42} = 0, \quad v_{43} = 0, \quad v_{44} = 0, \]

where the bounce process is turned on slowly, i.e. linearly with $V - J$, ensuring a small bounce probability in the algorithm for a moderate range of $V$ larger than the exchange. However, it is clear that the bounce process becomes negative for negative $V$ (i.e. $V < -J < 0$) and we hence need a different solution in this case. Again, we use a solution that turns the bounce processes on slowly, but in this case two non-zero bounces are required:

\[ v_{11} = C + J - 2|V|, \quad v_{12} = J/2, \quad v_{13} = J/2, \quad v_{14} = 2|V| - 2J, \]
\[ v_{21} = C + J - 2|V|, \quad v_{22} = 0, \quad v_{23} = 0, \quad v_{24} = |V| - J, \]
\[ v_{31} = J/2, \quad v_{32} = 0, \quad v_{33} = 0, \quad v_{34} = 0, \]
\[ v_{41} = J/2, \quad v_{42} = 0, \quad v_{43} = 0, \quad v_{44} = 0. \]

This last equation set imposes the requirement that $C > 2|V| - J$. In Eqs. (46) to (48), the actual exit probabilities for the directed-loop algorithm are obtained in the usual way by dividing the matrix elements by the vertex weights; $P_{ij}^e = v_{ij}/W_i$, where $W_i$ is the relevant matrix element.

Note again that when implementing a diagonal interaction such as the $V$ term, only the change required in the simulation code, relative to the pure J-K model, is the probability weights of only the specific relevant vertex-paths affected. In the case above for the plaquette $V$ term, only the vertex set shown in Fig. 17, and the related set with the other staggered vertex, will use the solutions outlined in Eqs. (46), (47) and (48). All other C to J vertex sets which do not contain fully-staggered diagonal vertices will use the original solution, Eq. (18).

\[ H = -J \sum_{(ij)} B_{ij} - K \sum_{ijkl} P_{ijkl} - h \sum_i S_i^z, \]

where we restrict $h > 0$. The diagonal term $H_{1,a}$ of Eq. (11) is modified to include the effects of the field,

\[ H_{1,a} = \frac{h}{4} (S_i^z + S_j^z + S_k^z + S_l^z) + CI_{ijkl}, \]

where this term now produces different matrix elements depending on the spins $S_i^z, S_j^z, S_k^z, S_l^z$, with an associated vertex weight, Eq. (18). We can ensure that each weight will remain positive by adjusting $C$, in particular, we write $C = h/2 + \epsilon$, where $\epsilon > 0$ is typically a
small constant. Representing the relevant plaquette of the state $|\alpha\rangle$ by a list of the spin states, we can calculate the weights of the 16 C-vertices using Eq. (50). The results are summarized in Table III.

In addition, with the Hamiltonian Eq. (49), the off-diagonal plaquette operators $H_{2a}$ to $H_{6a}$ in Eq. (11) remain unmodified. In this case, there are now four unique sets of directed loop equations for $C\rightarrow C$ and $C\rightarrow J$ vertices that are not related by trivial symmetry operations.

The first closed set of C and J vertex paths is illustrated in Fig. 4 with weights $a_{ij}$ which now also should include the bounce processes $a_{ij}$ left out in the figure. If we recall that the open circle in Fig. 5 denotes a spin down, or $S^z = -1/2$, then, the directed-loop equations corresponding to this set is now modified from Eq. (10) to read

\[
\begin{align*}
 a_{11} + a_{12} + a_{13} + a_{14} &= W_5^h = \epsilon, \\
 a_{21} + a_{22} + a_{23} + a_{24} &= W_4^h = h/4 + \epsilon, \\
 a_{31} + a_{32} + a_{33} + a_{34} &= W_3^h = J/2, \\
 a_{41} + a_{42} + a_{43} + a_{44} &= W_4^h = J/2.
\end{align*}
\]

(51)

We use the same detailed balance, Eq. (10) and symmetry arguments, Eq. (15), as previously to constrain the equation set and produce a unique solution. For fields $h < 4J$, we can obtain a solution which contains no bounce processes,

\[
\begin{align*}
 a_{11} &= h/8 - J/2 + \epsilon, \\
 a_{12} &= J/4 - h/16, \\
 a_{13} &= J/4 - h/16, \\
 a_{14} &= 0, \\
 a_{21} &= h/8 - J/2 + \epsilon, \\
 a_{22} &= J/4 + h/16, \\
 a_{23} &= J/4 + h/16, \\
 a_{24} &= 0, \\
 a_{31} &= J/4 - h/16, \\
 a_{32} &= J/4 - h/16, \\
 a_{33} &= 0, \\
 a_{34} &= 0, \\
 a_{41} &= J/4 - h/16, \\
 a_{42} &= J/4 + h/16, \\
 a_{43} &= 0, \\
 a_{44} &= 0.
\end{align*}
\]

(52)

The second independent closed set of vertex weights for the Hamiltonian Eq. (11) is obtained by taking the spin-reverse of the closed set illustrated in Fig. 5. The resulting directed-loop equations then contain the fully polarized vertex in Table III and are written as

\[
\begin{align*}
 c_{11} + c_{12} + c_{13} + c_{14} &= W_5^h = h + \epsilon, \\
 c_{21} + c_{22} + c_{23} + c_{24} &= W_4^h = 3h/4 + \epsilon, \\
 c_{31} + c_{32} + c_{33} + c_{34} &= W_3^h = J/2, \\
 c_{41} + c_{42} + c_{43} + c_{44} &= W_4^h = J/2.
\end{align*}
\]

(54)

This set is solved in the same way as set a above, employing analogous conditions for detailed-balance and vertex symmetries. The result is two sets of vertex weights; the first, for $h < 4J$ is

\[
\begin{align*}
 c_{11} &= 7h/8 - J/2 + \epsilon, \\
 c_{12} &= J/4 + h/16, \\
 c_{13} &= J/4 + h/16, \\
 c_{14} &= 0, \\
 c_{21} &= 7h/8 - J/2 + \epsilon, \\
 c_{22} &= J/4 + h/16, \\
 c_{23} &= J/4 - h/16, \\
 c_{24} &= 0, \\
 c_{31} &= J/4 + h/16, \\
 c_{32} &= J/4 - h/16, \\
 c_{33} &= 0, \\
 c_{34} &= 0, \\
 c_{41} &= J/4 + h/16, \\
 c_{42} &= J/4 - h/16, \\
 c_{43} &= 0, \\
 c_{44} &= 0.
\end{align*}
\]

(55)
where clearly, to keep \( c_{11} > 0 \) we require \( \epsilon \geq J/2 - 7h/8 \). We see that this solution is similar in form to the low-field solution for vertex set \( a \), Eq. (52). However, the \( c_{11} \) and \( c_{21} \) terms are modified, and also the other non-zero terms have the opposite sign of \( h \) (i.e. if \( a_{ij} = J/4 \pm h/16 \), then \( c_{ij} = J/4 \mp h/16 \)). The other solution corresponds to the large-field case, \( h > 4J \), and requires the inclusion of a non-zero weight for the bounce process \( c_{14} \),

\[
\begin{align*}
c_{11} &= \epsilon + 3h/4, \quad c_{12} = J/2, \quad c_{13} = J/2, \quad c_{14} = h/4 - J, \\
c_{21} &= \epsilon + 3h/4, \quad c_{22} = 0, \quad c_{23} = 0, \quad c_{24} = 0, \\
c_{31} &= J/2, \quad c_{32} = 0, \quad c_{33} = 0, \quad c_{34} = 0, \\
c_{41} &= J/2, \quad c_{42} = 0, \quad c_{43} = 0, \quad c_{44} = 0. \\
\end{align*}
\]

(56)

Again, the \( c_{11} \) and \( c_{21} \) terms are modified by the different vertex sets, and in addition the non-zero bounce process has moved to \( c_{14} \) from \( a_{24} \) in Eq. (53).

The third independent closed set of vertex weights does not include the fully spin-up or spin-down matrix elements of the previous two, sets \( a \) and \( c \). The diagrammatic representation is therefore not trivially related to these previous cases, and is illustrated in Fig. 18. In this case, the directed-loop equations are

\[
\begin{align*}
d_{11} + d_{12} + d_{13} + d_{14} &= W^h_4 = h/4 + \epsilon, \\
d_{21} + d_{22} + d_{23} + d_{24} &= W^h_3 = h/2 + \epsilon, \\
d_{31} + d_{32} + d_{33} + d_{34} &= W_3 = J/2, \\
d_{41} + d_{42} + d_{43} + d_{44} &= W_4 = J/2.
\end{align*}
\]

(57)

While the detailed balance conditions for this equation set is the same as before, Eq. (17), it can be noted that the additional symmetry conditions, Eq. (15), do not appear in the diagrams here. Although not immediately justifiable in terms of symmetry arguments, there is in general no reason why the same constrains cannot be used to solve equation set \( d \), and therefore we will continue to use Eq. (15) as it facilitates implementation of the algorithm (although there is no guarantee that this leads to the most efficient simulation). The low-field solution \( (h < 4J) \) is then given by the same equation set as solution \( a \), Eq. (52) with all \( d_{ij} = a_{ij} \) except the following:

\[
d_{11} = d_{21} = 3h/8 - J/2 + \epsilon. \quad (58)
\]

Here, it is quite obvious that we require \( \epsilon \geq J/2 - 3h/8 \) in order to keep all vertex weights positive. For the high-field case \( (h > 4J) \), we are forced to have a non-zero bounce process, and upon solving we again get an equation set similar to solution \( a \), Eq. (53), with the exception that

\[
d_{11} = d_{12} = \epsilon + h/4. \quad (59)
\]

The final set of vertex-weights used in the uniform-field solution is obtained by taking the spin-reverse of the closed set illustrated in Fig. 18 in an analogous manner to the way that set \( c \) was obtained from set \( a \). The result is the directed loop equations given by

\[
\begin{align*}
e_{11} + e_{12} + e_{13} + e_{14} &= W^h_2 = 3h/4 + \epsilon, \\
e_{21} + e_{22} + e_{23} + e_{24} &= W^h_3 = h/2 + \epsilon, \\
e_{31} + e_{32} + e_{33} + e_{34} &= W_3 = J/2, \\
e_{41} + e_{42} + e_{43} + e_{44} &= W_4 = J/2.
\end{align*}
\]

(60)

Again, we employ the detailed balance and symmetry conditions discussed above to find a unique low-field solution for \( h < 4J \), which in this case is the same as the solution set \( c \), Eq. (55) with the exception that

\[
e_{11} = e_{21} = 5h/8 - J/2 + \epsilon, \quad (61)
\]

where again the bounces have been eliminated, and to get \( e_{11} > 0 \), we need \( \epsilon \geq J/2 - 5h/8 \). The large-field \( (h > 4J) \) solutions are given by the analogous set, Eq. (56), with the exception that

\[
e_{11} = e_{21} = \epsilon + h/2. \quad (62)
\]

As before, the above four equations sets, \( a, c, d \) and \( e \), serve to uniquely define the exit probabilities, given by dividing the matrix elements by the vertex weights, e.g. \( P_{ij}^d = a_{ij}/W_i \), where the values of \( W_i \) are given either by Table I above, or by the previously-defined values of \( W_3 = W_4 = J/2 \). It is important, in the implementation of the directed-loop equations, that all diagonal vertices are weighted according to their proper equation set. The relation of a general \( C \) or \( J \) vertex to the proper equation set in some cases depends on the path that a loop
FIG. 19: Sublattice decoration of the two-dimensions square

segments takes through the vertex. For example, the
vertex in $a_{31}$ is related to $d_{31}$, however the path taken
by the loop in each case results in a C vertex which is
weighed differently by the field. Also, we note that the
common element of all of these equation sets is the con-
stant $\epsilon$. This $\epsilon$ must be chosen to keep all of the elements
$a_{11}, c_{11}$, $d_{11}$, $e_{11}$ and their symmetry related weights posi-
tive definite. The critical condition comes from Eq. (52),
where $a_{11} > 0$ in all cases for $\epsilon \geq J/2 - h/8$. It can
be seen that, if this condition is satisfied, then all of the
weights $c_{11}, d_{11}$ and $e_{11}$ will automatically be positive
definite, and it is therefore the $\epsilon$ that we choose in im-
plementation of the algorithm.

C. Staggered magnetic field

The final set of directed loop solutions that we will
present in this paper is for the J-K model in a staggered
Zeeman field. Motivation for this extension of the Hamilton-
ian comes directly from predictions in the theory of deconfining quantum criticality\textsuperscript{13,15} and its applicability to our microscopic model. In short, a staggered Zee-
man field on our spin model corresponds to a uniform
Zeeman field that couples to the $z$ component of $\hat{n}$ in the nonlinear-sigma model of relevance. The theory then
predicts a “split” transition between the VBS and super-
fluid phases, with an intermediate phase with neither order (but with a “background” field-induced staggered
magnetization).

The modified Hamiltonian is

$$ H = -J \sum_{(ij)} B_{ij} - K \sum_{ijkl} P_{ijkl} - h \sum_i ( -1)^{x_i+y_i} S_i^z, \quad (63) $$

where $x_i$ and $y_i$ are the Cartesian lattice coordinates of
the $i$th spin, and $h > 0$. The diagonal plaquette term
$H_{1,a}$ of Eq. (11) is modified to include the effects of the staggered field,

$$ H_{1,a} = ( -1)^{x_i+y_i} \frac{h}{4} ( S_i^z - S_j^z + S_k^z - S_l^z ) + CI_{ijkl}, \quad (64) $$

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
$|S_i^z S_j^z S_k^z S_l^z| H_{1,a} |S_i^z S_j^z S_k^z S_l^z|$ & A sublattice & B sublattice \\
\hline
$|↑↑↑↑⟩$ & $C$ & $C$ \\
$|↓↑↑↑⟩$ & $-h/4 + C$ & $h/4 + C$ \\
$|↑↓↑↑⟩$ & $-h/4 + C$ & $h/4 + C$ \\
$|↑↑↑↓⟩$ & $h/4 + C$ & $h/4 + C$ \\
$|↑↑↑↓⟩$ & $-h/4 + C$ & $h/4 + C$ \\
$|↓↑↑↓⟩$ & $h/4 + C$ & $h/4 + C$ \\
$|↓↑↑↓⟩$ & $h/4 + C$ & $h/4 + C$ \\
$|↑↑↓↑⟩$ & $-h/4 + C$ & $h/4 + C$ \\
$|↑↑↓↑⟩$ & $C$ & $C$ \\
$|↑↑↓↑⟩$ & $C$ & $C$ \\
$|↑↑↓↑⟩$ & $C$ & $C$ \\
$|↑↑↓↑⟩$ & $C$ & $C$ \\
$|↑↑↓↑⟩$ & $C$ & $C$ \\
$|↑↑↓↑⟩$ & $C$ & $C$ \\
$|↑↑→⟩$ & $h/2 + C$ & $-h/2 + C$ \\
$|↑↑↓↑⟩$ & $h/2 + C$ & $h/2 + C$ \\
\hline
\end{tabular}
\caption{The weight factors for the diagonal vertices in the staggered J-K model.}
\end{table}

and the other plaquette Hamiltonian terms remain un-
modified. Keeping $C$ arbitrary for now, we can easily calculate the weights for the 16 diagonal (C) vertices.
The approach we take in constructing the simulation is
the decorate the lattice with an “A” and “B” sublattice
in a checkerboard pattern (Fig. 19). The solution to each vertex weight in the directed loop equations will have two components, one if the vertex happens to fall on an “A” plaquette, and another for the same vertex on a “B” pla-
quette (see Table III).

Turning first to the closed set of C and J diagrams,
Fig. 5 we construct the directed-loop equations, which are now different from the forms Eq. (10) and Eq. (51).

$$ a_{11} + a_{12} + a_{13} + a_{14} = C, $$
$$ a_{21} + a_{22} + a_{23} + a_{24} = \mp h/4 + C, $$
$$ a_{31} + a_{32} + a_{33} + a_{34} = J/2, $$
$$ a_{41} + a_{42} + a_{43} + a_{44} = J/2. \quad (65) $$

Notice that we have suppressed the explicit definition
used before for the weights, $W$, in order to simplify no-
tation. The $\mp$ sign defines the convention that the corre-
sponding term is negative if it falls on an A plaquette,
and positive if it falls on a B plaquette. We can set the
bounce processes $a_{14} = a_{24} = 0$ as long as $J > h/4$,
giving a solution:
Again, the upper symbol of ± or \( \mp \) refers to the vertex weight on the A sublattice, and the lower symbol corresponds to the B sublattice. Note, however, that this sign in the first term in Eq. (66) must be found with a non-zero bounce,

\[
 a_{11} = C - J/2 \mp h/8, \quad a_{12} = J/4 \pm h/16, \quad a_{13} = J/4 \pm h/16, \quad a_{14} = 0,
 a_{21} = C - J/2 \mp h/8, \quad a_{22} = J/4 \pm h/16, \quad a_{23} = J/4 \mp h/16, \quad a_{24} = 0,
 a_{31} = J/4 \pm h/16, \quad a_{32} = J/4 \mp h/16, \quad a_{33} = 0, \quad a_{34} = 0,
 a_{41} = J/4 \pm h/16, \quad a_{42} = J/4 \mp h/16, \quad a_{43} = 0, \quad a_{44} = 0.
\]

For A-plaquettes, another form of the solution is needed, which is analogous to the solution Eq. (66) found for the diagonal interaction \( V < -J < 0 \). Setting \( a_{14} = h/2 - 2J \), and \( a_{24} = h/4 - J \) constrains the equations to give the solution \( h > 4J \) on A plaquettes:

\[
 a_{11} = C, \quad a_{12} = 0, \quad a_{13} = 0, \quad a_{14} = 0,
 a_{21} = C, \quad a_{22} = J/2, \quad a_{23} = J/2, \quad a_{24} = h/4 - J,
 a_{31} = 0, \quad a_{32} = J/2, \quad a_{33} = 0, \quad a_{34} = 0,
 a_{41} = 0, \quad a_{42} = J/2, \quad a_{43} = 0, \quad a_{44} = 0
\]

This imposes the requirement that \( C > h/2 - J \).

This outlines the basic method of constructing the directed-loop probabilities for the staggered magnetic field Hamiltonian. The only difficulty in completing the procedure is identifying all of the separate sets of closed vertex-path diagrams which contribute different vertex weights to the directed loop algorithm. Instead of explicitly illustrating and solving all of these different sets of equations, we simply present the solutions in a more concise form. To begin, note that we can abbreviate the illustration of the closed sets of C and J vertex-paths if we constrain the solutions to obey the same detailed balance, Eq. (17), and symmetry arguments, Eq. (45), used throughout this paper. In this case, one only needs to know the upper-left (reference) vertex \( a_{11} \) in Fig. 21 in order to uniquely define the entire closed set of C to J vertex paths. The rules for constructing the closed set, as discussed in section II E, can then be summarized by the schematic representation in Fig. 21, which illustrates the general relationship between the different vertex weights, and their corresponding transformations.
V. DISCUSSION

In summary, we have developed in this work an extensive algorithmic framework for SSE quantum Monte Carlo simulations of the $S = 1/2$ XY model with ring exchange – the J-K model – on a 2D square lattice. In addition to outlining the basic representation of the quantum

![Diagram](image)

**FIG. 21:** Schematic representation of the closed set of C and J vertex-paths used in solving the directed-loop equations for the J-K model. Blocks with the same shading represent equivalent vertex weights.

**TABLE IV:** Vertex weight equation set I, for the staggered-field J-K model. An example of the starting vertex, $a_{11}$, is illustrated in Fig. 21. The corresponding vertex weights appear in Table IV, and are equivalent to the symmetries of Fig. 21, however the full equation sets are recovered easily by using this figure or Eqs. (17) and (19).

| vertex | A/B ($h < 4J$) | A ($h > 4J$) | B ($h > 4J$) |
|--------|----------------|--------------|--------------|
| $a_{11}$ | $C - J/2 + h/8$ | $C + J - h/2$ | $C$ |
| $a_{12}$ | $J/4 + h/16$ | $J/2$ | 0 |
| $a_{14}$ | 0 | $h/2 - 2J$ | 0 |
| $a_{22}$ | $J/4 + h/16$ | $J/2$ | 0 |
| $a_{24}$ | 0 | $h/4 - J$ | $h/4 - J$ |
| $a_{33}$ | 0 | 0 | 0 |
| $a_{34}$ | 0 | 0 | 0 |

We can therefore easily construct an entire closed set of C and J vertex paths using Fig. 21 simply by defining the reference vertex. Following this procedure, we see that the number of unique vertex probability solution sets is narrowed down to six, unrelated by trivial symmetry operations. The reference vertices for these six unique sets are illustrated in Fig. 20. The corresponding vertex weights are summarized in the equation sets of Tables IV to IX. For example, the first reference vertex of Eq. set I in Fig. 20 corresponds to $a_{11}$ of Fig. 21. The corresponding vertex weights appear in Table IV and are equivalent to the solution sets Eqs. (10), (17) and (19). The tables are abbreviated to only include unique weights not related by the symmetries of Fig. 21, however the full equation sets are recovered easily by using this figure or Eqs. (17) and (19).

**TABLE V:** Vertex weight equation set II.

| vertex | A/B ($h < 4J$) | A ($h > 4J$) | B ($h > 4J$) |
|--------|----------------|--------------|--------------|
| $s_{11}$ | $C - J/2 + h/8$ | $C + J - h/2$ | $C$ |
| $s_{12}$ | $J/4 + h/16$ | 0 | $J/2$ |
| $s_{14}$ | 0 | 0 | $h/2 - 2J$ |
| $s_{22}$ | $J/4 + h/16$ | $J/2$ | 0 |
| $s_{24}$ | 0 | $h/4 - J$ | $h/4 - J$ |
| $s_{33}$ | 0 | 0 | 0 |
| $s_{34}$ | 0 | 0 | 0 |

**TABLE VI:** Vertex weight equation set III.

| vertex | A/B ($h < 4J$) | A ($h > 4J$) | B ($h > 4J$) |
|--------|----------------|--------------|--------------|
| $e_{11}$ | $C - J/2 + h/8$ | $C + J - h/2$ | $C$ |
| $e_{12}$ | $J/4 + h/16$ | $J/2$ | 0 |
| $e_{14}$ | 0 | $h/4 - J$ | $h/4 - J$ |
| $e_{22}$ | $J/4 + h/16$ | 0 | $J/2$ |
| $e_{24}$ | 0 | 0 | $h/2 - 2J$ |
| $e_{33}$ | 0 | 0 | 0 |
| $e_{34}$ | 0 | 0 | 0 |

**TABLE VII:** Vertex weight equation set IV.

| vertex | A/B ($h < 4J$) | A ($h > 4J$) | B ($h > 4J$) |
|--------|----------------|--------------|--------------|
| $f_{11}$ | $C - J/2 + h/8$ | $C + J - h/2$ | $C$ |
| $f_{12}$ | $J/4 + h/16$ | 0 | $J/2$ |
| $f_{14}$ | 0 | $h/4 - J$ | $h/4 - J$ |
| $f_{22}$ | $J/4 + h/16$ | $J/2$ | 0 |
| $f_{24}$ | 0 | $h/2 - 2J$ | 0 |
| $f_{33}$ | 0 | 0 | 0 |
| $f_{34}$ | 0 | 0 | 0 |

**TABLE VIII:** Vertex weight equation set V.

| vertex | A/B ($h < 4J$) | A ($h > 4J$) | B ($h > 4J$) |
|--------|----------------|--------------|--------------|
| $t_{11}$ | $C - J/2 + 3h/8$ | $C + h/4$ | $C + J - 3h/4$ |
| $t_{12}$ | $J/4 + h/16$ | 0 | $J/2$ |
| $t_{14}$ | 0 | 0 | $h/2 - 2J$ |
| $t_{22}$ | $J/4 + h/16$ | $J/2$ | 0 |
| $t_{24}$ | 0 | $h/4 - J$ | $h/4 - J$ |
| $t_{33}$ | 0 | 0 | 0 |
| $t_{34}$ | 0 | 0 | 0 |

**TABLE IX:** Vertex weight equation set VI.

| vertex | A/B ($h < 4J$) | A ($h > 4J$) | B ($h > 4J$) |
|--------|----------------|--------------|--------------|
| $j_{11}$ | $C - J/2 + 3h/8$ | $C + J - 3h/4$ | $C + h/4$ |
| $j_{12}$ | $J/4 + h/16$ | $J/2$ | 0 |
| $j_{14}$ | 0 | $h/2 - 2J$ | 0 |
| $j_{22}$ | $J/4 + h/16$ | 0 | $J/2$ |
| $j_{24}$ | 0 | $h/4 - J$ | $h/4 - J$ |
| $j_{33}$ | 0 | 0 | 0 |
| $j_{34}$ | 0 | 0 | 0 |
mechanical partition function as a power series expansion of plaquette-operators acting on a chosen basis in the $S^z$ representation, we have developed advanced implementations of the directed-loop and multi-branch cluster updates, designed to significantly increase algorithm efficiency in various parameter regimes of the Hamiltonian. We have studied the performance of the various updating procedures using autocorrelation functions. We have also outlined modifications of the directed-loop equations to account for extensions of the J-K Hamiltonian to include diagonal (potential energy) operators. Although several specific Hamiltonian terms are discussed, the procedure developed is sufficiently general to allow for easy extensions to other diagonal interactions.

**TABLE X:** Comparison of ground-state energy (per spin) of exact diagonalization and SSE quantum Monte Carlo results for various parameter values of the J-K Hamiltonian, on a $4 \times 4$ square lattice. The exchange was set to $J = 1/2$, and simulations were performed with 50 million Monte Carlo production steps each. The staggered field strength is represented by $h_z$.

| $K/J$ | $V/J$ | $h_z/J$ | $E_{exact}$ (1) | $E_{qmc}$ (1) |
|-------|-------|--------|----------------|--------------|
| 0     | 0     | 0      | -0.5624863     | -0.56249(1)  |
| 1     | 0     | 0      | -0.6803518     | -0.68034(1)  |
| 4     | 0     | 2      | -1.1530991     | -1.15311(2)  |
| 0     | 1/2   | 0      | -0.6239222     | -0.62392(1)  |
| 2     | 2     | 0      | -1.2864452     | -1.28643(2)  |
| 1     | -3    | 0      | -0.3983951     | -0.39838(1)  |
| 1     | 0     | 2      | -0.7434355     | -0.74343(1)  |
| 5     | 0     | 6      | -1.5000000     | -1.50001(1)  |
| 4     | 0     | 2      | -1.2547499     | -1.25476(2)  |
| 1     | 0     | 5      | -1.3859171     | -1.38590(1)  |

The last step needed to provide confidence in the rather complex implementation of our directed-loop algorithms discussed here is to carry out rigorous testing. We do this by comparing SSE data with results obtained by exact diagonalization of the Hamiltonian. Table X compares ground-state energies obtained in various algorithmic solution regimes of the quantum Monte Carlo schemes discussed here with exact diagonalization results for $4 \times 4$ lattices. In the simulations, the temperature $T_0$ was chosen sufficiently low for there to be no differences, within statistical errors, between simulations carried out at $T_0$ and $2T_0$. The absence of any detectable differences between the exact and SSE results to a relative statistical accuracy of $\approx 10^{-5}$ illustrates the unbiased nature of these calculations.

The SSE algorithm developed here can be extended straightforwardly to J-K models with four-spin exchange terms on other lattices. For example, implementation of the Hamiltonian on the triangular and kagome lattices is possible for some parameter regimes without being hampered by the sign problem. In particular, quantum Monte Carlo simulations at or near the RK-point ($J = 0, -K = V$) are anticipated to make explicit connection with predictions from analytical theories. Studies on these models are underway, and are expected to reveal a rich variety of ground state phenomenon.

In principle, the scheme can be extended also to multi-spin interactions on rings with more than four spins, for example the XY model with six-spin exchange on the pyrochlore lattice. However, it is clear that the directed-loop scheme will then become quite complex, and explicit solutions of the type we have presented here may not be practical.

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