Many-Configuration Markov-Chain Monte Carlo

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We propose a minimal generalization of the celebrated Markov-Chain Monte Carlo algorithm which allows for an arbitrary number of configurations to be visited at every Monte Carlo step. This is advantageous when a parallel computing machine is available, or when many biased configurations can be evaluated at little additional computational cost. As an example of the former case, we report a significant reduction of the thermalization time for the paradigmatic Sherrington-Kirkpatrick spin-glass model. For the latter case, we show that, by leveraging on the exponential number of biased configurations automatically computed by Diagrammatic Monte Carlo, we can speed up computations in the Fermi-Hubbard model by two orders of magnitude.

I. INTRODUCTION

The Markov-Chain Monte Carlo method [1] (MCMC) is a generic algorithm that allows to draw samples from a given unnormalized probability distribution. It has found applications in many areas of science, in particular in classical and quantum physics [2–4], and statistics [5].

The Markov-chain thermalization time is one of the critical properties of the MCMC algorithm [6]. Also known as mixing time, it is the time it takes for the Markov chain to approach the steady-state distribution, which is sometimes called the thermal-equilibrium distribution in statistical physics. In the context of a Monte Carlo calculation, the thermalization time is the time one needs to wait before accumulating statistics. If it is larger than the total number of Monte Carlo steps, the MCMC technique is not applicable. Another critical property is the autocorrelation time, which is defined as the time it takes to draw two uncorrelated samples from the Markov chain, after the thermalization time has passed. It can be reduced linearly by using a parallel computing machine running independent Markov chains, while the thermalization time cannot be reduced indefinitely with this approach. Introducing couplings between Markov chains has been shown to help reduce the thermalization time: one usually either considers chains at different temperatures [7,8], or constructs unbiased estimators [9]. Another strategy to reduce thermalization time is the use of irreversible Markov chains [10,11], a method that has recently been extended to allow for parallelization [12]. On the other hand, quasi-Monte Carlo techniques [13] do not have a thermalization time by construction, and have recently been successfully applied to quantum impurity problems [14], but their application to large configurations spaces has not yet been fully explored.

In some situations, one is able to generate many biased proposals for new configurations of the Markov chain with little or no additional computational effort. This is the case, for instance, with some variants of the Diagrammatic Monte Carlo technique as they automatically generate an exponential number of configurations at each Monte Carlo step at no additional cost [15–20]. Here, the MCMC algorithm can only consider one configuration at a given Monte Carlo step, and there is no way to use the information of the multiple biased configurations that have been generated.

In this paper, we propose a minimal generalization of the Markov-Chain Monte Carlo algorithm, which we call Many-Configuration Markov-Chain Monte Carlo (MCMCMC), that allows to consider multiple configurations at the same Monte Carlo step. This guarantees a straightforward parallelization of the computation in order to reduce the thermalization time, as well as allowing for the use of many biased configurations that might be available at a given Monte Carlo step.

The document is organized as follows: In Sec. II we formulate and motivate the problem which this work addresses; In Sec. III we present an intuitive picture of the MCMCMC technique by considering the case of two and three configurations explicitly; In Sec. IV we present benchmark results for the Sherrington-Kirkpatrick spin-glass model, showing how the use of a parallel machine can drastically reduce the thermalization time; In Sec. V we provide numerical results for the Fermi-Hubbard model within Diagrammatic Monte Carlo using a specifically designed version of the MCMCMC algorithm.

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II. PROBLEM STATEMENT

The MCMC method is based on the generation of a sequence of states, called Markov chain, such that the transition probability between these states depends only on the current state. The goal of a MCMC algorithm is to build a Markov chain such that, for every initial state, the probability of a given state converges to an arbitrary “equilibrium” probability distribution $P_{eq}$ in the long-time limit. The Markov chain is usually built by proposing a new state $c_1$ given the current state $c_0$ with a certain, arbitrary, proposal probability distribution, $P_{prp}(c_1 | c_0)$, which is easy to sample from; then, in the simplest form of MCMC, the proposed state is accepted or rejected according to the Metropolis rate satisfying detailed balance: \[ \min(1, \frac{P_{eq}(c_1)P_{prp}(c_0 | c_1)}{(P_{eq}(c_0)P_{prp}(c_1 | c_0))}). \]

While being an extremely general and powerful algorithm, there are situations where the sequential generation of new configurations leads to inefficiency. In the following, we will consider two such situations:

1. A parallel computing machine is available, and the thermalization time for the Markov chain is non-negligible
2. It is possible to compute a large number of biased configurations with little or no additional computational effort

In this paper, we present a solution to the following problem: What is a minimal modification of Markov-Chain Monte Carlo that allows to take advantage of one (or both) of these possibilities?

As already mentioned, the difficulty of MCMC in dealing with these situations can be traced back to its sequential definition: The Markov chain is built by considering only one new configuration at a given Monte Carlo step, and there is no way to simultaneously use the information from multiple configurations. Even if multiple configurations can be generated, only at most one of them can be accepted. In particular, in the presence of non-negligible thermalization time, there is little advantage in using a parallel computing machine over a single-core machine as any statistics accumulated before thermalization has completed cannot be used.

III. INTUITIVE PICTURE

Below, we aim at providing the reader with an intuitive picture of the novel algorithm presented in this work, Many-Configuration Markov-Chain Monte Carlo (MCMCMC hereafter), in the graph version [the set version is discussed in the Appendix, see Sec. A 3]. Here, we do not provide complete derivations and proofs, all of which can be found in Appendix A.

Let us first describe a standard version of MCMC in a language that will easily allow for its generalization. Using the notation of Fig. 1, let us suppose that, at a given Monte Carlo step, the Markov-chain state is the configuration $c_0$, which belongs to some configuration space we want to sample in. We propose a new configuration $c_1$ as the next state of the Markov chain, where $c_1$ is proposed given $c_0$ with some probability distribution $P_{prp}(c_1 | c_0)$.
\(P_{\text{prp}}\) can be freely chosen as long as it is guaranteed that the Markov chain is ergodic. We schematically depict this proposal process with a directed graph composed of the nodes \(c_0\) and \(c_1\), and of an arrow connecting \(c_0\) to \(c_1\) [see Fig. 1]. In order for the Markov chain to converge to a given equilibrium distribution \(P_{\text{eq}}\), it is sufficient to impose the detailed-balance condition:

\[
P_{\text{eq}}(c_i) P_{\text{prp}}(c_i | c_0) P_{\text{acc}}(c_1 | c_0) = P_{\text{eq}}(c_0) P_{\text{prp}}(c_0 | c_1) P_{\text{acc}}(c_1 | c_1),
\]

where \(P_{\text{acc}}(c_j | c_k)\) is the probability of accepting the proposed configuration \(c_k\) as the next Markov-chain state when proposing it from the configuration \(c_j\). In Fig. 1 we represent the detailed-balance process by an undirected graph with double arrows. After the acceptance/rejection process, the Markov-chain state is either \(c_0\) or \(c_1\), and this whole procedure is repeated at the next Monte Carlo step.

We now introduce the MCMCMC algorithm as a natural many-configuration generalization of MCMC. Let \(c_0\) be the Markov-chain state at a given Monte Carlo time step. We want to follow as closely as possible the MCMC procedure illustrated in Fig. 1. For this reason, we want to find a way to propose multiple configurations by repeatedly using the “two-body” probability distribution \(P_{\text{prp}}(c_k | c_j)\) introduced above. A natural way to achieve this is sketched in Fig. 2. We consider the configurations \(c_0, \ldots, c_5\) to be nodes of a directed graph; an arrow going from \(c_j\) to \(c_k\) means that the node \(c_k\) has been proposed using the probability distribution \(P_{\text{prp}}(c_k | c_j)\).

The graph structure and generation process are completely arbitrary; in the following we will detail some of the possible choices. In the MCMC procedure described above, once the graph is generated, one of the two configurations is chosen as the Markov-chain state at the next step. In the case of MCMCMC, as the graph we consider at each step can be very big, we want to make full use of all the proposed configurations. For this reason, we add a thermalization phase: All the nodes of the graph are visited a fraction of time proportional to the rate at which they would be chosen according to the detailed-balance condition between configurations belonging to the same undirected graph [see Fig. 2]. After this thermalization phase, a node of the graph is chosen with a probability proportional to the rate in which it is visited, and the process is iterated.

In the rest of this section we want to progressively motivate MCMCMC as a minimal extension of MCMC by considering the case of three proposed configurations per Monte Carlo step in detail. For this reason, we are going to present three algorithms that “interpolate” between MCMC and MCMCMC: the first is a rewriting of the standard MCMC with a heat-bath acceptance rate within the graph language we use in this paper, the second is a modification of the first where we visit multiple configurations at each Monte Carlo step, and the third is a MCMCMC algorithm for many configurations that we specialize to the case of three configurations.

\[R_{(0,1)} := c_0 \rightarrow c_1\]
\[R_{(1,0)} := c_0 \rightarrow c_2\]

\[T := c_0 \leftrightarrow c_1 \leftrightarrow c_2\]

FIG. 3. Top: in \(R_{(0,1)}\) the configuration \(c_1\) is generated from \(c_0\). Center: in \(R_{(1,0)}\) the configuration \(c_0\) is generated from \(c_1\). Bottom: the undirected graph \(T\) describes the two processes.

A. MCMC in the language of graphs

We now discuss in more detail the MCMC algorithm of Fig. 1 highlighting its graphical interpretation. We suppose that, at a given Monte Carlo step, the Markov-chain state is the configuration \(c_0\). As discussed above, we propose the configuration \(c_1\) as the next Markov-chain state given \(c_0\) with the probability distribution \(P_{\text{prp}}(c_1 | c_0)\). We can represent this process by a directed graph \(R_{(0,1)}\) with two nodes, \(c_0\) and \(c_1\), and an arrow connecting the configuration \(c_0\) to the configuration \(c_1\), as illustrated in Fig. 2.

As we want to use detailed balance, we also need to consider the inverse process in which the configuration \(c_0\) is proposed from \(c_1\). We can represent the inverse process by a directed graph \(R_{(1,0)}\) with the same nodes as \(R_{(0,1)}\) and opposite direction for the arrow [see Fig. 3]. Finally, we introduce the undirected graph \(T\) having the same nodes as \(R_{(0,1)}\) and \(R_{(1,0)}\) [see Fig. 3]. We define \(P_{\text{acc}}(c | T)\) as the probability of accepting a node \(c \in \{c_0, c_1\}\) of the undirected graph \(T\) as the next state of the Markov chain, which, for simplicity, we choose to be independent on the creation history of \(T\). We decide to impose the detailed balance condition independently on any such \(T\):

\[
P_{\text{eq}}(c_0) P_{\text{prp}}(T | c_0) P_{\text{acc}}(c_1 | T) = P_{\text{eq}}(c_1) P_{\text{prp}}(T | c_1) P_{\text{acc}}(c_0 | T),
\]

where we defined \(P_{\text{prp}}(T | c_0) := P_{\text{prp}}(c_1 | c_0)\) as the probability of proposing \(c_1 | c_0\) given \(c_0\), as discussed above. We remark that while Eq. 1 is equivalent to the interpretation is different: In Eq. 2 we have directly imposed the detailed balance condition independently on any such \(T\):

\[
P_{\text{acc}}(c | T) := \frac{P_{\text{eq}}(c) P_{\text{prp}}(T | c)}{\sum_{c' \in V(T)} P_{\text{eq}}(c') P_{\text{prp}}(T | c')},
\]

where \(V(T) := \{c_0, c_1\}\) is the set of nodes of \(T\). This is equivalent to standard MCMC with a “heat-bath” acceptance rate.
FIG. 4. The two directed graphs of configurations that can be generated starting from $c_0$.

$R_{\{(0,1),(0,2)\}} := \begin{array}{c}
\bullet \\
\rightarrow \\
\bullet
\end{array}$

$R_{\{(0,1),(1,2)\}} := \begin{array}{c}
\bullet \\
\bullet
\end{array}$

FIG. 5. Directed graphs that correspond to the same undirected graph $T$.

$R_{\{(0,1),(1,2)\}} := \begin{array}{c}
\bullet \\
\bullet
\end{array}$

$R_{\{(1,0),(1,2)\}} := \begin{array}{c}
\bullet \\
\bullet
\end{array}$

$R_{\{(1,0),(2,1)\}} := \begin{array}{c}
\bullet \\
\bullet
\end{array}$

$T := \begin{array}{c}
\bullet \\
\bullet \\
\bullet
\end{array}$

B. Generalization to three configurations per Monte Carlo step

In this section we generalize the procedure of Sec. III A to the case of three configurations per Monte Carlo step, for a particular graph-generation process. The main purpose of this section is to give the intuition behind the procedure, without providing a proof for all the statements, which is left to the Appendix [see Sec. A 2].

Suppose that, at a given Monte Carlo step, the Markov-chain state is $c_0$. We propose a new configuration $c_1$ with probability $P_{\text{prp}}(c_1 | c_0)$, analogously to what is done in Sec. III A. At this point, there are two possibilities: With probability $p$, we generate a new configuration $c_2$ from $c_0$ with generation probability $P_{\text{prp}}(c_2 | c_0)$; otherwise, with probability $q = 1 - p$, we generate a new configuration $c_1$ from $c_1$ with generation probability $P_{\text{prp}}(c_1 | c_1)$. We represent these two processes by two directed graphs, which we respectively denote by $R_{\{(0,1),(0,2)\}}$ and $R_{\{(0,1),(1,2)\}}$ [see Fig. 4]. Suppose that we have stochastically chosen to generate the first directed graph in Fig. 4, $R_{\{(0,1),(1,2)\}}$. Let $T$ be the undirected graph with the same nodes as $R_{\{(0,1),(1,2)\}}$ [see Fig. 5]. We consider all the directed graphs that have the same nodes as $T$, and edges that can be obtained from $T$ by removing one arrow per edge: these are $R_{\{(0,1),(2,1)\}}$, $R_{\{(1,0),(1,2)\}}$, and $R_{\{(1,0),(2,1)\}}$; they correspond to the different ways of generating the graph $T$ starting from one of the nodes [see Fig. 6 for the definition].

As the next Markov-chain state, we choose $c \in \{c_0, c_1, c_2\}$ with probability $P_{\text{acc}}(c | T)$, a quantity that only depends on the undirected graph $T$. In order to have a useful Monte Carlo process, we need to impose that the average time spent in a given configuration $c$ coincides with $P_{\text{eq}}(c)$. For this, it is sufficient to impose the detailed balance condition:

$$P_{\text{eq}}(c_j) \frac{P_{\text{prp}}(T | c_j)}{P_{\text{prp}}(T | c_k)} P_{\text{acc}}(c_k | T) = P_{\text{eq}}(c_k) \frac{P_{\text{prp}}(T | c_k)}{P_{\text{prp}}(T | c_j)} P_{\text{acc}}(c_j | T),$$  \hspace{1cm} (4)

FIG. 6. Discrete and continuous Monte Carlo time steps in MCMC. A discrete step corresponds to the generation of a new graph of configurations. A continuous step is a virtual update between two configurations which are connected by an edge within a given graph, a process which we refer to as “thermalization” of the undirected graph.

where $c_j$ and $c_k$ are nodes of the undirected graph $T$.

It can be shown [see Sec. A 2] that the following choice satisfies detailed balance:

$$P_{\text{acc}}(c | T) := \frac{P_{\text{eq}}(c) P_{\text{prp}}(T | c)}{\sum_{c' \in V(T)} P_{\text{eq}}(c') P_{\text{prp}}(T | c')},$$  \hspace{1cm} (5)

where $V(T) := \{c_0, c_1, c_2\}$ is the set of nodes of the graph $T$, and $P_{\text{prp}}(T | c)$ is the probability of generating the graph $T$ from $c$, which, for the specific stochastic graph generation process we consider in this section, is given by

$$P_{\text{prp}}(T | c_0) = P_{\text{prp}}(c_1 | c_0) q P_{\text{prp}}(c_2 | c_1)$$

$$P_{\text{prp}}(T | c_1) = 2 P_{\text{prp}}(c_0 | c_1) p P_{\text{prp}}(c_2 | c_1)$$

$$P_{\text{prp}}(T | c_2) = P_{\text{prp}}(c_1 | c_2) q P_{\text{prp}}(c_0 | c_1),$$  \hspace{1cm} (6)

where we have taken into account the two ways of generating $T$ given $c_1$.

C. Visiting many configurations in one Monte Carlo step by “thermalization” of the undirected graph

In order to render the algorithm more efficient when many configurations are simultaneously available, we introduce a modification of the Markov chain definition that allows to visit multiple configurations per Monte Carlo step. We call this extension the “thermalization” of the undirected graph [see Fig. 5]. As an intuitive picture, we can imagine that the generated undirected graph of configurations is the whole configuration space for one time step, and continuous-time Monte Carlo updates are made between nodes of the graph. Formally, this will be simply done by renaming the “probability of proposal of configurations”, $P_{\text{prp}}$, to the “probability of generation of configurations”, $P_{\text{gen}}$, and interpreting the probability of acceptance of a configuration $P_{\text{acc}}$ as the fraction of time spent in a node of the graph $P_{\text{node}}$.

A powerful way to formalize this concept is by considering a Markov chain of undirected graphs instead of the usual Markov chain of configurations. Suppose that at a given Monte Carlo step the Markov-chain state is the undirected graph $T$ consisting of the nodes $c_0$ and $c_1$ [see Fig. 6]. We generate the next state of the Markov
chain, $T'$, in the following way: We choose one of the nodes of $T$, say $c_0$, with a certain probability distribution $P_{\text{node}}(c_0|T)$ that coincides with $P_{\text{acc}}(c_0|T)$ [defined in Sec. II A]. We then generate the new state of the Markov chain, $T'$, with a probability $P_{\text{gen}}(T'|c_0)$ that coincides with $P_{\text{prp}}(T'|c_0)$ [$P_{\text{prp}}$ is introduced in Sec. II A]. To this discrete-time Markov chain of undirected graphs, we associate a Markov chain of configurations in continuous time in the following way: Suppose that the Markov-chain state at discrete time $j$ is $T$. For a continuous time $t$ such that $j \leq t < j + 1$, we spend a fraction of the time equal to $P_{\text{node}}(c|T)$ in a given configuration $c$ of the undirected graph $T$ [see Fig. 6 for an intuitive picture]. For any given $P_{\text{gen}} \equiv P_{\text{prp}}$, we adjust $P_{\text{node}}$ to achieve an average time of $P_{\text{eq}}(c)$ spent in each configuration $c$. It can be shown that substituting $P_{\text{acc}}$ with $P_{\text{node}}$ and $P_{\text{prp}}$ with $P_{\text{gen}}$ in Eq. (3) guarantees this equilibrium condition. In Sec. A 2 we provide a formal proof of this fact.

IV. APPLICATION TO A SPIN-GLASS MODEL

A. The Sherrington-Kirkpatrick model

We now present the implementation of the MCMCMC algorithm for the Sherrington-Kirkpatrick model, defined by the energy

$$E(\{J_{jk}\}, \{S_j\}) := \frac{1}{\sqrt{T}} \sum_{0 \leq j < k \leq L-1} J_{jk} S_j S_k$$

(7)

where $L$ is the system size, $S_j \in \{-1, 1\}$, and $J_{jk} \in \mathbb{R}$ are random gaussian numbers of zero mean and unit variance. We consider the average energy per site:

$$\langle E \rangle := \frac{\sum_{\{S_j\}} e^{-E(\{J_{jk}\}, \{S_j\})/T} E(\{J_{jk}\}, \{S_j\})/L}{\sum_{\{S_j\}} e^{-E(\{J_{jk}\}, \{S_j\})/T}}$$

(8)

where $T$ is the temperature. The model can be solved exactly in the thermodynamic limit \cite{22}, and at the critical temperature $T_c$ the system undergoes a replica-symmetry-breaking phase transition. The motivation to study it numerically is the fact that close but above the critical temperature, the system thermalizes very slowly, and can therefore be used as a benchmark for our technique. We consider here directly the critical case $T = T_c$.

B. Numerical results

We have compared the following algorithms for the Sherrington-Kirkpatrick model simulation: the simplest local MCMC algorithm; the MCMCMC extension of the local MCMC with the line-graph addition process [see Sec. B 1 for details]; and the graph populating process for a $k$-ary tree [see Sec. B 2 for details].

In Fig. 7 we present the results of the numerical comparison between the standard local Metropolis MCMC algorithm with a single update, and various MCMCMC techniques differing by graph structure. We see that the thermalization time is decreased by two orders of magnitude, proving therefore the success of the algorithm in dramatically reducing the thermalization time.

V. APPLICATION TO LATTICE FERMIONS

A. The Fermi-Hubbard model

We consider the doped two-dimensional fermionic Hubbard model \cite{22}:

$$H = \sum_{k, \sigma} (\epsilon_k - \mu) c_{k,\sigma}^\dagger c_{k,\sigma} + U \sum_i n_i \uparrow n_i \downarrow.$$  

(9)

Here $\mu$ denotes the chemical potential, $k$ the momentum, $\sigma \in \{\uparrow, \downarrow\}$ the spin, $U$ the onsite repulsion strength, $i$ labels lattice sites, and the (square lattice) dispersion is given by

$$\epsilon_k = -2t \cos(k_x) \cos(k_y),$$

(10)

where $t$ is the nearest-neighbor hopping amplitude (we set $t = 1$ in our units). We further define $T$ as the temperature and $n$ as the density.

In the chosen parameter regime of $T = 0.1$ and $n = 0.875$, one needs around ten well-computed expansion coefficients for the double occupancy (errorbars below 1%) to be able to resum the resulting series at interaction...
strength $U = 8$, which represents a much investigated strongly correlated regime of the model with stripe magnetic order in the ground state [25][27].

B. Numerical results

As traditional Quantum Monte Carlo techniques are affected from the fermionic sign problem when simulating the repulsive Hubbard model away from half filling, we use Diagrammatic Monte Carlo, which allows to circumvent this issue by sampling Feynman diagrams directly in the thermodynamic limit. We hereafter use a MCMCMC algorithm for sets we specifically developed for use within the Connected Determinant Diagrammatic Monte Carlo (CDet) [15] [see Sec. C for a CDet introduction]. The reader can find more details about the set generating process we use in the Appendix, Sec. D.

To assess relative performance of MCMCMC and MCMC we compare the stochastic error bars obtained after a given time (about one hour) on a single CPU processor [see Fig. 8]. For a given order we run the MCMCMC algorithm at order higher than the standard MCMC as this is optimal for the MCMCMC performance. Both algorithms spend around 10% of their time on normalisation. We report an improvement of up to two orders of magnitude in the computational time needed to reach a given stochastic error for the highest expansion coefficient 12, and, importantly, we observe that the improvement grows as a function of order.

![Graph showing improvement in computational time needed to reach a given stochastic error for a given expansion coefficient of the double occupancy as a function of expansion order for the Fermi-Hubbard model in the thermodynamic limit, at $T = 0$.](image)

FIG. 8. Improvement in computational time needed to reach a given stochastic error for a given expansion coefficient of the double occupancy as a function of order for the Fermi-Hubbard model in the thermodynamic limit, at $T = 0.1$ and 1/8 doping.

VI. CONCLUSION

In this paper we have introduced a minimal generalization of the Markov-Chain Monte Carlo algorithm that allows to consider multiple configurations at the same Monte Carlo step. This new technique permits straightforward parallelization, as well as giving the possibility of using an arbitrary number of biased configurations at the same Monte Carlo step.

After giving an intuitive picture of the algorithm based on a graphical interpretation, we have presented numerical results for spin-glass and quantum fermionic models, showcasing the generality and the potential of this new technique. More specifically, we have shown that, for the Sherrington-Kirkpatrick model, a very significant reduction of thermalization time can be achieved when many configurations are considered at each Monte Carlo step. We have further shown how we can use the knowledge from all subsets of diagram configurations within the Connected Determinant Diagrammatic Monte Carlo method to further improve its computational efficiency, and we have presented benchmark results for the paradigmatic Fermi-Hubbard model away from half-filling where a speedup of up to two orders of magnitude was observed at twelve Feynman loops.

We believe that our work has potential applications to areas where Markov-chain Monte Carlo techniques are often considered too computationally intensive due to their non-parallelizable nature, such as big data Bayesian inference [28]. More generally, the Markov-chain Monte Carlo algorithm for multiple configurations we have introduced in this paper will be potentially applicable to situations where the thermalization time is an issue and a parallel computing machine is available, or when many biased configurations can be evaluated at little computational effort.

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Appendix A: General theory

1. Markov chain of configurations

In this section we review the standard MCMC algorithm. We consider a discrete configuration space $S$. The Markov chain is usually defined as an infinite sequence of configurations $(c(j = 1), c(j = 2), ...), c(j) \in S$, indexed by a discrete “time” $j$, such that a configuration $c(j + 1)$ is generated stochastically using only $c(j)$ as input. Let
us define $P_{eq}(c)$ as the average time spent in the configuration $c \in S$:

$$P_{eq}(c) := \lim_{j \to \infty} \frac{1}{j} \sum_{j=1}^{J} \delta_{c,c(j)}$$ (A1)

We also define $P((c, j))$ as the probability of being in the configuration $c$ at discrete time $j$. We consider a Markov chain such that (at least on average)

$$\lim_{j \to \infty} P((c, j)) = P_{eq}(c).$$ (A2)

The MCMC algorithm is particularly useful to compute average values of an “observable” $O$, which takes as arguments elements of the configuration space $S$:

$$O := \frac{\sum_{c \in S} w(c) O(c)}{\sum_{c \in S} w(c)}$$ (A3)

where $w(c) \geq 0$ for every $c$. If the condition

$$P_{eq}(c) = \frac{w(c)}{\sum_{c' \in S} w(c')}$$ (A4)

is satisfied for every $c \in S$, then we can compute $O$ as a time average of $O(c(j))$, where $c(j)$ is the Markov-chain state at discrete time $j$:

$$O = \lim_{j \to \infty} \frac{1}{j} \sum_{j=1}^{J} O(c(j)).$$ (A5)

2. Markov chain of graphs of configurations

In this section, we generalize the standard MCMC formalism of Sec. [11] to a Markov chain consisting of an infinite sequence of undirected graphs of configurations $(T(j) = 1), T(j) = 2), \ldots$, such that the set of nodes of $T(j)$, $V(T(j))$, is contained in $S$, and such that $T(j + 1)$ is stochastically generated using only $T(j)$ as input. We can introduce the average time spent in a given graph $T \subseteq S$

$$P_{eq}(T) = \lim_{j \to \infty} \frac{1}{J} \sum_{j=1}^{J} \delta_{T,T(j)}.$$ (A6)

At a continuous time $t \in [j, j + 1], j \in \mathbb{N}$, we imagine visiting a configuration $c \in V(T(j))$ with a certain probability $P((c, t) | (T, j))$ which we impose to be time-independent, and we call it $P_{node}$:

$$P_{node}(c | T) := P((c, t) | (T, j)).$$ (A7)

We assume this probability to be normalized to one: If the graph $T$ belongs to the Markov chain at time $j \in \mathbb{N}$, then for every $t \in [j, j + 1]$, the system can be in only one node $c \in V(T)$ of the graph $T$ at at time, which is equivalent to imposing

$$\sum_{c \in V(T)} P_{node}(c | T) = 1$$ (A8)

for every undirected graph $T$.

The Markov chain of undirected graphs is built with the sole purpose of computing average values of functions defined in the nodes of the graph. Therefore, if we define

$$P_{eq}(c) = \sum_{T : V(T) \ni c} P_{eq}(T) P_{node}(c | T)$$ (A9)

and if we impose Eq. [A4], we can compute observables in configuration space from the Markov chain in graph space:

$$O = \lim_{j \to \infty} \frac{1}{J} \sum_{j=1}^{J} \sum_{c \in V(T(j))} P_{node}(c | (T(j))) O(c)$$ (A10)

where $O$ is defined in Eq. [A3]. The advantage of this formulation compared to Eq. [A5] is that we can consider multiple configurations at a given Monte Carlo step $j$, and visit each one of them.

We now show how to compute $P_{node}$ from the graph transition probability, which is a free parameter in this formulation. While we could choose an arbitrary graph transition probability, here we limit ourselves to the following choice: the new graph is generated starting from one of the vertices of the old graph

$$P((T', j + 1) | (T, j)) := \sum_{c \in V(T) \setminus V(T')} P_{node}(c | T) P_{gen}(T' | c),$$ (A11)

where $P_{gen}(T' | c)$ is the probability of generating a graph $T$ starting from a node $c$. $P_{gen}$ can be chosen in a completely arbitrary way, but a choice of $P_{gen}$ constrains the form of $P_{node}$. We will impose the detailed balance condition in configuration space, which is defined as

$$P((c, t), (c', t')) = P((c', t), (c, t')),$$ (A12)

where $c, c' \in S, t < t'$, and $t, t' \in \mathbb{R}^+$ are much larger than the thermalization time. First of all, we remark that in our Monte Carlo process there are no transitions at non-integer times; therefore, we can suppose $t' = j \in \mathbb{N}$, and $t = t' - 0^+$. We then obtain

$$P((c, j - 0^+), (c', j)) = \sum_{T : V(T) \ni c} P_{eq}(T) P_{node}(c | T) \times$$

$$\sum_{T' : V(T') \ni c'} P((T', j) | (T, j - 1)) P_{node}(c' | T).$$ (A13)

By using Eq. [A11], one can verify that the choice

$$P_{node}(c | T) := \frac{P_{eq}(c) P_{gen}(T | c)}{P_{eq}(T)}$$ (A14)
satisfies detailed balance [Eq. (A12)]. We remark that the probability of being in the undirected graph $T$, $P_{eq}(T)$, does not need to be computed as one can use the normalization condition [see Eq. (A8)].

3. Markov chain of sets of configurations

In this section we consider a version of the Markov chain algorithm for sets of configurations. We consider a Markov chain consisting of an infinite sequence of sets of configurations $(S(j = 1), S(j = 2), \ldots)$, such that $S(j)$ is a set of fixed cardinality $n \in \mathbb{N}$, $n > 0$, contained in $\mathcal{S}$, and such that the $S(j + 1)$ is stochastically generated using only $S(j)$ as input. We can introduce the average time spent in a given set $S \subseteq \mathcal{S}$ as

$$P_{eq}(S) = \lim_{J \to \infty} \frac{1}{J} \sum_{j=1}^{J} \delta_{S,S(j)}.$$  \hspace{1cm} (A15)

At a continuous time $t \in [j, j + 1], j \in \mathbb{N}$, we visit a subset $S' \subseteq S$ with a certain probability $P((S',t) | (S,j))$, which we impose to be time-independent:

$$P_{\text{subset}}(S'|S) := P((S',t)| (S,j)).$$ \hspace{1cm} (A16)

We assume this probability to be normalized to one: if $S$ is the Markov-chain state at discrete time $j$, then we must be in one and only subset $S' \subseteq S$ for every continuous time $t \in [j, j + 1]$, which is equivalent to imposing

$$\sum_{S' \subseteq S} P_{\text{subset}}(S'|S) = 1$$ \hspace{1cm} (A17)

for every $S \subseteq \mathcal{S}$ such that $|S| = n$. We would like to evaluate

$$O_u := \sum_{S \subseteq \mathcal{S} : |S| = u} w(S) O(S)$$ \hspace{1cm} (A18)

for $u \in \{0, 1, \ldots, n\}$, and $w(S) \geq 0$. We introduce $\lambda_u > 0$ for $u \in \{0, \ldots, n - 1\}$, and define

$$\mathcal{N}_n := \sum_{S \subseteq \mathcal{S} : |S| < n} \lambda_u |S| w(S).$$ \hspace{1cm} (A19)

We impose that the Markov chain thermalizes to the following probability distribution for sets of cardinality less than $n$

$$P_{eq}(S) = \frac{\lambda_u |S| w(S)}{\mathcal{N}_n},$$ \hspace{1cm} (A20)

for $S \subseteq \mathcal{S}, |S| < n$. We see that $\lambda_u$ is just a reweighting parameter between different cardinalities $u$. We can therefore estimate $O_u$ as

$$O_u = \lim_{J \to \infty} \frac{\mathcal{N}_n}{J} \sum_{j=0}^{J-1} \sum_{S' \subseteq S(j), |S'| = u} \frac{P_{\text{subset}}(S'|S(j)) O(S')}{\lambda_u},$$ \hspace{1cm} (A21)

for $u \in \{0, 1, \ldots, n - 1\}$, and

$$O_n = \lim_{J \to \infty} \frac{1}{J} \sum_{j=1}^{J} \frac{w(S(j)) O(S(j))}{|S|! P_{eq}(S(j))}.$$ \hspace{1cm} (A22)

We see therefore that we can consider many subset configurations at each Monte Carlo step.

We now show how to compute $P_{\text{subset}}$ from the set transition probability. We could choose an arbitrary set transition probability, but we limit ourselves to the case where the new set is generated starting from a subset:

$$P((S',j + 1) | (S,j)) = \sum_{S' \subseteq S} P_{\text{subset}}(S'|S) P_{\text{gen}}(S'|S')$$ \hspace{1cm} (A23)

where $S \neq S'$, and $|S'| = |S| = n$. The set generation function $P_{\text{gen}}$ can be chosen in an arbitrary way. As done in Sec. A2, we impose detailed balance, that is, the probability of being at $S$ at time $t$ and at $S'$ at time $t'$ is equal to the probability of being in $S'$ at time $t$ and being in $S$ at time $t'$

$$P((S,t), (S',t')) = P((S',t), (S,t'))$$ \hspace{1cm} (A24)

for $t < t'$, $t, t' \in \mathbb{R}^+$ are both much larger than the thermalization time, and $S, S' \subseteq \mathcal{S}, |S| \leq n, |S'| \leq n$. As there are no transitions at non-integer times, we can just consider the case where $t = j - 0^+$ and $t' = j$, where $j \in \mathbb{N}$. Let us consider $S, S' \subseteq \mathcal{S}$ of cardinality less than $n$, $|S| < n, |S'| < n$. One has

$$P((S,j - 0^+), (S',j)) = \sum_{S'' : S' \subseteq S'', |S''| = n} P_{eq}(S'') P_{\text{subset}}(S'|S'') \times \sum_{S'' : S' \subseteq S'', |S''| = n} P_{\text{gen}}(S''|S'') P((S'',j) | (S'',j - 1)) \times P_{\text{subset}}(S'|S'').$$ \hspace{1cm} (A25)

By using Eq. (A23), we can show that the following choice for $P_{\text{subset}}$ satisfies detailed balance [Eq. (A24)]:

$$P_{\text{subset}}(S | S') = \frac{P_{eq}(S) P_{\text{gen}}(S | S)}{P_{eq}(S')},$$ \hspace{1cm} (A26)

for $S, S' \subseteq \mathcal{S}, |S| < n, |S'| = n$. We can compute $P_{eq}(S)$ for sets $S$ of cardinality $n$ by using Equation (A26) and the normalization condition [Eq. (A19)]

$$P_{eq}(S) = \sum_{S' \subseteq \mathcal{S}, |S'| \leq n} P_{eq}(S') P_{\text{gen}}(S | S'),$$ \hspace{1cm} (A27)

for $|S| = n$.

Remark: Using Eq. (A26) and Eq. (A20), we see that the explicit $\lambda_u$ factor in Eq. (A21) simplifies to one and we can safely take the $\lambda_u \to 0^+$ limit for some $u \in \{0, 1, \ldots, n - 1\}$. This means that we can accumulate statistics for sets that are never visited by the Markov chain.
Appendix B: Generating graphs of configurations

In this section we describe some choices for the graph-generation probability $P_{gen}$ introduced in Sec. A3. We introduce two classes of graph-generation process: addition processes [Sec. B1], and populating processes [Sec. B2].

1. Line-graph addition process

We consider here the following process: starting from the configuration $c$, we create a new configuration $c'$ with a probability given by some function $P_{gen}(c' \mid c)$, and we consider the graph with an edge between $c$ and $c'$. Suppose now that we have created a graph consisting of $c_0, c_1, \ldots, c_{l-1}$ such that $c_k$ is connected by an edge to $c_{k+1}$, for $k \in \{0, 1, \ldots, l - 2\}$. With probability $\frac{1}{2}$, we add a new vertex $c'$ connected to $c_0$ with the probability distribution $P_{gen}(c' \mid c_0)$, otherwise we add the vertex $c'$ to the graph connecting it to $c_{l-1}$ with the probability distribution $P_{gen}(c' \mid c_{l-1})$. If $T$ is the line-graph with $c_0, c_1, \ldots, c_{L-1}$ as nodes, one therefore has

$$P_{gen}(T \mid c_k) = \frac{1}{2^L} \left( \begin{array}{c} L \\ k \end{array} \right) \left( \prod_{k_l=0}^{k-1} P_{gen}(c_{k_l} \mid c_{k_l+1}) \right) \times \left( \prod_{k_{l}=k+1}^{L-1} P_{gen}(c_{k_{l-1}} \mid c_{k_l}) \right).$$

(B1)

2. General graph populating process

We now present a graph-generation process that is amenable to analytic treatment. The key point is that, if we first generate an “empty” graph, where no node is assigned, and we then populate the graph nodes with configuration values in such a way that the computation of $P_{gen}(T \mid c)$ becomes straightforward. We consider specifically a tree $T$. We choose a root $r$ for the tree, $r \in \{0, 1, \ldots, |V(T)| - 1\}$, with a given probability distribution $p_r$, which determines a rooted tree $R$. From the root $r$, we can populate the tree by generating a configuration for each edge of the rooted tree with the probability distribution $P_{gen}(c' \mid c')$, where $c$ and $c'$ are connected with an edge going from $c$ to $c'$. We can therefore write, assuming that $c$ is the root of the rooted tree $R$

$$P_{gen}(T \mid c) = p_r \prod_{(c,c') \in E(R)} P_{gen}(c' \mid c').$$

(B2)

One has complete freedom on $p_r$: the uniform choice is just $p_r = \frac{1}{|V(T)|}$, which gives a self-thermalizing tree if $P_{gen}$ is symmetric.

Appendix C: Introduction to Connected Determinant Diagrammatic Monte Carlo

Below we provide a very brief overview of CDet. We are interested in computing a physical observable $\mathcal{C}(\xi)$, which we express in terms of an infinite power series

$$\mathcal{C}(\xi) := \sum_{n=0}^{\infty} c_n \xi^n,$$

(C1)

where the expansion coefficients $c_n$ are computed from the stochastic sampling of multi-dimensional integrals over a set of $n$ internal variables $\{X_1, \ldots, X_n\} =: S$ corresponding to vertex positions in some arbitrary space:

$$c_n = \frac{1}{N_n} \int_S c(S),$$

(C2)

where $N_n$ is a normalisation constant and $c(S)$ represents the sum of weights for all topologically distinct connected graphs $T$ constructed from vertices in $S$ and obeying additional rules imposed by the choice of model and observable. The weight of a particular graph is given by the product of the weights of its edges $E(S)[i, j]$, which are functions of two vertex positions $X_i$ and $X_j$. We can write:

$$c(S) = \sum_{T \in \{i,j\} \in T} E(S)[i,j].$$

(C3)

In general, the number of distinct connected graph topologies grows factorially with the number of vertices and so does the computational cost of evaluating $c(S)$. However, in many cases it is possible to compute the related sum of the weights for all connected and disconnected graphs $a(S)$ at only polynomial or exponential cost [29]. In order to obtain $c(S)$, one needs to eliminate all disconnected diagrams from $a(S)$ using the recursive formula:

$$c(S) = a(S) - \sum_{S' \subseteq S \setminus X_1} c(S') a(S \setminus S'),$$

(C4)

where, in order to properly define connectivity, the sum is over all subsets $S'$ containing the arbitrarily chosen vertex $X_1$ from $S$. The cost of evaluating Eq. (C4) scales as $\mathcal{O}(3^n)$ with the number of vertices and, sometimes together with the evaluation of $a(S)$, represents the computational bottleneck of the CDet algorithm. It is important to note from Eq. (C4) that in order to compute $c(S)$ for a given set of vertices, one is obliged to compute $c(S')$ for all of its subsets $S'$, which can be used in computing lower order expansion coefficients $c_{n'}$, where $n' < n$. This means that in the process of computing the weight at order $n$ we are generating an exponential $(2^n - 1)$ amount of a lower order weights as a side product.
Appendix D: Generating sets of configurations

1. Stochastic generation of the set

In this section we define the stochastic process that we perform to generate a set $S$ of cardinality $n \in \mathbb{N}_0$ given a subset $S' \subseteq S$ and $|S'| = m$. Let $S_0 = S'$. Given $S_k$, $k \in \{m, m+1, \ldots, n\}$, we generate $S_{k+1}$ by adding a vertex to $S_k$ in the following way: We choose one element $e' \in S_k$ randomly, we generate a new element $e$ with the same arbitrary probability distribution $P_{\text{gen}}(e' \mid e')$, and we add it to $S_k$ to generate $S_{k+1} = S_k \cup \{e\}$. We then identify $S_n = S$.

2. Recursive exponential formula for the generation probability

We now show how to compute $P_{\text{gen}}(S \mid S')$ for $S' \subseteq S$, for a given $S$ of cardinality $n \in \mathbb{N}_0$, $|S| = n$. This is needed to compute $P_{\text{subset}}$ [see Eq. (A2)]. A brute force approach would result in an algorithm that scales factorially with $n$. We are going to present a recursive algorithm whose computational cost scales only exponentially with $n$. We define

$$\tilde{P}_S(S') := P_{\text{gen}}(S \mid S \setminus S') \quad (D1)$$

for $S' \subseteq S$. One has

$$\tilde{P}_S(\{e'\}) = \frac{1}{|S|} \sum_{e'' \in S \setminus \{e'\}} P_{\text{gen}}(e' \mid e'') \quad (D2)$$

for $e \in S$. For $S' \subseteq S$, the Chapman-Kolmogorov equation can be written as

$$\tilde{P}_S(S') = \frac{1}{|S|^{|S'|}} \sum_{e' \in S \setminus S'} \sum_{e'' \in S'} P_{\text{gen}}(e' \mid e'') \cdot \tilde{P}_S(S' \setminus \{e'\}) \quad (D3)$$

which now has only computational cost of $O(n 2^n)$. This computational cost is negligible in comparison to $O(3^n)$, which is the asymptotic computational scaling for the CDet [15] algorithm used for the evaluation of connected Feynman diagrams.

We can express the previous equation in words: In order to generate the subset $S$ from the set $S \setminus S'$, we need to first generate an element $e'$ of $S'$ starting from one element $e''$ of $S \setminus S'$, then generate the set $S$ from the set $S \setminus S' \cup \{e'\}$. We note that that the cardinality of the l.h.s. of Eq. (D3) is one higher than the cardinality of the r.h.s and therefore this equation can be solved recursively. This leads to a computational cost of $O(n^2 2^n)$. It is possible to improve upon this scaling by introducing a “cumulative” probability distribution $\tilde{P}_{\text{gen}}(S', e')$ which we compute recursively as:

$$\tilde{P}_{\text{gen}}(S', e') = \begin{cases} \sum_{e', e'' \in S', e' \neq e''} P_{\text{gen}}(e' \mid e'') & \text{if } |S'| = 1 \\ P_{\text{gen}}(S' \setminus \{e_s', e'\}) - P_{\text{gen}}(e_s' \mid e') & \text{otherwise} \end{cases} \quad (D4)$$

where $e_s' \in S'$ can be chosen arbitrarily as long as $e_s' \neq e'$. Then we can rewrite Eq. (D3) into

$$\tilde{P}_S(S') = \frac{1}{|S|^{|S'|}} \sum_{e' \in S'} \tilde{P}_{\text{gen}}(S', e') \tilde{P}_S(S' \setminus \{e'\}) \quad (D5)$$

for all $S' \subseteq S$.

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