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Stochastic lists: Sampling multi-variable functions with population methods

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We introduce the method of stochastic lists to deal with a multi-variable positive function, defined by a self-consistent equation, typical for certain problems in physics and mathematics. In this approach, the function's properties are represented statistically by lists containing a large collection of sets of coordinates (or "walkers") that are distributed according to the function's value. The coordinates are generated stochastically by the Metropolis algorithm and may replace older entries according to some protocol. While stochastic lists offer a solution to the impossibility of efficiently computing and storing multi-variable functions without a systematic bias, extrapolation in the inverse of the number of walkers is usually difficult, even though in practice very good results are found already for short lists. This situation is reminiscent of diffusion Monte Carlo, and is hence generic for all population-based methods. We illustrate the method by computing the lowest-order vertex corrections in Hedin's scheme for the Fröhlich polaron and the ground state energy and wavefunction of the Heisenberg model in two dimensions.

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I. INTRODUCTION

We are interested in the solution $F(\mathbf{x})$ of equations of the type

$$F(\mathbf{x}) = F_0(\mathbf{x}) + K[F(\mathbf{x})], \quad (1)$$

where the coordinate \mathbf{x} is high-dimensional. The (generically nonlinear) functional K can involve a number of integrations, multiplications and summations, but we do not consider differentiations. Ultimately, the solution of (1) is often used to compute integrals involving F and some other, more simple, functions. A straightforward approach to solve Eq. (1) is by fixed point iterations: Starting from a guess $F^{(0)}$, one computes the right-hand side, plugs the newly obtained $F^{(1)}$ into the right-hand side, and continues this iteration until, ideally, convergence is reached. However, as soon as the dimension is higher than three it becomes very difficult to efficiently compute and store the function F .

Equations of the above type typically occur in the self-consistent formulation of quantum field theory, such as the Hedin equations,¹ the Schwinger-Dyson equations,^{2,3} parquet equations,^{4,5} etc. They can also occur in the presence of spontaneous symmetry breaking, such as the Bardeen-Cooper-Schrieffer theory, when the ordering field has to be determined self-consistently. Whereas

the Green function, the self-energy, the polarization, and the effective interaction are typically two-dimensional in case of rotational and translational symmetry [i.e., there is one spatial (or momentum) coordinate and one time (or frequency) coordinate] and can be stored efficiently with standard grids, the irreducible three-point vertex is already five-dimensional in 3D. Studies attempting to solve the Hedin equations therefore often treat the vertex function as just a bare vertex, leading to the GW -approximation. Alternatively, the full function is represented by an infinite number of contributions that only involve relatively simple integrals [cf. the expansion of the Luttinger-Ward functional⁶ in the Baym-Kadanoff effective action^{7,8} (or its generalization to bosons^{9,10}) popular in the context of electronic structure calculations].

This problem—sometimes referred to as the curse of dimensions—is among the most prominent ones faced by diagrammatic Monte Carlo (DiagMC) methods. This is unsatisfactory, because the premise of the DiagMC simulation is precisely to deal with high dimensions while maintaining the central limit theorem. In this work, we introduce *stochastic lists*, a method in which the high-dimensional function $F(\mathbf{x})$ is represented by a stochastic list of coordinates $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_P$, with P the length of the list. Specifically, a positive F is considered as a probabilistic function with norm \mathcal{N} and faithfully represented as

$$\frac{1}{N} \int F(\mathbf{x}) d\mathbf{x} \leftrightarrow \frac{1}{P} \sum_{j=1}^P \delta(\mathbf{x} - \mathbf{x}_j). \quad (2)$$

The entries in the stochastic list are obtained by some Markov process (to be discussed later; the key property is that the values of $F(\mathbf{x})$ do not explicitly enter into the equation used for generation of the list entries), and can be refreshed by some protocol, which is non-Markovian. The list provides a faithful statistical representation of $F(\mathbf{x})$: any quantity of interest which can be written as some integral over F can be computed. In this work we assume that F is positive.

We benchmark the approach by considering two different systems. First, we study the Hedin equations for the Fröhlich polaron by computing the lowest order vertex corrections self-consistently. Second, we formulate the power method to find the ground state of a Hamiltonian in the language of stochastic lists and study the ground-state energy and wavefunction of the two-dimensional Heisenberg model. We find that, in practice, short lists give already remarkably accurate results. Typically, a power law extrapolation can be attempted over several decades in $1/P$. However, we found deviations for longer lists (in our examples when $P \gg 10^6$), which makes any extrapolation difficult (unless the stochastic error dominates at this point).

As is clear from the power method example, stochastic lists share a number of properties with the diffusion Monte Carlo method. An exponential scaling for diffusion Monte Carlo was reported previously in the literature and was related to the correlation within the population of walkers as a consequence of the population control mechanisms.¹¹ It seems therefore that all population-based methods ultimately scale exponentially, implying that for sufficiently large (and hard) systems the extrapolation cannot be done reliably to eliminate the systematic bias. This outcome also questions the practicality of the method for arbitrary (bosonic) problems. Nevertheless, for many realistic cases this scaling will not be seen (due to the dominance of the stochastic error), and by sufficient insight into the problem (such as choosing a very good guiding wavefunction) the prefactor can be substantially reduced such that the scaling is not an issue. This we can also demonstrate for stochastic lists.

This paper is structured as follows. In Section II, we study the non-crossing approximation and the lowest non-trivial order vertex corrections for the Fröhlich polaron problem. In Section III, we proceed with the ground state energy of the two-dimensional Heisenberg model, with a special emphasis on the numerical convergence of the stochastic process. We conclude in Section IV.

II. THE HEDIN EQUATIONS FOR THE FRÖHLICH POLARON PROBLEM

As a first application, we consider the Hedin equations for the Fröhlich polaron. This system has a positive expansion, and is known to be convergent at any finite temperature. It is hence free from the most important restriction on the DiagMC method, which is the series convergence. (Since the DiagMC algorithms work by iteration, they typically require a finite region of convergence.) Sign-positive representation also implies that there is no need to take special care of the diagram topologies, and one can proceed with standard Metropolis-Hastings sampling techniques.^{12,13} Therefore, the study of the Fröhlich polaron provides an ideal opportunity to benchmark the idea of stochastic lists in the context of vertex corrections.

A. Model

The Fröhlich polaron model describes the interaction between an itinerant electron and longitudinal optical phonons in insulators. Historically, it was the first problem to which the DiagMC method was applied^{14–16} and for which it was able to provide definite answers regarding the polaron spectrum and arbitrarily precise polaron energies for any coupling strength. The Hamiltonian in the thermodynamic limit is given by ($\hbar = 1$)

$$\begin{aligned} H &= H_{\text{el}} + H_{\text{ph}} + H_{\text{el-ph}} \\ H_{\text{el}} &= \int \frac{d^3k}{(2\pi)^3} \frac{k^2}{2m} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \\ H_{\text{ph}} &= \int \frac{d^3q}{(2\pi)^3} \omega_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} = \omega_{\text{ph}} \int \frac{d^3q}{(2\pi)^3} b_{\mathbf{q}}^\dagger b_{\mathbf{q}}, \\ H_{\text{el-ph}} &= \int \frac{d^3k d^3q}{(2\pi)^6} V(\mathbf{q}) (b_{\mathbf{q}}^\dagger - b_{\mathbf{q}}) a_{\mathbf{k}-\mathbf{q}}^\dagger a_{\mathbf{k}}, \\ V(\mathbf{q}) &= \frac{i\omega_{\text{ph}}}{q (2m\omega_{\text{ph}})^{1/4}} \left(\frac{4\pi\alpha}{V} \right)^{1/2} = \frac{i\tilde{\alpha}}{q}. \end{aligned} \quad (3)$$

The operators $a_{\mathbf{k}}$ and $b_{\mathbf{q}}$ are annihilation operators for electrons of mass m with momentum \mathbf{k} and phonons with momentum \mathbf{q} , respectively. The phonon frequency $\omega_{\mathbf{q}} \equiv \omega_{\text{ph}}$ can be taken momentum-independent for optical, longitudinal phonons. The dimensionless coupling constant is α . Typical values for α vary from 0.023 for InSb over 0.29 for CdTe to 1.84 for AgCl.¹⁷

Here we focus on the $T = 0$ case. In the imaginary-time representation, the bare propagator reads $G_0(\mathbf{k}, \tau) = -\theta(\tau) \exp\left[-\left(\frac{k^2}{2m} - \mu\right)\tau\right]$. The phonon propagator $D(\mathbf{q}, \tau) = (\tilde{\alpha}/q)^2 \exp(-\omega_{\text{ph}}\tau)$ remains unrenormalized and is dispersionless. We absorbed the modulus squared of the electron-phonon interaction potential into the phonon propagator for convenience (the two factors always enter the technique as a product). The method of stochastic lists can not deal with momentum or frequency conservation because all coordinates of

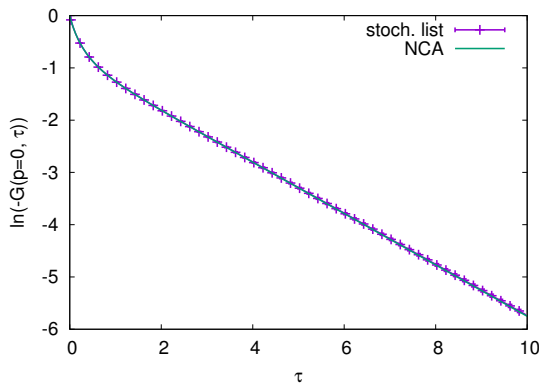


FIG. 1. (Color online.) Comparison of the Green function dependence on imaginary time at zero momentum, $-G(p=0, \tau)$, obtained in the NCA approximation between the stochastic list method (stoch. list) and an explicit evaluation. Data are shown for $\tilde{\alpha} = 5, \mu = -4$ and the list length $P = 10^6$.

the vertex function are generated by the list without restrictions. We therefore need to work in the imaginary-time, real-space representation, where the propagators for phonons and electrons read $D(\mathbf{r}, \tau) = \frac{\tilde{\alpha}^2}{4\pi r} \exp(-\omega_{\text{ph}}\tau)$ and $G_0(\mathbf{r}, \tau) = -\theta(\tau) \left(\frac{m}{2\pi\tau}\right)^{3/2} \exp(-\frac{mr^2}{2\tau} + \mu\tau)$, respectively.

B. The Non-Crossing Approximation

As a first application to set the ideas, we solve the Fröhlich polaron problem in the non-crossing approximation (NCA), which corresponds to the first-order skeleton diagram. The coupled set of NCA equations reads [we employ both (\mathbf{k}, ω_n) and (\mathbf{r}, τ) representations to simplify these equations]

$$\begin{aligned} \Sigma^{(1)}(\mathbf{r}, \tau) &= D(\mathbf{r}, \tau) G^{(1)}(\mathbf{r}, \tau), \\ G^{(1)}(\mathbf{k}, \omega_n) &= \frac{1}{G_0^{-1}(\mathbf{k}, \omega_n) - \Sigma^{(1)}(\mathbf{k}, \omega_n)}. \end{aligned} \quad (4)$$

Reference NCA data can be found in the lecture notes Ref. 18.

In order to solve these equations with stochastic lists, we cast the entire setup as a single self-consistent non-linear integral equation of the form (1):

$$G^{(1)}(X) = G_0(X) + \int \mathcal{I} d^4 X_1 d^4 X_2, \quad (5)$$

$$\mathcal{I} = G_0(X_1) G^{(1)}(X_2 - X_1) D(X_2 - X_1) G^{(1)}(X - X_2),$$

where we introduced the 4-dimensional space-time position vectors $X = (\mathbf{r}, \tau)$, $X_1 = (\mathbf{r}_1, \tau_1)$, and $X_2 = (\mathbf{r}_2, \tau_2)$. We then pretend that $G^{(1)}(X)$ cannot be evaluated and stored as a function, but its properties can be represented by a collection—the list—of X -coordinates generated stochastically by sampling the r.h.s. of (5) using

standard DiagMC techniques. There is no gain in using rotational symmetry for the coordinates in the list, since symmetrized elements will just be called more often from the list in order to sample the space possessing this symmetry.

The minimal set of updates consists of switching between the two sectors corresponding to the first and second terms in the r.h.s. of (5). The known integral over the first term, $\mathcal{N}_0 = \int |G_0(X)| d^4 X = 1/|\mu|$, is used for normalization: the Monte Carlo statistics for any property is properly normalized once multiplied by the factor \mathcal{N}_0/Z_1 , where Z_1 is the number of samples that belong to the first term. For example, the normalization integral $\mathcal{N}_G = \int |G^{(1)}(X)| d^4 X$ is obtained as $\mathcal{N}_G = \mathcal{N}_0(Z/Z_1)$, where Z is the total number of samples (no matter whether they belong to the first or the second term).

In order to go from the first to the second term, we draw a random variable τ_1 according to an exponential distribution $\propto |\mu| e^{-|\mu|\tau_1} d\tau_1$ and then generate three random numbers (x_1, y_1, z_1) according to a gaussian distribution with zero mean and variance τ_1/m ; the corresponding probability density is based on the G_0 function. Next, we choose coordinates X_3 and X_4 uniformly from the existing list; they define $X_2 = X_1 + X_3$ and $X = X_2 + X_4$, by translation invariance. The probability $1/P^2$ for selecting these two variables from the list is a faithful representation of the probability $G^{(1)}(X_2 - X_1) G^{(1)}(X - X_2) d^4 X_2 d^4 X / \mathcal{N}_G^2$, as follows from Eq. 2. In the reverse update taking the simulation from the second to the first term, the coordinates of the free propagator are again determined by the probability density based on G_0 : an exponential random number for the time and three gaussian random numbers for the space.

The key property behind the list technique is that all the values of the unknown function $G^{(1)}$ cancel in the acceptance ratio: The unknown full Green functions appear in both the proposed configuration weight and the probability density used to generate new variables. For the same reason all exponential and gaussian factors cancel $G_0(X_1)$. This results in an acceptance ratio $R = D(X_2 - X_1) \mathcal{N}_G^2$ (and $1/R$ for the reverse update). The update is then accepted with probability $\min(1, R)$, according to the Metropolis-Hastings algorithm. One thus arrives at a protocol of dealing with a function without knowing/revealing its explicit form.

In this implementation, we work with an existing list from which we draw random coordinates, while simultaneously preparing a new list which we consecutively fill after each Monte Carlo update by recording the current value of X (in both sectors). When the new list is full, it replaces the existing one and the new list is reset to zero. To initialize the procedure, we start with a short list based on random coordinates that we draw from the G_0 distribution, which we let grow by a small factor of the order of $1.001 \div 1.01$ till the maximum length is reached.

The results for a moderate coupling $\tilde{\alpha} = 5$ are shown in Fig. 1. Within the level of resolution of the plot, there

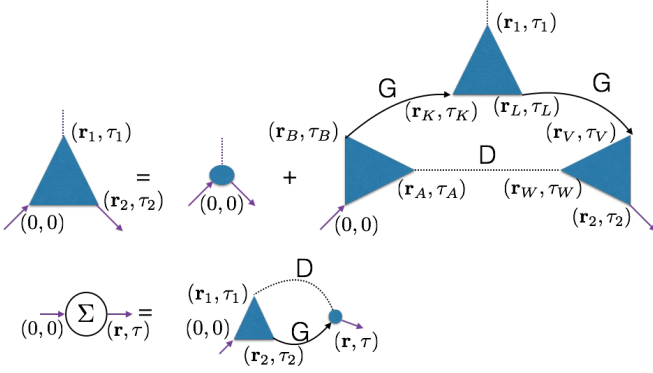


FIG. 2. (Color online.) *Upper pane:* Lowest-order contributions to the three-point vertex in the (imaginary-time, real-space) representation. *Lower pane:* Self-energy in terms of the three-point vertex in the (imaginary-time, real-space) representation.

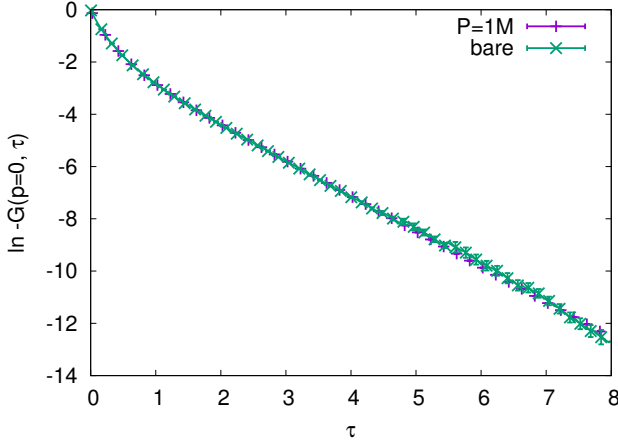


FIG. 3. (Color online.) Comparison of the Green function dependence on imaginary time at zero momentum, $-G(p=0, \tau)$, obtained by the stochastic list method applied to the scheme illustrated in Fig. 2 with a list of length $P = 10^6$ (“P=1M”) versus the result obtained by a conventional DiagMC simulation restricted to sample the same set of diagrams from the bare series (see text).

is no difference between the exact NCA result and the one obtained by stochastic lists of the length $P = 10^6$. We postpone the discussion of convergence properties till Sec. III. Here we simply note that for $P = 10^6$ any systematic bias was subdominant to the statistical noise. Also, there is no need for fast Fourier transforms (cf. Ref. 18) when employing lists and thus no need to take care of the asymptotic behavior of the Green function for large frequencies.

C. First-order vertex corrections

We now consider the Hedin scheme¹ where the vertex function takes into account both the zeroth-order

term and the first-order corrections. The system to solve consists of three equations, the two of which are shown graphically in Fig. 2, and the third one is the Dyson equation for the Green function. Our implementation involves two stochastic lists: one for the Green function $G(X)$, as before, and the other one for the three-point vertex $\Gamma(X_1, X_2)$, the latter containing 6 spatial and 2 temporal coordinates. (As before, there is no gain in exploiting symmetries to reduce the number of spatial coordinates.) We set up one stochastic Markov-chain process to sample both quantities. The algorithm itself is a straightforward extension of the one discussed above, and we will not elaborate here on minute technical details.

Reference data were obtained from the algorithms discussed in Ref. 18, where we used the bare-series code with the updates “insert-remove” and “dress-undress” switched on and the “swap” update switched off. Starting from an arbitrary Green function diagram, the “insert” update attempts to insert a new D -propagator without dressing any of the existing vertices; i.e., none of the vertices covered by the new D -propagator remains unlinked on the updated time interval. “Remove” is the complementary update. The “dress” update attempts to insert a new D -propagator that covers precisely one vertex; the “undress” update is its complementary partner. This set of updates is not ergodic for the full problem (e.g., no diagrams in which a D -propagator covers two or more non-linked vertices can be reached), but it accounts for all diagrams covered by Fig. 2.

The results of benchmark comparison are shown in Fig. 3. We see that perfect agreement is reached for the Green function at zero momentum as a function of imaginary time for a list of length $P = 10^6$ (the same length is used for both G and Γ). The method of stochastic lists seems thus promising to study vertex corrections in the context of (bosonic) dynamical mean-field theory and its cluster extensions. However, as we will see in the next section, establishing the convergence of the answer can only be done on a case by case basis, at best.

III. GROUND STATE OF THE ANTIFERROMAGNETIC HEISENBERG MODEL

In this section, we consider the spin-1/2 Heisenberg antiferromagnet (HAF) on a square lattice

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = \frac{J}{2} \sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_i^- S_j^+ + 2S_i^z S_j^z), \quad (6)$$

with spin exchange amplitude $J > 0$. The sum is over nearest neighbor sites, and the lattice is of size $L \times L$. By performing the unitary transformation $S_i^x \rightarrow -S_i^x$, $S_i^y \rightarrow -S_i^y$, $S_i^z \rightarrow S_i^z$ on one of the sublattices, the sign of the amplitude in front of the raising and lowering term is reversed. The matrix elements of $C - H$, for an appropriately chosen constant $C = JL^2/2$, are then all positive in the usual S^z basis. The eigenvalue problem

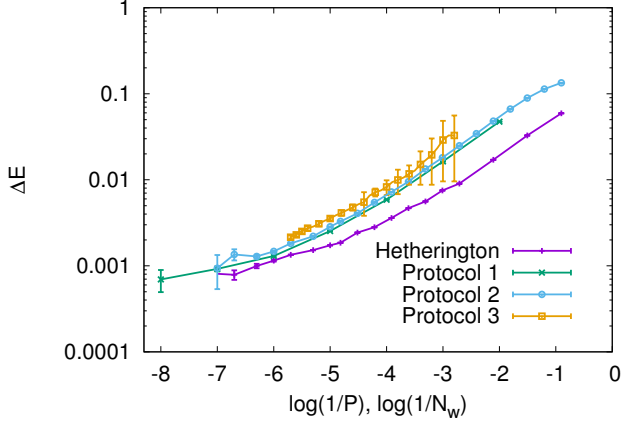


FIG. 4. (Color online.) Difference between the exact energy per site (taken from Ref. 19) and the one obtained with either a stochastic list of length P (see text for an explanation of the different protocols), or in a diffusion Monte Carlo simulation with N_w walkers (“Hetherington,” with $k = 128$; see text). The system is a 2D Heisenberg model with linear size $L = 10$ with $J = 1$.

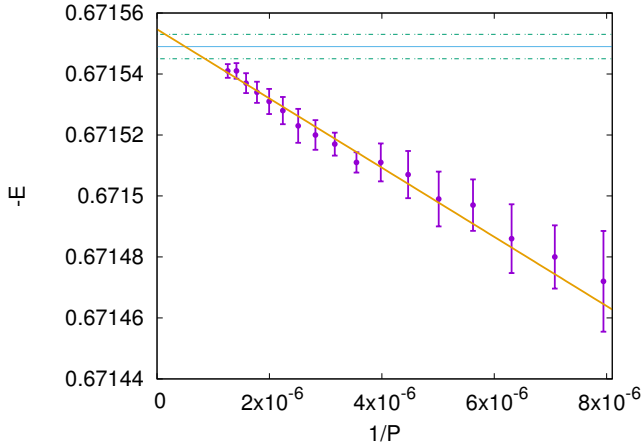


FIG. 5. (Color online.) Minus the energy per site as a function of $1/P$ using protocol 3 (with $\kappa = 1$) with a Gutzwiller guiding wavefunction with $b = 0.8$, which is (close to) optimal. The error bars have been obtained from 10 independent runs. The data are compared with the value $E/J = -0.671549(4)$ per spin, plotted as a thin blue line and its error bars as a thin dot-dashed green line, obtained by A. Sandvik using the stochastic series expansion method¹⁹. The data have been extrapolated linearly (shown as a full line in the plot) according to $E(x) = E_0 - bx$ with $x = 1/P$, resulting in $a = 0.671555(4)$ and $b = 11.3(4)$. The system is a 2D Heisenberg model with linear size $L = 10$ with $J = 1$.

$$(C - H)\psi = (C - E_0)\psi, \quad (7)$$

can be considered a power method when the state ψ is iteratively represented by the stochastic list. It yields the absolute value of the largest eigenvalue in magni-

tude, whose eigenfunction can always be chosen positive for a positive matrix. With the above transformations, this corresponds to projecting onto the antiferromagnetic ground state (and not the ferromagnetic anti-groundstate). This problem is challenging because of the gapless spectrum of elementary excitations in the thermodynamic limit and the large dimension of the Hilbert space, growing exponentially with system size.

The coordinates in the list consist now of L^2 bits representing the spins on the lattice. We add to the sampled configuration space a dummy spin-independent term for normalization purposes; the equation to solve thus contains a normalization constant C_N as well as the matrix-vector multiplication term. The key updates are switching between these two terms. To go from the former to the latter, we pick randomly an entry from the stochastic list of length P , which provides us a coordinate (Fock state) j . The probability of this selection is $1/P$ or, according to Eq. 2, $|\psi_j|/\mathcal{N}_\psi$, where $\mathcal{N}_\psi = \sum_j |\psi_j|$ is the normalization sum (estimated using the same procedure as described above for \mathcal{N}_G). Next, we have to determine all non-zero Hamilton matrix elements H_{ij} when acting on the state corresponding to coordinate j . We assume that the Hamiltonian is too large to be stored explicitly, so that this step must be repeated in every Monte Carlo update. For sparse matrices, there are very few possible final coordinates i . We choose the final coordinate i according to the heatbath algorithm, i.e. with probability $p_i = H_{ij}/\bar{H}_j$, where $\bar{H}_j = \sum_i H_{ij}$. The resulting Metropolis-Hastings acceptance ratio is just $R = \mathcal{N}_\psi \bar{H}_j / C_N$ (and $1/R$ for the reverse update). The update is accepted with probability $\min(1, R)$. We also occasionally employed the Metropolis-like algorithm, in which one of the non-zero matrix elements H_{ij} is chosen with uniform probability instead of the heatbath algorithm. It did not lead to significant differences in the autocorrelation times. A good choice for the dummy term constant is $C_N = 2JL^2$ (to compensate the typical value of the \bar{H}_j sum). Measurements of the parameter \mathcal{N}_ψ and recordings of the new list entries are performed only in the matrix-vector multiplication sector.

Apart from the previously discussed protocol (“protocol 1”) where the current list is replaced by the new one once the latter is completed, we also applied “protocol 2.” Here there is only one list updated at each Monte Carlo step by drawing a random integer in the interval $m \in [0, P[$ and replacing the existing entry m with the new coordinate. In “protocol 3” the list is continuously growing as a function of the Monte Carlo steps according to $P = \sqrt{\tau_{MC}/\kappa}$. The list grows then by one entry whenever the integer part of $\sqrt{\tau_{MC}/\kappa}$ increases by one; otherwise an existing entry is overwritten when measuring the list. As will be clear from the results, the differences between these protocols are not of leading importance.

The above algorithm works remarkably well for small matrices, even if they are poorly conditioned. For a system of size $L = 4$, the systematic error can easily be made smaller than the statistical noise. When P exceeds

1000, we find that the systematic error decreases as $1/P$. However, at larger system size (speaking of $L = 10$ and larger), this extrapolation law is no longer valid: Longer lists are needed, which need to be iterated much longer to converge. We also observe that the converged results cannot be extrapolated as a power law in $1/P$ (even though the results are remarkably accurate already for short lists). This gets worse with increasing system size, and the marginal gain of using longer lists diminishes further. We also see in Fig. 4 that the scaling does not depend on which protocol we use, suggesting that the reason for the inefficiency of the simulation must be found in the build-up of autocorrelations scaling unfavorably with the system size: due to the overwriting of the entries in the stochastic list, a few Fock states tend to dominate and the superposition of those is not the exact ground state. Protocol 3 appears to yield results that can be extrapolated by a single power law over several decades in $1/P$ and may hence look superior. Some care with this observation is however needed because we could not reach lists that are as long as in protocols 1 and 2; *i.e.*, it might be that the law $P = \sqrt{\tau_{\text{MC}}/\kappa}$ is still too fast when $P \gg 10^5$.

The method of stochastic lists applied to the power method is highly reminiscent of diffusion Monte Carlo, which has also been applied to the Heisenberg model with impressive results.^{20–25} We compare here with an implementation motivated by the original algorithm by Hetherington²⁰ and the reconfiguration ideas of Ref. 25. In this scheme, N_w walkers propagate through the Fock space but, instead of satisfying a detailed balance condition, they acquire multiplicative weight factors (these are the previously introduced \bar{H}_j sums), which fluctuate at an extensive scale. After a number of generations k , a population-control mechanism is applied to keep the number of walkers fixed. Walkers with high weight are more likely to reproduce and walkers with a low weight are more likely to be eliminated. The resulting bias is compensated by global factors $\langle \bar{H}(1) \rangle, \dots, \langle \bar{H}(k) \rangle$ (*i.e.*, the \bar{H} values averaged over all walkers in every generation), see Refs. 20 and 25 for details. In Fig. 4 we see that the above algorithm with $k = 128$ yields results that are more accurate than the list when there are few walkers, but that the scaling is the same as for the list. We checked that the same holds for $k = 12$. It has been known since the early days of diffusion Monte Carlo that the population size might easily lead to the dominant source of error; more recently, Nemec claimed an exponential scaling,¹¹ and population size bias was also found by Boninsegni and Moroni.²⁶ The explanation given by Nemec apparently also applies to stochastic lists.

It is well known that diffusion Monte Carlo can significantly be enhanced by using a good guiding wavefunction. For the HAF model, and certainly for small system sizes, excellent variational Jastrow wavefunctions are known.²⁷ We employed here a simpler but faster to evaluate Gutzwiller ansatz, reminiscent of perturbation

theory,

$$\psi_G \sim \prod_{\langle i,j \rangle} \exp(-b S_i^z S_j^z), \quad (8)$$

where b is a variational parameter (Note however that we have no proof that our final answer for the ground state energy is variational). For $b > 0$ antiferromagnetic correlations are enhanced. The only change to the code is that the Hamiltonian matrix element is replaced by $H_{ij} = \psi_G(i) H_{ij} / \psi_G(j)$ where $\psi_G(i)$ denotes Eq. 8 evaluated for spin configuration i . We performed the simulation for various values of b using protocol 3. We show in Fig. 5 the convergence for $b = 0.8$, which is very close to optimal. We find that the energies differ by an amount 8×10^{-6} for the longest lists we have studied, $P \sim 8 \times 10^5$. The figure makes however clear that the energy still drifts as a function of $1/P$. If we extrapolate, the results agree within error bars (of the order of 4×10^{-6}) with Sandvik's stochastic series expansion results¹⁹ and with the diffusion Monte Carlo results of Ref. 25. These results are hence up to two orders of magnitude more precise than the results without using the guiding wavefunction. However, a poor guiding wavefunction can lead to severe slowing down and, recalling our main goal of studying vertex corrections, one has to recognize that good (and easy to evaluate) guiding schemes are not available in general.

IV. CONCLUSION

We have introduced the method of stochastic lists, which allows one to accurately emulate properties of a multi-variable function $F(\mathbf{x})$. The repeatedly refreshed list consists of a large set of coordinates \mathbf{x} distributed according to the $F(\mathbf{x})$ values. The list of length P represents only a tiny fraction of the full coordinate space of F , but after it is refreshed multiple times, a faithful representation of the entire $F(\mathbf{x})$ function is obtained. The method was benchmarked by computing vertex corrections self-consistently for the Fröhlich polaron model and by applying the power method for obtaining the ground-state energy and wave function of the antiferromagnetic Heisenberg model. The method gives reasonably accurate results for most problems in practice, and can apparently be extrapolated as a power law over several decades in the inverse list length. However, for very long lists we could observe deviations rendering a controlled extrapolation for an arbitrary problem difficult. This behavior seems inherent to all population-based methods. Nevertheless, stochastic lists are extremely promising for many problems where clever guiding functions for the stochastic sampling are known. Here the systematic error can be reduced to such a degree that it becomes irrelevant in practice.

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Science Foundation under the grant DMR-1720465. The open data for this project, including an open source implementation for Fig. 5, can be found at <https://gitlab.lrz.de/QSIMCORR/StochList>.

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