Quantum Monte Carlo methods (QMC) allow an in principle exact simulation of quantum many-body systems. Over the past decade, cluster updates have increased the efficiency of lattice-QMC methods dramatically. They proved particularly useful near phase transitions, where the traditional algorithms suffered from a critical slowing down. Based on an analogy with the Swendsen-Wang algorithm for classical systems, the first loop algorithm for QMC constructed clusters in the form of loops, which then could be flipped to obtain new configurations. An important development was the formulation in continuous imaginary time, which eliminated discretization errors. The worm algorithm established the link between the construction of the loops and the sampling in an extended configuration space, thereby allowing a direct evaluation of the one-body Green’s function. The loop updates have also been implemented in the stochastic series expansion method (SSE). A further optimization of the loop construction process was developed in the form of directed loops. These turned out to be a special case of a more general locally optimal strategy, which tries to optimize the loop construction by using the optimal stochastic transition kernel at each local step of the process. The aforementioned loop algorithms all lead to fluctuations in particle number (or in magnetization for spin systems). Therefore they sample the grand canonical ensemble. There are cases where particle-number conservation plays an important role and where one would like to sample directly the canonical ensemble: e.g. lattice systems at commensurate fillings or finite systems such as ultrasmall superconducting grains or atomic nuclei. Results for the canonical ensemble can be obtained from loop algorithms by by using only those configurations in the sample which have the right particle number or by explicitly throwing out the loop updates which change particle number. However, this is impractical because a lot of effort is wasted on the discarded configurations or updates and because it requires a good estimate of the chemical potential. In this letter, we present a class of loop updates which explicitly conserve particle number. The algorithm results in moves that are always accepted, which makes it easier to code and more efficient to run than other loop-update schemes. Furthermore, one can impose the conservation of other symmetries.

Like most QMC methods, our algorithm starts from a decomposition of the imaginary time propagator, \( U(\beta) = \exp(-\beta H) \). Generally one can write the Hamiltonian as \( H = H_0 - V \), consisting of an easy part \( H_0 \) and a residual interaction \( V \) (note the minus sign in front of \( V \), in order to ease notations further on). For such a Hamiltonian, one can make a perturbative expansion in \( V \) using the following integral expression:

\[
U(\beta) = \sum_{m=0}^{\infty} \int_0^\beta \cdots \int_0^\beta V(t_1)V(t_2)\cdots V(t_m) e^{-\beta H_0} dt_1 dt_2 \cdots dt_m, \tag{1}
\]

with \( V(t) = \exp(-tH_0)V\exp(tH_0) \). Instead of sampling the representations of the operator \( U(\beta) \) directly, our method will perform a Markovian random walk in an extended configuration space, related to the decomposition of the operator \( U'(\beta, \tau) = e^{-\tau H} A e^{-(\beta - \tau) H} \), where \( A \) is the worm operator, to be defined later on. An alternative would be to insert a creation and an annihilation operator at different imaginary times. This forms the basis of the continuous-time loop algorithm and the worm algorithm. Here we will show that it is advantageous to work with a single worm operator, provided that it commutes with the residual interaction: \( AV = VA \). If the operator \( A \) furthermore commutes with the generator of a symmetry of \( H_0 \) and \( V \), then one can restrict the configurations to specific symmetry representations, such that symmetry-projected results are obtained. In particular one can sample the canonical ensemble with a worm operator that conserves particle number.

By taking the trace (restricted to the wanted particle number and symmetry) and inserting complete sets of eigenstates of \( H_0 \) between all operators in the integral representation of \( U'(\beta, \tau) \), one assigns a weight \( W(m, l, t, \tau) \) to the configurations specified by an order \( m \), a set of inserted eigenstates \( l_0, l_1, \ldots, l_m \), interaction times \( t_1, t_2, \ldots, t_m \), and the worm insertion time \( \tau \). Let \( l_k \) and \( i_k \) denote the states to left and right of the worm operator. We will call the configurations for which \( l_k = i_k \) diagonal configurations. One can choose the worm operator \( A \) such that its diagonal elements are constant, i.e. \( \langle i | A | i \rangle = c \) for all basis states \( i \). Then the sum of the weights of all the diagonal configurations is proportional to the particle-number projected trace of the operator \( U(\beta) \), which is nothing else than the canonical partition function.
Hence, the sampling of the configurations proportional to their weight $W(m, i, t, \tau)$ leads to a sampling of the canonical ensemble.

To this end a Markov process is used for which the stationary distribution reflects the contribution of the configurations to the extended partition sum $Z^\prime_N(\beta) = \text{Tr}_N[U(\beta, \tau)]$. Let us assume that a diagonal configuration is given. We are free to choose a new insertion time $\tau$ for the worm operator because the weight is independent of $\tau$. Then we perform a number of Markov steps according to the following rules, until the move halts again in a diagonal configuration. We present the Markov rules in terms of a set of parameters $q_D, c_D, N_{DD}^D, \varepsilon_D, g_D, a_D$ and $s_D$, which are defined in detail in table I.

- Evaluate the diagonal energy to the left ($E_L$) and to the right ($E_R$) of the worm operator, and evaluate the values of $q_L$ and $q_R$.
- Choose a direction $D$, either left (L) or right (R), proportional to the relative weights $q_L$ and $q_R$. Let $D'$ denote the opposite direction.
- With probability $c_D$, insert an interaction term $V$ and choose a new intermediate state $i$ according to the distribution $P_{DD'}(i) = \langle i_D|A|i_i\rangle \langle i_i|V|i_{D'}\rangle / \langle i_D|AV|i_{D'}\rangle$.
- Move the worm in direction $D$ over a step size $\Delta \tau$ chosen according to a Poisson distribution: $\Delta \tau \propto \exp(-\varepsilon_D \Delta \tau)$. Assume periodic boundaries in imaginary time.
- If the worm would pass an interaction term in the time step $\Delta \tau$, there are three options: (a) With probability $s_D$: remove the interaction and halt the worm. Then the Markov step ends here. (b) With probability $a_D$: remove the interaction, adjust the parameters and continue the worm move in the same direction. (c) With probability $1 - s_D - a_D$, or if the interaction can not be removed: let the worm pass the interaction, but choose a new intermediate state according to $P_{DD'}(i)$. Adjust the parameters and continue the worm move in the same direction.
- When the worm has reached the end of the time step $\Delta \tau$, then with probability $1 - s_D$ the worm is halted and the Markov step ends here. With probability $s_D$, insert an interaction and choose a new intermediate state according to $P_{DD'}(i)$. Adjust the parameters, draw a new time step $\Delta \tau$ and continue the worm move in the same direction.

There is considerable freedom in the definition of the sampling parameters. Guided by the principle of locally optimal moves \[14, 17\], we propose the definitions as given in table I. These rules assure that the Markov chain satisfies the detailed balance condition for the weight $R_{LR}W(m, i, t, \tau)$, with $R_{LR} = q_R + q_L$. One could use the Metropolis-Hastings algorithm \[18, 19\] in order to sample according to the weights $W(m, i, t, \tau)$. Because the factors $R_{LR}$ fluctuate only mildly in practice, one can accept all moves and take the extra weighting factor $R_{LR}$ into account when evaluating observables. This speeds up the algorithm and reduces the complexity of the code. Note that during a Markov step the worm keeps moving in the same direction, even after passing, inserting or removing interactions. This is possible while maintaining detailed balance because $A$ and $V$ commute. Otherwise one would have to consider so-called bounces: the worm could return on the path it came from and undo its last changes. This is one of the reasons why our new algorithm is more efficient than the worm and loop algorithms of Refs. \[2, 6, 7, 9\].

| Parameters | Diagonal Configurations | Non-Diagonal Configurations |
|------------|-------------------------|-----------------------------|
| $E_D$      | $\langle i_D|H_0|i_D\rangle$ | $\langle i_D|VA|i_{D'}\rangle/\langle i_D|A|i_{D'}\rangle$ |
| $E_D'$     | $\langle i_D'|H_0|i_{D'}\rangle$ | |
| $N_{DD}^D$ | $\langle i_D|VA|i_{D'}\rangle/\langle i_D|A|i_{D'}\rangle$ | |
| $q_D$      | $\phi$                  | $0$                         |
| $q_D'$     | $\phi$                  | $E_D - E_D$                 |
| $c_D$      | $1$                     | $0$                         |
| $c_D'$     | $1$                     | $\min\left(1, \frac{N_{DD}^D}{\varepsilon_D}\right)$ |
| $\varepsilon_D$ | $0$            | $E_D - E_D$                 |
| $\varepsilon_D'$ | $0$            | $0$                         |
| $g_D$      | $0$                     | $\min\left(1, \frac{N_{DD}^D}{\varepsilon_D}\right)$ |
| $g_D'$     | $0$                     | $0$                         |
| $a_D$      | $0$                     | $0$                         |
| $a_D'$     | $0$                     | $\min\left(1, \frac{E_{D} - E_D}{N_{DD}^D}\right)$ |
| $s_D$      | $\phi/N_{DD}^D$         | $0$                         |
| $s_D'$     | $\phi/N_{DD}^D$         | $0$                         |
| $R_{DD}$   | $2\phi$                | $|E_{D'} - E_D|$             |

TABLE I: Definitions for the sampling parameters, assuming that $E_D \leq E_{D'}$ (interchange $D$ and $D'$ otherwise). The global parameter $\phi$ should be taken small (such that $\phi \leq N_{DD}^D$ for all diagonal configurations) but not zero, to make sure that the worm halts in diagonal configurations that are sufficiently decorrelated.

While each Markov step is based on local changes, the chain of steps between two diagonal configurations corresponds to a global loop update: if one follows the creation and annihilation part of the worm operator as they move through the world-line representation of the configurations, one sees that they describe a loop which closes again when the configuration becomes diagonal. By keeping track of the worm operator at the intermediate steps, one can collect statistics for the expectation values of non-diagonal operators, similar to the way one evaluates the one-body Green’s function in the worm algorithm \[7\]. The advantage of our method is that the operators are always evaluated at equal imaginary times, leading to much better statistics for non-diagonal operators.

As an illustration we have applied our method to the...
one-dimensional Bose-Hubbard Hamiltonian, given by \( H = -t \sum_i b_i^{\dagger} b_{i+1} + U \sum_i n_i (n_i - 1)/2 \), with \( n_i = b_i^{\dagger} b_i \). It models the low-energy degrees of freedom of various physical systems: cold bosonic atoms in an optical lattice \([20, 4]^{\text{He}}\) atoms on graphite \([21]\), and superconducting islands or grains connected by Josephson junctions \([22]\). Various many-body techniques have been deployed to study its phase diagram. Without trying to be complete, we mention here algebraic \([23]\), mean-field \([11]\), perturbative \([24]\), renormalization-group \([25]\) and QMC approaches \([26]\). For our method we take \( V = \sum_i b_i^{\dagger} b_{i+1} \) and \( A = \sum_i b_i^{\dagger} b_i \). At commensurate fillings, this model can undergo a quantum phase transition from a superfluid to a Mott isolator. With grand-canonical methods it is difficult to simulate this transition because one has to determine the chemical potential such that the exact density is obtained. Fig. 1 shows the superfluid and condensed fraction for a uniform one-dimensional system of 128 sites at nearly zero temperature (\( \beta = T^{-1} = 128t^{-1} \)) at a density of exactly one particle per site. The superfluid fraction was derived from the winding numbers \([27]\), while the condensed fraction was obtained from the one-body equal-time Green’s function.

Fermionic models can be handled too, provided that there is a symmetry which guarantees that all matrix elements are positive, such that the sign problem is absent. This is the case for the pairing Hamiltonian:

\[
H = \sum_{\alpha,j,m} e_{\alpha,j,m} a_{\alpha,j,m}^{\dagger} a_{\alpha,j,m} - \frac{G}{4} \sum_{\alpha,j,m,m'} a_{\alpha,j,m}^{\dagger} a_{\alpha,j,m}^{\dagger} a_{\alpha,j,m'} a_{\alpha,j,m'},
\]

where \( a_{\alpha,j,m}^{\dagger} \) creates a particle in a state with quantum numbers \( \alpha, j, m \), and \( a_{\alpha,j,m} \) a particle in the time-conjugated state. The pairing model has been used extensively in nuclear physics to model the pair correlations between nucleons and to explain the particular odd-even effects found in nuclear spectroscopy \([28, 29]\). Canonical QMC methods for the pairing Hamiltonian have been presented before: Cerf’s world-line QMC method \([30]\) does not have a sign problem, but it does not sample the full phase space of broken pairs \([31]\), which makes it impractical for finite temperature calculations. The shell model Monte Carlo method overcomes this problem \([14, 15, 32]\), but has a sign problem for odd particle numbers. For a constant pairing strength \( G \), the eigenstates can be calculated exactly \([33, 34]\). Our method supplements these algebraic solutions with finite temperature results. It can also be applied to level-dependent pairing interactions, for which no algebraic solution is available. Here, we take \( V \) to be the non-diagonal part of the pairing interaction and we take \( A \) equal to \( V \) plus a constant diagonal term. A pair-breaking term has to be added to \( A \) and \( V \) in order to ensure ergodicity \([17]\). Note that the worm operator conserves angular momentum. Therefore one can restrict the intermediate states to a specific value of the quantum numbers \( J \) and \( J_z \). Fig. 2 shows how the \( J_z \)-projected finite-temperature results converge to the exact eigenvalues at low temperature, for a model that describes neutron pair correlations in \(^{56}\text{Fe}\) \([15]\).

The pairing model where all levels are double degenerate \((j = 1/2 \text{ for all } \alpha)\) and equally spaced (with level spacing \( d \)), is called the picket fence model. It applies to ultrasmall metallic grains, provided that a canonical approach is used \([12, 13, 35]\). One has found that grand-canonical approaches lead to an abrupt but unphysical suppression of the superconductive correlations for level spacings larger than the bulk gap \( \Delta \). The extension of the exact ground-state calculations to finite temperatures was cited as an open problem in Ref. \([13]\), and has only been treated at the mean-field level \([36]\) (except for the smallest systems). Our method provides exact finite-temperature results both for odd and even particle numbers. Therefore we can study the odd-even asymmetry, which is a key indicator of superconductive correlations. An illustrative quantity is the canonical pairing gap \( \Delta_{\text{can}} \), as defined by Eq.(92) of Ref. \([13]\). It is a measure of

![Fig. 1: Superfluid (\( \rho_s \)) and condensed fraction (\( \rho_c \)) for the one-dimensional Bose-Hubbard model on a uniform lattice of 128 sites, at an inverse temperature \( \beta = 128t^{-1} \).](image)

![Fig. 2: \( J_z \)-projected internal energies as a function of temperature for 10 neutrons in the \( p_f + sdg \) shell, for a constant pairing interaction with \( G = 0.286 \) and single-particle energies as in Ref. \([13]\). On the left hand side the exact eigenvalues are shown \([14]\).](image)
the change in energy due to pairing correlations. Its deviation from the BCS bulk gap indicates the difference between the canonical and grand-canonical ensemble. In Fig. 3 one sees the canonical pairing gap converging to the bulk gap with increasing system size. There is a clear odd-even effect at lower temperatures that disappears at higher temperatures, and this transition temperature decreases with increasing system size.

These applications show the versatileness of the canonical loop updates. Our method can be used to sample configurations with specific symmetries and in particular to sample the canonical ensemble. It leads to a very efficient sampling scheme with all moves accepted and without 'bounces' or critical slowing down. It can be applied to bosons and fermion pairs in discrete model spaces and to spin systems at fixed magnetization. Off-diagonal observables such as the equal-time one-body Green’s function can be evaluated with high efficiency. This opens new perspectives for the study of quantum many-body systems where particle number and other symmetries play an important role, such as the nuclear shell model and ultrasmall superconducting grains.

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[1] D.M. Ceperley, Rev. Mod. Phys. 71, 438 (1999).
[2] H.G. Evertz, G. Lana, and M. Marcu, Phys. Rev. Lett. 70, 875 (1993).
[3] H.G. Evertz, Adv. Phys. 52, 1 (2003); N. Kawashima and K. Harada, J. Phys. Soc. Jpn. 73, 1379 (2004).
[4] W. von der Linden, Phys. Rep. 220, 53 (1992).
[5] R. H. Swendsen and J. S. Wang, Phys. Rev. Lett. 58, 86 (1987); N. Kawashima and J.E. Gubernatis Phys. Rev. E 51, 1547 (1995).
[6] B.B. Beard and U.-J. Wiese, Phys. Rev. Lett. 77, 5130 (1996).
[7] N.V. Prokof’ev, B.V. Svistunov, and I.S. Tupitsyn, Phys. Lett. A 238, 253 (1998); Sov. Phys. - JETP 87, 310 (1998).
[8] A.W. Sandvik, Phys. Rev. B 59, 14157 (1999).
[9] O.F. Syljuåsen and A.W. Sandvik, Phys. Rev. E 66, 046701 (2002); O.F. Syljuåsen, ibid. 67, 046701 (2003).
[10] L. Pollet, S.M.A. Rombouts, K. Van Houcke, and K. Heyde, Phys. Rev. E 70, 056705 (2004).
[11] M.P.A. Fisher, P.B. Weichman, G. Grinstein, and D.S. Fisher, Phys. Rev. B 40, 546 (1989); K. Sheshadri, H.R. Krishnamurthy, R. Pandit, and T.V. Ramakrishnan, Europhys. Lett. 22, 257 (1993).
[12] J. Dukelsky and G. Sierra, Phys. Rev. Lett. 83, 172 (1999).
[13] J. von Delft and D.C. Ralph, Phys. Rep. 345 61 (2001).
[14] S.E. Koonin, D.J. Dean and K. Langanke, Phys. Rep. 278, 1 (1997).
[15] S. Rombouts, K. Heyde and N. Jachowicz, Phys. Rev. C 58, 3295 (1998).
[16] P. Roos and S. Miyashita, Phys. Rev. B 59, 13782 (1999).
[17] K. Van Houcke, S.M.A. Rombouts, and L. Pollet, unpublished, submitted to Phys. Rev. E.
[18] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller, and E. Teller, J. Chemical Physics 21, 1087 (1953).
[19] W.K. Hastings, Biometrika 57, 97 (1970).
[20] D. Jaksch, C. Bruder, J.I. Cirac, C.W. Gardiner, and P. Zoller, Phys. Rev. Lett. 81, 3108 (1998); M. Greiner, O. Mandel, T. Esslinger, T. Hänsch and I. Bloch, Nature (London) 415, 39 (2002).
[21] G.T. Zimanyi, P.A. Crowell, R.T. Scalettar, and G.G. Batrouni, Phys. Rev. B 50, 6515 (1994).
[22] A. van Oudenaarden and J.E. Mooij, Phys. Rev. Lett. 76, 4947 (1996).
[23] E.H. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1960).
[24] J.K. Freericks and H. Monien, Europhys. Lett. 26, 545 (1994); N. Elstner and H. Monien, Phys. Rev. B 59, 12184 (1999); K. Sengupta and N. Dupuis, Phys. Rev. A 71, 033629 (2005).
[25] T.D. Kühner, S.R. White, and H. Monien. Phys. Rev. B 61, 12474 (2000); C. Kollath, U. Schollwöck, J. von Delft, and W. Zwerger, Phys. Rev. A 69, 031601 (2004); L. Pollet, S. Rombouts, K. Heyde, and J. Dukelsky, ibid. 69, 043601 (2004).
[26] R.T. Scalettar, G.G. Batrouni and G.T.Zimanyi, Phys. Rev. Lett. 66, 3144 (1991); G.G. Batrouni and R.T. Scalettar, Phys. Rev. B 46, 9051 (1992); W. Krauth and N. Trivedi, Europhys. Lett. 69, 627 (1991); M.V. Zyubin and V.A. Kashurnikov, Phys. Rev. E 69, 036701 (2004); L. Pollet, S.M.A. Rombouts, and P.J. H. Denteneer, Phys. Rev. Lett. 93, 210401 (2004).
[27] E.L. Pollock and D.M. Ceperley, Phys. Rev. B 36, 8343 (1987).
[28] K.L.G. Heyde, The nuclear shell model, Springer Verlag, Berlin (1990).
[29] D.J. Dean and M. Hjorth-Jensen, Rev. Mod. Phys. 75, 607 (2003).
[30] N.J. Cerf, Phys. Rev. Lett. 76, 2420 (1996).
[31] S. Rombouts and K. Heyde, Phys. Rev. Lett. 80, 885 (1998).
[32] S.M.A. Rombouts, K. Heyde, and N. Jachowicz, Phys.Rev.Lett. 82, 4155 (1999).
[33] R.W. Richardson, Phys. Lett. 3, 277 (1963); R.W. Richardson and N. Sherman, Nucl. Phys. 52, 221 (1964).
[34] S. Rombouts, D. Van Neck, and J. Dukelsky, Phys. Rev. C 69, 061303 (2004).
[35] G. Sierra, J. Dukelsky, G. G. Dussel, J. von Delft, and F. Braun, Phys. Rev. B 61, 11890 (2000).
[36] R. Rossignoli, N. Canosa, and J.L. Egido, Phys. Rev. B 64, 224511 (2001).