

Inchworm quasi Monte Carlo for quantum impurities

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The inchworm expansion is a promising approach to solving strongly correlated quantum impurity models due to its reduction of the sign problem in real and imaginary time. However, inchworm Monte Carlo is computationally expensive, converging as $1/\sqrt{N}$ where N is the number of samples. We show that the imaginary-time integration is amenable to quasi Monte Carlo, with parametrically better $1/N$ convergence, by mapping the Sobol low-discrepancy sequence from the hypercube to the simplex with the so-called Root transform. This extends the applicability of the inchworm method to, e.g., multiorbital Anderson impurity models with off-diagonal hybridization, relevant for materials simulation, where continuous-time hybridization expansion Monte Carlo has a severe sign problem.

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Quantum impurity models are key for describing the physics of low-dimensional quantum systems such as quantum dots [1], molecular junctions [2], and cold atom systems [3] which can exhibit quantum many-body effects such as Coulomb blockade [4] and Kondo screening [5,6]. Quantum impurity models are also central for the *ab initio* simulation of correlated quantum materials where they appear as auxiliary problems within dynamical mean-field theory [7] and its extensions [8–11]. Therefore, efficient simulation of quantum impurity models is of paramount importance in improving our understanding of quantum dots, correlated materials, and their emergent collective phenomena, such as anomalous superconductivity [12], metal-insulator transitions [13], and magnetic order [14,15].

In thermal equilibrium, continuous-time quantum Monte Carlo [16–18] provides numerically exact solutions to a wide range of quantum impurity problems, e.g., multichannel quantum dots connected to separate reservoirs and correlated materials with high symmetry. For multichannel and multiorbital impurities, the continuous-time hybridization expansion algorithm (CTHYB) [19–21] has been particularly important for progress in the field. However, for intermixed reservoirs, low crystal symmetry, and materials with relativistic mixing of spin and orbital momentum, the majority of continuous-time quantum Monte Carlo algorithms suffer from a sign problem [18].

One notable exception is inchworm quantum Monte Carlo [22,23], a strong-coupling bold-line diagrammatic Monte Carlo [24–28], where causality is exploited to reorder the diagram summation. The reordering has been shown to give subexponential decay of the average sign in real time [22], as well as a drastic improvement in the sign for low-symmetry equilibrium problems, where CTHYB suffers from a dire sign problem [23]. However, the attainable accuracy is limited by the $1/\sqrt{N}$ convergence of the integration with the number of Monte Carlo steps N . Additionally, the order-by-order Monte Carlo integrals are normalized by overlaps with low order diagrams, which becomes difficult at low temperatures [29].

In this Letter, we show that by using quasi Monte Carlo integration [30–32] in imaginary time the convergence rate can be parametrically improved from $1/\sqrt{N}$ to $1/N$, greatly increasing the efficiency of the algorithm (see Fig. 1).

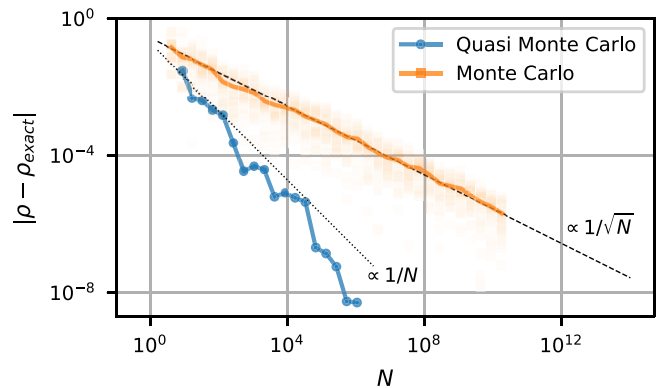


FIG. 1. Absolute error $|\rho - \rho_{\text{exact}}|$ in the many-body density matrix ρ as a function of the number of samples N for the proposed inchworm quasi Monte Carlo algorithm (blue circles) with $1/N$ scaling (dotted line) compared to the Monte Carlo based continuous-time hybridization expansion [19–21,33,34] (orange squares) with $1/\sqrt{N}$ scaling (dashed line).

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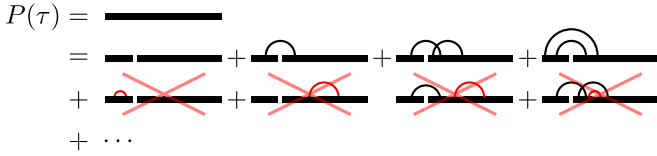


FIG. 2. Modified inchworm expansion for the pseudoparticle propagator $P(\tau)$ with bold propagators on both sides of τ_w .

Additionally, since quasi Monte Carlo is a direct integration technique there is no need for order-by-order normalization. We benchmark our quasi Monte Carlo inchworm algorithm on several impurity models computing both the local many-body density matrix as well as single- and two-particle response functions.

Inchworm algorithm. In its original formulation, the inchworm quantum Monte Carlo method is a stochastic strong-coupling technique for solving general quantum impurity models [22]. The algorithm relies on the causality property of the pseudoparticle propagator $P(\tau)$ [35], which is computed step by step starting at $\tau_i = 0$ and ending at $\tau_f = \beta$ where β is the inverse temperature. At each step, a short (compared to β) new segment $[\tau_w; \tau_f]$ is attached to the previously computed segment $[0; \tau_w]$ (see Fig. 2). Once $P(\tau)$ has been determined, the single-particle Green's functions $G_{\alpha\beta}(\tau) = -\langle \mathcal{T} c_\alpha(\tau) c_\beta^\dagger(0) \rangle$ is computed as a sum over another set of diagrams [29].

Quasi Monte Carlo integration on the simplex. For each step of the inchworm algorithm all possible *inchworm proper* [22,29] diagrams have to be integrated over the internal imaginary times. The internal times τ_j are ordered, i.e., $\tau_f \geq \tau_1 \geq \tau_2 \geq \dots \geq \tau_d \geq 0$, and the integration domain is a d -dimensional simplex. However, the low-discrepancy sequences used for quasi Monte Carlo integration, such as the Sobol sequence [36] used in our calculations, are commonly defined in the d -dimensional hypercube $\vec{x} \in [0, 1]^d$. Hence, a transformation that maps the d -dimensional hypercube to the d -dimensional simplex, while preserving the low-discrepancy property of the transformed sequence is required. We adopt the Root transformation [37]

$$\tau_1 = \tau_f x_1^{1/d}, \quad \tau_2 = \tau_1 x_2^{1/(d-1)}, \quad \dots, \quad \tau_d = \tau_{d-1} x_d, \quad (1)$$

which is continuous, has a constant Jacobian $\tau_f^d/d!$, and—with linear complexity in the dimension d —is computationally feasible in high dimensions. Figure 3 shows the distribution of points in the two- and three-dimensional τ simplex obtained by Root-transforming the first 1024 points of the Sobol sequence.

Unlike the transformation used for the real-time weak-coupling expansion [38], the Root transformation has no free adjustable parameters and does not discard any points from the input low-discrepancy sequence. The latter feature has recently been shown to be of crucial importance [39], as skipping even one point spoils the digital net property of the sequence and can worsen the convergence rate. Furthermore, numerical experiments with individual low-order inchworm diagrams showed that it outperforms the alternatives from Refs. [37,38] in terms of the relative error scaling with the number of taken samples.

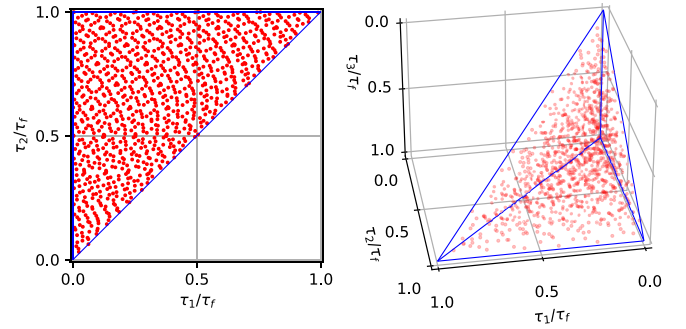


FIG. 3. Sobol sequences with 1024 points mapped from the hypercube to the simplex in two (left panel) and three (right panel) dimensions using the Root transform [37] in Eq. (1).

Inchworm quasi Monte Carlo. Our implementation of the inchworm algorithm does not rely on any form of importance sampling. Instead, the imaginary-time integrals are computed using quasi Monte Carlo integration [30–32]. The remaining discrete parameters labeling various contributions to the strong-coupling series—such as expansion order, spin projections, and orbital indices—are explicitly summed over. This approach is straightforward, well controlled yet fast enough for the moderate expansion orders $n_{\max}$ explored here ($n_{\max} \lesssim 7$). We also consider a special class of single high-order diagrams ($n_{\max} \leq 8192$) (see Supplemental Material [40]).

At a given inchworm step defined by (τ_w, τ_f) , the accumulation of the bold pseudoparticle propagators proceeds as follows. For each expansion order n up to a fixed $n_{\max}$, a list of $n!$ diagram topologies is generated. A topology is a partition of the tuple $\{1, \dots, 2n\}$ into pairs. Diagrammatically, it can be thought of as a set of n undirected hybridization lines connecting pairs of vertices located at positions $\{1, \dots, 2n\}$ on the segment $[0; \tau_f]$. If each hybridization line is connected by crossings to a line that overarches τ_w , the corresponding topology is *inchworm proper* [22,29] (cf. Fig. 2). Note, this differs slightly from previous definitions because we choose to use the *bold* rather than the bare propagator also between τ_w and τ_f . This adjustment marginally reduces the number of diagrams appearing in the expansion. All the proper topologies are then transformed into diagrams by replacing the paired vertices with all possible pairs of operators c_α and $c_\beta^\dagger$ (swapping c and $c^\dagger$ within a pair results in a different diagram). Finally, a sum of all contributing diagrams of order n is integrated over the imaginary time domain by evaluating it at the first $N = 2^m$ Root-transformed points of a $2n$ -dimensional Sobol sequence. The power-of-two sample size restriction to N is essential to preserve the digital net property of the Sobol sequence; using other sample sizes, e.g., 10^m , severely degrades accuracy [39].

As is known in the context of hybridization expansion methods [21], a significant fraction of diagrams stemming from a retained topology do not actually contribute due to symmetry considerations. We employ the autopartition algorithm [34] to reveal invariant subspaces of the atomic Hamiltonian and to unitarily transform the matrix-valued bare pseudoparticle propagator $P_0(\tau)$ into a block-diagonal form. The choice of the invariant subspaces accounts for any

potential symmetry breaking caused by a nondiagonal hybridization function. This way, we ensure that the subspace partition is not too restricted, and that the boldified propagator $P(\tau)$ possesses the same block-diagonal form.

A JULIA package implementing the proposed method is publicly available at Ref. [41]. It relies on the `Keldysh.jl` framework [42] for handling pseudoparticle propagators and Green's functions, and on the `KeldyshED.jl` package [43] for solving the atomic problem and construction of the bare atomic propagators $P_0(\tau)$.

Benchmarks. The theory of quasi Monte Carlo integration [30–32] only promises $1/N$ convergence for well-behaved integrands [44]. Hence, it is important to perform a direct investigation of the convergence rate when applying quasi Monte Carlo to a new class of problems.

To establish the convergence rate we study the impurity problem of a single fermionic state hybridized with a semi-infinite chain at $\beta = 8$, with the action

$$S = - \int_0^\beta d\tau d\tau' c^\dagger(\tau) [-\delta(\tau - \tau') \partial_\tau - \Delta(\tau - \tau')] c(\tau'), \quad (2)$$

where $c^\dagger$ and c are fermion creation and annihilation operators, and $\Delta(\tau)$ is the hybridization function with a semicircular density of states with bandwidth $W = 2$ and the lower band edge at the Fermi level, coupled to the impurity with the hybridization strength $V = 1/4$. This system is non-interacting and—while it can be solved exactly—it is also a worst-case scenario for the strong-coupling expansion, far from the atomic limit.

The convergence rate of the many-body density matrix $\rho = P(\beta)$ as a function of number of samples N per inchworm step, in Fig. 1, has clear $1/N$ scaling. The improved convergence rate is key to reach high-precision results, e.g., at absolute accuracy 10^{-8} it gives a *six orders of magnitude* reduction in both the required number of samples N and runtime (see Fig. 1 and Supplemental Material [40], respectively) compared to the parametrically worse Monte Carlo with $1/\sqrt{N}$ convergence.

Computing dynamical response functions is central for the application of an impurity solver in many-body methods such as dynamical mean-field theory [7]. Therefore, we compute the single-particle Green's function $G(\tau) = -\langle \mathcal{T} c(\tau) c^\dagger(0) \rangle$ [29] and study the convergence for the action in Eq. (2) with $W = 4$ and $V = 1$. To see the effect of the expansion order we perform calculations including all diagrams up to a given order $n_{\max}$ and observe a rapid convergence of $G(\tau)$ with respect to $n_{\max}$ [see Fig. 4(b)]. Already at order four the inchworm result for $G(\tau)$ in Fig. 4(a) is indistinguishable from the exact result. Looking in detail at the order by order convergence in Fig. 4(b), we observe rapid exponential convergence setting in at order 4. For a fixed order, the inchworm expansion (circles) is markedly more accurate than the bare expansion (squares) recently combined with tensor train decomposition (TTD) [45]. We also study the convergence rate of $G(\tau)$ with respect to the number of quasi Monte Carlo integration points. For fixed order we generically observe an initial $1/N$ rate of convergence followed by a plateau as the error becomes

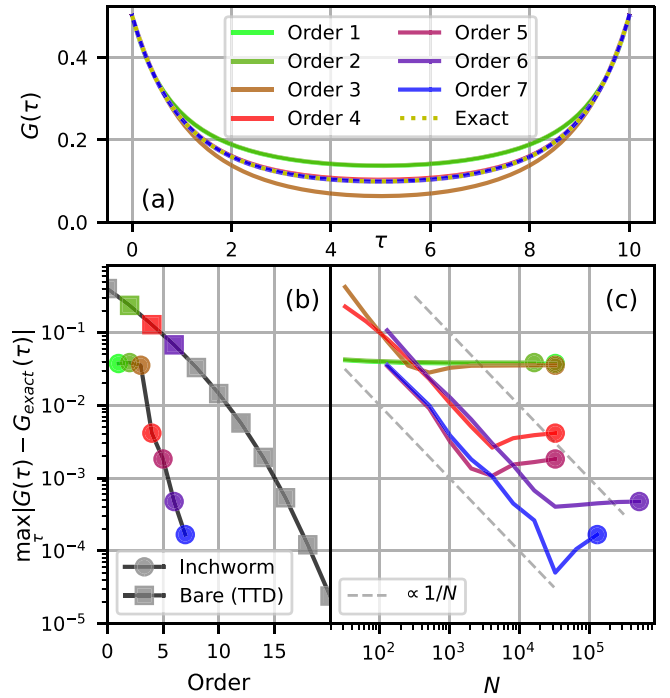


FIG. 4. (a) Imaginary-time single-particle Green's function $G(\tau)$ from inchworm quasi Monte Carlo at expansion orders $n_{\max} = 1-7$ (solid lines) compared to the exact solution (dashed line) at $\beta = 10$. (b) Expansion order convergence of the error $\max_\tau |G(\tau) - G_{\text{exact}}(\tau)|$ (circles) compared to the bare TTD expansion error (at $\tau = \beta/2$) (squares) [45]. (c) Convergence with respect to quasi Monte Carlo samples N at fixed order.

dominated by the difference between the fixed-order result and the exact infinite-order solution [see Fig. 4(c)].

Note that the difference in order-by-order convergence in Fig. 4(b) is not related to the quasi Monte Carlo (and the TTD of Ref. [45]) but rather coming from the difference between the inchworm and bare strong-coupling perturbation expansions. In terms of the amount of diagrams per order, the bare expansion only contains diagrams up to a given order while the inchworm expansion contains infinite resummations of bare diagrams. In the benchmark we see that the inchworm expansion with more diagrams converges faster with respect to order. However, this comes at the cost of the factorial scaling in the number of diagrams, while the bare expansion has a Wick's theorem and can use a determinant approach to avoid the factorial scaling [19]. Note, however, that the inchworm factorial scaling can be reduced to exponential using summation based on the inclusion-exclusion principle [46].

For the general applicability of quasi Monte Carlo imaginary-time integration, a central question is whether the $1/N$ convergence deteriorates with increased expansion order [44]. To assess this, we have studied one diagram topology class up to order 8192 and found robust $1/N$ convergence, independent of order (see Supplemental Material [40]).

Having established the $1/N$ convergence we now turn to benchmark our inchworm quasi Monte Carlo solver for a non-trivial multiorbital impurity model relevant for real-materials simulation within dynamical mean-field theory. To this end we study a spinful two-band impurity model with a local

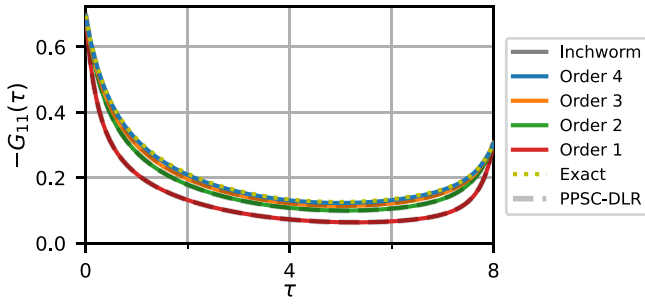


FIG. 5. Single-particle Green's function $G_{11}(\tau)$ for the two-band Kanamori model [Eq. (3)] with off-diagonal hybridization at $\beta = 8$. The inchworm quasi Monte Carlo result (solid lines) is compared to the exact result from exact diagonalization (yellow dotted line) and the first-, second-, and third-order result of bold pseudoparticle self-consistent perturbation theory using the discrete Lehmann representation (PPSC-DLR) [49] (gray dashed lines).

Kanamori interaction [47,48]

$$H = \sum_{i=1}^2 U n_{\uparrow,i} n_{\downarrow,i} + \sum_{\sigma,\sigma'} [U - (3 - \delta_{\sigma,\sigma'}) J] n_{\sigma,1} n_{\sigma,2} - J(c_{\uparrow,1}^\dagger c_{\downarrow,1}^\dagger c_{\uparrow,2} c_{\downarrow,2} + c_{\uparrow,1}^\dagger c_{\downarrow,1}^\dagger c_{\uparrow,2} c_{\downarrow,1} + \text{H.c.}), \quad (3)$$

where $c_{\sigma,i}^{(\dagger)}$ creates (annihilates) a fermion in state $i = 1, 2$ with spin $\sigma = \uparrow, \downarrow$, with Hubbard interaction $U = 2$ and Hund's coupling $J = 1/5$, chemical potential $\mu = (3U - 5J - 3)/2$, and a *nondiagonal* hybridization function, $\Delta_{i\sigma,j\sigma'}(\tau) = \delta_{\sigma,\sigma'} \Delta(\tau)$, where $\Delta(iv_n) = 1/(iv_n + \epsilon) + 1/(iv_n - \epsilon)$ and $\epsilon = 2.3$. This class of impurity models is out of reach for a standard partition function continuous-time hybridization expansion Monte Carlo, since the off-diagonal hybridization produces a severe sign problem [18]. Previously this model has been used to showcase that stochastic inchworm Monte Carlo is not impacted by such a sign problem [23]. Using inchworm *quasi* Monte Carlo we observe a rapid convergence of the solution with expansion order, with order 4 already being remarkably close to the exact solution, obtainable by exact diagonalization since the hybridization function is a discrete set of poles (see Fig. 5). We also compare the first-, second-, and third-order inchworm result (extrapolated to zero step size) with bold pseudoparticle perturbation theory recently obtained from a direct integration approach [49] using the discrete Lehmann representation [50,51]. The agreement confirms that the two expansions are equivalent at fixed perturbation order.

The inchworm approach is not limited to computing single-particle response functions and is able to compute arbitrary dynamical response functions [29]. As an example we study the spin-polarized Anderson impurity model with action $\mathcal{S}_B = \sum_{\sigma=\uparrow,\downarrow} \mathcal{S}[c_\sigma, c_\sigma^\dagger] - \int_0^\beta d\tau B c_\uparrow^\dagger(\tau) c_\uparrow(\tau)$ where the field $B = 2$ couples to the spin-up component and $\mathcal{S}[c_\sigma, c_\sigma^\dagger]$ [see Eq. (2)] has a spin-diagonal hybridization function $\Delta_\sigma(\tau) = \Delta(\tau)$ with semicircular density of states, bandwidth $W = 2$, and hybridization $V = 1/2$. Since the model is noninteracting, it amounts to a worst-case scenario for strong-coupling expansions such as the inchworm approach, which expands in the hybridization function. The single-particle Green's function

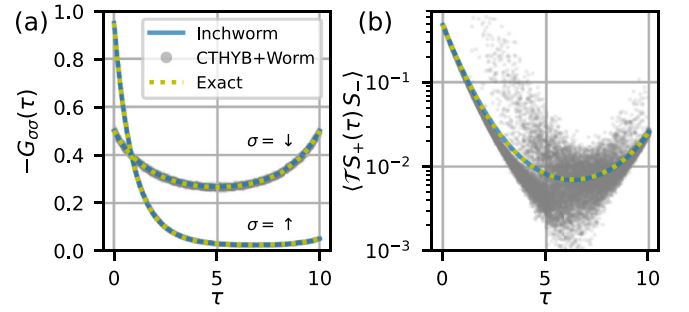


FIG. 6. (a) Single-particle Green's function for the spin-polarized Anderson impurity model at inverse temperature $\beta = 10$. (b) Out-of-plane spin response $\langle TS_+(\tau)S_- \rangle = \langle T(c_\uparrow^\dagger c_\downarrow)(\tau)(c_\downarrow^\dagger c_\uparrow) \rangle$. The inchworm result (blue lines) at order 5 is shown together with the exact analytic solution (dotted yellow lines), and the continuous-time hybridization expansion worm sampling (CTHYB+Worm) [52–54] (gray circles) where the ergodicity problem induces an extremely large variance between bins adjacent in time.

$G_{\sigma,\sigma}(\tau) = -\langle T c_\sigma(\tau) c_\sigma^\dagger \rangle$ is shown in Fig. 6(a) with $G_{\downarrow\downarrow}$ half filled and $G_{\uparrow\uparrow}$ almost unoccupied. The inchworm expression for dynamical response functions is agnostic to the kind of operators [29], so computing the transverse spin response $\langle TS_+(\tau)S_- \rangle$ is straightforward [see Fig. 6(b)]. On the other hand, this correlator cannot be sampled in partition function continuous-time hybridization expansion Monte Carlo since in this case S_+ and S_- do not commute with the local Hamiltonian [33,34]. This limitation can, in part, be overcome by worm sampling [52–54]. However, for some higher-order correlators such as $\langle TS_+(\tau)S_- \rangle$ also worm sampling has ergodicity problems, as shown in Fig. 6(b).

Discussion and conclusions. In conclusion, we have demonstrated a quantum impurity solver based on quasi Monte Carlo integration techniques [30–32] applied to the inchworm method [22,23,29]. Using quasi Monte Carlo, a $1/N$ convergence rate with the number of samples is achievable, which is parametrically better than the $1/\sqrt{N}$ convergence of previous Monte Carlo methods. In order to achieve this convergence rate, the smooth Root transformation [37] of the Sobol sequence from the unit hypercube to the simplex is used, which maintains the low discrepancy property. We demonstrate the improved convergence of our method on simple single-orbital problems where exact results are available, as well as on a more challenging multiorbital problem, and single diagrams at very high order [40]. These results show the usefulness of quasi Monte Carlo for achieving high accuracy of imaginary-time integrals arising in diagrammatic expansions for quantum systems.

We also point out that stochastic inchworm quantum Monte Carlo previously has been applied to nonequilibrium real-time dynamics of quantum impurity problems, with considerable success in taming the dynamical sign problem [22,29]. Hence, the extension of the quasi Monte Carlo integration approach to out-of-equilibrium real-time simulations is an interesting venue for further research.

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