Alternating-basis quantum Monte Carlo method for correlated electrons on a lattice

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We devise and benchmark a numerically exact quantum Monte Carlo (QMC) method for interacting electrons on a lattice, that we dub the alternating-basis QMC (ABQMC). The method is uniquely suited to evaluate charge and spin density and the corresponding correlation functions, in both direct and reciprocal space, imaginary or real time. The formalism applies in and out of thermal equilibrium, described by either the canonical or grand-canonical ensemble. The method relies on Suzuki-Trotter decomposition (STD) and owes flexibility to the representation of the kinetic and interaction terms in the many-body bases in which they are diagonal. We formulate a Monte Carlo (MC) update scheme that respects both the momentum and particle-number conservation laws, to restrict the configuration space and thus improve the efficiency of the sampling. To test the method, we perform various calculations for the Hubbard model on finite square lattices of up to 48 sites. We obtain the equation of state (density vs. chemical potential curve) in agreement with reference methods. We also evaluate the (real-time) dynamics of the survival probability of pure density-wave-like states: At small lattice sizes, where the exact diagonalization results are available, we demonstrate the validity of our method at short times; We then proceed to investigate this dynamics on the $4 \times 4$ Hubbard cluster. Finally, we discuss the extent of the fermionic sign problem and the current limitations of our method, both primarily related to the number of time-slices that we take in the STD.

I. INTRODUCTION

Last two decades have witnessed remarkable developments in laser and ultracold-atom technologies that have enabled experimental studies of the nonequilibrium dynamics of strongly correlated electrons. Ultrafast pump-probe spectroscopies can unveil complex excitation and relaxation pathways in strongly correlated materials (e.g., the cuprates, transition-metal oxides, and organic salts) and also provide means to manipulate their electronic phases. Ultracold atoms in optical lattices and optical-tweezer arrays have been used as quantum simulators of paradigmatic models of condensed-matter physics, such as the Hubbard model. Recent experiments with ultracold fermionic atoms have probed both equilibrium (e.g., the equation of state, charge and spin correlation functions, identification of string patterns) and transport properties (by monitoring charge, mass, or spin diffusion) of the two-dimensional Hubbard model.

These great strides on the experimental side should be accompanied by the development of computational methods capable of accurately describing the motion of correlated electrons in real time. The nonequilibrium dynamical properties of strongly correlated electronic systems have been studied using a host of theoretical approaches, among others the exact diagonalization, nonequilibrium dynamical mean-field theory, time-dependent density-matrix renormalization group, reduced density matrix approaches, quantum kinetic equations based on the nonequilibrium Green’s functions formalism, real-time path-integral techniques, and different flavors of the continuous-time QMC. Each of these methods has its own weaknesses that seriously affect its practical applicability. For example, the density matrix approaches need an exponentially large number of auxiliary operators to produce the results of a preset accuracy. The QMC simulations of the long-time dynamics of strongly correlated fermions are exponentially hard due to the so-called dynamical sign problem. These weaknesses generally limit the applications of the above-listed methodologies to relatively short-time dynamics, weak-correlation regimes or small systems (e.g., quantum impurity models). Even though substantial efforts have been invested to overcome these limitations, simulations of large systems are still intractable. Very recently, a time-dependent generalization of the auxiliary-field QMC has been proposed as a viable route towards the dynamics of correlated fermions on two-dimensional lattices.

Furthermore, the available numerical methods are yet to fully catch up with the multitude of novel kinds of experimental measurements that have become feasible recently, especially in the quantum simulator setups. An excellent example is the recent ultracold-atom experiment in Ref. 19. In this study, and as later confirmed in Ref. 54, solid agreement between theory and an optical-lattice simulation of the Hubbard model was reached regarding the temperature dependence of dc resistivity. However, the resistivity was not directly accessible to experimentalists. What was measured is the temporal evolution of spatially resolved particle density, following a quench of an external density-modulating field. The interpretation of the raw measurement data was based on an assumption of hydrodynamic behavior of charge density at long wavelengths that could not have been inde-
pendently checked by available microscopic theory. It is, therefore, of utmost importance to devise novel theoretical tools that can be used to directly cross-check measurements in cold-atom experiments (such as those of the time-evolution of the spatially resolved charge density). This work is intended to be a step in this direction.

We develop and test a QMC procedure termed the alternating-basis QMC method. The ABQMC method belongs to the class of discrete-time QMC methods,\textsuperscript{55,56} which use the STD as the first step in the computation of some quantity of interest.\textsuperscript{57–59} In the ABQMC method, the infinitesimal propagators of the kinetic and interaction term are then represented in the many-body bases in which they are diagonal. In the case of the Hubbard model, the kinetic-term eigenstates are constructed out of plane waves, while the interaction-term eigenstates feature electrons localized at individual lattice sites. The time evolution may then be seen as a sequence of basis alternations between the momentum and coordinate eigenbasis, hence the name of the method. At any given MC step, such a construction makes measurements of the density of spin and charge (in both direct and inverse space) or spatially uniform current, algorithmically trivial and computationally cheap. The STD may be applied along the entire Kadanoff–Baym 3-piece contour, which allows access to real-time evolution of densities and, at least in principle, any corresponding n-point correlation function. Our ABQMC method has the additional flexibility that it can treat the canonical ensemble, in contrast to the Green’s function based methods (such as continuous-time interaction-expansion QMC (CT-INT),\textsuperscript{38,60} or diagrammatic MC\textsuperscript{61,62}) where only grand-canonical ensemble can be straightforwardly treated. The ABQMC method can also be straight-forwardly applied to the time-evolution of pure states in either the plane-wave or coordinate many-body bases, which is highly relevant for recent experiments on optical-tweezer arrays.\textsuperscript{9–11}

Our results for the average charge density in the Hubbard model show agreement with numerically exact results in multiple examples, thus validating our implementation. At moderate coupling of the order of half bare bandwidth, we observe that only two imaginary-time slices suffice to obtain excellent results in the temperature range relevant for optical lattice experiments. In parameter regime where we are unaware of other readily applicable approaches, we study the time evolution of the survival probability of several pure states, which is generally relevant for ultracold-atom experiments. The survival probability, which monitors the relaxation of a quantum system prepared in a state that is not the eigenstate of the Hamiltonian governing time evolution,\textsuperscript{63,64} can hold insight into correlations and other properties.\textsuperscript{53,65} Similarly to observations made in Ref. 66, we find in general that the survival probability decays over longer times, when interactions are stronger. At shorter times, we find that the behavior depends strongly on the type of the initial state, likely related to the average density. Finally, we find that the main obstacle in the ABQMC method is the fermionic sign problem, which we document in detail. The severity of the sign problem scales with the average density, lattice size, but most importantly the number of time slices. The method may be readily useful in few-body or weak coupling calculations where the average sign is manageable and a low number of time slices does not introduce a serious systematic error. However, further algorithmic developments are needed to access parameter regimes of primary interest (large lattices, strong coupling, low temperature, density close to half-filling).

The paper is organized as follows. The ABQMC method is developed in Sec. II and applied to equilibrium and out-of-equilibrium setups in Sec. III. Section IV discusses the ABQMC method in light of other widely used QMC algorithms. Section V summarizes our main findings, indicates their implications, and discusses possible improvements of our method.

II. MODEL AND METHOD

A. Hubbard Hamiltonian

We study the Hubbard model on a square-lattice cluster containing $N_c = N_x N_y$ sites under periodic boundary conditions (PBC). The Hamiltonian reads as

$$H = H_0 + H_{\text{int}}.$$  

The noninteracting (single-particle) part $H_0$ of the Hamiltonian describes a band of itinerant electrons

$$H_0 = -J \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} c_{\mathbf{r} \sigma}^{\dagger} c_{\mathbf{r}' \sigma} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} n_{\mathbf{k} \sigma},$$  

where $J$ is the hopping amplitude between the nearest-neighbor lattice sites $\mathbf{r}$ and $\mathbf{r}'$, while the operators $c_{\mathbf{r} \sigma}^{\dagger}$ ($c_{\mathbf{r} \sigma}$) create (destroy) an electron of spin $\sigma$ on lattice site $\mathbf{r}$. Under PBC, $H_0$ is diagonal in the momentum representation; the wave vector $\mathbf{k}$ may assume any of the $N_c$ allowed values in the first Brillouin zone of the lattice. The free-electron dispersion is given by

$$\varepsilon_{\mathbf{k}} = -2J(\cos k_x + \cos k_y).$$

The density operator is

$$n_{\mathbf{k} \sigma} = c_{\mathbf{k} \sigma}^{\dagger} c_{\mathbf{k} \sigma},$$

where $U$ is the interaction strength, while

$$n_{\mathbf{r} \sigma} = c_{\mathbf{r} \sigma}^{\dagger} c_{\mathbf{r} \sigma}.$$

If the number of particles is not fixed, Eq. (1) additionally features the chemical-potential term $-\mu \sum_{\mathbf{k} \sigma} n_{\mathbf{k} \sigma}$, so that the free-electron dispersion $\varepsilon_{\mathbf{k}}$ appearing in Eq. (2) is replaced by $\varepsilon_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$.

B. ABQMC method

Finding viable approximations to the exponential of the form $e^{-\alpha H}$ is crucial to many QMC methods. With
$\alpha = 1/T$ ($T$ denotes temperature), this is the Boltzman operator, which will play a role whenever the system is in thermal equilibrium. In the formulation of dynamical responses, the time-evolution operator will also have this form, with $\alpha = it$, where $t$ is the (real) time. One possible way to deal with these is the lowest-order STD\cite{STD}

$$e^{-\alpha H} \approx \left(e^{-\Delta H_0} e^{-\Delta H_{\text{int}}}ight)^{N_\alpha}$$ (4)

where the interval of length $|\alpha|$ is divided into $N_\alpha$ subintervals of length $|\Delta \alpha|$ each, where $\Delta \alpha = \alpha/N_\alpha$. The error of the approximation is of the order of $|\Delta \alpha|^2 ||[H_0, H_{\text{int}}]||$, where the norm $||[H_0, H_{\text{int}}]||$ may be defined as the largest (in modulus) eigenvalue of the commutator $[H_0, H_{\text{int}}]$\cite{STD}. The error can in principle be made arbitrarily small by choosing $N_\alpha$ large enough. However, the situation is complicated by the fact that the RHS of Eq. (4) contains both single-particle and two-particle contributions. Employing the discrete Hubbard–Stratonovich transformation,\cite{HST} two-particle contributions are commonly recast as sums over one-particle contributions characterized by discrete auxiliary-field variables that are sampled using auxiliary-field QMC methods\cite{AFQMC1,AFQMC2,AFQMC3,AFQMC4}.

In contrast to these methods, our ABQMC approach is based on another fundamental difference between $e^{-\Delta H_0}$ and $e^{-\Delta H_{\text{int}}}$. While the former is diagonal in the momentum representation, the latter is diagonal in the coordinate representation. The spectral decomposition of $e^{-\Delta H_0}$ is performed in terms of totally antisymmetric states in the momentum representation

$$|\Psi_k\rangle = \prod_{\sigma}^{N_\sigma} \prod_{j=1}^{N_j} \epsilon_0^{e_j^\sigma} |0\rangle,$$ (5)

where $|0\rangle$ denotes the vacuum. The state $|\Psi_k\rangle$ contains $N_\sigma$ electrons of spin $\sigma$ whose momenta $k_1^\sigma, \ldots, k_{N_\sigma}^\sigma$ are ordered according to a certain rule and we define $\epsilon_0(|\Psi_k\rangle) = \langle \Psi_k|H_0|\Psi_k\rangle$. Analogously, the spectral decomposition of $e^{-\Delta H_{\text{int}}}$ is performed in terms of totally antisymmetric states in the coordinate representation

$$|\Psi_i\rangle = \prod_{\sigma}^{N_\sigma} \prod_{j=1}^{N_j} \epsilon_{\text{int}}^{e_j^\sigma} |0\rangle$$ (6)

that contain $N_\sigma$ electrons of spin $\sigma$ whose positions $r_1^\sigma, \ldots, r_{N_\sigma}^\sigma$ are ordered according to a certain rule. We define $\epsilon_{\text{int}}(|\Psi_i\rangle) = \langle \Psi_i|H_{\text{int}}|\Psi_i\rangle$.

Further developments of the ABQMC method somewhat depend on the physical situation of interest. We formulate the method first in equilibrium, and then in out-of-equilibrium situations. To facilitate discussion, in Figs. 1(a)–1(d) we summarize the contours appropriate for different situations we consider.

1. ABQMC method for thermodynamic quantities

The equilibrium properties at temperature $T = \beta^{-1}$ follow from the partition function $Z \equiv \text{Tr} e^{-\beta H}$, which may be computed by dividing the imaginary-time interval $[0, \beta]$ into $N_\tau$ slices of length $\Delta \tau \equiv \beta/N_\tau$, employing Eq. (4), and inserting the spectral decompositions of $H_0$ and $H_{\text{int}}$. One eventually finds

$$Z \approx \sum_{\mathcal{C}} \mathcal{D}(\mathcal{C}) e^{-\Delta \tau \epsilon(\mathcal{C})},$$ (7)

The configuration

$$\mathcal{C} = \{ |\Psi_{k,1}\rangle, \ldots, |\Psi_{k,N_\tau}\rangle, |\Psi_{i,1}\rangle, \ldots, |\Psi_{i,N_\tau}\rangle \}$$ (8)

resides on the contour depicted in Fig. 1(a) and consists of $N_\tau$ totally antisymmetric states $|\Psi_{k,l}\rangle$ ($l = 1, \ldots, N_\tau$) in the momentum representation and $N_\tau$ totally antisymmetric states $|\Psi_{i,l}\rangle$ in the coordinate representation. $\mathcal{D}(\mathcal{C})$ is the product of $2N_\tau$ Slater determinants

$$\mathcal{D}(\mathcal{C}) \equiv \prod_{l=1}^{N_\tau} \prod_{\sigma}^{N_\sigma} \langle \Psi_{i,l}|\Psi_{k,l}\rangle/\langle \Psi_{i,l}|\Psi_{k,l=1}\rangle$$ (9)

that stem from the sequence of basis alternations between the momentum and coordinate eigenbasis. The cyclic subtraction in Eq. (9) is the standard subtraction for $l = 2, \ldots, N_\tau$, while $1 \equiv 1 = N_\tau$. Using the notation of Eqs. (5) and (6), the most general Slater determinant $\langle \Psi_i|\Psi_k\rangle$ entering Eq. (9) is given as

$$\langle \Psi_i|\Psi_k\rangle = \prod_{\sigma} \text{det} S(\Psi_i, \Psi_k, \sigma)$$ (10)

$$[S(\Psi_i, \Psi_k, \sigma)]_{j_1,j_2} = \langle r_{j_1}^\sigma | r_{j_2}^\sigma \rangle = \frac{\exp(ik_{j_2}^\sigma \cdot r_{j_1}^\sigma)}{\sqrt{N_c}}$$ (11)
where $1 \leq j_1, j_2 \leq N_\sigma$. The symbol $\varepsilon(C)$ stands for
\begin{equation}
\varepsilon(C) \equiv \sum_{l=1}^{N_\tau} \left[ \varepsilon_0(\Psi_{k,l}) + \varepsilon_{\text{int}}(\Psi_{i,l}) \right] .
\end{equation}

By virtue of the cyclic invariance under trace, the thermodynamic expectation value of an observable $A$ can be expressed as
\begin{equation}
\langle A \rangle = \frac{1}{N_\tau} \sum_{l=0}^{N_\tau-1} \frac{1}{Z} \text{Tr} \left\{ (e^{-\Delta \tau H})^l A (e^{-\Delta \tau H})^{N_\tau-l} \right\} .
\end{equation}

In the most relevant cases, $A$ is diagonal in either the coordinate (e.g., the interaction energy $H_{\text{int}}$) or the real-space density $n_{x a}$ or the momentum (e.g., the kinetic energy $H_0$) representation, which is further signalized by adding the subscript $a = i, k$ denoting the representation in which $A_a$ is diagonal. Equation (13), combined with the lowest-order STD [Eq. (4)], then reduces to
\begin{equation}
\langle A_a \rangle \approx \frac{1}{Z} \sum_{C} D(C) e^{-\Delta \tau \varepsilon(C)} \frac{1}{N_\tau} \sum_{l=1}^{N_\tau} A_a(\Psi_{a,l}) ,
\end{equation}

where
\begin{equation}
A_a(\Psi_{a,l}) \equiv \langle \Psi_{a,l} | A_a | \Psi_{a,l} \rangle .
\end{equation}

The evaluation of Eq. (14) using the importance-sampling MC procedure is complicated by the fact that $D(C)$ is a complex number defined by its modulus and phase. While the modulus can be included in the weight of configuration $C$, the phase gives rise to the so-called phase problem, which is generally much harder to curb than the ordinary sign problem. However, since the STD preserves the equality $Z = Z^*$, Eq. (7) can be replaced by
\begin{equation}
Z \approx \sum_{C} \text{Re} \{ D(C) \} e^{-\Delta \tau \varepsilon(C)} ,
\end{equation}
and we remain with the ordinary sign problem. Equation (14) should then be replaced by
\begin{equation}
\langle A_a \rangle \approx \frac{\sum_{C} \text{Re} \{ D(C) \} e^{-\Delta \tau \varepsilon(C)} \frac{1}{N_\tau} \sum_{l=1}^{N_\tau} A_a(\Psi_{a,l}) }{\sum_{C} \text{Re} \{ D(C) \} e^{-\Delta \tau \varepsilon(C)}} .
\end{equation}

Defining the weight $w(C)$ of configuration $C$ as
\begin{equation}
w(C) \equiv |\text{Re} \{ D(C) \}| e^{-\Delta \tau \varepsilon(C)} ,
\end{equation}
Eq. (17) is rewritten as
\begin{equation}
\langle A_a \rangle \approx \frac{\langle \text{sgn}(C) \frac{1}{N_\tau} \sum_{l=1}^{N_\tau} A_a(\Psi_{a,l}) \rangle_w }{|\text{sgn}(C)|_w} ,
\end{equation}
where $\langle \ldots \rangle_w$ denotes the weighted average over all $C$ with respect to the weight $w(C)$; $\text{sgn}(C) \equiv \text{Re} \{ D(C) \} / |\text{Re} \{ D(C) \}|$ is the sign of configuration $C$, while $|\langle \text{sgn} \rangle| \equiv |\langle \text{sgn}(C) \rangle_w|$ is the average sign of the ABQMC simulation.

By construction, our ABQMC approach yields exact results for the noninteracting electrons (ideal gas, $U = 0$) and in the atomic limit ($J = 0$). In both limits, due to $[H_0, H_{\text{int}}] = 0$, the ABQMC method with arbitrary $N_\tau$ should recover the exact results. Nevertheless, the performance of the method, quantified through the average sign of the simulation, deteriorates with increasing $N_\tau$.

For $N_\tau = 1$, our ABQMC algorithm is sign-problem-free because $D(C) = |\langle \Psi_{k,1} | \Psi_{k,1} \rangle|^2$ for any configuration $C = \{ \langle \Psi_{k,1}, | \Psi_{1,1} \rangle \}$, see Eq. (9).

An important feature of the above-presented methodology is its direct applicability in both the grand-canonical and canonical ensemble. Allowing the electron number to fluctuate according to the fixed chemical potential is essential for the formulation of the majority of theoretical approaches addressing the equilibrium properties of the Hubbard model. For example, in the auxiliary-field QMC; the fluctuating electron number is at the crux of the transformation of complicated traces over electrons to the product of determinants. To extract equilibrium quantities for a fixed number of electrons, one has to resort to particle-projection codes68,69 or many-body recursive methods70,71 whose numerical cost may greatly exceed that of grand-canonical techniques. In contrast to these approaches, the formulation of our ABQMC method does not depend on whether the electron number is fixed or not. However, the selection of MC updates does depend on the ensemble we work in. In the canonical ensemble, the updates should conserve the number of electrons; In the grand-canonical ensemble, we need to include also the updates that insert/remove electrons. In both cases, we design the MC updates so as to respect the particle-number and momentum conservation laws across the (imaginary-)time evolution. The particle-number conservation demands that all the states $|\Psi_{k,1}, \Psi_{1,1} \rangle \in C$ have the same numbers of electrons of each spin projection. Furthermore, the momentum conservation demands that all the momentum-space states $|\Psi_{k,1} \rangle \in C$ have the same total electron momentum $K \equiv \sum_{k,a} k |\Psi_{k,a} | \Psi_{k,a} \rangle$. Our MC updates, together with the procedure used to extract MC results and estimate their statistical error, are presented in great detail in Sec. SI of the Supplementary Material.

2. ABQMC method for time-dependent quantities

Ideally, numerical simulations of quench experiments such as those from Refs. 19, 21, and 22 should provide the time-dependent expectation value $\langle A_a(t) \rangle$ of an observable $A_a$ at times $t > 0$ after the Hamiltonian undergoes a sudden change from $H(0)$ for $t < 0$ to $H$ for $t > 0$. Again, the most relevant observables are diagonal in the coordinate or momentum representation, which is
emphasised by the subscript $a = i, k$. The computation proceeds along the Kadanoff–Baym contour:

$$
\langle A_a(t) \rangle = \frac{\text{Tr} \left( e^{-\beta H(0)} e^{iHt} A_a e^{-iHt} \right)}{\text{Tr} \left( e^{-\beta H(0)} \right)}
$$

(20)

where one may employ the above-outlined alternating-basis approach after dividing the whole contour into a number of slices, see Fig. 1(b). While $H$ is the Hubbard Hamiltonian given in Eqs. (1)–(3), $H(0)$ describes correlated electrons whose charge (or spin) density is spatially modulated by external fields.

The immediate complication (compared to the equilibrium case) is that there are now three operators (instead of one) that need to be decomposed via the STD. A preset accuracy determined by the size of both $\Delta \tau$ and $\Delta t$ will therefore require a larger number of time-slices. In turn, this will enlarge the configuration space to be sampled, and potentially worsen the sign problem in the MC summation.

To simplify the task, and yet keep it relevant, we consider the evolution from a pure state $|\psi(0)\rangle$ that is an eigenstate of real-space density operators $n_{q,\sigma}$, so that its most general form is given by Eq. (6). Such a setup has been experimentally realized.\textsuperscript{10,11,19,22} Replacing $e^{-iHt} \rightarrow |\psi(0)\rangle\langle\psi(0)|$ in Eq. (20) leads to the expression for the time-dependent expectation value of observable $A_a$

$$
\langle A_a(t) \rangle = \frac{\langle \psi(0)| e^{iHt} A_a e^{-iHt} |\psi(0)\rangle}{\langle \psi(0)|\psi(0)\rangle}.
$$

(21)

Still, the STD should be applied to both the forward and backward evolution operators, see Fig. 1(c), which requires a larger number of time-slices to reach the desired accuracy (in terms of the systematic error). A further simplification is to consider the overlap of the state at time $t > 0$ with the initial state, which amounts to replacing $A_a \rightarrow |\psi(0)\rangle\langle\psi(0)|$ in Eq. (21). We are then left with the dynamics of the so-called survival probability $P(t)$

$$
P(t) = \left| \frac{\langle \psi(0)| e^{-iHt} |\psi(0)\rangle}{\langle \psi(0)|\psi(0)\rangle} \right|^2
$$

(22)

which is the probability of finding the system in its initial state after a time $t$ has passed. Evaluating Eq. (22) by the ABQMC method necessitates only one STD, see Fig. 1(d). The survival probability is thus the simplest example on which the applicability of our ABQMC method to out-of-equilibrium setups can be systematically studied.

Generally speaking, the symmetries of the model should be exploited to enable as efficient as possible MC evaluation of Eqs. (20)–(22). Recent experimental\textsuperscript{20} and theoretical\textsuperscript{22} studies have discussed the dynamical symmetry of the Hubbard model, according to which the temporal evolution of certain observables is identical for repulsive and attractive interactions of the same magnitude. The symmetry relies on specific transformation laws of the Hamiltonian $H$, the initial state $|\psi(0)\rangle$, and the observable of interest $A_a$ under the combined action of two symmetry operations. The first is the bipartite lattice symmetry or the $\pi$-boost\textsuperscript{20} operation, which exploits the symmetry $\varepsilon_k = -\varepsilon_{k+\pi,\pi}$ of the free-electron dispersion and which is represented by the unitary operator $B$. The second is the time reversal symmetry represented by the antiunitary operator $T (T iT = -i)$ that reverses electron spin and momentum according to $T c_{\downarrow}^{(i)} T = (1)^{\delta_{s,\uparrow}} c_{\uparrow}^{(i)}$ and $T c_{\sigma}^{(i)} T = (1)^{\delta_{s,\uparrow}} - e^{-i\pi \sigma} c_{\sigma}^{(i)}$. In Appendix A, we formulate our ABQMC method to evaluate Eqs. (21) and (22) in a way that manifestly respects the dynamical symmetry of the model (each contribution to MC sums respects the symmetry). Here, we only cite the final expressions, starting from the technically simpler case [Eq. (22)] on which we focus our MC simulations. The ABQMC method to evaluate Eq. (20) is developed in Sec. SII of the Supplementary Material.

The ABQMC expression for the survival probability of state $|\psi(0)\rangle$ that satisfies $TB|\psi(0)\rangle = e^{i\chi}|\psi(0)\rangle$ ($\chi \in \mathbb{R}$) reads as

$$
P(t) \cong \sum_c \text{Re} \left( D(C) \right) \cos[\varepsilon_0(C)\Delta t] \cos[\varepsilon_{\text{int}}(C)\Delta t] \left/ \sum_c \text{Re} \left( D(C) \right) \right.^2.
$$

(23)

The configuration $C$ resides on the contour depicted in Fig. 1(d) and consists of $N_t$ totally antisymmetric states $|\Psi_{l,1}\rangle$ ($l = 1, \ldots, N_t$) in the momentum representation and $N_t - 1$ totally antisymmetric states $|\Psi_{l,\downarrow}\rangle$ ($l = 2, \ldots, N_t$) in the coordinate representation, while $|\Psi_{l,1}\rangle \equiv |\psi(0)\rangle$. The length of a single real-time slice $\Delta t \equiv t/N_t$ increases with $t$. $D(C)$ is defined in Eq. (9), in which $N_t$ is replaced with $N_t$. The symbols $\varepsilon_0(C)$ and $\varepsilon_{\text{int}}(C)$ stand for

$$
\varepsilon_0(C) = \sum_{l=1}^{N_t} \varepsilon_0(\Psi_{l,1}), \quad \varepsilon_{\text{int}}(C) = \sum_{l=1}^{N_t} \varepsilon_{\text{int}}(\Psi_{l,\downarrow}).
$$

(24)

We note that each term in Eq. (23) is invariant under transformations $\varepsilon_0(C) \rightarrow -\varepsilon_0(C)$ and $\Delta t \rightarrow -\Delta t$, which reflect the action of the bipartite lattice symmetry and the time reversal symmetry, respectively. Being term-by-term invariant under the transformation $\varepsilon_{\text{int}}(C) \rightarrow -\varepsilon_{\text{int}}(C)$, Eq. (23) explicitly satisfies the requirement that the dynamics of $P(t)$ for repulsive and attractive interactions of the same magnitude are identical. Defining the weight of the configuration $C$ as $w(C) \equiv |\text{Re} \left( D(C) \right)|$, Eq. (23) is recast as

$$
P(t) \approx \left| \frac{\langle \text{sgn}(C) \cos[\varepsilon_0(C)\Delta t] \cos[\varepsilon_{\text{int}}(C)\Delta t] \rangle \omega}{\langle \text{sgn}(C) \rangle \omega} \right|^2.
$$

(25)

This choice for $w$ is optimal in the sense that it minimizes the variance of $\langle \text{sgn}(C) \rangle \omega$\textsuperscript{73} whose modulus is the average sign of the ABQMC simulation.

We now cite the ABQMC expression for the time-dependent expectation value of an observable $A_a$ that satisfies $TB A_a B T = A_a$ when the evolution starts from
a state $|\psi(0)\rangle$ that satisfies $TB|\psi(0)\rangle = e^{i\chi}|\psi(0)\rangle$
\[
(A_a(t)) \approx \frac{1}{\sum_C \text{Re}(D(C))} \sum_C \text{Re}(D(C)) A_a(\Psi_a, l_a) \times \cos [\Delta \varepsilon_0(C) \Delta t] \cos [\Delta \varepsilon_{\text{int}} \Delta t].
\] (26)

Here, the configuration resides on the Keldysh contour, see Fig. 1(c), which is divided into $2N_t$ slices in total, and contains $2N_t - 1$ independent states. We assume that states $|\Psi_{i,k,l}\rangle$ for $l = 1, \ldots, N_t$ ($l = N_t + 1, \ldots, 2N_t$) lie on the forward (backward) branch of the contour, while $|\psi_{i,1}\rangle \equiv |\psi(0)\rangle$. The index $l_a$ assumes the value $N_t + 1$ when the observable $A_a$ is diagonal in the coordinate representation ($a = i$) and the value $N_t$ when the observable $A_a$ is diagonal in the momentum representation ($a = k$). $A_a(\Psi_a, l_a)$ is defined as in Eq. (15), while
\[
\Delta \varepsilon_0(C) \equiv \sum_{l=1}^{N_t} [\varepsilon_0(\Psi_{i,k,l+N_t}) - \varepsilon_0(\Psi_{i,k,l})],
\] (27)
\[
\Delta \varepsilon_{\text{int}}(C) \equiv \sum_{l=1}^{N_t} [\varepsilon_{\text{int}}(\Psi_{i,k,l+N_t}) - \varepsilon_{\text{int}}(\Psi_{i,k,l})].
\] (28)

Equation (26) is term-by-term invariant under the transformations $\Delta \varepsilon_0(C) \rightarrow -\Delta \varepsilon_0(C)$, $\Delta t \rightarrow -\Delta t$, and $\Delta \varepsilon_{\text{int}}(C) \rightarrow -\Delta \varepsilon_{\text{int}}(C)$ that respectively reflect the transformation properties under the bipartite lattice symmetry, the time reversal symmetry, and the fact that the dynamics of $(A_a(t))$ is identical in the repulsive and the attractive model. Defining the weight of the configuration $C$ as $w(C) \equiv |\text{Re}(D(C))|$, Eq. (26) is recast as
\[
(A_a(t)) \approx \frac{\langle \text{sgn}(C) A_a(\Psi_a, l_a) \rangle \cos [\Delta \varepsilon_0(C) \Delta t] \cos [\Delta \varepsilon_{\text{int}} \Delta t] w}{\langle \text{sgn}(C) w \rangle}.
\] (29)

It is important to note that $w(C)$ in Eqs. (25) and (29) does not depend on either $\Delta t$ or any other property of configuration $C$ ($\varepsilon_0, \varepsilon_{\text{int}}, \Delta \varepsilon_0, \Delta \varepsilon_{\text{int}}$). Therefore, the MC evaluation of Eqs. (25) and (29) may be performed simultaneously (using a single Markov chain) for any interaction strength $U$ and any real time $t$. This is different from the equilibrium case, Eq. (19), where the configuration weight does depend on $\varepsilon(C)$ and the temperature, so that MC evaluations for different values of $U$ and $T$ (and the chemical potential $\mu$ if the particle number is not fixed) should be performed separately.

We now discuss the application of conservation laws in the evaluation of Eqs. (25) and (29). In both cases, the particle-number conservation demands that throughout the time evolution, the total number of electrons of each spin species remains unchanged from that in the initial state $|\psi(0)\rangle$. Next, in the case of the survival probability [Eq. (25)], the momentum conservation poses the restriction that all the momentum-space states $|\Psi_{k,i}\rangle$ have the same total electron momentum $K$. The application of the momentum conservation to the evaluation of Eq. (29) depends on the representation in which the observable of interest is diagonal. If we deal with the observable $A_k$ diagonal in the momentum representation, then all momentum-space states $|\Psi_{k,1}\rangle, \ldots, |\Psi_{k,2N_t}\rangle$ should have the same momentum $K$. On the other hand, the observable $A_i$ diagonal in the coordinate representation breaks the momentum conservation along the whole contour into two conservation laws that are satisfied separately on the two branches. Namely, the momenta of $N_t$ momentum-space states on the forward branch are all equal to $K_{\text{fwd}}$, the momenta of $N_t$ momentum-space states on the backward branch are all equal to $K_{\text{bwd}}$, while $K_{\text{fwd}}$ and $K_{\text{bwd}}$ need not be mutually equal.

Specifically in the calculation of $P(t)$, further symmetries can be employed to improve performance of the method for a very broad class of pure density-wave-like initial states. These states correspond to extreme spin- and charge-density wave patterns, which one obtains by applying strong external density-modulating fields. The SDW-like state can be written as
\[
|\psi_{\text{SDW}}\rangle = \prod_{\mathbf{r} \in G} c_{\mathbf{r}, \uparrow} \prod_{\mathbf{r} \not\in G} c_{\mathbf{r}, \uparrow} |\varnothing\rangle
\] (30)
where $G$ denotes the multitude of sites on which the electron spins are polarized up, while set $U \not\subset G$ contains all sites of the cluster studied. The electron spins on sites belonging to $U \not\subset G$ are thus polarized down. Such states have been experimentally realized in Ref. 22.

The CDW-like states have also been realized in experiment, and they read as
\[
|\psi_{\text{CDW}}\rangle = \prod_{\mathbf{r} \in G} c_1 c_{\mathbf{r}, \uparrow} |\varnothing\rangle.
\] (31)

The sites belonging to $G$ are doubly occupied, while the remaining sites are empty. The state $|\psi_{\text{CDW}}\rangle$ can be obtained from a corresponding $|\psi_{\text{SDW}}\rangle$ state by applying the partial particle–hole transformation that acts on spin-down electrons only
\[
|\psi_{\text{SDW}}\rangle = \prod_{\mathbf{r}} \left( c_{\mathbf{r}, \downarrow} (1 - n_{\mathbf{r}, \downarrow}) + c_{\mathbf{r}, \uparrow} n_{\mathbf{r}, \downarrow} \right) |\psi_{\text{CDW}}\rangle,
\] (32)
see also Refs. 74 and 75. The dynamics of the survival probabilities of states $|\psi_{\text{SDW}}\rangle$ and $|\psi_{\text{CDW}}\rangle$ are identical, i.e.,
\[
|\langle \psi_{\text{SDW}}| e^{-iHt} |\psi_{\text{SDW}}\rangle|^2 = |\langle \psi_{\text{CDW}}| e^{-iHt} |\psi_{\text{CDW}}\rangle|^2.
\] (33)

The formal demonstration of Eq. (33), which relies on the partial particle–hole and bipartite lattice symmetries, is deferred for Appendix B. It is possible to combine the Markov chains for the $P(t)$ calculations starting from these two symmetry-related states to achieve improved convergence. We summarize this procedure in Appendix B [see the text below Eq. (B6)] and apply it in all corresponding computations presented in Sec. III B.

Similarly, in the calculation of the time-evolution of spatially-resolved density, starting from $|\psi_{\text{CDW}}\rangle$ and
\[ |\psi_{SDW}\rangle \text{ states, the following symmetry holds:} \]
\[
\langle \psi_{CDW}|e^{iHt}(n_{r\uparrow} + n_{r\downarrow} - 1)e^{-iHt}|\psi_{SDW}\rangle = \langle \psi_{SDW}|e^{iHt}(n_{r\uparrow} - n_{r\downarrow})e^{-iHt}|\psi_{SDW}\rangle.
\]

Once, again, efficiency is gained by combining the Markov chains for the two symmetry-related evolutions. This procedure is described in Appendix B and we employ it in the corresponding computations in Sec. III C.

III. NUMERICAL RESULTS

We first apply the ABQMC method to equilibrium situations (the particle number is not fixed), see Sec. III A, and then in out-of-equilibrium setups (evolution of pure states), see Secs. III B and III C. For the implementation of the full Kadanoff–Baym contour [Eq. (20)], we give benchmarks in Sec. SII of the Supplementary Material.

A. Equilibrium results: Equation of state

We start by considering the Hubbard dimer, the minimal model capturing the subtle interplay between electron delocalization and electron–electron interaction. We opt for moderate temperature \( T/J = 1 \) and interaction \( U/J = 4 \), so that the expected number of imaginary-time slices needed to obtain convergent ABQMC results is not very large. Figure 2 presents the equation of state (i.e., the dependence of the electron density \( \rho_e = \frac{\langle \hat{N}_\uparrow + \hat{N}_\downarrow \rangle}{N_e} \) on the chemical potential \( \mu \)) for a range of \( \mu \) below the half filling. Here, \( \hat{N}_\uparrow \) and \( \hat{N}_\downarrow \) are the operators of the total number of spin-up and spin-down electrons, respectively. The symbols present the results of our ABQMC method with \( N_\tau = 2 \) (circles) and \( N_\tau = 4 \) (squares) imaginary-time slices, while the solid line presents the exact-diagonalization results. Figure 2 suggests that already \( N_\tau = 2 \) imaginary-time slices suffice to obtain very good results in the considered range of \( \mu \), while increasing \( N_\tau \) from 2 to 4 somewhat improves the accuracy of the ABQMC results.

We now apply our ABQMC method to evaluate the equation of state on larger clusters. We focus on a 4 × 4 cluster, which may already be representative of the thermodynamic limit at \( T/J \geq 1 \). \(^{14}\) We compare our \( \rho_e(\mu) \) results with the numerical linked-cluster expansion (NLCE) method.\(^{78-80} \) The NLCE results are numerically exact and converged with respect to the control parameter, i.e., the maximal cluster-size used. NLCE is commonly used to benchmark methods and understand experimental data.\(^{14,15} \) Again, we keep \( U/J = 4 \), but we take \( T/J = 1.0408 \) to be able to compare results to the data of Ref. 78. Figure 3(a) reveals that the ABQMC results with only \( N_\tau = 2 \) imaginary-time slices agree very well with the NLCE results over a wide range of chemical potentials. This is a highly striking observation. It is unclear whether other STD-based methods would reach here the same level of accuracy with only two time-slices. This may be a specific property of ABQMC. We also calculate the double occupancy \( \sum_{\tau}(n_{r\uparrow}n_{r\downarrow})/N_e \) and compare to the reference NLCE results, see Fig. 3(c). Although qualitative behavior is well captured, the agreement with the reference data is less favorable, as one would expect in the case of such modest imaginary-time discretization. Unfortunately, we are currently unable to converge results for the 4 × 4 lattice at \( N_\tau > 2 \) due to increasing severity of the sign problem.

The extent of the sign problem encountered in the above calculation is summarized in Fig. 3(b). The average sign strongly depends on the average electron density: it is minimal around the half filling, and (roughly) monotonically increases as the density is lowered. Between \( \rho_e = 1 \) and \( \rho_e = 0.06 \) it grows by three orders of magnitude. The average sign above the half-filling \( \rho_e = 1 \) mirrors that below the half-filling. The particle–hole symmetry ensures that \( \rho_e(\mu) = 2 - \rho_e(U - \mu) \), but that it also governs the average sign is not immediately obvious from the construction of the method. A formal demonstration of the electron-doping–hole-doping symmetry of the average sign is, however, possible (see Appendix C). Note that we restrict our density calculations to \( \rho_e < 1 \) because in this case the numerical effort to manipulate the Slater determinants is lower (size of the Slater determinants is given by the number of particles of a given spin). The performance of the ABQMC algorithm to compute \( \rho_e(\mu) \) (average time needed to propose/accept an MC update and acceptance rates of individual MC updates) is discussed in Sec. SIII of the Supplementary Material.

We further benchmark our method in the case of very strong coupling, \( U/J = 24 \) and, again, \( T/J = 1.0408 \). Figure 4(a) compares the ABQMC results on a 4 × 4 cluster using \( N_\tau = 2 \) imaginary-time slices with the NLCE,
Figure 3. (Color online) (a) Equation of state $\rho_e(\mu)$ for the Hubbard model on a $4 \times 4$ cluster with the following values of model parameters: $U/J = 4$, $T/J = 1.0408$. The solid line is a guide to the eye. (c) The double occupancy $\sum (n_{r\uparrow} n_{r\downarrow})/N_c$ as a function of the electron density $\rho_e$. In (a) and (c), full dots are obtained using the ABQMC method with $N_{\tau} = 2$ imaginary-time slices, while the solid line shows the NLCE data taken from Ref. 78. The estimated statistical error of the ABQMC data is in all cases smaller than the symbol size.

Figure 4. (Color online) (a) Equation of state $\rho_e(\mu)$ for the Hubbard model on a $4 \times 4$ cluster with the following values of model parameters: $U/J = 24$, $T/J = 1.0408$. Full dots represent ABQMC results using $N_{\tau} = 2$ imaginary-time slices, the solid line shows the NLCE data taken from Ref. 78, the dashed line shows the atomic-limit results, while the dash-dotted line shows the ideal-gas results. The estimated statistical error of the ABQMC data is in all cases smaller than the symbol size. (b) The average sign as a function of the ABQMC estimate $\rho_e,\text{ABQMC}$ for the electron density. (c) The average sign as a function of the cluster size $N_c$ for the following values of model parameters: $U/J = 24$, $T/J = 1.0408$, $\mu/J = -5$. The dashed lines in (b) and (c) are guides to the eye. Next to each point in (c), we provide information on cluster shape, as well as the converged value of $\rho_e$ accompanied by its statistical error. The referent NLCE result is $\rho_e,\text{NLCE} = 0.0602$. The estimated statistical error of the ABQMC data is in all cases smaller than the symbol size.}

atomic-limit, and corresponding $U = 0$ results. At extremely low fillings $\rho_e \lesssim 0.1$, the relative importance of the interaction term with respect to the kinetic term is quite small, and both the ABQMC and NLCE results are very close to the ideal-gas result, see the results for $\mu/J = -5$ and $-4$ in Fig. 4(a). As the filling is increased, the interaction effects become increasingly im-
important, and our ABQMC results follow quite closely the NLCE results up to fillings $\rho_e \sim 0.5$. Above this density, the predictions of the ABQMC method are consistently closer to the atomic-limit than to the NLCE results, see the top right part of Fig. 4(a). The imaginary-time discretization employed here is too coarse to accurately describe the competition between the kinetic and interaction terms at higher fillings.

At this strong coupling, the dependence of the average sign on the density is somewhat modified [see Fig. 4(b)]. The minimal sign is no longer reached at half-filling but at around $\rho_e \sim 0.7$. Comparing Fig. 4(b) with Fig. 3(b), we see that the average sign does not become smaller with increasing interaction, in sharp contrast with methods such as CT-INT.\textsuperscript{38,60} Indeed, at half-filling, we find that the average sign is an order of magnitude larger at $U/J = 24$ than at $U/J = 4$.

Finally, we discuss the applicability of ABQMC to larger clusters. Here we take the most favorable, low-density case, i.e. $\mu/J = -5$, and again take $N_e = 2$ imaginary-time slices. Figure 4(c) shows that the average sign exhibits an exponential decrease with the cluster size $N_c$. Apart from the largest, 8 × 6 cluster, we have been able to converge the $\rho_e$ results down to a reasonable statistical error bar, and obtain results in agreement with NLCE value $\rho_e = 0.0602$. The obtained values are given alongside average-sign data points.

### B. Time-dependent results: Survival probability

#### 1. Benchmarks on small clusters

We first benchmark our ABQMC method on Hubbard dimers and tetramers for different ratios $U/D$, where $D$ is the half-bandwidth of the free-electron band ($D = J$ for the dimer and $D = 2J$ for the tetramer). The initial states are schematically summarized in Table I. In both cases, we are at half filling.

| system  | $|\psi_{CDW}\rangle$ | $|\psi_{SDW}\rangle$ |
|---------|---------------------|---------------------|
| dimer   |                     |                     |
| tetramer|                     |                     |

Table I: Schematic representations of the initial states of small systems on which the ABQMC method for $P(t)$ is benchmarked.

Figures 5(a1)–5(e2) present time evolution of the survival probability of the initial CDW-like and SDW-like states depicted in Table I for the dimer (left panels) and tetramer (right panels) for different values of $U/D$ starting from the limit of weakly nonideal gas ($U/D = 0.05$) and approaching the atomic limit ($U/D = 20$). The results are obtained using $N_t = 2$ (full red circles) and $N_t = 4$ (blue stars) real-time slices and contrasted with the exact result (solid black lines). The ABQMC results with $N_t = 2$ agree both qualitatively (oscillatory behavior) and quantitatively with the exact result up to $t_{\text{max}} \sim 1/U$. Increasing $N_t$ from 2 to 4 may help decrease the deviation of the ABQMC data from the exact result at later times. Even when finer real-time discretization does not lead to better quantitative agreement, it may still help the ABQMC method qualitatively reproduce gross features of the exact result. The converged values of $|\langle \text{sgn} \rangle|$ for the dimer and tetramer for $N_t = 2, 3, 4$ are summarized in Table II. For the dimer, increasing $N_t$ by one reduces $|\langle \text{sgn} \rangle|$ by a factor of 2. In contrast, in the case of the tetramer, increasing $N_t$ by one reduces $|\langle \text{sgn} \rangle|$ by almost an order of magnitude.

#### 2. Results on larger clusters

We move on to discuss the survival-probability dynamics of different 16-electron and 8-electron states on a $4 \times 4$ cluster. Figures 6(a) and 6(b) present $P(t)$ for 16-electron states schematically depicted in their respective insets. These states are representative of CDW patterns formed by applying strong external density-modulating fields with wave vectors $q = (\pi, 0)$ in Fig. 6(a) and $q = (\pi, \pi)$ in Fig. 6(b). Figures 6(c) and 6(d) present $P(t)$ for 8-electron states schematically depicted in their respective insets. The ABQMC method employs $N_t = 2$ real-time slices. The results are shown up to the maximum time $D t_{\text{max}} = 2.5$, which we chose on the basis of the results presented in Fig. 5(c2).

As a sensibility check of our ABQMC results, we first compare the exact result in the noninteracting limit, see solid lines in Figs. 6(a)–6(d), with the corresponding ABQMC prediction, see full circles in Figs. 6(a)–6(d). While the exact and ABQMC result agree quite well in Figs. 6(b) and 6(c), the agreement in Figs. 6(a) and 6(d) is not perfect. Since no systematic errors are expected in ABQMC at $U = 0$, the discrepancy must be due to statistical error. Regarding the data in Fig. 6(a), we confirm this expectation in Fig. 7 where we see that the obtained curve tends to the exact one with the increasing number of MC steps. The average sign cited in Fig. 6(d) suggests that more MC steps are needed to obtain fully converged results. Even though the converged average sign in Figs. 6(a)–6(c) is of the same order of magnitude, we find that the rate of convergence depends on both the number and the initial configuration of electrons.

In Figs. 6(a)–6(d), we observe that weak interactions ($U/D \lesssim 0.5$) do not cause any significant departure of $P(t)$ from the corresponding noninteracting result. On the other hand, the effect of somewhat stronger inter-
Figure 5. (Color online) Time dependence of the survival probability of the initial state $|\psi_{\text{CDW}}\rangle$ or $|\psi_{SDW}\rangle$ (see Table I) for the dimer [(a1)–(e1)] and tetramer [(a2)–(e2)] for five different interaction strengths starting from the noninteracting limit and approaching the atomic limit: $U/D = 0.05$ [(a1) and (a2)], $U/D = 0.25$ [(b1) and (b2)], $U/D = 1$ [(c1) and (c2)], $U/D = 5$ [(d1) and (d2)], and $U/D = 20$ [(e1) and (e2)]. The ABQMC results with $N_t = 2$ (red full circles) and $N_t = 4$ (blue stars) are compared with the exact result (black solid lines). The dotted/dashed lines connecting subsequent circles/stars are guides to the eye. In most cases, the MC error bars are smaller than the linear size of the symbols.

actions on $P(t)$ depends crucially on the filling. In the 16-electron case, the increasing interactions speed up the initial decay of $P$, see Figs. 6(a) and 6(b), while in the 8-electron case interactions have little effect at $Dt < 1$, see Figs. 6(c) and 6(d). This we attribute to the essential difference in the overall electron density and the relative role of the interaction term in the Hamiltonian. In the 16-electron case, starting from the moderate coupling $U/D \sim 1$, there is a clear revival of the initial state in Fig. 6(a), while no such a revival is observed in Fig. 6(b). Furthermore, the memory loss of the initial density-wave pattern is more rapid in Fig. 6(a) than in Fig. 6(b), even at $U = 0$. The revival of the initial state is observed in the 8-electron case as well: at $t < 1/D$ there is barely any
Figure 6. (Color online) Survival-probability dynamics of the 16-electron states [in (a) and (b)] and 8-electron states [in (c) and (d)] that are schematically depicted in the respective insets. ABQMC results are shown for five different interaction strengths (symbols) and compared with the noninteracting result (solid line). We cite the converged value of the average sign $\langle|\text{sgn}|\rangle$, as well as the total number $N_{\text{MC}}$ of MC steps completed.

effect of the interaction, yet at longer times it boosts $P$. However, in contrast to the 16-electron case, the results in Figs. 6(c) and 6(d) exhibit a weaker dependence of the survival-probability dynamics on the initial density-wave pattern. Indeed, the exact results in the noninteracting case are identical for both patterns in Figs. 6(c) and 6(d). Except in the case of the $(\pi,\pi)$ wave, the interactions lead to a persistence of the initial pattern at longer times, $t > 1/D$. The precise form of temporal correlations that develop due to interactions apparently depends on the initial spatial arrangement of the electrons.

Figure 8 shows $P(t)$ for the 16-electron initial state schematically depicted in Fig. 6(a) in regimes that are close to the atomic limit. In these regimes, the natural energy unit is $U$, so that the time is measured in units $1/U$. The time range is chosen on the basis of the results in Figs. 5(d1)–(e2), which suggest that the ABQMC method with $N_t = 2$ real-time slices produces a qualitatively correct behavior of $P(t)$ up to times $Ut \approx 6$. $P(t)$ exhibits oscillations whose amplitude decreases in time. There is almost no difference between $P(t)$ for $D/U = 0.05$ and 0.1 during the first oscillation, while $P(t)$ for $D/U = 0.2$ is at all times below $P(t)$ for stronger $U$. While for the strongest $U$ the maxima reached by $P(t)$ are always close to 1, the maxima for weaker $U$ are smaller than 1 and decrease with time. All these observations can be rationalized by an increased importance of the kinetic over the interaction term as $U/D$ is decreased.

The outcomes of our attempts to compute $P(t)$ on a larger cluster or using a finer time discretization are summarized in Secs. SIV and SV of the Supplementary Material.

C. Time-evolution of local charge and spin densities

In this section, we test the ABQMC method [Eq. (26)] on the more difficult example of time evolution of spatially resolved charge and spin density. As already mentioned in Sec. II B 2, and previously discussed in Ref. 76, the evolution of charge density starting from $|\psi_{\text{CDW}}\rangle$ state is equivalent to the evolution of spin starting from the corresponding $|\Psi_{\text{SDW}}\rangle$. Once again we take $N_t = 2$ in the STD of each evolution operator, which adds up to 4 real-time slices in total, i.e., the forward and the backward branch are divided into $N_t = 2$ identical slices each. Because of this complication, we can at present only reach the lattice size $N_c = 4$, and thus focus on the case of the Hubbard tetramer (equivalent to the $2 \times 2$ plaquette). Fig-
Figure 7. (Color online) (a) Average sign as a function of the number of MC steps in the ABQMC simulation of $P(t)$ for the 16-electron initial state schematically depicted in Fig. 6(a). (b) Time dependence of the survival probability for $U=0$ extracted using the first 1/30 of the total number of MC steps completed (1.29 $\times$ 10$^9$ steps, full red circles), the first 1/3 of the total number of MC steps completed (1.29 $\times$ 10$^{10}$ steps, full blue squares), and all the MC steps completed (3.87 $\times$ 10$^{11}$ steps, full green up-triangles). These results are compared to the exact result in the noninteracting limit, which are represented by the solid line. The vertical lines in (a), whose colors match the colors of the symbols in (b), denote the ending points of the simulations.

Figure 8. (Color online) Survival-probability dynamics of the 16-electron initial state schematically depicted in Fig. 6(a) for three values of the interaction strength that are close to the atomic limit.

Figure 9. (Color online) Time-dependent population of the initially doubly occupied sites in the CDW state $|\psi_{\text{CDW}}\rangle$ of the Hubbard tetramer, see Table I. The results are presented for different values of the electron–electron interaction $U$. The ABQMC results are represented by full symbols, while the exact results are represented by solid lines.

IV. RELATION TO OTHER ALGORITHMS

The ABQMC method that we develop here was initially imagined as an alternative to the Hirsch–Fye (HF) QMC method, in the context of the Hubbard model. The HF method is similarly based on the STD, and there is a relatively large configuration space to be sampled, with the size scaling as $2^{N_c N_\tau}$ (configuration is defined by $N_c N_\tau$ Ising—up or down—auxilliary spins; $N_\tau$ here denotes the total number of time slices, be it imaginary or real time, or both). Similarly to the ABQMC method, the MC weight of any given configuration in the HF method requires computation of a determinant of a matrix, the dimension of the matrix being $N_c N_\tau$. The large size of the matrix in the HF method often represents an obstacle, and the calculation of the determinant is the bottleneck of the procedure. In our method, the configuration space is a priori much bigger ($2^{N_c N_\tau}$), but it is also substantially reduced by the conservation laws that we
employ. On the other hand, we compute determinants of much smaller matrices, with their size equal to the total number of particles of a given spin. For this reason, a single MC step is much cheaper in the ABQMC than in the HF method, with complexity scaling only linearly with \(N_c\) (compared to \(\sim N_c^2\) in HF). Additional difference is that in the HF method, calculation of density is not as straightforward as in the ABQMC method. The local auxiliary Ising spin only distinguishes between singly-occupied and doubly-occupied/empty site. In the ABQMC method, the densities in both coordinate and momentum space can be simply read off the configuration. Most importantly, the ABQMC method can readily be applied to canonical ensembles and pure states, which may not be possible with the HF method. In our implementation, the evolution of pure states can be even performed for multiple values of \(U\) and multiple times \(t\) using a single Markov chain. However, we find that the poor scaling of the average sign in the ABQMC method offsets its relative advantages. The HF calculations in the half-filled particle-hole-symmetric Hubbard model are manifestly sign-problem-free. At present, we are unable to transform the ABQMC algorithm in such a way to ensure \(|\langle \text{sgn} \rangle| = 1\) in any case.

Our algorithm is also similar in spirit to auxiliary-field QMC, as presented in Refs. 50–52. These algorithms, similarly to the HF, make use of the Hubbard–Stratonovich transformation and, ultimately, the time-evolution is described as a random walk in the space of Slater determinants. This construction generally allows for a larger number of time-steps, because the random-walk paths can be constructed time-step by time-step. However, to the best of our understanding, this approach cannot be as easily applied in thermal equilibrium calculations without invoking certain approximations such as the constrained-path approximation or the phaseless approximation. Additionally, like in world-line algorithms, one must algorithmically ensure that the path connects two identical states (\(Z = \sum_\Psi \langle \Psi | \text{path} | \Psi \rangle\)), allowing also for particle exchanges. In the ABQMC algorithm, there is no such issue, and the method is readily applicable to the full range of equilibrium and out-of-equilibrium setups.

V. SUMMARY AND OUTLOOK

We devise, implement, benchmark, and make first use of a numerically exact QMC method, aimed at calculations relevant for the recent ultracold-atom simulations of the Hubbard model. The algorithm formally applies to the calculation of densities of spin, charge, or uniform current, and the corresponding correlation functions in the full range of equilibrium and out-of-equilibrium setups. In the present work, we have demonstrated the validity of our method in the calculation of the average density in equilibrium, as well as in the calculation of survival probability and charge density in the evolution of pure states. We make use of the method in the calculation of survival probability of pure density-wave-like states for the Hubbard model on a \(4 \times 4\) square-lattice. Our study is timely because there are not many reference results, or other algorithms that are readily applicable to this problem. For example, finite-temperature Lanczos method can treat 16-site Hubbard model, but real-time dynamics is difficult to implement. The auxiliary-field QMC method has been generalized to real-time calculations only very recently. Our results reveal a clear trend that interactions speed up the initial decay of the survival probability, but facilitate a persistence of the initial charge-pattern at longer times. Additionally, we observe a characteristic value of the coupling constant, \(U \sim 0.5D\), below which the interaction makes no visible effect on time-evolution. These findings bare qualitative predictions for future ultracold-atom experiments, but are limited to dynamics at the shortest wave-lengths, as dictated by the maximal size of the lattice that we can treat.

We find that our method is heavily plagued by the fermionic sign-problem and may not be easily pushed to bigger lattices or finer time-discretizations. In the attempt to curb this problem, we have identified some of the symmetries of the ABQMC configuration space related to the particle-hole, time-reversal, and bipartite lattice symmetry of the Hubbard model; These findings have enabled us to formulate the ABQMC in a way that several symmetries of the Hubbard model are manifestly satisfied. We have also been able to alleviate the “phase problem” and reduce it to the standard sign problem. It is likely that there are symmetry structures in the ABQMC configuration space that we have not yet exploited to further speed up convergence. To this end, one may attempt to use quasi MC methods, which sample the configuration space using highly structured and deterministic quasi-random sequences (in contrast to the pseudo-random numbers employed in this study). Another promising direction is the many-configuration Markov-chain MC, which is capable of visiting an arbitrary number of configurations at every MC step. This possibility is particularly appealing when the properties of the configurations to be visited at a given MC step can be obtained at a small computational cost, which may be true of configurations linked by symmetry operations. Finding viable ways of integrating these ideas into our ABQMC method is left as another challenge for future work.

Finally, we make a striking observation that even a tiny number of time slices can be sufficient to properly describe the time-evolution of density in the parameter regime relevant for the optical-lattice experiments \((U \sim 1D, T \sim 0.25D)\). This finding suggests that discrete-time methods (such as Hirsch–Fye or possibly a discrete-time version of CT-INT) should be revisited in the context of the Kadanoff–Baym (3-piece) contour calculations. In thermal equilibrium calculations, HF is often performed with as many as 80 time slices, with
the intent to properly resolve the imaginary-time Green’s function \(G(\tau)\). However, the requirement for the proper description of the instantaneous correlator \(\langle n \rangle = \langle c\dagger c \rangle\) might be much lower. In strongly incoherent regimes, the thermalization of the system is expected to be quick, and the dynamical sign problem may not come into play in the description of the relevant transient regimes, such as the one studied in Ref. 19.

SUPPLEMENTARY MATERIAL

See the supplementary material for (a) a detailed description of MC updates that respect momentum and particle-number conservation laws and more details on the extraction of the MC results, (b) benchmarks of quench calculations along the Kadanoff–Baym contour performed on small systems, (c) a detailed performance analysis of the ABQMC method applied to evaluate the equation of state, and (d) a discussion on the applicability of the ABQMC method to larger clusters/finer discretizations.

AUTHORS’ CONTRIBUTIONS

J.V. conceived the research. V.J. developed the formalism and computational codes under the guidance of J.V., conducted all numerical simulations, analyzed their results, and prepared the initial version of the manuscript. Both authors contributed to the submitted version of the manuscript.

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DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Appendix A: Derivation of the ABQMC formulae that manifestly respect the dynamical symmetry of the Hubbard model

Here, we derive the ABQMC expressions for the survival probability [Eq. (23)] and the expectation value of an observable [Eq. (26)] that manifestly respect the dynamical symmetry of the Hubbard model.

We start by defining the action of the bipartite lattice symmetry, which is represented by a unitary, hermitean, and involutive operator \(B (B \dagger = B^{-1})\) whose action on electron creation and annihilation operators in the real space is given as

\[
Bc_{r \sigma}^{(i)} B = (-1)^{r_x + r_y + x_{r_x}} c_{r \sigma}^{(i)}.
\] (A1)

In the momentum space, \(B\) is actually the so-called \(\pi\)-boost\(^{20}\)

\[
Bc_{k \sigma}^{(i)} B = c_{k + Q, \sigma}^{(i)}
\] (A2)

that increases the electronic momentum by \(Q = (\pi, \pi)\). The time reversal operator \(T\) is an antiunitary (unitary and antilinear), involutive, and hermitean operator whose action on electron creation and annihilation operators in the real space is given as

\[
Tc_{r \sigma}^{(i)} T = c_{r \sigma}^{(i)}, \quad Tc_{r \uparrow}^{(i)} T = -c_{r \downarrow}^{(i)}.
\] (A3)

while the corresponding relations in the momentum space read as

\[
Tc_{k \sigma}^{(i)} T = c_{-k \sigma}^{(i)}, \quad Tc_{k \downarrow}^{(i)} T = -c_{-k \uparrow}^{(i)}.
\] (A4)

Using Eqs. (A1)–(A4), it follows that

\[
BH_0 B = -H_0, \quad BH_{\text{int}} B = H_{\text{int}}, \quad TH_0 T = H_0, \quad TH_{\text{int}} T = H_{\text{int}}.
\] (A5)
In Sec. II B 2, we assumed that the initial state $|\psi(0)\rangle$ is an eigenstate of local density operators $n_{r\sigma}$, which means that $B|\psi(0)\rangle = e^{i\lambda T}|\psi(0)\rangle$, see Eq. (A1). In the following discussion, we additionally assume that the time reversal operation changes $|\psi(0)\rangle$ by a phase factor, $T|\psi(0)\rangle = e^{i\chi T}|\psi(0)\rangle$, so that

$$TB|\psi(0)\rangle = e^{i\chi}|\psi(0)\rangle \quad (A6)$$

The CDW-like states $|\psi_{\text{CDW}}\rangle$ summarized in Table I and Figs. 6(a)–6(d) are one example of states satisfying Eq. (A6). On the contrary, the corresponding SDW-like states $|\psi_{\text{SDW}}\rangle$ [Eq. (32)] generally do not satisfy Eq. (A6). Examples of SDW-like states that satisfy Eq. (A6) are spin-balanced states corresponding to CDW-like states in Table I and Figs. 6(a) and 6(b).

Let us first discuss the survival probability. Equations (A5) and (A6) imply that the survival probabilities

$$P_{\pm U}(t) = \left| \langle \psi(0)| e^{-i(H_0 \pm H_{\text{int}})t} |\psi(0)\rangle \right|^2 \quad (A7)$$

for the interactions $+U$ and $-U$ are mutually equal, $P_{+U}(t) = P_{-U}(t)$. Moreover, considering the time reversal symmetry alone, we conclude that the survival probability amplitude $\langle \psi(0)| e^{-iHt} |\psi(0)\rangle$ is purely real. Starting from

$$\langle \psi(0)| e^{-iHt} |\psi(0)\rangle \approx \frac{1}{2} \left( \langle \psi(0)| (e^{-iH_0 t} e^{-iH_{\text{int}} t})^N |\psi(0)\rangle + \frac{1}{2} \left( \langle \psi(0)| (e^{-iH_{\text{int}} t} e^{-iH_0 t})^N |\psi(0)\rangle \right), \quad (A8)$$

where $\Delta t = t/N_t$, we obtain

$$\langle \psi(0)| e^{-iHt} |\psi(0)\rangle = \sum_c \text{Re} \{|D(C)| e^{-i[\epsilon_0(C) + \epsilon_{\text{int}}(C)]\Delta t} \rangle \quad (A9)$$

In order for Eq. (A9) to manifestly respect the above-described dynamical symmetry, we rewrite it as follows

$$\langle \psi(0)| e^{-iHt} |\psi(0)\rangle = \frac{1}{2} \sum_c e^{-i[\epsilon_0(C) + \epsilon_{\text{int}}(C)]\Delta t} \text{Re} \{|D(C)| \rangle + \frac{1}{2} \sum_c e^{i[\epsilon_0(C) - \epsilon_{\text{int}}(C)]\Delta t} \text{Re} \{|D(C)| \rangle \quad (A10)$$

In the second sum on the right-hand side of Eq. (A10), we have introduced the following variable substitution

$$C \rightarrow C' = \{|\Psi_{k,l}\rangle = B|\Psi_{k,l}\rangle, |\Psi_{l,k}\rangle = B|\Psi_{l,k}\rangle|l = 1, \ldots, N_t\} \quad (A11)$$

under which $D(C') = D(C)$ and $\epsilon_0(C') = -\epsilon_0(C)$. The invariance under the time reversal implies that Eq. (A10) should not change upon replacing $\Delta t$ by $-\Delta t$. The last requirement transforms Eq. (A10) into

$$\langle \psi(0)| e^{-iHt} |\psi(0)\rangle = \sum_c \text{Re} \{|D(C)| \cos[\epsilon_0(C)\Delta t] \cos[\epsilon_{\text{int}}(C)\Delta t], \quad (A12)$$

and Eq. (23) then follows immediately. If the initial state is invariant under the bipartite lattice symmetry, but not under the time reversal, the ABQMC method uses the expression after the second equality in Eq. (A10).

In the case of $\langle A_n(t)\rangle$, we start from the fact that it is purely real

$$\langle A_n(t)\rangle = \frac{1}{2} \left( \langle \psi(0)| (e^{-iH_0 t} e^{-iH_{\text{int}} t})^N A_n (e^{-iH_0 t} e^{-iH_{\text{int}} t})^N |\psi(0)\rangle \right) + \frac{1}{2} \left( \langle \psi(0)| (e^{-iH_{\text{int}} t} e^{-iH_0 t})^N A_n (e^{-iH_{\text{int}} t} e^{-iH_0 t})^N |\psi(0)\rangle \right), \quad (A13)$$

and obtain

$$\langle A_n(t)\rangle = \sum_c \text{Re} \{|D(C)| A_n (\psi_{a,N_t}) \{\cos[\Delta \epsilon_0(C)\Delta t] \cos[\Delta \epsilon_{\text{int}}(C)\Delta t] - \sin[\Delta \epsilon_0(C)\Delta t] \sin[\Delta \epsilon_{\text{int}}(C)\Delta t]\} - \sum_c \text{Im} \{|D(C)| A_n (\psi_{a,N_t}) \{\sin[\Delta \epsilon_0(C)\Delta t] \cos[\Delta \epsilon_{\text{int}}(C)\Delta t] + \cos[\Delta \epsilon_0(C)\Delta t] \sin[\Delta \epsilon_{\text{int}}(C)\Delta t]\} \quad (A14)$$

and Eq. (32) generally do not satisfy Eq. (A6). Examples of SDW-like states that satisfy Eq. (A6) are spin-balanced states corresponding to CDW-like states in Table I and Figs. 6(a) and 6(b).
We first use the transformation laws under the bipartite lattice symmetry, $B A_a B = A_a$, and $B |\psi(0)\rangle = e^{i H t} |\psi(0)\rangle$. We rewrite Eq. (A14) as a sum of its two halves, and in one of them we introduce the variable substitution analogous to Eq. (A11) (with $N_t$ replaced by $2 N_t$). Because of $D(C) = D(C)$ and $\Delta \epsilon_0(C) = -\Delta \epsilon_0(C)$, Eq. (A14) reduces to

$$
\langle A_a(t) \rangle = \sum_c \Re \{ D(C) \} A_a(\psi_{a,N_t}) \cos [\Delta \epsilon_0(C) \Delta t] \cos [\Delta \epsilon_{\text{int}}(C) \Delta t] - \sum_c \Im \{ D(C) \} A_a(\psi_{a,N_t}) \cos [\Delta \epsilon_0(C) \Delta t] \sin [\Delta \epsilon_{\text{int}}(C) \Delta t].
$$

(A15)

The transformation laws under the time reversal symmetry imply that Eq. (A15) should contain only contributions that are invariant under the change $\Delta t \rightarrow -\Delta t$. This requirement equates the second sum on the right-hand side of Eq. (A15) to zero, and we remain with Eq. (26). If the time reversal changes the initial state by more than a phase factor, the ABQMC method uses Eq. (A15).

**Appendix B: Survival-probability dynamics of the CDW-like and SDW-like states**

Here, we provide a formal demonstration of Eq. (33) and explain how we combine Markov chains for the survival probability amplitudes of states $|\psi_{\text{CDW}}\rangle$ and $|\psi_{\text{SDW}}\rangle$ to efficiently and accurately evaluate their survival probabilities.

We first introduce the partial particle–hole transformation that is represented by a unitary, hermitean, and involutive operator $P$ ($P^\dagger = P = P^{-1}$) whose action on electron creation and annihilation operators in the real space is given as$^{74,75}$

$$
P_{c\uparrow} P = c_{\uparrow}, \quad P_{c\downarrow} P = c_{\downarrow},
$$

(B1)

$$
P_{c\uparrow} P = (-1)^{r_x + r_y} c_{\uparrow}, \quad P_{c\downarrow} P = (-1)^{r_x + r_y} c_{\downarrow},
$$

(B2)

The interaction Hamiltonian $H_{\text{int}}$ thus transforms under the partial particle–hole transformation as follows

$$
P H_{\text{int}} P = U N \widetilde{N} - H_{\text{int}}.
$$

(B3)

The action of the partial particle–hole transformation in the momentum space read as $[Q = (\pi, \pi)]$

$$
P_{c\uparrow} P = c_{\uparrow} P, \quad P_{c\downarrow} P = c_{\downarrow} P,
$$

(B4)

$$
P_{c\uparrow} P = c_{\downarrow} P, \quad P_{c\downarrow} P = c_{\uparrow} P.
$$

(B5)

The kinetic energy, therefore, remains invariant under the partial particle–hole transformation, i.e., $P H_0 P = H_0$. Equations (B1) and (B2) imply that $P |\psi\rangle = \prod_r c_r^\dagger |\psi\rangle$, where the product is taken over all the sites of the cluster studied. We then find that $P |\psi_{\text{CDW}}\rangle = |\psi_{\text{SDW}}\rangle$, i.e., the partial particle–hole transformation transforms the CDW state defined in Eq. (31) into the SDW state defined in Eq. (30) and vice versa.$^{76}$ The states $|\psi_{\text{CDW}}\rangle$ and $|\psi_{\text{SDW}}\rangle$ have the same number of spin-up electrons, while their numbers of spin-down electrons add to $N_c$. Using the combination of the partial particle–hole transformation $P$ and bipartite lattice transformation $B$ defined in Appendix A, one obtains

$$
|\psi_{\text{CDW}}| e^{-i H t} |\psi_{\text{CDW}}\rangle = e^{-i N_c (\psi \dagger U) / \epsilon} |\psi_{\text{SDW}}| e^{-i H t} |\psi_{\text{SDW}}\rangle^*,
$$

(B6)

where $N_c (\psi) = \langle \psi_{\text{CDW}}| \widetilde{N}_{\text{CDW}} |\psi_{\text{CDW}}\rangle = \langle \psi_{\text{SDW}}| \widetilde{N}_{\text{SDW}} |\psi_{\text{SDW}}\rangle$ is the total number of spin-up electrons in CDW and SDW states. Equation (33) then follows immediately from Eq. (B6).

We now explain how we use Eq. (B6) to efficiently and accurately compute the survival probability of states $|\psi_{\text{CDW}}\rangle$ and $|\psi_{\text{SDW}}\rangle$. The state $|\psi_{\text{CDW}}\rangle$ is invariant under $TB$ (up to a phase factor), so that the ABQMC computation of the left-hand side of Eq. (B6) employs Eq. (A12). The state $|\psi_{\text{SDW}}\rangle$ is in general changed under $TB$ by more than a phase factor, so that the ABQMC computation of the right-hand side of Eq. (B6) employs Eq. (A10). Suppose that we obtained Markov chains (of length $N_{\text{CDW}}$) $\{ N_{1 \text{CDW}}(t), \ldots, N_{N_{\text{CDW}} \text{CDW}}(t) \}$ and $\{ D_{1 \text{CDW}}, \ldots, D_{N_{\text{CDW}} \text{CDW}} \}$ for the numerator and denominator of the importance-sampling MC expression corresponding to Eq. (A12), respectively. Suppose also that we obtained Markov chains (of length $N_{\text{SDW}}$) $\{ N_{1 \text{SDW}}(t), \ldots, N_{N_{\text{SDW}} \text{CDW}}(t) \}$ and $\{ D_{1 \text{SDW}}, \ldots, D_{N_{\text{SDW}} \text{SDW}} \}$ for the numerator and denominator of the importance-sampling MC expression corresponding to Eq. (A10), respectively. Using these Markov chains, we found that the best result for the survival probability is obtained by joining them into one Markov chain $\{ e^{-i N_c (\psi \dagger U)} N_{1 \text{SDW}}(t)^*, \ldots, e^{-i N_c (\psi \dagger U)} N_{N_{\text{CDW}} \text{SDW}}(t)^*, N_{N_{\text{SDW}} \text{CDW}}(t)^*, N_{N_{\text{SDW}} \text{CDW}}(t) \}$ and another Markov chain $\{ D_{1 \text{SDW}}, D_{N_{\text{SDW}} \text{SDW}}, D_{N_{\text{SDW}} \text{CDW}}, D_{N_{\text{SDW}} \text{CDW}} \}$ of length $N_{\text{SDW}} + N_{\text{CDW}}$ for the numerator, and another Markov chain $\{ D_{1 \text{CDW}}, D_{N_{\text{CDW}} \text{CDW}}, D_{N_{\text{CDW}} \text{CDW}}, D_{N_{\text{CDW}} \text{CDW}} \}$ of length $N_{\text{CDW}} + N_{\text{CDW}}$ for the denominator. If individual chain lengths $N_{\text{CDW}}$ and $N_{\text{SDW}}$ are sufficiently large, the manner in which the chains are joined is immaterial; here, we append the CDW chain to the SDW chain, and we note that other joining possibilities lead to the same final result (within the statistical error bars).
Appendix C: Using the particle–hole symmetry to discuss the average sign of the ABQMC method for chemical potentials $\mu$ and $U-\mu$

The (full) particle–hole transformation is represented by a unitary, hermitean, and involutive operator $P_f$ ($P_f^\dagger = P_f = P_f^{-1}$) whose action on electron creation and annihilation operators in the real space is defined as

$$P_f c_r^{\sigma} P_f = (-1)^{r_x + r_y} c_r^{\dagger \sigma}.$$  \hfill (C1)

The corresponding formula in the momentum space reads as

$$P_f c_{\mathbf{k}\sigma} P_f = c_{\mathbf{Q}_{-\mathbf{k}}\sigma}.$$  \hfill (C2)

Let us fix $J, U,$ and $T$ and compute the equation of state $\rho_e(\mu)$ using Eq. (17) in which $A_a(\Psi_{a,l}) = [N_\uparrow(C) + N_\downarrow(C)]/N_c$.

It is convenient to make the $\mu$-dependence in $\tilde{\varepsilon}(C, \mu)$ explicit. In the sums entering Eq. (17) we make the substitution

$$C \rightarrow C' = \{ |\Phi_{k,l}\rangle = P_f |\Psi_{k,l}\rangle, |\Phi_{i,l}\rangle = P_f |\Psi_{i,l}\rangle |l = 1, \ldots, N_r\}$$  \hfill (C3)

under which

$$D(C) = D(C'), \quad \tilde{\varepsilon}(C, \mu) = \tilde{\varepsilon}(C', U-\mu) + (U-2\mu) N_r N_c, \quad N_\sigma(C') = N_c - N_\sigma(C).$$  \hfill (C4)

It then follows that

$$\frac{\sum_C \text{Re}\{D(C)e^{-\Delta \tilde{\varepsilon}(C, \mu)}[N_\uparrow(C) + N_\downarrow(C)]/N_c\}}{\sum_C \text{Re}\{D(C)e^{-\Delta \tilde{\varepsilon}(C, \mu)}\}} = 2 - \frac{\sum_{C'} \text{Re}\{D(C')e^{-\Delta \tilde{\varepsilon}(C', U-\mu)}[N_\uparrow(C') + N_\downarrow(C')]/N_c\}}{\sum_{C'} \text{Re}\{D(C')e^{-\Delta \tilde{\varepsilon}(C', U-\mu)}\}}. \hfill (C5)$$

The ABQMC simulations of the ratios in the last equation are performed for chemical potentials $\mu$ and $U-\mu$, which are symmetric with respect to the chemical potential $U/2$ at the half-filling. Since $\tilde{\varepsilon}(C, \mu)$ and $\tilde{\varepsilon}(C', U-\mu)$ differ by a constant additive factor, the corresponding configuration weights differ by a constant multiplicative factor, and the average signs of the two ABQMC simulations are thus mutually equal.
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SI. MONTE CARLO UPDATES

Here, we present the Monte Carlo updates we use to move through the configuration space of our ABQMC method. One important feature of all the updates to be presented is that they respect the particle-number and momentum conservation laws.

The configuration space is sampled through Markov chains starting from an, in principle arbitrary, configuration $C_0$. For convenience, all the momentum-space states $|\Psi^0_{k,l}\rangle \in C_0$ are assumed to be identical (the momentum conservation then trivially holds). On the other hand, the initial real-space states $|\Psi^0_{i,l}\rangle \in C_0$ are chosen completely arbitrarily. The Metropolis–Hastings algorithm is used to determine the probability of transferring from configuration $C_n$ at Monte Carlo step $n$ to configuration $C_{n+1}$ at the subsequent Monte Carlo step $n+1$. The transition probability $W_{n\rightarrow n+1}$ is

$$W_{n\rightarrow n+1} = W_{n\rightarrow n+1}^{\text{prop}}W_{n\rightarrow n+1}^{\text{acc}}$$

where $W_{n\rightarrow n+1}^{\text{prop}}$ is the probability of proposing the update from configuration $C_n$ to configuration $C_{n+1}$, while $W_{n\rightarrow n+1}^{\text{acc}}$ determines the probability with which such a proposal is accepted. The Metropolis–Hastings acceptance rate reads as

$$W_{n\rightarrow n+1}^{\text{acc}} = \min\{1, R_{n\rightarrow n+1}\}$$

where the acceptance ratio $R_{n\rightarrow n+1} = 1/R_{n+1\rightarrow n}$ depends on the weights of the configurations involved, as well as on the proposal probabilities in both directions $C_n \leftrightarrow C_{n+1}$ in the following manner

$$R_{n\rightarrow n+1} = \frac{w(C_{n+1})W_{n\rightarrow n+1}^{\text{prop}}}{w(C_n)W_{n\rightarrow n+1}^{\text{prop}}}.$$

While the proposal probabilities $W_{n\rightarrow n+1}^{\text{prop}}$ for many of the QMC algorithms can be determined relatively straightforwardly (even analytically), their determination for the ABQMC algorithm may be quite challenging due to the explicit momentum conservation. For all the moves involving changes in the momentum-space states, we can give no analytical expression for $W_{n\rightarrow n+1}^{\text{prop}}$, and we have to devise computer algorithms capable of precisely enumerating all possible propositions that comply with the momentum (and also particle-number) conservation.

A. Updates that conserve the number of particles

(1a) $\text{add}_q$—used in the equilibrium ABQMC and the ABQMC for the survival probability

The momentum $K$ of each of the states $|\Psi^0_{k,l}\rangle$, $l = 1, \ldots, N_{\tau/t}$, is increased by a randomly chosen momentum $q \neq 0$, thereby obtaining new states $|\Psi^{n+1}_{k,l}\rangle$, $l = 1, \ldots, N_{\tau/t}$, with momentum $K + q$. The real-space states are not changed, i.e., $|\Psi^{n+1}_{k,l}\rangle = |\Psi^{n+1}_{k,l}\rangle$. In each momentum-space state, momentum $q$ is added to an electron of spin $\sigma$ that carries momentum $k_{j,l}^{\sigma}$ under the condition that the state $(\sigma, k_{j,l}^{\sigma} + q)$ is unoccupied in $|\Psi^0_{k,l}\rangle$. All possible momentum-accepting states $(\sigma, k_{j,l}^{\sigma} + q)$ have to be explicitly enumerated and their number is denoted as $p_{\tau/l}^{\sigma+q}$.  

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The inverse move starts from states $|\Psi_{k,l}^{n+1}\rangle$, $l = 1, \ldots, N_{\tau/t}$, with momentum $K + q$, and adds momentum $-q$ to each of them. All possible momentum-accepting states in $|\Psi_{k,l}^{n+1}\rangle$ have to be explicitly enumerated and their number is denoted as $p_l^{q}$. The ratio of the proposal probabilities is then

$$W_{n \rightarrow n+1}^{\mathrm{prop}} = \prod_{l} \frac{p_l^q}{p_l^{-q}}.$$ 

This move ensures that we sample configurations from sectors featuring different electronic momenta.

(1b) add $-q$—used in the ABQMC for local electron or spin densities, when the momentum conservation law is broken into two independent conservation laws on the two branches of the Keldysh contour

We randomly choose momentum $q \neq 0$ and the branch (forward or backward) on which the move is applied.

If the forward branch is chosen, the momenta of the states $|\Psi_{k,l}^{n}\rangle$, $l = 1, \ldots, N_{\tau}$, which are all equal to $K_{\text{fwd}}$, are increased by $q$ in the same manner as in (1a).

If the backward branch is chosen, the momenta of the states $|\Psi_{k,l}^{n}\rangle$, $l = N_{\tau} + 1, \ldots, 2N_{\tau}$, which are all equal to $K_{\text{bwd}}$, are increased by $q$ in the same manner as in (1a).

In both cases, the real-space states are kept intact, i.e., $|\Psi_{k,l}^{n}\rangle = |\Psi_{k,l}^{n+1}\rangle$.

The inverse move operates on the same branch as the direct move and attempts to add momentum $-q$ to all the momentum-space state on the chosen branch in the same manner as in (1a).

(2) exchange $-q$

We randomly choose one momentum-space state $|\Psi_{k,j_1}^{n}\rangle$ in which we select two electrons of spins $\sigma_1$ and $\sigma_2$ and momenta $k_{j_1}^{\sigma_1}$ and $k_{j_2}^{\sigma_2}$, which are ordered so that $k_{j_1,y} + N_yk_{j_1,x} > k_{j_2,y} + N_yk_{j_2,x}$. The momenta are subsequently changed using $k_{j_1}^{\sigma_1} \rightarrow k_{j_1}^{\sigma_1} + q$, $k_{j_2}^{\sigma_2} \rightarrow k_{j_2}^{\sigma_2} - q$ ($q \neq 0$). As a consequence, the net momentum of $|\Psi_{k,j_1}^{n}\rangle$ remains unchanged. Obviously, the move may be realized only when the states $(\sigma_1, k_{j_1}^{\sigma_1} + q)$ and $(\sigma_2, k_{j_2}^{\sigma_2} - q)$ are both unoccupied in $|\Psi_{k,j_1}^{n}\rangle$.

We note that enumerating all possible momenta $q \neq 0$ that may be transferred between the electrons is relatively simple for $\sigma_1 \neq \sigma_2$ ($\sigma_2 = 17$), when the two electrons can be distinguished by their spins. It is then enough to go through all empty states $(\sigma_1, k')$ to which the electron $(\sigma_1, k_{j_1}^{\sigma_1})$ can be moved and to determine the corresponding momentum transfer $q = k' - k_{j_1}^{\sigma_1}$. We then ask if the state $(\sigma_1, k_{j_2}^{\sigma_2} - q)$ is empty; in the affirmative case, we memorize the current $q$ as one possible momentum transfer. The inverse move proceeds in a completely analogous manner by explicitly enumerating possible back-transfers.

On the other hand, two electrons of the same spin are indistinguishable, and special care should be exercised to avoid double counting. For given $k_{j_1}$ and $k_{j_2}$ (we now omit $\sigma_1 = \sigma_2$), possible values of $q$ follow from the construction that is schematically summarized in Fig. S1. We make use of the periodic boundary conditions to construct a new unit cell (in the momentum space) such that the electron of momentum $k_{j_1}$ is in its “center”, while its vertices are at $k_{j_2}$, and its periodic copies $k_{j_1} + 2\pi(1,0), k_{j_2} + 2\pi(0,1)$, and $k_{j_1} + 2\pi(1,1)$. The “central point” and the four vertices partition the unit cell into four rectangular regions that are colored yellow (bottom left), green (top left), cyan (top right), and magenta (bottom right). The vectors $q$ that may be added to $k_{j_1}$ and subtracted from $k_{j_2}$ are to be selected so that the final states $k_{j_1} + q$ and $k_{j_2} - q$ belong to just one half of each of the regions, the two halves being separated by the line connecting the “central” point and the vertices. The halves from which possible final states $k_{j_1} + q$ and thus possible momentum transfers $q$ are selected is shaded. Choosing the momentum transfer such that the final state $k_{j_1} + q$ belongs to the other (unshaded) half is equivalent to assigning momentum $k_{j_1}$ to the blue electron and $k_{j_2}$ to the red electron, i.e., to exchanging momentum labels $k_{j_1}$ and $k_{j_2}$, which produces the setup equivalent to that presented in Fig. S1. The momentum transfer $q$ along the edges of the four shaded triangles should be counted only once because of the periodic boundary conditions. For example, if we enumerate possible $q$s along the vertical edge of the green shaded triangle, then we should not enumerate possible $q$s along the vertical edge of the cyan shaded triangle. Moreover, if any of the lines connecting the “center” and the four edges contains any other lattice point, possible $q$s along that line are subjected to the condition $|q| \leq |k_{j_1} - k_{j_2} - 2\pi(a_x, a_y)|/2$, where $(a_x, a_y) \in \{(0,0), (1,0), (0,1), (1,1)\}$. While this construction is appropriate for $k_{j_1,x} \neq k_{j_2,x}$ and $k_{j_1,y} \neq k_{j_2,y}$, further discussion is needed when either $k_{j_1,x} = k_{j_2,x}$ or $k_{j_1,y} = k_{j_2,y}$. In the inverse move, we start from the two electrons carrying momenta $k_{j_1}' = k_{j_1} + q$ and $k_{j_2}' = k_{j_2} - q$, we order them so that $k_{j_1,y} + N_yk_{j_1,x} > k_{j_2,y} + N_yk_{j_2,x}$, and repeat the above-described procedure.

This move ensures that we sample configurations belonging to the sector of the chosen total electron momentum.
(3) change_r_local

We randomly choose one real-space state $|\Psi_{i,l_0}^n\rangle$ in all the time-dependent computations we perform, $l_0 \neq 1$ due to $|\Psi_{i,l_0}^n\rangle \equiv |\psi(0)\rangle$ at each Monte Carlo step $n$ and move an arbitrarily chosen electron (spin $\sigma$, position $r_i^0$) to a new position $s_j^0$ under the condition that the state $(\sigma, s_j^0)$ is unoccupied in $|\Psi_{i,l_0}^n\rangle$.

The inverse move proceeds in the same manner as described above. The ratio of proposal weights is $W_{n+1 \to n}^{\text{prop}} / W_{n \to n+1}^{\text{prop}} = 1$.

This move ensures that we sample configurations with different real-space electron patterns.

(4) change_r_global

We randomly choose one real-space state $|\Psi_{i,l_0}^n\rangle$ in all the time-dependent computations we perform, $l_0 \neq 1$ due to $|\Psi_{i,l_0}^n\rangle \equiv |\psi(0)\rangle$ at each Monte Carlo step $n$ and replace it with a new state $|\Psi_{i,l_0}^{n+1}\rangle \neq |\Psi_{i,l_0}\rangle$. While the effects of this “global” move can be mimicked by multiple applications of its “local” version change_r_local, we found this move very useful in evenly sampling real-space configurations.

The inverse move proceeds in the same manner as described above. The ratio of proposal weights is $W_{n+1 \to n}^{\text{prop}} / W_{n \to n+1}^{\text{prop}} = 1$.

(5) spin_flip—used only in the equilibrium ABQMC because it does not separately conserve the number of spin-up and spin-down electrons, yet it conserves the total electron number

We randomly choose spin $\sigma$ and attempt to increase/decrease the number of electrons of spin $\sigma/\overline{\sigma}$ by one. In each imaginary-time slice $l = 1, \ldots, N_r$, we explicitly enumerate the momentum states $(\sigma, k) \in |\Psi_{k,l}^n\rangle$ such that $(\overline{\sigma}, k) \notin |\Psi_{k,l}^n\rangle$. This is the simplest possible update that changes the spin of an electron and yet keeps the total momentum of the configuration fixed. The state $|\Psi_{k,l}^{n+1}\rangle$ is then obtained from the state $|\Psi_{k,l}^n\rangle$ by removing the electron in the state $(\sigma, k)$ and adding the electron in the state $(\overline{\sigma}, k)$. The inverse move proceeds in an analogous manner: we explicitly enumerate momentum the states $(\overline{\sigma}, k') \in |\Psi_{k,l}^{n+1}\rangle$ such that $(\sigma, k') \notin |\Psi_{k,l}^{n+1}\rangle$.

In each imaginary-time slice $l = 1, \ldots, N_r$, we choose an electron of spin $\sigma$ at position $r$ from the real-space state $|\Psi_{i,l}^n\rangle$ and construct the real-space state $|\Psi_{i,l}^{n+1}\rangle$ by changing the electron’s position $r \to s$ and spin $\sigma \to \overline{\sigma}$. The ratio of the proposal probabilities in the real space can be directly computed as $W_{n+1 \to n}^{\text{prop}} / W_{n \to n+1}^{\text{prop}} = N_\sigma(N_\sigma - N_\overline{\sigma}) / (1 + N_\sigma)(N_\sigma - N_\overline{\sigma} + 1)$, where $N_\sigma$ and $N_\overline{\sigma}$ are numbers of electrons of spin $\sigma$ and $\overline{\sigma}$ in $|\Psi_{i,k,l}^n\rangle$.

This move is very useful once the ABQMC starts sampling the configurations whose total electron number (the sum of the numbers of spin-up and spin-down electrons) fluctuates around the value predicted by the fixed temperature and chemical potential. One value of the total electron number may be realized via many different
combinations of numbers of spin-up and spin-down electrons, and it is precisely this move that enables efficient sampling through all these combinations.

B. Updates that do not conserve the number of particles

The updates \texttt{add\_particle} and \texttt{remove\_particle} are used only in the equilibrium ABQMC, when the number of particles fluctuates according to the fixed chemical potential and temperature.

The move \texttt{add\_particle/remove\_particle} adds/removes one electron from the configuration. These two moves are inverses of one another. While analogous moves are relatively simply implemented in other QMC algorithms, here, special care is to be exercised because of the particle-number and momentum conservation. In more detail, the spin \( \sigma \) of the electron added to/removed from the imaginary-time slice \( l = 1 \) fixes that an electron added to/removed from the remaining imaginary-time slices \( l = 2, \ldots, N_\tau \) must have the same spin \( \sigma \). Furthermore, the momentum \( q \) of the electron added to/removed from the imaginary-time slice \( l = 1 \) fixes that momentum change upon addition/removal of an electron in the remaining imaginary-time slices \( l = 2, \ldots, N_\tau \) must be precisely \( q \). This requirement may be realized in many different ways. One trivial possibility is to add/remove the electron to/from the state \( (\sigma, q) \) if this state is empty/occupied. On the other hand, we may add/remove the electron to/from state \( (\sigma, k) \), in which case we should find another electron \( (\sigma_{\text{comp}}, k_{\text{comp}}) \) of arbitrary spin \( \sigma_{\text{comp}} \) to compensate for the difference in the momentum change from \( +q \), where \( +/− \) sign is for electron addition/removal. The electron in the state \( (\sigma_{\text{comp}}, k_{\text{comp}}) \) that may receive the momentum difference \( ±(q−k) \) will be termed the compensating electron. The situation is relatively simple when the spin of the compensating electron is \( \bar{\sigma} \) because the added electron and the compensating electron may be distinguished by their spins. When the spins of the added and compensating electrons are both equal to \( \sigma \), these two electrons cannot be distinguished in the sense that their roles (added/compensating) may be reverted. Special care should thus be taken to avoid double counting. An elaborate analysis reveals that the double counting is avoided by ordering the momenta of:

(\texttt{add}) the added electron \( k \) and the compensating electron \( k_{\text{comp}} + q − k \) after the compensation;

(\texttt{rmv}) the removed electron \( k \) and the compensating electron \( k_{\text{comp}} \) before the compensation.

The ordering is the same as in the update \texttt{exchange\_q}.

While the above discussion regards the momentum-space states \( |\Psi_{ik,l}^n\rangle \rightarrow |\Psi_{ik,l}^{n+1}\rangle \), the situation with the real-space states \( |\Psi_{i,l}^n\rangle \rightarrow |\Psi_{i,l}^{n+1}\rangle \) is far less complicated because only the particle-number conservation should be satisfied. The spin of the electron to be added to/removed from each \( |\Psi_{i,l}^n\rangle \) is determined by the spin \( \sigma_{\text{comp}} \) of the compensating electron: \( q = \pm |\Psi_{i,k,l}^n\rangle \). The ratio of the backward and forward proposal probabilities for the real-space parts of the configuration may be directly computed as:

\[
\begin{align*}
\text{(add)} & \quad \frac{W_{n+1\rightarrow n}^{\text{prop},i,l}}{W_{n\rightarrow n+1}^{\text{prop},i,l}} = \frac{N_\sigma - N_{\bar{\sigma}}}{1 + N_{\bar{\sigma}}}, \\
\text{(rmv)} & \quad \frac{W_{n+1\rightarrow n}^{\text{prop},i,l}}{W_{n\rightarrow n+1}^{\text{prop},i,l}} = \frac{N_\sigma}{N_\sigma - N_{\bar{\sigma}} + 1},
\end{align*}
\]

where \( N_\sigma \) is the number of electrons of spin \( \sigma \) in all the states \( |\Psi_{i,k,l}^n\rangle \) (before the update).

C. Fast determinant updates used to reduce the time needed to propose MC updates

The determinant \( D(C) \) is the product of a number of Slater determinants. Since all the moves can be seen as a single row/column change potentially combined with addition/removal of a single row/column, changes in individual Slater determinants may be efficiently computed using the formulae for fast determinant updates. These formulae, which provide the determinant ratio before and after the update, deal with the inverses of the Slater determinants, whose total number in the equilibrium ABQMC and the ABQMC for the survival probability is \( 2 \times 2N_{\tau} = 4N_{\tau} \), where the first factor of 2 comes from two spin orientations.

D. Extraction of the Monte Carlo results

Here, we describe in some detail the procedure we employ to extract ABQMC results from raw MC data. The number of MC steps needed to obtain converged results is inversely proportional to the average sign \(|\langle \text{sgn} \rangle|\), which is
generally much smaller than unity. To reach a relative (statistical) accuracy of \( r \), one has to complete \( \sim (r|\langle sgn \rangle|)^{-2} \) MC steps.\(^1\) All relevant quantities are measured at every MC step, and the individual-step data are grouped into bins of length \( L_b \), where \( L_b \sim 10^5 - 10^6 \), depending on the total number of MC steps completed. The convergence of the ABQMC is generally slow, which is illustrated in Fig. S2 for an equilibrium simulation (the situation is similar in time-dependent simulations). In the lower panel, which shows the average sign as a function of the number of MC steps, we observe that the very steep initial decay of \(|\langle sgn \rangle|\) (first \( \sim 2 \times 10^8 \) MC steps) is followed by quite a slow equilibration phase (up to \( \sim (5 - 6) \times 10^9 \) MC steps) characterized by multiple episodes of somewhat less steep decay and growth. It is for this reason that we have to discard many initial MC steps. In practice, we discard first 80% of the simulation. The data in the last 20% of the simulation are delimited by vertical lines. The average of the binned data in the final 20% of the simulation is taken as the MC estimate of the quantity of interest. The statistical error is estimated as the root-mean-square deviation of the binned data in the final 20% of the simulation from the above-computed average value. Such an estimate of the error is appropriate for statistically independent MC data. While we have not performed a systematic binning analysis, we may expect that the bin length we chose is sufficiently large that the data from different bins may be considered as statistically independent.

Figure S2. Upper panel: evolution of the electron density \( \rho_e \) in MC time. Lower panel: evolution of the average sign \(|\langle sgn \rangle|\) in MC time. ABQMC simulation is performed on a \( 4 \times 4 \) cluster with the following values of model parameters: \( U/J = 4, T/J = 1.0408, \mu/J = 2 \).
SII. ABQMC METHOD TO EVALUATE TIME-DEPENDENT EXPECTATION VALUES ALONG THE KADANOFF–BAYM CONTOUR

We start from

$$\langle A_\alpha(t) \rangle = \frac{\text{Tr} \left( e^{-iH(0)} e^{iHt} A_\alpha e^{-iHt} \right)}{\text{Tr} \left( e^{-iH(0)} \right)}$$  \hspace{1cm} (S4)$$

where $H$ is the Hubbard Hamiltonian, while $H(0)$ additionally contains terms that modulate charge or spin density. For example, to simulate the response recorded in Ref. 2, the following $H(0)$ may be appropriate:

$$H(0) = \sum_{k\sigma} \varepsilon_k n_{k\sigma} + U \sum_r n_{r\uparrow} n_{r\downarrow} - \sum_{r\sigma} v_r n_{r\sigma}$$  \hspace{1cm} (S5)$$

where $v_r$ is the external harmonic potential that modulates electron density, e.g.,

$$v_r = V_0 \cos(q \cdot r).$$  \hspace{1cm} (S6)$$

Inspired by Ref. 2, we assume that $q = q e_z$, i.e., we assume that the electron density is modulated along one direction with the wavelength $\lambda = 2\pi/q$. We also assume that $\lambda \leq N_x$ and that $N_x \text{mod} \lambda = 0$, i.e., the cluster’s linear dimension along $x$ axis is spanned by an integer number of wavelengths.

There are at least two manners in which the ABQMC method in the presence of external density-modulating potential (at $t < 0$) can be formulated. They differ by the choice of the contributions that are diagonal in the coordinate and momentum representations.

1. The part diagonal in the momentum representation is

$$[H(0)]_{\text{mom}} = \sum_k \varepsilon_k n_{k\sigma},$$

while the part diagonal in the coordinate representation

$$[H(0)]_{\text{coord}} = U \sum_r n_{r\uparrow} n_{r\downarrow} - \sum_{r\sigma} \mu_r n_{r\sigma}$$

contains position-dependent chemical potential $\mu_r = \mu + v_r$. Such a decomposition provides exact results in the atomic limit ($J = 0$) and is expected to provide reasonable results when the electron–electron interaction dominates over the electronic hopping.

2. The part diagonal in some momentum representation is

$$[H(0)]_{\text{mom}} = \sum_{k\sigma} \varepsilon_k n_{k\sigma} - \frac{V_0}{2} \sum_{k\sigma} \left( c_{(k_x+q, k_y)\sigma}^\dagger c_{(k_x, k_y)\sigma} c_{(k_x+q, k_y)\sigma}^\dagger c_{(k_x, k_y)\sigma} + c_{(k_x-q, k_y)\sigma}^\dagger c_{(k_x, k_y)\sigma} c_{(k_x-q, k_y)\sigma}^\dagger c_{(k_x, k_y)\sigma} \right)$$

while the part diagonal in the coordinate representation is

$$[H(0)]_{\text{coord}} = U \sum_r n_{r\uparrow} n_{r\downarrow}.$$

Such a decomposition provides exact results in the noninteracting limit ($U = 0$) and is expected to provide reasonable results when the electronic hopping dominates over the electron–electron interaction. Our further developments will be focused on this decomposition.

The external harmonic potential introduces the coupling between different $k$ states which results in a reduction of the Brillouin zone along $x$ axis by a factor of $\lambda$. The wave vector $k$ in the full Brillouin zone $[0, 2\pi) \times [0, 2\pi)$ is not a good quantum number anymore. Its role is taken by the wave vector $\tilde{k}$ in the reduced Brillouin zone $[0, 2\pi/\lambda) \times [0, 2\pi)$, whose $x$ projection $\tilde{k}_x$ may assume any of the $n_{\tilde{q}_x} = N_x \text{div} \lambda$ allowed values in the interval $[0, 2\pi/\lambda)$ ($p \times 2\pi/N_x$, where $p = 0, \ldots, n_{\tilde{q}_x} - 1$) and whose $y$ projection $\tilde{k}_y$ may assume any of the $N_y$ allowed values in the interval $[0, 2\pi)$ ($p \times 2\pi/N_y$, where $p = 0, \ldots, N_y - 1$). In addition to $\tilde{k}$, there is another degree of freedom that will be denoted by
ν and that may assume values 0, ..., λ − 1. The Hamiltonian $H_{\text{mom}}$ has a block-diagonal structure and the blocks defined by the wave vector $\mathbf{k}$ can be diagonalized separately. There are $n_q N_q$ such blocks and the dimension of each of them is $\lambda \times \lambda$.

The Hubbard Hamiltonian $H$ appears in combination $e^{i H t} \cdots e^{-i H t}$, meaning that the chemical-potential term $-\mu \sum_{\sigma} n_{\sigma} = -\mu \sum_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma}$ is not effective (we assume that $A_\sigma$ conserves the total particle number, which is a reasonable assumption) and there is no ambiguity regarding the part $H_{\text{mom}}$ or $H_{\text{coord}}$ to which it should be associated. Therefore, the partition of the Hubbard Hamiltonian in parts that are diagonal in the momentum and coordinate representation is the same as in the main body of the paper

$$H_{\text{mom}} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma}, \quad H_{\text{coord}} = U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}. \quad (S7)$$

Let us now exploit symmetries to develop as efficient as possible ABQMC algorithm to evaluate Eq. (S4). Since $H(0)$ is not invariant under the bipartite lattice symmetry, we use only the time-reversal symmetry, according to which $\langle A_\sigma(-t) \rangle = \langle A_\sigma(t) \rangle$. Furthermore, we note that both the numerator and the denominator of Eq. (S4) are purely real. Using the strategy described in the main text, one may derive the ABQMC counterpart of Eq. (S4)

$$\langle A_\sigma(t) \rangle = \frac{\sum_c \text{Re}\{D(C)\} e^{-\Delta \varepsilon_{\text{M}(C)}} \cos \{[\Delta \varepsilon_{0}(C) + \Delta \varepsilon_{\text{int}}(C)] \Delta t\} A_\sigma(\Psi_{a,l_c})}{\sum_c \text{Re}\{D(C)\} e^{-\Delta \varepsilon_{\text{M}(C)}}} \quad (S7)$$

The configuration $C$ consists of $2N_t + N_r$ many-body states $|\Psi_{l,i}\rangle$ ($l = 1, \ldots, 2N_t + N_r$) composed of single-particle momentum eigenstates and $2N_t + N_r$ many-body states $|\Psi_{l,i}\rangle$ composed of single-particle coordinate eigenstates. While momenta of states $|\Psi_{k,1}\rangle, \ldots, |\Psi_{k,2N_t+1}\rangle$ are defined in the full Brillouin zone, states $|\Psi_{k,2N_t+1}\rangle, \ldots, |\Psi_{k,2N_t+N_r}\rangle$ have their momenta defined in the reduced Brillouin zone. The symbols $D(C)$, $\Delta \varepsilon_{0}(C)$, and $\Delta \varepsilon_{\text{int}}(C)$ are defined as in the main text, while $\varepsilon_{\text{M}(C)}$ is the sum of energies of $2N_t$ states along the Matsubara part of the contour, i.e.,

$$\varepsilon_{\text{M}(C)} = \sum_{l=2N_t+1}^{2N_t+N_r} \left[ \varepsilon_0(\Psi_{l,i}) + \varepsilon_{\text{int}}(\Psi_{l,i}) \right]. \quad (S8)$$

The slice on which the expectation value $A_\sigma(\Psi_{a,l_c}) = \langle \Psi_{a,l_c} | A_\sigma | \Psi_{a,l_c} \rangle$ is evaluated depends on the representation $a = i, k$ in which the observable $A_\sigma$ is diagonal, so that $l_i = N_i + 1$ and $l_k = N_i$.

The structure of Eq. (S7) is intuitively clear as it is a combination of the ABQMC formula for thermodynamic quantities [Eq. (17) of the main text] and the ABQMC formula for the time-dependent expectation value along the Keldysh contour [Eq. (26) of the main text]. However, since we cannot exploit the bipartite lattice symmetry in this setup, the time-dependent part of the numerator in Eq. (S7) is $\cos \{[\Delta \varepsilon_{0}(C) + \Delta \varepsilon_{\text{int}}(C)] \Delta t\}$ instead of $\cos[\Delta \varepsilon_{0}(C) \Delta t] \cos[\Delta \varepsilon_{\text{int}}(C) \Delta t]$. Configuration weight may be chosen as $w(C) = |\text{Re}\{D(C)\}| e^{-\Delta \varepsilon_{\text{M}(C)}}$ and Eq. (S7) is recast as

$$\langle A_\sigma(t) \rangle = \frac{\langle \text{sgn}(C) \cos \{[\Delta \varepsilon_{0}(C) + \Delta \varepsilon_{\text{int}}(C)] \Delta t\} A_\sigma(\Psi_{a,l_c}) \rangle_w}{\langle \text{sgn}(C) \rangle_w}. \quad (S9)$$

Markov-chain MC evaluation of Eq. (S9) suffers from the sign problem that does not depend on time $t$ (it is not dynamical). Still, it becomes more pronounced when the cluster size $N_c$ or the number of slices ($N_t$ and $N_r$) is increased. Similarly to equilibrium ABQMC calculations, the weight $w(C)$ depends on all model parameters ($U$, $T$, $\mu$, $V_0$, $t$). Therefore, the calculations for different values of these parameters have to be performed using different Markov chains, which is different from the computation of $P(t)$ or $\langle A_\sigma(t) \rangle$ starting from a pure state $|\psi(0)\rangle$.

The application of conservation laws on the Kadanoff–Baym contour is somewhat more involved than on simpler contours studied in the main body of the paper. The particle-number conservation demands that all the many-body states constituting configuration $C$ have the same number of spin-up and spin-down electrons. We discuss the momentum conservation under the assumption that the observable $A_\sigma$ is diagonal in the coordinate representation (e.g., $A_\sigma = \sum_{\sigma} \varepsilon_{\mathbf{r}\sigma} n_{\mathbf{r}\sigma}$). From the main text, we know that the momentum conservation along the horizontal parts of the contour (Keldysh branch) is broken into two conservation laws that are satisfied separately on the forward and backward branch. In other words, the momenta (in the full Brillouin zone!) of $N_t$ momentum-space states $|\Psi_{k,1}\rangle, \ldots, |\Psi_{k,N_t}\rangle$ on the forward branch are all equal to $K_{\text{fwbd}}$, while the momenta of $N_t$ momentum-space states $|\Psi_{k,2N_t+1}\rangle, \ldots, |\Psi_{k,2N_t+N_r}\rangle$ on the backward branch are all equal to $K_{\text{bwbd}}$. In contrast to the situation encountered in the main text, $K_{\text{fwbd}}$ and $K_{\text{bwbd}}$ are not completely independent because states $|\Psi_{k,1}\rangle$ and $|\Psi_{k,2N_t}\rangle$ are “in contact” with states $|\Psi_{k,2N_t+1}\rangle$ and $|\Psi_{k,2N_t+N_r}\rangle$ on the Matsubara branch. Therefore, the relation between $K_{\text{fwbd}}$ and $K_{\text{bwbd}}$ is determined by the momentum-conservation law along the Matsubara branch, which is formulated in the reduced Brillouin zone. Namely,
the momenta (in the reduced Brillouin zone!) of \(N\tau\) momentum-space states \(|\Psi_{k,2Nt+1}\rangle, \ldots, |\Psi_{k,2Nt+N\tau}\rangle\) are all equal to \(\tilde{K}_M\). The momenta \(K_{\text{fwd}}, K_{\text{bwd}},\) and \(\tilde{K}_M\) are related as follows:

\[
K_{\text{fwd}} \cdot e_y = K_{\text{bwd}} \cdot e_y = \tilde{K}_M \cdot e_y,
\]

\[
\frac{K_{\text{bwd}} \cdot e_x}{2\pi/N_x} \mod \frac{N_x}{\lambda} = \frac{\tilde{K}_M \cdot e_x}{2\pi/N_x}, \quad \frac{K_{\text{bwd}} \cdot e_x}{2\pi/N_x} \mod \frac{N_x}{\lambda} = \frac{\tilde{K}_M \cdot e_x}{2\pi/N_x}.
\]

Due to the more complicated momentum-conservation law, MC updates presented in Sec. SI have to be amply modified. Instead of describing modified MC updates in detail, we demonstrate the correctness of our implementation by benchmarking it on small clusters. Motivated by Ref. 2, we limit the discussion to the electron occupation dynamics on individual sites.

We start from the noninteracting electrons, where already \(N\tau = 1\) imaginary-time slice and \(2Nt = 2\) real-time slices \((2Nt + N\tau = 3\) slices in total\) are expected to reproduce the exact result. Trivial as they may seem, the benchmarks on the noninteracting case are quite important, because densities of individual sites are expected to display nontrivial oscillatory behavior. The fact that our ABQMC results reproduce these oscillations quite accurately strongly suggests that our implementation is correct. In Fig. S3 we present results for the Hubbard dimer initially subjected to the external density-modulating field \(v_{r_x} = V_0 \cos(\pi r_x)\) with \(r_x = 0, 1\). Figure S4 displays results for the Hubbard tetramer initially subjected to the external density-modulating field of wavelength \(\lambda = 4\), \(v_{r_x} = V_0 \cos(\pi r_x/2)\), with \(r_x = 0, 1, 2, 3\). Figure S5 displays results for the Hubbard tetramer initially subjected to the external density-modulating field of wavelength \(\lambda = 2\), \(v_{r_x} = V_0 \cos(\pi r_x)\), with \(r_x = 0, 1, 2, 3\).

![Figure S3. Time-dependent site populations of the Hubbard dimer with the following values of model parameters: \(\mu/D = 1.3\), \(V_0/D = 2\), \(U = 0\), \(T/D = 0.57\). The external potential at \(t < 0\) is \(v_{r_x} = V_0 \cos(\pi r_x)\) with \(r_x = 0, 1\).]
We conclude this section by applying the ABQMC algorithm to interacting electrons. We first discuss the Hubbard dimer in the canonical ensemble, where we can obtain converged results with as many as \(2N_t + N_\tau = 12\) slices in total at half-filling \((N_\uparrow = N_\downarrow = 1)\). The results are presented in Fig. S6. We observe that ABQMC results qualitatively reproduce the exact result in the whole time window considered. The quantitative agreement is reasonable up to \(Dt \approx 2\). Figure S7 presents results for the Hubbard tetramer in the grand-canonical ensemble, where we obtain converged results using only \(N_t = 1\) and \(N_\tau = 2\). Further increase in \(N_t\) reduces the average sign by orders of magnitude: for \(N_t = 1\), \(N_\tau = 2\) we obtain \(|\langle \text{sgn} \rangle| = 1.2 \times 10^{-2}\), while for \(N_t = 2\), \(N_\tau = 2\) we find \(|\langle \text{sgn} \rangle| \sim 10^{-4}\).
While $N_\tau = 2$ is enough to reproduce equilibrium populations in the external field at $t = 0$, a single real-time slice leads to the quantitative agreement between the ABQMC and exact results only at shortest times.

Figure S6. Dynamics of electron populations on individual sites of the Hubbard dimer that at $t < 0$ is subjected to the density-modulating potential $v_{rx} = V_0 \cos(\pi r_x)$ with $r_x = 0, 1$. We work in the canonical ensemble with $N^\uparrow = N^\downarrow = 1$. The model parameters assume the following values: $V_0/D = 1$, $U/D = 0.6$, $T/D = 0.45$. 
Figure S7. Dynamics of electron populations on individual sites of the Hubbard tetramer that at \( t < 0 \) is subjected to the density-modulating potential \( v_{\tau_x} = V_0 \cos(\pi \tau_x) \) with \( \tau_x = 0, 1, 2, 3 \). We work in the grand-canonical ensemble with \( N_t = 1, N_\tau = 2 \) (\( 2N_t + N_\tau = 4 \) slices in total), and the following values of model parameters: \( \mu/D = -0.325, V_0/D = 0.5, U/D = 0.5, T/D = 0.5 \).

SIII. DETAILED PERFORMANCE OF THE ABQMC METHOD APPLIED TO EVALUATE THE EQUATION OF STATE

A. \( U/J = 4, T/J = 1.0408 \)

Figure S8. Average time needed to propose (black circles) and accept (red squares) one Monte Carlo update as a function of the ABQMC electron density. The averaging is performed over all updates used in ABQMC simulations to evaluate the equation of state: \texttt{add\_particle}, \texttt{remove\_particle}, \texttt{spin\_flip}, \texttt{add\_q}, \texttt{exchange\_q}, \texttt{change\_r\_local}, and \texttt{change\_r\_global}. 
Figure S9. Acceptance rates of individual Monte Carlo updates as a function of the ABQMC electron density. Being inverses of one another, the acceptance rates of moves add_particle and remove_particle are mutually equal. The acceptance rates of moves add_particle, remove_particle, spin_flip, add_q, and exchange_q exhibit weak dependence on the filling, while moves involving changes in the real-space part of configurations tend to be accepted less frequently as the filling is increased.

B. \( U/J = 24, \ T/J = 1.0408 \)

Figure S10. Average time needed to propose (black circles) and accept (red squares) one Monte Carlo update as a function of the ABQMC electron density. The averaging is performed over all updates used in ABQMC simulations to evaluate the equation of state: add_particle, remove_particle, spin_flip, add_q, exchange_q, change_r_local, and change_r_global.
Figure S11. Acceptance rates of individual Monte Carlo updates as a function of the ABQMC electron density. Being inverses of one another, the acceptance rates of moves `add_particle` and `remove_particle` are mutually equal. The acceptance rates of moves `add_q` and `exchange_q` exhibit weak dependence on the filling, while moves `add_particle`, `remove_particle`, `spin_flip`, `change_r_local`, and `change_r_global` tend to be accepted less frequently as the filling is increased.

SIV. APPLICABILITY OF THE ABQMC METHOD TO A $4 \times 4$ CLUSTER WITH $N_t = 4$ REAL-TIME SLICES

This section addresses the applicability of the ABQMC method to compute the survival probability of the 16-electron CDW-like/SDW-like state on a $4 \times 4$ square-lattice cluster when the number of real-time slices is increased from $N_t = 2$ to $N_t = 4$. In Fig. S12 we compare the behavior of the average sign for $N_t = 2$, when we make $3.87 \times 10^{10}$ steps, and $N_t = 4$, when we make $1.16 \times 10^{10}$ steps. Increasing the number of real-time slices from 2 to 4 decreases $|\langle \text{sgn} \rangle|$ after $10^{10}$ MC steps by an order of magnitude. With $N_t = 4$, the stabilization of the average sign takes much more than $10^{10}$ MC steps, and its overall decrease as the simulation proceeds may be very well described by a power law with the exponent of $-1/2$, see the dashed line in Fig. S12.

Figure S12. Magnitude of the average sign as a function of the number of MC steps during the ABQMC simulation of the survival probability of the 16-electron CDW/SDW state on a $4 \times 4$ square-lattice cluster using $N_t = 2$ and $N_t = 4$ real-time slices. The overall behavior of $|\langle \text{sgn} \rangle|$ for $N_t = 4$ may be fitted very well by the function $5 / \sqrt{N_{\text{MC}}}$ that is shown by the dashed line.
This section addresses the applicability of the ABQMC method to compute the survival probability of a 16-electron initial state on an $8 \times 4$ cluster with $N_t = 2$ real-time slices. The initial CDW-like state is schematically depicted in Fig. S13(a), while Fig. S13(b) shows the evolution of the average sign during the MC simulation. We perform $10^{10}$ MC steps, during which the magnitude of the average sign shows no signals of stabilization, but steadily decreases in a power-law fashion with the exponent $-1/2$, see the dashed line in Fig. S13(b). Even though the final stages of our MC simulation may suggest that $|\langle \text{sgn} \rangle|$ stabilizes on the level of $\sim 4 \times 10^{-5}$, a very noisy behavior of $|\langle \text{sgn} \rangle|$ throughout the simulation casts doubts on such a conclusion. We observe in Fig. S13(b) that $|\langle \text{sgn} \rangle|$ displays pronounced dips whose duration may be as long as a couple of billions of steps, which is in stark contrast with the rather smooth decrease of $|\langle \text{sgn} \rangle|$ observed, e.g., in Fig. S12. These dips suggest that there may be problems with the configuration-space sampling. The dimension of the configuration space of our ABQMC method is much larger than the dimension of the Hilbert space of the model, which is astronomically large for the Hubbard model on an $8 \times 4$ cluster. To further illustrate the last point, in Fig. S13(c) we present the survival probability of the initial state in the noninteracting case. In contrast to the $4 \times 4$ cluster, for which perfect collapses and revivals in $P(t)$ are observed already on relatively short time scales, there is no such a regular behavior on the $8 \times 4$ cluster, see Fig. S13(c). On general grounds, the noninteracting system is bound to display perfect collapses and revivals in $P(t)$, while the time scale on which the pattern in $P(t)$ repeats itself is inversely proportional to the dimension of the system’s Hilbert space.

Figure S13. (a) Schematic view of the 16-electron initial state on an $8 \times 4$ square-lattice cluster whose survival probability is computed. (b) Magnitude of the average sign as a function of the number of MC steps during the ABQMC simulation of the survival probability of the initial state depicted in (a). $N_t = 2$ real-time slices are used. The overall behavior of $|\langle \text{sgn} \rangle|$ may be fitted very well by the function $2/\sqrt{N_{\text{MC}}}$ that is shown by the dashed line. (c) Time dependence of the survival probability of the initial state depicted in (a) in the noninteracting case $U = 0$. The dimensionality of the system’s Hilbert space is so large that no perfect revival in $P(t)$ (which is bound to occur since $U = 0$) is observed up to $Dt = 250$.

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