Beating the efficiency of both quantum and classical simulations with semiclassics

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While rigorous quantum dynamical simulations of many-body systems are extremely difficult (or impossible) due to the exponential scaling with dimensionality, corresponding classical simulations completely ignore quantum effects. Semiclassical methods are generally more efficient but less accurate than quantum methods, and more accurate but less efficient than classical methods. We find a remarkable exception to this rule by showing that a semiclassical method can be both more accurate and faster than a classical simulation. Specifically, we prove that for the semiclassical dephasing representation the number of trajectories needed to simulate quantum fidelity is independent of dimensionality and also that this semiclassical method is even faster than the most efficient corresponding classical algorithm. Analytical results are confirmed with simulations of quantum fidelity in up to 100 dimensions with $2^{1700}$-dimensional Hilbert space.

Introduction. Correct description of many microscopic dynamical phenomena, such as ultrafast time-resolved spectra or tunneling rate constants, requires an accurate quantum (QM) simulation. While classical (CL) molecular dynamics simulations are feasible for millions of atoms, solution of the time-dependent Schrödinger equation scales exponentially with the number $D$ of degrees of freedom (DOF) and is feasible for only a few continuous DOF. An apparently promising solution is provided by semiclassical (SC) methods, which use CL trajectories, but attach to them phase information, and thus can approximately describe interference and other QM effects completely missed in CL simulations. Unfortunately, SC methods suffer from the “dynamical sign problem” due to the addition of rapidly oscillating terms, resulting in the requirement of a huge number of CL trajectories for convergence. Consequently, most SC methods are much less efficient than CL simulations and in practice were used for at most tens of DOF. Even though several techniques have explored this issue [1], the challenge remains open. Below we turn this challenge around by showing that in simulations of QM fidelity (QF) [2, 3], a SC method called “dephasing representation” (DR) is not only more accurate but, remarkably, also faster than the most efficient corresponding CL algorithm [4].

Quantum and classical fidelity. QF was introduced by Peres [5] to measure the stability of QM dynamics (QD). He defined QF $F_{QM}(t)$ as the squared overlap at time $t$ of two QM states, identical at $t = 0$, but subsequently evolved with two different Hamiltonians, $H_0$ and $H_e = H_0 + eV$:

$$F_{QM}(t) := |f_{QM}(t)|^2,$$  
$$f_{QM}(t) := \langle \psi | U_{t}^e U_t^0 | \psi \rangle,$$  

where $f_{QM}(t)$ is the fidelity amplitude and $U_t^e := \exp(-i H_t t / \hbar)$ the QM evolution operator. Rewriting Eq. (2) as $f_{QM}(t) = \langle \psi | U_t^e | \psi \rangle$ with the echo operator $U_t^e := U_{-t}^e U_t^0$, it can be interpreted as the Loschmidt echo, i.e., an overlap of an initial state with a state evolved for time $t$ with $H_0$ and subsequently for time $-t$ with $H_e$. (In general, we write time $t$ as a superscript. Subscript $e$ denotes that $H_e$ was used for dynamics. If an evolution operator, phase space coordinate, or density lacks a subscript $e$, Loschmidt echo dynamics is implied.) QF amplitude (2) is ubiquitous in applications: it appears in NMR spin echo experiments [6], neutron scattering [7], ultrafast electronic spectroscopy [8, 9], etc. QF (1) is relevant in QM computation and decoherence [10], and can be used to measure nonadiabaticity [11] or accuracy of molecular QD on an approximate potential energy surface [12].

Definition (1) can be generalized to mixed states in different ways [2, 13–15], but we assume that the initial states are pure. In this case, one may write QF (1) as $F_{QM}(t) = \text{Tr}(\hat{\rho}_t^e \hat{\rho}_0^0)$ where $\hat{\rho}_t^e := U_t^e \hat{\rho} U_{-t}^e$ is the density operator at time $t$. In the phase-space formulation of QM mechanics, QF becomes $F_{QM}(t) = \hbar^{-D} \int dx \hat{\rho}_s(x) \hat{\rho}_0^0(x)$ where $x := (q, p)$ is a point in phase space and $A_W(x) := \int dξ (q - ξ/2) \hat{A} q + ξ/2 e^{i pξ/\hbar}$ is the Wigner transform of $\hat{A}$. This form of QF suggests its CL limit, called CL fidelity (CF) [16, 17]:

$$F_{CL}(t) := F_{id}(t) = \hbar^{-D} \int dx \hat{\rho}_s(x) \hat{\rho}_0^0(x)$$  
$$= F_{echo}(t) = \hbar^{-D} \int dx \hat{\rho}(x) \hat{\rho}_0(x)$$

where the first and second line express CF in the fidelity and Loschmidt echo pictures, respectively. If $F$ or $ρ$ lack the subscript “CL”, “QM”, or “DR”, “CL” is implied.

Dephasing representation. There were several attempts at describing QF semiclassically. Most were analytical [3, 18] and valid only under special circumstances because the numerical approaches were overwhelmed with the sign problem. Extending a numerical SC method for localized Gaussian wavepackets (GWPs) [19], the DR was introduced as a more accurate and general approximation of QF [13–15]. The DR of QF amplitude is an interference integral:

$$f_{DR}(t) := \hbar^{-D} \int dx \hat{\rho}(x) \exp[i \phi(x, t)],$$  
$$\phi(x, t) := -\Delta S(x, t) / \hbar = (\epsilon / \hbar) \int_0^t dτ V(x_τ^e),$$
where the phase $\phi$ is determined by the action $\Delta S$ due to the perturbation along a trajectory propagated with the average Hamiltonian $H_{1/2}$ [20]. Above, $x^j := \Phi^j(x^0)$ where $\Phi^j$ is the Hamiltonian flow of $H_c$ and the perturbation $V$ can, in general, depend on both $q$ and $p$. The DR of fidelity, computed as $F_{\text{DR}} := |f_{\text{DR}}|^2$, was successfully used to describe stability of QD in integrable, mixed, and chaotic systems [13–15], nonadiabaticity [11] and accuracy of molecular QD on an approximate potential energy surface [12], and the local density of states and the transition from the Fermi-Golden-Rule (FGR) to the Lyapunov regime of QF decay [21]. The same approximation was independently derived and used in electronic spectroscopy [8]. Recently, the range of validity of the DR was extended with a SC prefactor [20]. The remarkable efficiency of the original DR observed empirically in applications led us to analyze this property rigorously here and to compare it with the efficiencies of the QM and CL calculations of QF.

**Algorithms.** The most general and straightforward way to evaluate Eqs. (3–4) and (5) is with trajectory-based methods. While the DR (5) is already in a suitable form, Eqs. (3–4) for CF must be rewritten using the Liouville theorem as

$$F_{\text{fid}}(t) = h^{-D} \int dx^0 \rho(x^{-t}_0)\rho(x^{-t}_0)$$

and

$$F_{\text{echo}}(t) = h^{-D} \int dx^0 \rho(x^{-t}_0)\rho(0).$$

Above, $x^t := \Phi^t(x^0)$ where $\Phi^{-t} := \Phi^{-t} \phi_0$ is the Loschmidt echo flow. Since it is the phase space points rather than the densities that evolve in expressions (7)-(8), we can take $\rho = \rho_{\text{W}}^{\text{t=0}}$. For numerical computations, Eqs. (5) and (7-8) are further rewritten in a form suitable for Monte Carlo evaluation, i.e., as an average

$$\langle A(x^0), t \rangle_{W(x^0)} := \frac{\int dx^0 A(x^0, t)W(x^0)}{\int dx^0 W(x^0)}$$

where $W$ is the sampling weight for initial conditions $x^0$. Using $W = \rho_{W}(x^0)$, the DR algorithm becomes [13–15]

$$f_{\text{DR}}(t) = \langle \exp [i\phi(x^0, t)] \rangle_{\rho_{W}(x^0)}.$$ (9)

Sampling is straightforward for $\rho_{W} \geq 0$, but can be done also for general pure states [15]. While previously used CL algorithms sampled from $W = \rho$ [17–22], Ref. [4] considered more general weights $W = W_M(x^0) := \rho(x^0)^M$ and $W = W_M(x^{-t}_0) = (\rho(x^{-t}_0)^M)$ for the echo and fidelity dynamics, respectively. These weights yield four families of $M$-dependent algorithms [4]

$$F_{\text{fid-M}}(t) = I_M \langle \rho(x^0^{-t})\rho(x^0^{-t})^{1-M}\rangle_{\rho(x^0)^M},$$

$$F_{\text{echo-M}}(t) = I_M \langle \rho(x^0^{-t})\rho(x^0)^{1-M}\rangle_{\rho(x^0)^M},$$

$$F_{\text{fid-N-M}}(t) = \frac{\langle \rho(x^{-t})\rho(x^{-t})^{1-M}\rangle_{\rho(x^{-t})^M}}{\langle \rho(x^0)^{2-M}\rangle_{\rho(x^0)^M}},$$

$$F_{\text{echo-N-M}}(t) = \frac{\langle \rho(x^{-t})\rho(x^0)^{1-M}\rangle_{\rho(x^0)^M}}{\langle \rho(x^0)^{2-M}\rangle_{\rho(x^0)^M}},$$

where $I_M := h^{-D} \int \rho(x^0)^M dx^0$ is a normalization factor. Conveniently, the “normalized” (N) algorithms (12–13) do not require the normalization factor $I_M$ which is, for general states, known explicitly only for $M \in \{0, 1, 2\}$ ($I_0 = n_0$, $I_1 = I_2 = 1$). For further details, see Ref. [4] where it was found that the echo-2 algorithm is optimal since it is already normalized (i.e., echo-2 = echo-N-2), applies to any pure state (in particular, $\rho$ does not have to be positive definite), and—most importantly—is by far the most efficient CL algorithm.

**Efficiency.** The reader does not have to be persuaded of the exponential scaling of QD with $D$. We just note that the direct diagonalization of the Hamiltonian leads to a QD algorithm with a cost $O(t^D n_1^2)$ which $n_D = n_1^2$ is the dimension of the Hilbert space of $D$ DOF. Despite the independence of $t$, the scaling with $D$ is overwhelming. More practical is the split-operator algorithm requiring the fast Fourier transform (FFT) at each step. The complexity of FFT is $O(n_D \log n_D)$, hence the overall cost is $O(tDn_1^2 \log n_1)$. The effective $n_1$ is reduced in increasingly popular methods with evolving bases, but the exponential scaling remains.

Regarding the CF and DR algorithms, efficiency of trajectory-based methods depends on two ingredients: First, what is the cost of propagating $N$ trajectories for time $t$? Second, what $N$ is needed to converge the result to within a desired discretization error $\sigma_{\text{discr}}$? As this analysis was done for the CL algorithms in Ref. [4], here we only outline the main ideas and apply them to analyze the efficiency of the DR.

The cost of a typical method propagating $N$ trajectories for time $t$ is $O(\epsilon_t N)$ where $\epsilon_t$ is the cost of a single force evaluation. However, among the above mentioned algorithms, this is only true for the fidelity algorithms with $M = 0$ (i.e., fid-0 and fid-N-0) and for the DR! Remarkably, in all other cases, the cost is $O(\epsilon_t N^2)$. The cost is linear in time for a single time $t$, but becomes quadratic if one wants to know $\rho$ for all times up to $t$. For the echo algorithms, it is due to the necessary full backward propagation for each time between 0 and $t$. For the fidelity algorithms, it is because the weight function $\rho(x^{-t})^M$ changes with time and the sampling has to be redone for each time between 0 and $t$.

The number $N$ of trajectories required for convergence can depend on $D$, $t$, dynamics, initial state, and method. Below we estimate $N$ for the DR analytically using the technique proposed in Ref. [4]. The expected systematic component of $\sigma_{\text{discr}}$ is zero for $f_{\text{DR}}$ and $O(N^{-1})$ for $F_{\text{DR}}$ and is negligible to the expected statistical component $\sigma = O(N^{-1/2})$ which therefore determines convergence. Expected statistical error of $A(N)$ is computed as $\sigma_A^2(N) = |A(N)|^2 - \langle A(N) \rangle^2$ where the overline denotes an average over infinitely many independent simulations with $N$ trajectories.

The discretized form of Eq. (9) is $f_{\text{DR}}(t, N) = N^{-1} \sum_{j=1}^N \exp \{i\phi(x_j^0, t)\}$, from which $f_{\text{DR}}(t, N)^2 = N^{-1} \sum_{j=1}^N f_{\text{DR}}(t, j)^2 = F_{\text{DR}}(t)$, and $\sigma_{\text{fdr}}^2 = N^{-1}(1 - F_{\text{DR}})$. The analogous calculation for $F_{\text{DR}}$ is somewhat more involved but straightforward. Inverting the results
for \( \sigma_{F_{\text{for}}}^2 \) (exact) and \( \sigma_{F_{\text{for}}}^2 \) (to leading order in \( N \)) gives

\[
N_{F_{\text{for}}} = \sigma^{-2} (1 - F_{\text{DR}}) \quad \text{and} \quad \sigma_{F_{\text{for}}}^2 \geq \frac{2}{\sigma^2} \left[ \text{Re} \left( \langle e^{i2\phi} \rangle_{\rho_{\text{w}}} \langle e^{-i\phi} \rangle_{\rho_{\text{w}}}^2 \right) + F_{\text{DR}} - 2F_{\text{DR}}^2 \right].
\]

Result (14) for \( N_{F_{\text{for}}} \) is completely general. As for \( N_{F_{\text{for}}} \), using the inequality \( |\langle e^{i2\phi} \rangle_{\rho_{\text{w}}}| \leq 1 \) and Eq. (9), we can find a completely general upper bound,

\[
N_{F_{\text{for}}} \leq 4\sigma^{-2} F_{\text{DR}} (1 - F_{\text{DR}}).
\]

Estimate (14) and upper bound (16) show, remarkably, that without any assumptions, the numbers of trajectories needed for convergence of both \( f_{\text{DR}} \) and \( F_{\text{DR}} \) depend only on \( \sigma \) and \( F_{\text{DR}} \), and are independent of \( D, t, \) initial state, or dynamics. Estimate (15) of \( N_{F_{\text{for}}} \) can be evaluated analytically for normally distributed phase \( \phi \). This is satisfied very accurately in the chaotic FGR and integrable Gaussian regimes [2,3], and exactly for pure displacement dynamics of GWP.

Using a similar analysis, in Ref. [4] it was found that for CF algorithms (10)-(13) and \( D > 1 \), one needs \( N = \sigma^{-2} \alpha(F)\beta^D \) trajectories where \( \alpha \) and \( \beta \) depend on the method, initial state, and dynamics. For all methods with \( M \neq 2 \), there are simple examples [4] with \( \beta > 1 \), implying an exponential growth of \( N \) with \( D \). Remarkably, for any dynamics and any initial state, \( \beta = 1 \) for the echo-2 algorithm, implying, as for the DR, that \( N \) is independent of \( D \) [4].

**Numerical results and conclusion.** To illustrate the analytical results, numerical tests were performed in multidimensional systems of uncoupled displaced simple harmonic oscillators (SHOs, for pure displacement dynamics) and perturbed kicked rotors (for nonlinear integrable and chaotic dynamics). The last model is defined, modulo \( 2\pi \), by the map \( q_{j+1} = q_j + p_j, p_{j+1} = p_j - \nabla W(q_{j+1}) - \epsilon \nabla V(q_{j+1}) \) where

\[
W(q) = -k \cos q \text { is the potential and } V(q) = -\cos(2q) \text { the perturbation of the system; } \kappa \text { and } \epsilon \text { determine the type of dynamics and perturbation strength, respectively. Uncoupled systems were used in order to make QF calculations feasible (as a product of } D \text { 1-dimensional calculations); however, both CF and DR calculations were performed as for a truly } D\text{-dimensional system. The initial state was always a multidimensional GWP. Expected statistical errors were estimated by averaging actual statistical errors over 100 different sets}
FIG. 3. Regardless of dynamics, statistical error of the DR is independent of dimensionality \( D \), time \( t \), and is proportional to \( N^{-1/2} \). Errors are compared for 10 kicked rotors in the chaotic FGR regime \(( k = 18, \epsilon = 6.4 \times 10^{-6}, n_1 = 131072)\), 100 kicked rotors in the integrable Gaussian regime \(( k = 0.2, \epsilon = 6.4 \times 10^{-6}, n_1 = 131072)\), and a single kicked rotor in the quasi-integrable algebraic regime \(( k = 0.2, \epsilon = 6.4 \times 10^{-4}, n_1 = 131072)\). Time \( t \) was chosen separately for each system so that \( F \approx 0.94 \).

of \( N \) trajectories. No fitting was used in any of the figures, yet all numerical results agree with the analytical estimates. Note that the figures show also results for algorithm echo-1’, \( F_{\text{echo-1}'}(t) = 1 + \langle \rho(x^{-}) - \rho(x^{0}) \rangle_{\rho(x^{0})} \), which is a variant of echo-1 accurate for high fidelity [4].

Figure 1 displays fidelity in a 100-dimensional system of kicked rotors. It shows that both echo-2 and DR algorithms converge with several orders of magnitude fewer trajectories than the echo-1, echo-1’, and echo-N-1 algorithms but while the DR agrees with the QM result, even the fully converged CF (computed as a product of 100 one-dimensional fidelities) cannot reproduce QM effects. Figure 2 confirms that whereas the statistical errors of the echo-1, echo-1’, and echo-N-1 algorithms grow exponentially with \( D \), statistical errors of the DR and echo-2 algorithms are independent of \( D \). Figure 3 shows that for several very different dynamical regimes, \( \sigma_{\text{DR}} \) is independent of \( t \), \( D \) and \( n_1 \), in agreement with the general upper bound (16) and—in the FGR and Gaussian regimes—also in agreement with the analytical estimate (17). Finally, figure 4 exhibits the superior computational efficiency of the DR compared to all CF algorithms: thanks to the linear scaling with \( t \) and independence of \( D \), the DR is orders of magnitude faster already for quite a small system and short time.

To conclude, in the case of QF, a SC method can be not only more accurate, but also more efficient than a CL simulation of QD. This counterintuitive result should be useful for future development of approximate methods for QD of large systems. This research was supported by Swiss NSF grant No. 200021L124936 and NCCR MUST, and by EPFL. We thank T. Seligman and T. Zimmermann for discussions.

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FIG. 4. Computational cost as a function of simulation time \( t \) for different algorithms. The CPU time grows quadratically with \( t \) for all CL algorithms while it is only linear with \( t \) for the DR and fid-0 algorithms. Dynamics is of pure displacement type given by a \( D \)-dimensional system of displaced SHOs for which all algorithms converge to the exact result. Fidelity was computed at fidelity revival times at which \( F \approx 0.9 \). Number of trajectories \( N \) was selected for each algorithm separately so that the statistical error \( \sigma \approx 0.01 \) for all methods. (a) \( D = 20 \). (b) \( D = 1 \).
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