Beating the efficiency of both quantum and classical simulations with semiclassics

Cesare Mollica\textsuperscript{1} and Jiri Vanicek\textsuperscript{1}

\textsuperscript{1}Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne, Lausanne, 1015, Switzerland
e-mail: jiri.vanicek@epfl.ch

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 \cite{1}. Specifically, we prove that for the semiclassical dephasing representation \cite{2,3} (a method closely related to Hubbard and Miller’s semiclassical perturbation approximation \cite{4}), 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 \cite{5}. Analytical results are confirmed with simulations of quantum fidelity in up to 100 dimensions with $2^{1700}$-dimensional Hilbert space. Applications of the dephasing representation that will be discussed include evaluation of the nonadiabaticity of molecular quantum dynamics \cite{6,7} and calculation of the ultrafast time-resolved electronic spectra \cite{8}.

\begin{thebibliography}{9}


\end{thebibliography}