A new mixed quantum/semiclassical propagation methodology
STEVEN SCHWARTZ, Albert Einstein College of Medicine — We present a new propagation algorithm for the evolution of a highly quantum subsystem coupled to a more classical like bath. The quantum system is treated exactly, while the bath is evolved with a frozen Gaussian evolution. An evolution operator correction scheme we recently developed is then applied to compute the coupling between the quantum systems and the semiclassical bath. The scheme is applied to test problems and found to be accurate and not significantly more difficult to implement than standard classical molecular dynamics. The approach also admits the possibility of higher order correction to obtain exact quantum results.

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