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Commutator Magnus Development Integrators

Mahendran Rajat*

Department of Mathematics, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Tamilnadu, India

Commentary

Hybrid quantum-classical systems combine both classical and quantum degrees of freedom. Typically, in chemistry, molecular physics, or materials science, the classical degrees of freedom describe atomic nuclei (or cations with frozen core electrons), whereas the quantum particles are the electrons. Although many possible hybrid dynamical models exist, the essential one is that the so-called Ehrenfest dynamics that results from the simple partial classical limit applied to the complete quantum Schrödinger equation. Few numerical methods are developed specifically for the mixing of this sort of systems. Here we present a preliminary study of the performance of a family of recently developed propagators: the (quasi) commutator-free Magnus expansions. These methods, however, were initially designed for non-autonomous linear equations. We employ them for the nonlinear Ehrenfest system, by approximating the state value at whenever step within the propagation, using an extrapolation from previous time steps.

The right procedure, and even the likelihood, of producing classical and quantum physics into a physically consistent hybrid quantum-classical theory are extensively researched, and remains a topic of debate. There could also be fundamental reasons to think about these hybrids, that is, it's been speculated that hybrid systems may very well exist. for instance , a uniform scientific theory valid for cosmology problems remains not available, and it's been argued that Newtonian mechanics should be considered because the fundamental description; therefore the coupling of those systems to quantum matter should be modelled with a hybrid theory. Furthermore, hybrid models are proposed to elucidate the measurement process: the “wave function collapse” should be explained through the interaction of the quantum system with a classical measurement device.

However, the foremost important reason to affect hybrid models is that they're essential to permit the approximation of fully quantum systems that are overlarge to model exactly. If the classical approximation could also be taken for variety of particles of a quantum system, but not for others, the matter involves a hybrid quantum-classical model representation which will significantly reduce the computational cost with reference to the complete quantum treatment. Within the extreme case, the quantum degrees of freedom can actually be integrated out completely, resulting in a purely classical system, formed by particles that interact through forces that contain in an approximate way the influence of the quantum particles. This is often the realm of classical molecular dynamics (MD). The matter then reduces to the mixing of Newton's equations and is not any longer hybrid but merely classical and is therefore not the target of this work.

Broadly speaking, the drastic reduction within the complexity of the matter that results in classical MD can only be done when the quantum particles (hereafter, the electrons) are constantly within the state of the Hamiltonian like each instantaneous configuration of the classical particles (hereafter, the nuclei). This amounts to assuming the so-called adiabatic approximation. Outside its domain of validity, a non-adiabatic sort of MD must be used, during which the phase space does contain both the electrons and nuclei, which must be evolved simultaneously—hence constituting a real hybrid system. There could also be two reasons to necessitate a non-adiabatic MD: First, when the goal is to compute equilibrium properties, if the temperature is sufficiently high so on populate the electronic excited states. Second, for time-dependent problems out of equilibrium, if the intensity of the perturbation is robust and fast enough to induce the electronic transitions. Indeed, within the past decades, the arrival and fast development of high-intensity ultra-fast laser pulses has created the fields of femto- and atto-chemistry, whose theoretical study naturally involves a non-adiabatic treatment.

A number of hybrid quantum-classical non-adiabatic MD models are proposed over the years, but perhaps the foremost fundamental of all of them is given by the so-called Ehrenfest equations- oftentimes simply called the mixed quantum-classical dynamics. This fundamental role played by Ehrenfest dynamics (ED) could also be understood in two ways. First, it's the results of the simple application of the classical limit, for a subset of the particles, to the complete Schrödinger equation. Second, it's the Hamiltonian system that results of the straightforward composition of two Hamiltonian systems that represent both a classical and a quantum part: because it is documented, Schrödinger dynamics could also be written in terms of a Poisson bracket, and is therefore a Hamiltonian system. ED is thus symplectic, and it's desirable that the numerical integrator wont to solve the ED equations preserves this geometrical structure. Moreover, the norm of the quantum wave function must even be preserved in time.

Recently, a number of authors have demonstrated the great performance of the commutator free (CF) Magnus expansion based propagators for the time-dependent Kohn-Sham equations, which are the set of equations that stem of time-dependent density-functional theory (TDDFT). This theory is one among the various alternatives that exist to tackle the many-electron problem, substituting the Schrödinger equation by more manageable equations. This substitution reduces the dimension of the matter, making it computationally feasible, but also makes it nonlinear. The CF Magnus propagators were originally designed for linear equations, yet we proved that they will be used for the nonlinear TDDFT equations by performing an easy extrapolation predictor step.

In this proceedings article, we extend this idea to hybrid quantum-classical systems, and present preliminary results on the performance of two orders and two order CF Magnus expansion propagators applied to ED- for the case in which the quantum problem is handled directly by Schrödinger's equation. The goal is to use the same propagator for both electrons and nuclei and apply the CF expansions formula to the full ED, which is also a nonlinear problem. In a forthcoming publication, we will present the application of these methods to the ED TDDFT combination, a more detailed analysis of the performance of the schemes, and a deeper theoretical analysis.

***Address for Correspondence:** Mahendran Rajat, Department of Mathematics, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Tamilnadu, India, E-mail: mahendran.r@gmail.com*

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