SIMULATING QUANTUM DYNAMICS OF MANY- ELECTRON SYSTEMS

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We present a novel Quantum monte Carlo (QMC) approach based on the Real Time Path Integrals (RTPI), for simulations of many-particle systems. As a test case we simulate the response of a two-electron system to a short time pulse external electric field. Also, we demonstrate some distinguished features, which are not typical for QMC methods, like straightforward treatment of fermions and finding the stationary eigenstates of the system in time-independent case.

We present results and demonstrate finding the lowest excited states, and also, dynamics as a response to the time dependent external electric fields. Our test bench is sc. Hooke's atom: two electrons in a harmonic potential. This is a case of very strong correlation: Coulomb interaction of the electrons splits the space of relative motion into two independent parts. We analyse the role of relevant approximations, Monte Carlo method and numerical parameters. We also assess the accuracy in comparison with the exact analytical data [1].

We have shown that RTPI method [2, 3] is capable of incorporating the Coulombic electronic correlations exactly within numerical accuracy. Furthermore, combined with Monte Carlo sampling of paths RTPI becomes a robust method.

The improved Trotter kernel is shown to be useful with large enough number of Monte Carlo walkers, in cases where exact propagators are not available. We find that the accuracy and stability of RTPI are tunable with the number of Monte Carlo walkers and the real time step size. Regarding ground states, the computational cost of RTPI is significantly higher than that of Diffusion Monte Carlo. However, one of the advantages of RTPI is that it provides the wave function explicitly, and thus, the evaluation of local multiplicative operator expectation values becomes straightforward. Moreover, RTPI is capable of locating the nodal surfaces of excited states, which is promising for fermion simulations.

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[2] Ilkka Ruokosenmäki, Tapio T. Rantala, Comm. in Comp. Phys. 18, 91 (2015).
[3] Ilkka Ruokosenmäki, Hossein Gholizade, Tapio T. Rantala, Computer Physics Communications 210, 45 (2017).