Quantum Diffusion Monte Carlo Method for strong field time dependent problems

MATT KALINSKI, Utah State University — We formulate the Quantum Diffusion Quantum Monte Carlo (QDMC) method for the solution of the time-dependent Schrödinger equation for atoms in strong laser fields. Unlike for the normal diffusion Monte Carlo the wave function is represented by walkers with two kinds or colors which solve two coupled and nonlinear diffusion equations. Those diffusion equations are coupled by the potentials similar to those introduced by Shay which must be added to Schrödinger’s equation to obtain classical dynamics equivalent to the quantum mechanics [1]. The potentials are calculated semi-analytically similarly to smoothing methods of smooth particle electrodynamics (SPD) with Gaussian smoothing kernels. We apply this method to strong field two electron ionization of Helium. We calculate two electron double ionization rate in full six-dimensional configuration space quantum mechanically. Comparison with classical mechanics and the low dimensional grid models is also provided. [1] D. Shay, Phys. Rev A 13, 2261 (1976)

Matt Kalinski
Utah State University

Date submitted: 19 Jan 2006

Electronic form version 1.4