

# REAL TIME DIFFUSION MONTE CARLO METHOD (FOR TIME DEPENDENT SCHRÖDINGER EQUATION)

The Schrödinger equation is

$$[-\frac{\partial^2}{\partial x^2} + V(x)]\psi(xt) = \dot{\psi}(xt) \quad (1)$$

It can be rewritten without the need of complex numbers

$$[-\frac{\partial^2}{\partial x^2} + V(x)]\phi_1 = -\dot{\phi}_2 \quad (2)$$

$$[-\frac{\partial^2}{\partial x^2} + V(x)]\phi_2 = \dot{\phi}_1 \quad (3)$$

Those are equivalent to two coupled Hartree-like imaginary time Schrödinger equations we have ones readily solved [1]

$$[-\frac{\partial^2}{\partial x^2} + V(x) + V_{Q1}(x)]\phi_1 = \dot{\phi}_1 \quad (4)$$

$$[-\frac{\partial^2}{\partial x^2} + V(x) + V_{Q2}(x)]\phi_2 = \dot{\phi}_2 \quad (5)$$

$$V_{Q1}(x) = -\gamma(x)\frac{1}{\phi_2}\frac{\partial^2}{\partial x^2}\phi_2 + \frac{1}{\phi_1}\frac{\partial^2}{\partial x^2}\phi_1 + (1/\gamma(x) - 1)V(x) \quad (6)$$

$$V_{Q2}(x) = \frac{1}{\gamma(x)}\frac{1}{\phi_1}\frac{\partial^2}{\partial x^2}\phi_1 + \frac{1}{\phi_2}\frac{\partial^2}{\partial x^2}\phi_2 - (\gamma(x) + 1)V(x) \quad (7)$$

Those can be solved as coupled diffusion equations (Hartree-like) (the standard Monte Carlo Gaussian diffusion) since the coupling potentials are of type of Shay (Hydrodynamical Quantum Potentials) and should be easily calculated with the SPH Gaussian smoothing Kernels [1].

[1] M. Kalinski, J. H. Eberly, J. A. West, and C. R. Stroud, Phys. Rev. A **67** 032503 (2003).