Implementation and application of Vector Hartree-Fock equations in Electron-Nuclear Dynamics theory

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Electron-Nuclear Dynamics (END) [1] is a theory to simulate Molecular Dynamics (MD) computationally, where the evolution of nucleus and electron happen at the same time and without using a potential surface. The ENDyne program [2] implements a first version of END theory, with electrons in a simple determinantal state - only one spin-orbital configuration - and classic nuclei. A possible upgrade of this basic implementation is permit more than one spin-orbital configuration for the same geometry, in other words, electron represented by a multi-determinantal state. For this work will be developed and implemented Verctor Hartree-Fock wave-function, a kind of electronic Complete-Active-Space (CAS) wave function, and with this new implementation will be possible analyze ressonant structures, like ozone.

[1] E. Deumens, A. Diz, H. Taylor, and Y. Öhrn, 1992, *J. Chem. Phys.* **96**, 6820.
[2] E. Deumens, A. Diz, R. Longo, and Y. Öhrn, 1994, *Rev. Mod. Phys.* **66(3)**, 917.