

# Multi-configuration electron-nuclear dynamics: An approach for open-shell systems

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The multi-configuration electron-nuclear dynamics (MCEND) is formulated by a second quantization approach [1]. The mean fields are evaluated from the reduced density matrices. The computations are simplified as compared with those in previous work [2]. A spin-unrestricted approach is derived for open-shell systems. To calibrate the accuracy of the present method, molecular structures, dipole moments, absorption spectra, and von Neumann entropies for light-element diatomic molecules are compared with experimental data and *ab initio* results.

## References

1. *J. Chem. Phys.* **155**, 154103, 2021
2. *Phys. Rev. A* **100**, 023406, 2019