# Symmetry Breaking and Restoration

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Symmetries play a crucial role in electronic structure theory. I will discuss our recent developments regarding the self-consistent variation-after-projection optimization of symmetry-projected wave functions **[1,2]** for number, spin $S^2$ and $S_z$, complex conjugation, point group, and lattice translation. The resulting method yields a comprehensive black-box treatment of static correlation with mean-field computational cost. The ensuing wave function is of high quality multireference character competitive with CASSCF. The method can be applied to excited states and spectral functions **[3]** and has been extended to non-orthogonal multi-references **[4]**. Applications to both molecules and lattice systems will be presented. The curse of the thermodynamic limit and the quest for a low-cost treatment of residual correlations will also be addressed.

[1] Projected quasiparticle theory for molecular electronic structure, G. E. Scuseria, C. A. Jimenez-Hoyos, T. M. Henderson, J. K. Ellis, and K. Samanta, *J. Chem. Phys.* **135**, 124108 (2011).

[2] Projected Hartree-Fock theory, C. A. Jimenez-Hoyos, T. M. Henderson, and G. E. Scuseria, *J. Chem. Phys.* **136**, 164109 (2012).

[3] Symmetry-projected variational approach for ground and excited states of the two-dimensional Hubbard model, R. Rodrıguez-Guzman, K. W. Schmid, C. A. Jimenez-Hoyos, and G. E. Scuseria, *Phys. Rev.* **B 85**, 245130 (2012).

[4] Multi-reference symmetry-projected variational approaches for ground and excited states of the one-dimensional Hubbard model, R. R. Rodríguez-Guzmán, C. A. Jiménez-Hoyos, R. Schutski, and G. E. Scuseria, *Phys. Rev*. **B 87**, 235129 (2013).