

# Keeping Quantum Chemistry Simple: Two Tales

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Complexity is a natural consequence of modern quantum chemistry, both in terms of theory and computational implementation. But, there is still a great deal of merit in heeding the old adage, "Keep it Simple Stupid". Here are presented two case studies in employing simplicity in quantum chemistry. The first is a simple method of treating spin-adaptation in closed-shell systems, as applied to equation-of-motion coupled cluster theory. It is demonstrated that deriving arbitrarily spin-adapted EOM-CC theories even at high levels of excitation can be made simple by utilizing the non-orthogonal spin-adaptation framework and common-sense choices for the amplitude representations. The second is a study in the implementation of tensor contraction, a ubiquitous and critical computational kernel in coupled cluster methods. It is shown that implementing tensor contraction as a trivial tweak on matrix multiplication at a very low level yields a simple to understand, simple to implement, and simple to use (not to mention highly performant) kernel.