Development of multireference coupled-cluster methods from singlestate and multistate bivariational principles

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The bivariational principle due to Arponen and Löwdin [1,2] is a useful reformulation of the Schrödinger equation and a natural foundation for single-reference coupled-cluster theory and state-specific multireference theory [3]. It also provides a framework for mathematical a priori error analysis [4], and is a natural starting point for introducing internal corrections to externally corrected coupled-cluster methods such as tailored coupled-cluster theory using tensor-network states [5, 6]. After discussing the singlestate case, I describe a novel multistate bivariational principle which could be a natural foundation for multistate (state-universal) multireference coupled-cluster methods. I discuss some multireference coupled-cluster approaches that are under investigation inour team.

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