

Flexible Ansatz for N-body Perturbation Theory

Rugwed Lokhande, Pratiksha Balasaheb Gaikwad, David Kim T, Ramón Miranda-Quintana

Quantum theory project, Dept. of Chemistry, University of Florida, Gainesville, FL

We propose a new Perturbation Theory framework that can be used to help with the projective solution of the Schrödinger equation for arbitrary wavefunctions. This Flexible Ansatz for N-body Perturbation Theory (FANPT) is based on our previously proposed Flexible Ansatz for N-body Configuration Interaction (FANCI). We derive recursive FANPT expressions including arbitrary orders in the perturbation hierarchy. We show that the FANPT equations are well-behaved across a wide range of conditions, including static correlation-dominated configurations and highly non-linear wavefunctions.