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Taming Negative Ion Resonances Using Nonlocal Exchange-Correlation Functionals

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Abstract

The characterization of negative ion resonances poses a fundamental challenge to density functional methods due to the unbound nature of resonances. To overcome this challenge, we propose one-particle nonlocal exchange-correlation (xc) potentials combining the exact-exchange (EXX) and the random phase approximation (RPA) correlation potentials. The negative ion resonances are identified by perturbing the real Hermitian nonlocal xc potentials using complex absorbing local potentials. Our studies show that the nonlocal EXX+RPA potential significantly enhances the description of positions and widths of negative ion resonance states compared to potentials that exclude dynamic polarization in RPA or include only EXX. The use of low-scaling algorithms simplifies the computation of the RPA potential, thereby providing a practical solution for resonance-state characterization within the density functional framework. A theoretical framework and the underlying assumptions required for combining real Hermitian nonlocal xc potentials with complex local potentials are discussed.