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Universal extension to the Becke-Johnson exchange potential ESA RASANEN, Nanoscience Center, Department of Physics, University of Jyvaskyla, Finland, STEFANO PITTALIS, Department of Physics and Astronomy, University of Missouri, Columbia, USA, CESAR PROETTO, Institut fur Theoretische Physik, Freie Universitat Berlin, Germany — The Becke-Johnson exchange potential [J. Chem. Phys. **124**, 221101 (2006)] has been successfully used in electronic structure calculations within density-functional theory. However, in its original form the potential may dramatically fail in systems with non-Coulombic external potentials, or in the presence of external electric or magnetic fields. Here we present a system-independent extension to the Becke-Johnson approximation by (i) enforcing its gauge-invariance and (ii) making it exact for any single-electron system. The resulting approximation is then better designed to deal with current-carrying states, and recovers the correct asymptotic behavior for systems with arbitrary number of electrons. Our approximation is shown to give very good results for atoms, atomic chains, and molecules with and without external electric or magnetic fields.

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