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Linked-cluster formulation of screened electron-hole interaction from explicitly-correlated geminal functions without using unoccupied states ARINDAM CHAKRABORTY, Syracuse Univ, MICHAEL BAYNE, Department of Chemistry, Syracuse Univ — The accurate determination of the electron-hole interaction kernel remains a significant challenge for precise calculations of optical properties in the GW+BSE formalism. The inclusion of unoccupied states has long been recognized as the leading computational bottleneck that limits the application of this approach for large finite systems. In this work, we present an alternative derivation that avoids using unoccupied states to construct the electron-hole interaction kernel. The central idea of our approach is to use explicitly correlated geminal functions for treating electron-electron correlation for both ground and excited state wave functions. We demonstrate with diagrammatic techniques that the frequency-dependent electron-hole kernel can be expressed in terms of connected closed-loop diagrams. We show that the cancelation of disconnected diagrams is a consequence of the linked-cluster theorem in real-space representation and the resulting renormalized operators are equivalent to infinite-order summations of particle-hole diagrams. The derived electron-hole interaction kernel was used to calculate excitation energies in atoms, molecules, clusters and quantum dots and the results for these systems were compared with CIS, TDHF, TDDFT, EOM-CCSD, and GW+BSE calculations.

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