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Iterative diagonalization of non-Hermitian eigenproblems in time-dependent density-functional and many-body perturbation theory[1] ZHAOJUN BAI, DARIO ROCCA, UC Davis, REN-CANG LI, UT Arlington, GIULIA GALLI, UC Davis — We present a technique for the iterative diagonalization of random-phase approximation (RPA) matrices, which are encountered in the framework of time-dependent density-functional theory (TDDFT) and in the solution of the Bethe-Salpeter equation (BSE) [1]. The non-Hermitian character of these matrices does not permit a straightforward application of standard iterative techniques used, i.e., for the diagonalization of ground state Hamiltonians. We first introduce a new block variational principle for RPA matrices. We then develop an algorithm for the simultaneous calculation of multiple eigenvalues and eigenvectors, with convergence and stability properties similar to techniques used to iteratively diagonalize Hermitian matrices. The algorithm is validated by computing multiple low-lying excitation energies of molecules at both the TDDFT and BSE level.

[1] D. Rocca, Z. Bai, R.-C. Li, and G. Galli, submitted to J. Chem. Phys.

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