Electronic Excitations in Strong Magnetic Fields

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The London program is a code designed for solving quantum chemical problems involving molecules in very strong magnetic fields. Magnetic properties are determined non-perturbatively, and associated gauge-origin problems are avoided by employing London orbitals instead of the traditional Gaussian orbitals commonly used.

In this work, a solver for determining electronic excitation energies in the Random Phase Approximation (RPA) has been implemented in the London code, applicable to restricted, unrestricted and generalized Hartree–Fock wave functions. The RPA generalized eigenvalue problem is solved in the atomic orbital basis using a subspace-accelerated iterative procedure that yields excitation energies and corresponding excitation operator matrices. From these matrices associated transition properties are calculated.

Some illustrative applications of the code are presented, focusing on basis set convergence of transition and excited state properties with London orbitals compared to Gaussian orbitals.