Advances in many-body perturbation and Green's function theories

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We present three new advances made in the diagrammatic and size-consistent formalisms of many-body perturbation (MBPT) and Green's function (MBGF) theories:

Monte Carlo MBPT (with Soohaeng Willow). With a Laplace transform, we convert the canonical expressions of MBPT and explicitly correlated MBPT into sums of a few high-dimensional dimensional integrals, which are then evaluated by highly scalable Monte Carlo integration. Good weight functions for importance sampling are identified that are analytically integrable, are finite and nonnegative everywhere, and share the same singularities as the integrands. This stochastic algorithm does away with the integral transformation as the hotspot of the conventional algorithm, displays near linear size dependence of cost per Monte Carlo step even for small molecules, and does not suffer from the fermion sign problem. It can also compute correlation corrections to the self-energies (i.e., quasiparticle energy bands in the entire Brillouin zone) directly for molecules and solids and not as small differences between two large, noisy quantities.

Finite-temperature MBPT (with Xiao He). In 1960, Kohn and Luttinger showed that the textbook finite-temperature extension of MBPT(2) had the incorrect zero-temperature limit in a metal and, on this basis, argued that the theory was incorrect. We show that this arises from the noninclusion of temperature effects in the energies of the zeroth-order eigenstates, which also causes another inconsistency, namely, the different rate of divergence of the correlation energy in a metal. We propose a renormalized finite-temperature MBPT(2) derivable from thermal Wick's theorem and show that this new formalism has the correct zero-temperature limit and the same rate of divergence in a metal as the zero-temperature counterpart. We apply both the conventional and new finite-temperature MBPT(2) as well as finite-temperature Hartree–Fock theory to the Peierls and charge-density-wave transitions in one-dimensional solids.

General-order MBGF (with Matt Hermes, Jack Simons, and Vince Ortiz). We introduce a determinant-based, general-order algorithm of MBGF and present the nth-order self-energies of small molecules up to n=30. Here, the nth-order "self-energy" is defined as the difference in the MBPT(n) energy between the neutral and ionized (electron-attached) species expanded by the same set of orbitals. They are found to show the following fascinating behavior: The self-energies up to n=3 are found to agree with those in the frequency-independent, diagonal approximation, but as $n \to \infty$, they converge at the exact self-energies, which are frequency-dependent and non-diagonal. We present a diagrammatic analysis at low n to argue that the frequency dependence and off-diagonal elements of the self-energy are included via the disconnected (but linked) diagrams and semi-reducible diagrams, respectively.