A direct approach to the calculation of many-body Green' s functions

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Many-body perturbation theory is a powerful approach to understand and predict many properties of materials. However, sometimes low-order perturbation expressions for the self-energy, like the GW approximation [1] and related approaches, are not sufficient. For example, satellite structure beyond the quasi-particle peaks in the spectral function is often not well described in GW, and in the case of strong coupling, where the quasi-particle picture is no longer adequate, other approaches are needed. We explore an alternative route to the calculation of interacting electron Green's functions. It is based on a set of functional differential equations relating the one-body Greens function to its functional derivative with respect to an external perturbing potential [2]. This set of equations can be used to generate the perturbation series. Here we will show that working directly with the differential equations, instead of some low order approximation to the solution, yields precious insight concerning fundamental questions, guidelines for practical calculations, and methods that lead to an improved description of spectra and total energies. Results will be illustrated on various levels of approximation, ranging from simple models [3] to full ab inito calculations [4].

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