

Failures of the Feynman–Dyson diagrammatic perturbation expansion of one-particle many-body Green’s function

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In many areas of physics, the dynamics of many interacting particles is described graphically and compellingly by Feynman diagrams. These diagrams denote perturbation corrections to a mean-field theory adopted as the zeroth-order description. Hence, a diagram consists of vertexes, designating interactions, and of edges, each describing the propagation of a mean-field particle or hole from one spacetime position to another. Mathematically, the propagator is written as a time-ordered Green’s function of the Schrödinger equation in the case of quantum chemistry.

In this talk, using a general-order many-body Green's-function method for molecules [1], I will numerically illustrate three pathological behaviors of the Feynman–Dyson diagrammatic perturbation expansion of one-particle many-body Green's functions as electron propagators [2].

(1) The perturbation expansion of the frequency-dependent self-energy is nonconvergent at the exact self-energy in many frequency domains. (2) The Dyson equation with an odd-order self-energy has a qualitatively wrong shape and, as a result, most of their satellite roots are complex and nonphysical. (3) The Dyson equation with an even-order self-energy has an exponentially increasing number of roots as the perturbation order is raised, which quickly exceeds the correct number of roots. (4) Infinite partial summation of diagrams by vertex or edge modification exacerbates these problems.

Not only does the nonconvergence render higher-order perturbation theories useless for satellite roots, but it also makes it impossible to use higher-than-second-order Green’s-function method in the ansätze requiring the knowledge of all poles and residues. Such ansätze include the Galitskii–Migdal identity, self-consistent Green's-function methods, Luttinger–Ward functional, and some models of the algebraic diagrammatic construction.

More importantly, this pathology calls into question the validity or at least the robustness of the Feynman–Dyson diagrammatic perturbation theory as the principal mathematical foundation of quantum field theory, which has dominated much of modern physics, ranging from quantum chemistry to solid state physics to quantum electrodynamics to nuclear physics.

[1] S. Hirata, A. E. Doran, P. J. Knowles, and J. V. Ortiz, *J. Chem. Phys.* **147**, 044108 (2017).

[2] S. Hirata, I. Grabowski, and R. J. Bartlett, arXiv:2312.03157 (2023).