Thermodynamically consistent conserving approximations for correlated electrons: Feynman and Schwinger approaches combined

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Strong electron correlations lead to emerging low-temperature macroscopic phenomena in solids that can be explained only via microscopic quantum laws. The most famous are itinerant metallic magnetism and superconductivity. The generic microscopic models for these phenomena were introduced a long time ago, but their full solution remains unavailable. Hence, approximations must be employed. Presently, there are two approaches with which one can reach a non-perturbative microscopic description of strongly correlated electrons. One is based on renormalizations of the perturbation expansion of the thermodynamic functional and/or of Green functions (Feynman). The other relies on the exact equations for Green functions and relations between their different types (Schwinger). The former approach leads to explicit representations of thermodynamic and dynamic quantities but does not guarantee thermodynamic consistency. The latter construction obeys all consistency restrictions but does not tell us how to preserve them in approximate solutions.

Approximate solutions cannot guarantee all exact relations but reliable ones must be conserving and preserve thermodynamic consistency. The way to derive conserving approximations of interacting quantum particles was introduced within the Feynman theory by Baym and Kadanoff [1, 2]. This construction gives recipes on how to construct thermodynamic quantities, including thermodynamic potential, so that macroscopic conservation laws are obeyed. What is, however, not guaranteed is thermodynamic consistency between the critical behavior of the conserving response functions (susceptibility) and the dynamical and thermal ones (heat capacity). It is a consequence of the general inability of approximate solutions to match the conserving vertex of the Feynman construction with the dynamical vertex from the Schwinger theory [3]. Matching of the ordered and disordered phases at the critical points then fails, the application of the renormalization group on the critical behavior is impeded, and the scaling relations between the critical exponents do not hold.

We recently opened a new path towards the construction of thermodynamically consistent approximations of the critical behavior and phase transitions of strongly correlated electrons by combining the Schwinger equations for the Green functions with the input from the Feynman diagrammatic approach [4, 5]. The fundamental idea is to use the diagrammatic input for the two-particle irreducible vertex functions from the Bethe-Salpeter equations with a critical behavior instead of the one-particle self-energy of the Baym-Kadanoff scheme. We use the exact relations between the one-particle and two-particle Green functions from the Schwinger theory to obtain the self-energy that is split into two parts according to the symmetry-breaking field responsible for the critical behavior. The even self-energy, controlling quantum dynamics, is determined from the two-particle irreducible vertex from the Schwinger-Dyson equation, while the odd self-energy, the quantum analog of the order parameter, is obtained from the critical Bethe-Salpeter equation and the linearized Ward identity.

Knowing the self-energy is not enough to guarantee thermodynamic consistency. The thermodynamic, Luttinger-Ward functional must be the ultimate result of the consistent approximations. We presently focus on constructing the Luttinger-Ward functional from the generating two-particle irreducible vertex. It is done so that the conserving vertex of the Baym-Kadanoff construction coincides with the dynamical one from the Schwinger-Dyson equation inducing the critical behavior of the heat capacity. To achieve this goal, supplementary and compensating terms, not derived from the diagrammatic expansion, must be added to the thermodynamic functional. In this way, the ordered phase is properly attached to the disordered phase at the critical point, and the two-particle irreducible vertex derived from the thermodynamic functional in the Schwinger theory equals the one from the Feynam diagrammatic construction.

The new scheme of constructing thermodynamically consistent conserving approximations with unrestricted quantum dynamics offers excellent possibilities to make tangible progress in quantum many-body theory. It significantly improves the existing approximate schemes with various levels of self-consistency and sets the description and understanding of quantum critical behavior on a qualitatively higher level. The benefits are: first, it is the extension of the self-consistent approximations into the magnetically ordered and superconducting phases; second, it is the possibility to include the full two-particle vertex renormalization in the thermodynamically consistent description of quantum criticality such as the Kondo effect whereby both magnetic and thermal fluctuations are treated on the same footing and display the same critical behavior; third, it allows us to go beyond the dynamical mean-field theory and to describe with affordable computational means quantum critical behavior in low-spatial dimensions where static long-range order is realizable only at zero temperature and is forbidden above absolute zero. And finally, the achieved thermodynamic consistency opens the way to the application of the renormalization group technique to the quantum-critical behavior of correlated electrons.

The project is open and suitable for Ph.D. students as well as for post-doctoral young researchers. The prerequisites for becoming an active and useful member of this project are a good knowledge of quantum mechanics, statistical and many-body physics, complex and functional analysis, proficiency in scientific programming, and experience with coding large-scale program packages.

The benefits for the participants in this project are being involved in the forefront research of the basic microscopic quantum origins of the observable macroscopic phenomena, understanding the role of strong electron correlations in forming low-temperature dynamical and thermodynamic properties of solids, and learning modern non-perturbative methods of quantum many-body theory.

Bibliography

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