M2 project: Combining the correlation channels of many-body perturbation theory

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Many-body Green's function methods are a set of powerful theoretical techniques used in condensed matter physics and quantum chemistry to study the behavior of interacting particles in a many-body system [2]. These methods are based on the concept of Green's functions, which are mathematical objects that describe the propagation of one or more quantum particles. In many-body perturbation theory, Green's functions are used to describe the response of a quantum system to external perturbations, and they provide a way to compute various physical observables.

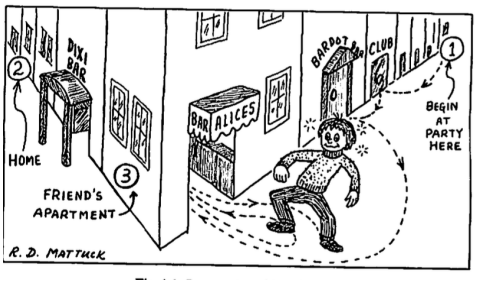

Figure 1: Concept of propagation [1].

The quasiparticle picture is the central concept of many-body perturbation theory as it provides a means to understand the behavior of electrons within a material or a molecule. It emerges as an effective mapping from the complex many-body system to a simplified effective one-body system. Within the quasiparticle framework, the effects of collective excitations are incorporated by adding a dynamical correction to an effective one-body operator obtained from a simpler system.

Different effective mappings, based on so-called correlation channels, do exist in many-body perturbation theory and each of them corresponds to an elegant resummation of Feynman diagrams [3–7]. For example, the well-known GW method corresponds to the infinite summation of bubble diagrams while the T-matrix approximation sums separately particle-particle and electron-hole ladder diagrams up to infinity [1]. Advanced methods, like FLEX (Fluctuation Exchange Approximation) and parquet [8], are employed in condensed matter physics to study strongly correlated electron systems, where traditional perturbation theory approaches break down. They provide a way to simultaneously consider different correlation channels and offer a more complete understanding of the electronic structure and response properties of materials.

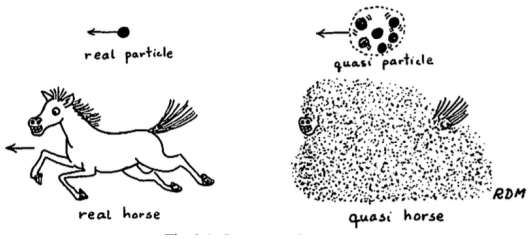

Figure 2: Concept of quasiparticle [1].

This project aims to investigate the combination of these correlation channels via approximation schemes such as FLEX and parquet, and to apply them to realistic molecular systems. Specifically, the project consists of the formulation of relevant equations and their subsequent implementation, followed by rigorous testing through computational calculations applied to molecular systems. **As an extension of this Master's project, a three-year PhD scholarship is available within our research group, allowing for the continuation of this research project.** The candidate should have a solid background in Physics and Mathematics and it is desirable that he/she is familiar with electronic structure theory.

This project is supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 863481)

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