Laboratoire des Solides Irradiés, UMR 7642

Soutenance de thèse

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Amphi Becquerel - 10h00

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THEORY OF ELECTRON SPECTROSCOPY BEYOND THE STATE-OF-THE-ART

An improved description of fermion-plasmon coupling in Green's function calculations

The topic of this thesis is situated in the framework of theoretical spectroscopy. In particular, I propose a new ab-initio derivation to find approximations for the one-body Green's function (GF). This approach leads to an improved description of fermion-plasmon coupling in the framework of many-body perturbation theory (MBPT), which can be used to study direct and inverse photoemission spectroscopy. Although the observed phenomena have been well known before, my formulation yields a better description than previous state-of-the-art approaches. It answers several open questions, cures some fundamental shortcomings and suggests a way for systematic improvement.

In photoemission spectroscopy, a sample is irradiated by photons and electrons are emitted. From the energy difference of the incoming photon and outgoing electron, a great deal of information on the properties of the sample can be obtained, e.g. the band structures or lifetimes of excitations. In an independent-particle picture, this energy difference corresponds to the one-particle energy level that the emitted electron was occupying before the measurement. This leads to a sharp peak in the spectrum, with weight normalized to one. In reality, photoemission is not just photons in and independent electrons out, because the sample is an interacting many-body system. The Coulomb interaction and the anti-symmetric nature of fermions give rise to the so-called exchange correlation effects, which makes the problem fundamentally difficult to solve. The description, understanding and prediction of the effects of the Coulomb interaction on the properties of materials has been one of the big challenges of theoretical condensed matter physics for ages. In the framework of this thesis one can imagine that first, the photoemission creates a hole (i.e., a missing electron) in the sample, which causes all remaining electrons to relax. Due to the attractive interaction between positively charged holes and negatively charged electrons, the electrons move towards to the holes and dress them to create "quasi-particles". The effective interaction between quasi-particles is the dynamically screened Coulomb interaction. It is in general weaker than the bare Coulomb interaction. Consequently, the observed band structure is a quasi-particle band structure, which differs from the result of an independent-particles band structure calculation. Second, when the hole propagates in the sample the remaining electrons can show collective oscillations, the density response to the perturbation. These are neutral excitations with approximately bosonic nature, because they are constituted by pairs of fermions. The coupling of the hole to the neutral excitations leads to additional structures in the photoemission spectrum, called satellites. This reduces the quasi-particle weight that is now fractional. Most often, the dominant satellites are due to plasmons, collective long-range oscillations, but one can also observe interband transitions or excitons, or other satellites that are due to more complicated couplings.

This overview shows that in order to have a good description of photoemission spectroscopy, we should study the propagation of particles, as well as the interaction between particles and plasmonsor other excitations. The Green's function gives the probability amplitude of particles propagating from one point to another. Its imaginary part yields the spectral function that has a direct link to the spectrum measured in a photoemission experiment. The derivations and approximations proposed in this thesis give a new way to calculate the Green's function, which improves the description of photoemission spectroscopy. Moreover, it gives access to other quantities that can be obtained from the one-body Green's function, in particular total energies.