SOUTENANCE DE THESE

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Towards an improved description of spectroscopies for materials with localized electrons: Effective potentials and interactions

Spectroscopic measurements are often used to get information about many properties of materials. Since their interpretation can be difficult, theory plays an important role for analysis and predictions. In a theoretical description a major challenge is to capture the many-body effects. One way to formulate the problem is in terms of screening, by introducing the screened Coulomb interaction W. Common approximations treat screening in low-order perturbation theory and in the linear response approximation; such examples are the GW approximation and cumulant expansions [1, 2].

These methods (GW, cumulant) work often well for metallic and semiconducting systems with delocalized electrons, while for systems with localized electrons there is room for improvement. When electrons are localized, and when they have small overlap with other electrons, their potential can be captured in a classical description. For example, in the photoemission of a localized electron screening enters through the response of the density of the other electrons. In this case,the removal of an electron might be a strong perturbation to the system and non-linear effects need to be taken into account in the screened interaction.

In my presentation I will discuss the framework of approximations for systems with localized electrons and present a formulation of many-body perturbation theory where the screened interaction can be obtained from Time-Dependent Density-Functional Theory (TDDFT). In this formulation the first point that I will discuss is the solution of the Kadanoff-Baym equation, for a coreelectron, which yields a cumulant where non-linear screening appears explicitly. The second point that I will discuss is a vertex correction to Hedin's GW approximation, which goes beyond the simple approximations derived from Time-Dependent Density-Functional Theory (TDDFT) [3] and leads to non-locality corrections to photoemission spectra.

References

[1] L. Hedin. Phys. Rev., 139:A796–A823, Aug 1965.

[2] F. Aryasetiawan, L. Hedin, and K. Karlsson. Phys. Rev. Lett., 77:2268–2271, Sep 1996; M. Guzzo et al. Phys. Rev. Lett., 107:166401, Oct 2011; J. Sky Zhou et al. The Journal of Chemical Physics, 143(4):109, 2015.

[3] R. Del Sole, L. Reining, and R. W. Godby. Phys. Rev. B, 49:8024–8028, Mar 1994.

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