Freie Universität Berlin

Colloquium
Dahlem Center for Complex Quantum Systems

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On the response of large systems to electrostatic fields

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Abstract:

The fact that materials respond in a characteristic way to external electromagnetic fields forms the basis of a large variety of spectroscopic methods for characterizing the materials. Moreover, the responses can also be exploited in different technological applications. In both cases, a detailed understanding and description of the interactions between the fields and the materials are mandatory. It may therefore surprise that even the simple case of an electrostatic field interacting with an extended system poses a number of fundamental theoretical, conceptual, and methodological challenges that only partially have been met satisfactorily.

In this presentation, the challenges related to the treatment of extended systems exposed to an electrostatic field are discussed. Subsequently, the basic principles behind a theoretical method for treating infinite, periodic systems exposed to an external electrostatic field are outlined. The approach, that can be derived through different approaches, including the vector-potential description of the external field, leads to single-particle Hartree-Fock or Kohn-Sham equations that differ from the field-free counterparts in several aspects. In particular, solving them is only possible through a careful so-called smoothing procedure. In that case it is possible to derive a numerically stable and efficient approach that, moreover, allow for an automatic structure optimization in the presence of the field. Results of model studies for quasi-one-dimensional systems are reported in order to illustrate the approach. A surprising outcome is that the surfaces (terminations) have a definite effect on the responses, although these can be included in the infinite-system calculations. Finally, extensions and open issues are briefly discussed.