Numerical Methods for Correlated Electrons

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Electron correlation physics has two aspects: the extent to which the ground state wave function is significantly different from the single Slater determinant that characterizes the non-interacting many-electron wave function, and the extent to which the frequency dependence of the electron spectral function deviates significantly from the single delta function characteristic of non-interacting particles. Similarly, methods for dealing with correlated electron problems may be crudely divided into those designed to capture ground state properties (especially the energy) and those primarily aimed at calculating excitations.

A taxonomy of correlated electron systems is:

1. Approximately free electrons. Here the key physics is the long-ranged part of the Coulomb interaction and the essential parameter is r_S, roughly the inter-electron distance expressed in units of the effective Bohr radius For $r_S \lesssim 1$ (very high density) the interactions may be treated perturbatively; typical wide-band metals have $2 \lesssim r_S \lesssim 6$ and the Wigner crystallization transition occurring at an $r_S \sim 30 - 80$ (with the range depending on dimensionality). The Dirac dispersion means graphene presents a special case.

2. Materials with partially filled but strongly localized (tight-binding-like) orbitals (transition metal oxides, sulfides, pncitides), rare earth and actinide compounds, certain organic conductors. Here the key role is played by short ranged (intra-orbital) interactions and the physics is driven by suppression of certain electronic configurations of the localized orbitals and concomitant enhancement of the importance of emergent, typically slowly fluctuating degrees of freedom such as electron spins. We further distinguish

   (a) Mott-Hubbard systems, where the key physics is Coulomb blockade (suppression of charge configurations by an on-site density-density repulsion U) and correlation effects are maximized when the density of electrons is high (d-shells with nearly integer filling).

   (b) Charge-transfer systems (mainly oxides comprising first-row transition metals), where the physics is controlled by the energy difference between ligand states and transition metal d-levels

(c) 'Hunds metals' where the physics is controlled by states of very high total spin with slowly fluctuating local moments. This correlation effect is not tied to the proximity to a Mott transition.

3. Heavy fermions, where the physics is of a broad band of weakly correlated electrons coupled to local moments

4. Special cases, including the quantized Hall states, one dimensional (spin chain and Luttinger liquid) materials, and quantum impurity models (a fininte number of interacting degrees of freedom coupled to a non-interacting band of states).

Density functional theory is both an algorithm (in principle exact, in practice approximate) for computing the ground state energy and charge distribution and an approximation (with no formal status at all) to the ground state wave function as a Slater determinant of Kohn-Sham eigenfunctions and to excitation energies (as differences of Kohn-Sham eigenvalues) and matrix elements (as overlaps of operators and Kohn-Sham eigenfunctions). In the physics community, discussions of failures of density functional theory often focus on the eigenstates. Here I present two examples where DFT gives substantially incorrect energy differences and structures, as well as a quantitatively incorrect electronic excitation spectrum: a 'spin crossover molecule' [Jia Chen, C. Marianetti and A. J. Millis, Phys. Rev. **B91** 241111 (2015)] and the rare earth nickelates [Hyowon Park, Andrew J. Millis, Chris A. Marianetti, Phys. Rev. **B89**, 245133 (2014); Hyowon Park, Andrew J. Millis, Chris A. Marianetti, Phys. Rev. **B90**, 235103 (2014) and E. A. Nowadnick, J. P. Ruf, H. Park, P. D. C. King, D. G. Schlom, K. M. Shen, A. J. Millis, Phys. Rev. **B92**, 245109 (2015)].

Improvements to density functional theory may be viewed as quantum embedding algorithms, in which a subset of orbitals and matrix elements are treated by an exact many-body method, while the other degrees of freedom are treated by density functional theory. Embedding methods include dynamical mean field theory [Antoine Georges, Gabriel Kotliar, Werner Krauth and Marcelo Rozenberg, Rev Mod Phys **68** 13 (1996)] (DFT +U is just the Hartree approximation to this), Density Matrix Embedding theory [G. Knizia and G. Chan, Phys. Rev. Lett. **109** 106484 (2012)] and Self Energy Embedding Theory [T. N. Land, A. A. Kananenka and D. Zgid, J. Chem Phys. **143** 241102 (2015)]. The formalism and physics associated with embedding, in particular the physics of the "double counting correction" will be discussed.

A brief discussion of the ideas behind the different ideas for solution of quantum many body models will be given, including wave function methods such as CI and its generalizations and DMRG/matrix product methods and the different Monte Carlo approaches, in particular diagrammatic Monte Carlo and FCI-QMC. Looking toward the future the importance of benchmarking and comparison of different algorithms is stressed (with examples from the Simons Foundation Hubbard benchmarking project) and also the need for developing the methods needed to manage the large computational overhead of realistic interaction matrix elements and orbitals.