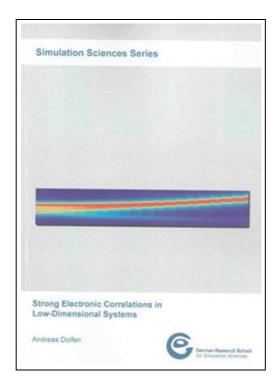
Strong Electronic Correlations in Low-Dimensional Systems



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Reviews

Very beneficial to all category of folks. We have study and that i am sure that i will planning to go through yet again again in the future. Its been printed in an extremely straightforward way in fact it is just soon after i finished reading this pdf where actually changed me, alter the way i really believe.

(Emmett Mann)

STRONG ELECTRONIC CORRELATIONS IN LOW-DIMENSIONAL SYSTEMS



Shaker Verlag Mai 2011, 2011. Buch. Condition: Neu. Neuware - Understanding strongly correlated systems is one of the most challenging problems of physics. Their properties often sensitively depend on the delicate interplay of kinetic and Coulomb energy rendering them susceptible to external perturbations. To understand and predict experimental results we need methods to reliably describe these materials. In this thesis we tackled the problem from two different perspectives: the construction of appropriate models and the evaluation of dynamical lattice response functions. At first we derive realistic material-specific Hubbard model parameters for organic crystals. We extract the simplest parameters, the hopping integrals t, from the bonding/anti-bonding splitting of the relevant orbitals in a tight-binding dimer. The main challenge is the proper evaluation of the screening for the Coulomb integrals, which we tackle with a three-step approach. At first we calculate the Hartree-integrals. To assess the screening of the electrons within the molecules alone we calculate DFT total energies for additional charges in the molecules. The orbital relaxation effect in the self-consistent calculation yields the screening energy. The final step captures the effect of all molecules. With a quantum mechanical treatment being infeasible we resort to a classical electrostatic method which effectively describes a non-polar molecular crystal in terms of a microscopic point-dipole model. We apply this method to two organic crystals: TTF-TCNQ and (BEDT-TTF)_2 I_3. Having the parameters of the former we solve a long standing problem in the interpretation of its spectra. One of the most successful methods to treat strongly correlated systems is DMFT. It provides a good approximation to local correlations and direct access to quantities such as the local self-energy. While lattice spectral functions follow directly from the self-energy, general lattice susceptibilities are difficult to obtain. To make the evaluation feasible we rewrit



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