Une nouvelle approche pour la détermination des fonctionnalités statiques et dynamiques des systèmes d'électrons fortement corrélés

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Abstract

In this work, a specific instance of a slave boson representation—originally introduced in the context of the Hubbard model by Kotliar and Ruckenstein—is put to use to investigate the effect of electronic interactions on two classes of properties of condensed matter systems described by extended Hubbard models. In the first place, an original extension to the Hubbard model, entailing a spatially modulated single-particle potential along with nearest-neighbour electronic interactions, is introduced. Its static properties, namely the competing ground states in its zero-temperature phase diagram, as well as its quasiparticles band structure, are investigated at half filling by means of a saddle-point approximation to the Kotliar-Ruckenstein representation. A competition between two symmetry broken phases, both featuring a checkerboard charge order, and distinguished by the presence or absence of a Néel ordering of the spins, is evidenced. Strongly discontinuous transitions are revealed by an analysis of the relevant order parameters at all coupling scales. Coexistence between both phases, with one phase slightly higher in energy than the ground state, is found in large regions of the parameter space. The band structure of the phases, and more precisely the sizable difference in their band gap, is analyzed, putting forward possible applications of putative experimental realizations of the model as candidate functional materials. In the second place, a Hubbard model, extended by long range Coulomb interactions between electrons, is analyzed by means of an alternative form of the Kotliar-Ruckenstein representation. An instance of dynamical property, namely the model’s zero-temperature charge excitation spectrum, is computed in the form of the electron energy loss function. Specifically, Gaussian fluctuations of the slave boson fields around the paramagnetic saddle-point of the alternative representation are calculated, ultimately allowing for a derivation of an analytical formula for the dynamical charge susceptibility, and thus for the loss function as well as the optical conductivity. The spectrum, generically comprising a particle-hole excitation continuum as well as two collective modes, the plasmon and a signature of the upper Hubbard band, is then compared with standard random phase approximation in order to evidence strong correlation features. Focus is put on the plasma frequency, the energy of the plasmon mode at long wavelengths, emphasizing lattice effects as well as the relevance of the interaction-driven renormalization of the inverse effective mass.