On the existence and nature of the excitonic insulator phase in the extended Falicov-Kimball model

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We act on the suggestion that an excitonic insulator (EI) state might separate — at very low critical temperatures — a semimetal (SM) from a semiconductor (SC) and ask for the nature of these transitions. Thereby the EI constitutes an exciton condensate in equilibrium. To analyze the EI instability, triggered by the Coulomb interaction between conduction band electrons and valence band holes, we study the half-filled Falicov-Kimball model extended by a finite f-bandwidth, by means of various analytical and numerical methods. For the 1D extended Falicov-Kimball model, we present exact DMRG results for the ground-state phase diagram and show that the criticality of the EI state with power-law correlations shows up in the von Neumann entropy [1]. In 3D, the momentum-resolved exciton numbers clearly reveal the BCS-like mechanism at the SM-EI transition, whereas at the SC-EI transition a Bose-Einstein condensation (BEC) of preformed electron-hole pairs occurs [2]. Thus, the composite nature of the excitons is of vital importance. We furthermore calculate the bound-state fractions and the exciton density to characterize the composition of the normal phase and to identify the so-called halo phase (surrounding the EI above the critical temperature), which realizes a three-component plasma consisting of electrons, holes, and excitons. The coherence length and the single-particle spectral functions show the continuous crossover from a BCS- to a BEC-type pairing by tuning the Coulomb attraction within the EI phase. The precursor of this crossover in the normal phase might cause the transport anomalies observed in several mixed-valence compounds. We also comment on spontaneous coherence in double-layer exciton systems [3].

References

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