Thermodynamics of the generalized spin-one-half Falicov-Kimball model in two dimensions

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9.7 cm

The extrapolation of small-cluster exact-diagonalization calculations and the Monte-Carlo method is used to study the spin-one-half Falicov-Kimball model extended by the spin-dependent Coulomb interaction (J) between the localized f and itinerant d electrons as well as the on-site Coulomb interaction (U_{ff}) between the localized f electrons. It is shown that in the symmetric case, when the chemical potential μ equals to U (where U is the spin-independent on-site Coulomb interaction between the f and d electrons) the ground-state phase diagram of the model has an extremely simple structure that consists of only two phases, and namely, the charge-density-wave (CDW) phase (with local f-electron pairs on one of the two sublattices of a bipartite lattice) and the spin-density-wave (SDW) phase. The nonzero temperature studies of the specific heat showed that these phases persist also at finite temperatures. The critical temperature T_c for a transition from the low-temperature ordered phases to the high-temperature disordered one is calculated numerically for various values of J and U_{ff}. It was found that in the CDW area the maximum value of the critical temperature is for $J = 0$ and in the SDW area for $J \sim U$.

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