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Superconductivity, Charge Density Wave and Charge Kondo States in Systems of Coexisting Itinerant Electrons and Local Pairs

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The properties of a system of coexisting local pairs and itinerant electrons described by the (hard-core) boson–fermion model are discussed. For the first time we include into analysis of the model not only the superconducting and non-ordered (normal) states but also the charge density wave phases as well as the so-called charge Kondo state. Within an extended mean-field approximation, a mutual stability of charge density wave, superconducting and charge Kondo states are determined at $T = 0$ in the case of half-filled fermionic and bosonic bands.

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1. Introduction

The purpose of the present paper is analysis of the phase diagrams and electron orderings of a system of coexisting local electron pairs and itinerant electrons described by the (hard-core) boson–fermion model. The Hamiltonian of itinerant c electrons and the d electrons creating local pairs (LP) has the form

$$\hat{H} = \sum_i \Delta_0 n_i^d + \sum_{\langle ij\rangle\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + I_0 \sum_i (c_{i\uparrow}^+ c_{i\downarrow}^+ \rho_{id}^- + \mathrm{h.c.}) + \frac{1}{2} V_0 \sum_i n_i^d n_i^c. \quad (1)$$

The model takes into account both the intersubsystem charge coupling I_0 as well as the density–density interaction V_0, $n_i^c = n_{i\uparrow}^c + n_{i\downarrow}^c$, $n_i^d = n_{i\uparrow}^d + n_{i\downarrow}^d$, a total number of particles per site is $n = n_c + n_d = (\sum_i \langle n_i^c\rangle + \sum_i \langle n_i^d\rangle)/N$. $\Delta_0 - D$ measures the relative position of the LP level with respect to the bottom of c-electron band, $2D = 2zt$ is the band width of c-electron band in the absence of interactions, z is the number of nearest neighbours (nn). The Hamiltonian (1) is defined in the subspace excluding single occupancy of sites by d electrons. In this subspace the charge operators $\{\boldsymbol{\rho}_{id}\}$, defined by $\rho_{id}^+ = d_{i\uparrow}^+ d_{i\downarrow}^+ = (\rho_{id}^-)^+$, $\rho_{id}^z = \frac{1}{2}(n_{id} - 1)$, obey the Pauli spin $\frac{1}{2}$ commutation relations and the following relations are fulfilled:

$$n_{i\uparrow}^{d} n_{i\downarrow}^{d} = \rho_{id}^{z} + \frac{1}{2}, \quad \left(n_{i\uparrow}^{d} - n_{i\downarrow}^{d}\right)^{2} = 0.$$

Up to now the studies of the model have been concentrated on the superconducting (SC) and non-ordered (normal) phases [1–5]. We extend the previous investigation and include into the analysis the charge density wave (CDW) phases as well as the so-called charge Kondo state (CKS). The CKS being an analogue of the magnetic Kondo state in the systems of the periodic Kondo lattice is characterized by a compensation of a local charge moment (isospin singlet) [1, 4–6]. One finds that such a state can be realized in the present model if the intersubsystem charge exchange interaction is increased, and it can compete with SC and CDW orderings.

We have performed a detailed analysis of the phase diagrams and thermodynamic properties of the model (1) for d-dimensional hypercubic lattices and arbitrary, positive and negative I_0 and V_0 [6]. In the analysis we have used an extended mean-field approximation (MFA-HFA), analogous to that used in the treatment of the Kondo lattice model [7, 8]. Below we only quote the main results of this investigation, concentrating on the case of half-filled bands: $n_c = n_d = 1$ which is realized for $n = 2$ and $\Delta_0 = 0$. We will restrict our analysis to the pure phases and assume rectangular density of states (DOS) for c-electron band.

Definitions of the phases considered and the corresponding order parameters are the following:

superconducting phase (SC) $\rho_0^x \neq 0,\ x_0 \neq 0$, where

$$\rho_0^x = \frac{1}{2N}\sum_i \left\langle \rho_{id}^{+} \right\rangle \text{ and } x_0 = \frac{1}{N}\sum_k \left\langle c_{k\uparrow}^{+} c_{-k\downarrow}^{+} \right\rangle,$$

charge-ordered phase (CDW) $\rho_Q^z \neq 0,\ n_Q \neq 0$, where

$$\rho_Q^z = \frac{1}{N}\sum_i \left\langle n_i^d \right\rangle \mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\boldsymbol{R}_\mathrm{i}} = \frac{1}{N}\sum_i \left\langle 2\rho_{id}^z \right\rangle \mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\boldsymbol{R}_\mathrm{i}}, \quad n_Q = \frac{1}{N}\sum_{k\sigma} \left\langle c_{k+Q\sigma}^{+} c_{k\sigma} \right\rangle,$$

$$\boldsymbol{Q} = \left(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}\right),$$

charge Kondo state (CKS)

$$\lambda = \frac{1}{2N}\sum_i \left(\left\langle d_{i\sigma}^{+} c_{i\sigma} \right\rangle + \text{h.c.}\right).$$

2. Results and discussion

For $n = 2$ and $\Delta_0 = 0$ one finds that the chemical potential $\mu = V_0/2$ and $n_c = n_d = 1$ for any T. In such a case the ground state diagram of the model (1), taking into account only pure phases and calculated for rectangular DOS, is plotted in Fig. 1.

In Figs. 2–4 we present the evolution of the order parameters and the quasiparticle gap in the excitation spectrum E_g at $T = 0$ with increasing interactions.

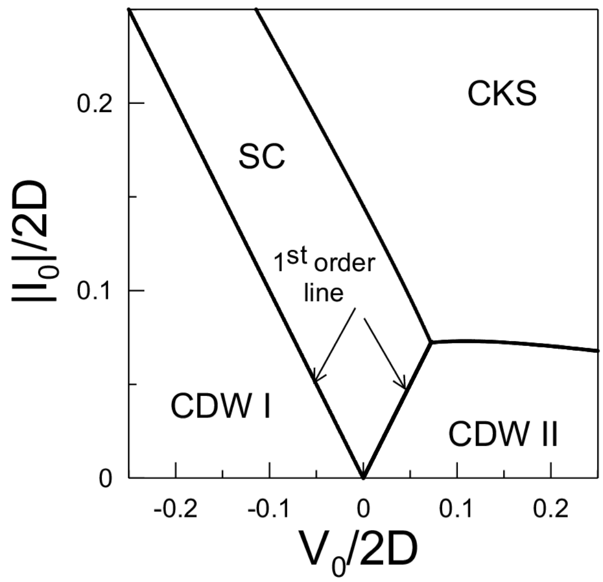

Fig. 1. Ground state phase diagram of the model (1) at half-filling plotted as a function of $I_0/2D$ and $V_0/2D$, for $n = 2,\ \Delta_0/2D = 0,\ n_c = n_d = 1$, for rectangular DOS.

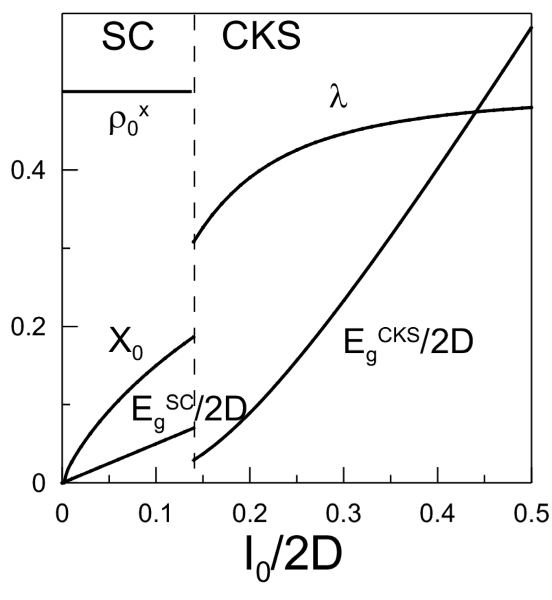

Fig. 2. Variation of the SC and CKS order parameters and the quasiparticle gap at $T = 0$ as a function of $I_0/2D$ for $n = 2,\ \Delta_0/2D = 0,\ V_0/2D = 0$.

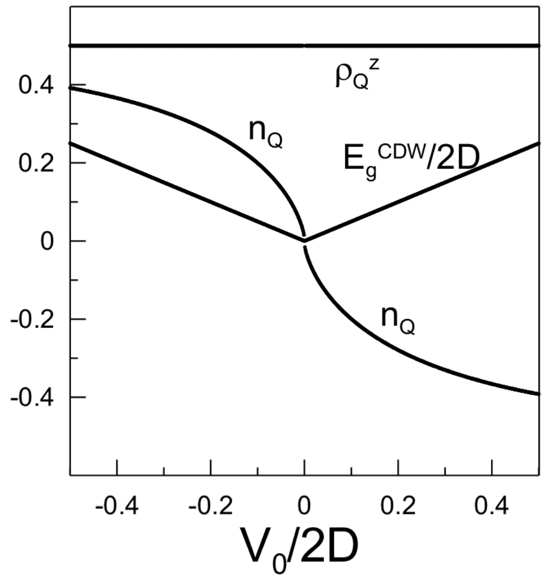

Fig. 3. Variation of the CDW order parameter ρ_Q^z and n_Q and the quasiparticle gap $E_{\mathrm{g}}^{\mathrm{CDW}}/2D$ at $T=0$ as a function of $V_0/2D$ for $n=2,\ \Delta_0/2D=0,\ I_0/2D=0$.

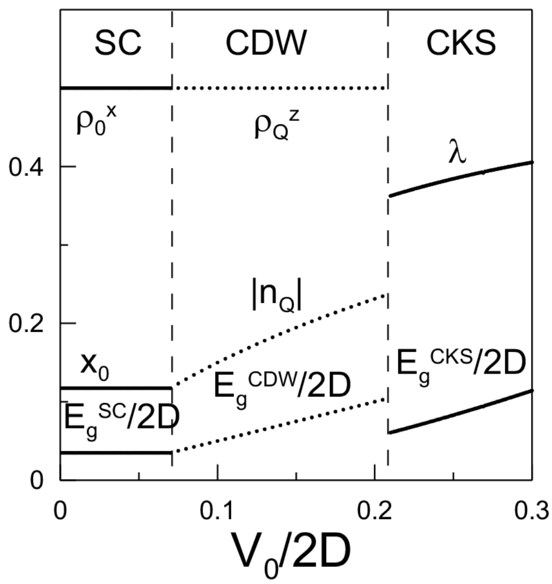

Fig. 4. Variation of the SC, CDW and CKS order parameters and the quasiparticle gaps at $T=0$ as a function of $V_0/2D$ for $n=2,\ \Delta_0/2D=0,\ I_0/2D=0.07$.

3. Summary

Let us shortly summarize our main findings.

1. For small values of $I_0/2D$ and $V_0/2D$ the ground state is SC, if $|I_0| > |V_0|$ and CDW if $|I_0| < |V_0|$, for both signs of I_0 and V_0 (cf. Fig. 1).
2. For $|I_0| > |V_0|$ and $T = 0$, with increasing $|I_0|/2D$ the system exhibits a transition from SC to CKS state at $(|I_0|/2D)_c$ (cf. Figs. 1 and 2). The value of $(|I_0|/2D)_c$ depends on the lattice structure of the system and the strength of V_0: repulsive V_0 ($V_0 > 0$) reduces this critical value whereas attractive V_0 ($V_0 < 0$) enhances it.
3. For $|I_0| < |V_0|$ and $T = 0$ the system remains in the CDW state for any $|V_0|/2D$, if $V_0 < 0$, whereas for repulsive V_0 ($V_0 > 0$) the increase in $|I_0|/2D$ yields a transition CDW $\rightarrow$ CKS, and the critical value $(|I_0|/2D)_c$ slowly decreases with increasing $V_0/2D$ (cf. Fig. 1).
4. The phases CDW and CKS are nonmetallic and at the borders of these phases with SC the system exhibits the nonmetal–superconductor transition.
5. The CDW ordering is stabilized by the intersubsystem density interaction V_0 (both the repulsive and attractive one). It involves spatial modulation of charge in both subsystems and the order parameters ρ^z_Q and n_Q have the same signs for $V_0 < 0$ and the opposite signs for $V_0 > 0$, which maximizes (minimizes) the total amplitude of charge modulation for $V_0 < 0$ ($V_0 > 0$) (cf. Fig. 3) and we call the CDW phases realized for $V_0 < 0$ and $V_0 > 0$ as CDW I and CDW II, respectively.
6. The plots of CDW order parameters and the gap in the c-electron spectrum at $T = 0$ as a function of $|V_0|/2D$ for $|I_0|/2D = 0$ are shown in Fig. 2.
7. With increasing $V_0/2D$ ($-\infty < V_0/2D < \infty$) for a fixed value of $I_0/2D$ the system can exhibit the following sequences of transitions: CDW I $\rightarrow$ SS $\rightarrow$ CDW II $\rightarrow$ CKS, if $0 < I_0/2D < (I_0/2D)_c$, and CDW I $\rightarrow$ SS $\rightarrow$ CKS, if $I_0/2D > (I_0/2D)_c$.

At present we study the case of arbitrary particle concentrations and include into consideration the mixed ordered phases. Our preliminary results clearly indicate that the deviation from the half-filling (i.e. from $n_c = n_d = 1$) with a change of n or/and Δ_0 can strongly extend the range of stability of SC phase with respect to other phases.

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