Vol. **106** (2004) *ACTA PHYSICA POLONICA A* No. 5

Proceedings of the School Superconductivity and Other Phenomena in Perovskites, Warsaw 2004

Superconducting Properties of the η-Pairing State in the Penson–Kolb–Hubbard Model

W.R. Czart and S. Robaszkiewicz

Institute of Physics, Adam Mickiewicz University
Umultowska 85, 61-614 Poznań, Poland

The Penson–Kolb–Hubbard model, i.e. the Hubbard model with the pair-hopping interaction J is studied. We focus on the properties of the superconducting state with the Cooper-pair center-of-mass momentum $\boldsymbol{q} = \boldsymbol{Q}$ (η-phase). The transition into the η-phase, which is favorized by the repulsive J ($J < 0$) is found to occur only above some critical value $|J_{\mathrm{c}}|$, dependent on band filling, on-site interaction U and band structure, and the system never exhibits standard BCS-like features. This is in obvious contrast with the properties of the isotropic s-wave state, stabilized by the attractive J and attractive U, which exhibit at $T = 0$ a smooth crossover from the BCS-like limit to that of tightly bound pairs with increasing pairing strength.

PACS numbers: 74.20.–z, 71.28.+d, 74.25.Ha

1. Introduction

The Penson–Kolb–Hubbard (PKH) model is one of the conceptually simplest effective models for studying superconductivity of the narrow band systems with short-range, almost unretarded pairing [1–5]. Its Hamiltonian has the form

$$H = -t \sum_{\langle ij \rangle \sigma} \left(c^{+}_{i\sigma} c_{j\sigma} + \mathrm{h.c.} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \frac{1}{2} J \sum_{\langle ij \rangle} \left(c^{+}_{i\uparrow} c^{+}_{i\downarrow} c_{j\downarrow} c_{j\uparrow} + \mathrm{h.c.} \right),$$

where $n_{i\sigma} = c^{+}_{i\sigma} c_{i\sigma}$, t is the single electron hopping integral, U is the on-site density interaction, J is the pair hopping (intersite charge exchange) interaction. $\langle ij \rangle$ restricts the sum to nearest neighbors (nn) and $n = \frac{1}{N} \sum_{i\sigma} \langle n_{i\sigma} \rangle$.

The model includes a nonlocal pairing mechanism (the pair hopping term J) that is distinct from the on-site interaction in the attractive Hubbard (AH) model and that is the driving force of pair formation and also of their condensation.

The PKH model has been investigated only in a few particular limits till now [1–7]. The main efforts concerned the ground state properties of the model in one dimension ($d = 1$) at half-filling ($n = 1$) [1, 2, 4]. For d-dimensional hypercubic lattices the ground state diagrams of the half-filled PKH model have been determined by means of the (broken symmetry) Hartree–Fock approximation (HFA) and by the slave-boson mean field method in Ref. [2]. For $d = 1$ the diagrams are shown to consist of at least nine different phases including superconducting states, site and bond-located antiferromagnetic and charge-density-waves states, as well as mixed phases with coexisting site and bond orderings. The stability range of the bond-type orderings shrinks with increasing lattice dimensionality and for $d = \infty$ the phase diagram involves exclusively site-located orderings.

Recently, we have studied superconducting characteristics of the PK model [6] and the PKH model [5] in the case of *attractive* J ($J > 0$), which stabilizes s-wave pairing state (S) analogous to that driven by the on-site attraction in the AH model.

In the following we will conclude the properties of the PKH model in the case of *repulsive* J ($J < 0$). Such an interaction can stabilize the η-phase, i.e. the superconducting state with the Cooper-pair center of mass momentum $\boldsymbol{q} = \boldsymbol{Q}$ ($\boldsymbol{Q} = \Pi/a, \Pi/a, \ldots$), with the order parameter $x_\eta = \sum_i \exp(\mathrm{i}\boldsymbol{Q} \cdot \boldsymbol{R}_i) \times \langle c^+_{i\uparrow} c^+_{i\downarrow} \rangle \neq 0$ [2–4, 7].

2. Results and discussion

We performed an extended analysis of the thermodynamic and electromagnetic properties of the η-phase of the model for d-dimensional hypercubic lattices and arbitrary electron concentration ($0 < n < 2$) [8]. In the analysis we used a linear response theory and the electromagnetic kernel was evaluated within the HFA-RPA scheme. The effects of phase fluctuations on T_c for $d = 2$ lattices were estimated within the Kosterlitz–Thouless (K–T) scenario in the same way as it was done previously for the case of S-phase [5, 6]. Moreover, the properties of the zero-bandwidth limit of the model were determined using the variational approach which treats the on-site interaction term exactly.

Below we only quote the main results of this study.

1. The transition into the η-phase is found to occur only above some critical value $(|J|/B)_\mathrm{c}$ ($J < 0$ and B is the band width), and the system never exhibits standard BCS-like features. The critical value J_c depends on the form of the density of states (DOS), the value of U and the band filling n (Figs. 1, 2).

2. At any fixed n and U there exists also a second characteristic value of $|J|/B$, which we call $(|J|/B)_{\mathrm{c}1}$ and $(|J|/B)_{\mathrm{c}1} \geq (|J|/B)_\mathrm{c}$. For all the DOS

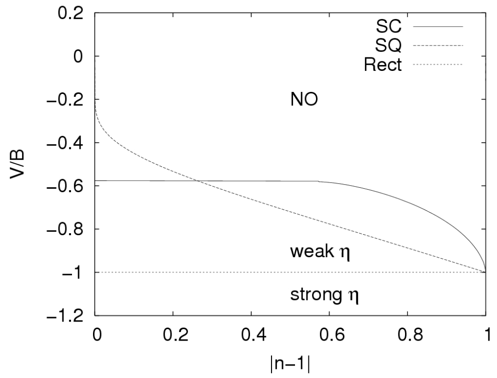

Fig. 1. Ground state phase boundaries between the η-phase and the NO (normal) state calculated within (broken symmetry) HFA for $d = 2$: SQ (square) $d = 3$: SC (simple cubic) lattices and for rectangular DOS: Rect. $V = J_0 + U$, $B = 2zt$, $J_0 = zJ$. z is the number of n.n. (*strong*-η and *weak*-η regions are defined in the text).

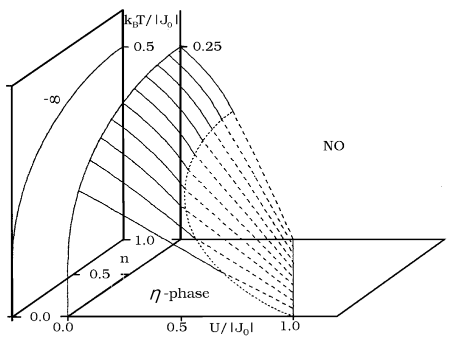

Fig. 2. Finite temperature phase diagram of the PKH model with $J < 0$ in the zero--band width limit ($t = 0$) calculated within the variational approach which treats the U-term exactly and J-term within HFA. The second- and first-order transitions are indicated, respectively, by the solid and the dashed curves. Tricritical points are shown as a dotted line.

considered and $U = 0$ $(|J|/B)_{c1} = 1/z$ at any n. For $|J/B| > (|J|/B)_{c1}$ the ground state of the system is characterized by a nonzero gap between the lower and higher quasiparticle band, i.e. $E_g^m(T = 0) \equiv \min E_k^+ - \max E_k^- > 0$ and by the order parameter which takes its maximum value (the same as in the zero band width limit) $x_\eta^{\max} = \frac{1}{2}\sqrt{n(2-n)}$. We define this state as the *strong η-pairing* phase (in analogy with strong ferromagnet). For $|J|/B > (|J|/B)_{c1}$, $T_c > 0$ for any n $(0 < n < 2)$. On the contrary, for $(|J|/B)_c < |J|/B < (|J|/B)_{c1}$: $E_g^{\min} \le 0$ and $x_\eta < x_\eta^{\max}$ at $T = 0$. Consequently, we define this state as the *weak η-pairing* phase (in analogy with weak ferromagnet). This phase exists only in a restricted range of n, which shrinks to zero with decreasing $|J|$ (Fig. 1).

3. For $E_{\rm g}^{\rm m}(T) < 0$ the quasiparticle DOS in the η-phase is finite for arbitrary energy but a local minimum in the DOS can occur at the Fermi surface and the system will exhibit a pseudogap behavior [9].

4. The electromagnetic and thermodynamic properties of the η-phase (for $J < 0$) become similar to those of the S-phase (for $J > 0$) only in the large $|J|$ limit: $B/|V| \ll 1$, $|U| \ll |J_0|$ (compare Figs. 3a, b with Fig. 4 of Ref. [5]). In this limit $H_{\rm c}^2$, $1/\lambda^2(0)$, and $T_{\rm c}$ become proportional to $|J|$, the coherence length $\xi_{\rm GL}$ tends to a constant value $a/\sqrt{2z}$, while the Ginzburg ratio $\kappa = \lambda/\xi_{\rm GL} \sim 1/\sqrt{|J|}$ and the energy gap $E_{\rm g}^{\rm min} \Rightarrow |J_0|$, for any n. With decreasing $|J_0|/B$, $\xi_{\rm GL}$ increases and becomes n-dependent, going to infinity at $(|J|/B)_{\rm c}$ i.e. at the border with NO state.

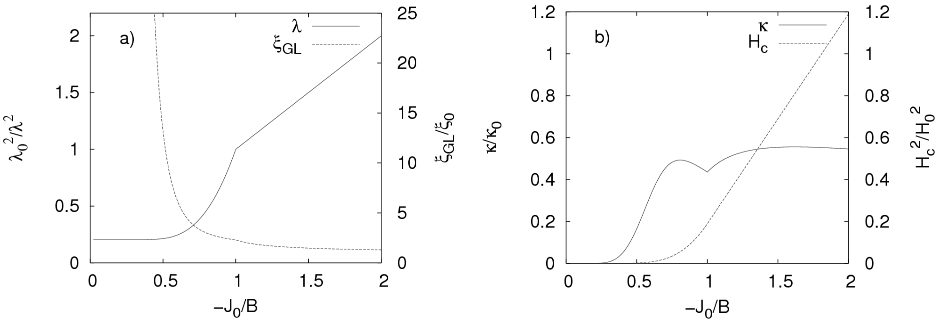

Fig. 3. (a) Inverse square penetration depth $1/\lambda^2$ ($\lambda_0 = \frac{\hbar c}{e}\sqrt{a^{d-2}/4\pi B}$) and the Ginzburg–Landau (G–L) coherence length $\xi_{\rm GL}/\xi_0$ ($\xi_0 = a/\sqrt{2z}$) and (b) the Ginzburg ratio κ/κ_0 ($\kappa_0 = \frac{\hbar c}{e}\sqrt{2/\pi B a^{4-d}}$) and $H_{\rm c}^2/H_0^2$ ($H_0^2 = 4\pi B/a^d$) at $T = 0$ plotted as a function of $-J_0/B$ for SQ lattice and $n = 1$, $U = 0$.

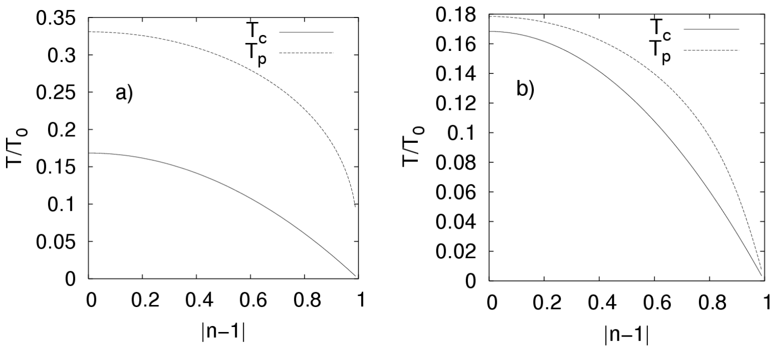

Fig. 4. Transition temperatures for η-pairing calculated within HFA ($T_{\rm p}$) and within K–T approach ($T_{\rm c}$), plotted as a function of $|n-1|$ for SQ lattice: (a) $-J_0/B = 1.5$ and $U/B = 0$, (b) $-J_0/B = 1.5$ and $U/B = 0.5$ ($T_0 = B/k_{\rm B}$).

5. There are strong effects of phase fluctuations on the η-phase in $d = 2$. As we see from Fig. 4 the K–T transition temperature T_{c} can be substantially lower than T_{p}, which in $d = 2$ gives only the estimation of the pair formation temperature.

6. Attractive U ($U < 0$) expands the range of stability of η-phase at $T = 0$ towards lower values of $|J|$. Moreover, the η-phase can survive also for repulsive values of U ($0 < U < U_{\mathrm{c}}$). In the narrow band regime ($t_{ij} \to 0$) one finds that the increasing repulsive U changes first the nature of the η-pairing transition from a continuous to a discontinuous type, resulting in the tricritical point, then it suppresses superconductivity for low $|n-1|$ and finally, for $U/|J_0| > 1$ the system remains in a normal state at any T and n (cf. Fig. 2).

Acknowledgments

We thank R. Micnas and B. Bułka for helpful discussion. This work was supported in part by the State Committee for Scientific Research, grant no. 1 P03B 084 26; 2004–2006.

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