SUPERCONDUCTIVITY IN THE TWO-DIMENSIONAL EXTENDED HUBBARD MODEL WITH PAIR-HOPPING INTERACTION*

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The extended Hubbard model with pair-hopping (intersite charge exchange) interaction is studied. The effects of phase fluctuations on the s-wave superconductivity of this system are discussed within the Kosterlitz–Thouless scenario. For two-dimensional (SQ) lattice the evolution of the superconducting critical temperature $T_{\rm c}$, the pair formation temperature $T_{\rm p}$ and the Uemura-type plots (*i.e.* the plots of $T_{\rm c}$ *vs* superfluid stiffness at $T = 0$) with pairing strength is determined.

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1. General formulation

The extended Hubbard model with pair hopping interaction *i.e.* the so-called Penson–Kolb–Hubbard (PKH) model is one of the conceptually simplest phenomenological models for studying correlations and for description of superconductivity of narrow band systems with short-range, almost unretarded pairing [1,2]. The model Hamiltonian has the form:

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

where t is the single electron hopping integral, U is the on-site density–density interaction, J is the pair hopping (intersite charge exchange) interaction, μ is the chemical potential, the limit $\langle ij\rangle$ restricts the sum to nearest

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neighbors (nn). The Peierls factors in Eq. (1) account for the coupling of electrons to the magnetic field via its vector potential $\vec{A}(\vec{r})$:

$$\Phi_{ij} = -\frac{e}{\hbar c}\int\limits_{R_i}^{R_j} d\vec{r}\vec{A}(\vec{r}) \,,$$

and e is the electron charge.

In the absence of the U term the Hamiltonian (1) reduces to the Penson–Kolb (PK) model [3–5], whereas for $J=0$ and $U<0$ one gets the Hamiltonian of the Attractive Hubbard (AH) model [6–8].

Till now the PKH model has been investigated only in a few particular limits [1,2]. The main efforts concerned the ground state properties of the model in one dimension ($d=1$) at half-filling ($n=1$) [2]. For d-dimensional hypercubic lattices the ground state diagrams of the Penson–Kolb–Hubbard model have been determined by means of the (broken symmetry) Hartree–Fock Approximation (HFA) and by the slave-boson mean field method in Ref. [1]. At half filling 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 d and for $d=\infty$ the phase diagram involves exclusively site-located orderings.

In this paper we extend the investigations of the PKH model to the case of finite temperatures. We will focus on the two-dimensional case with arbitrary particle concentration ($0<n<2$) and $J>0$ and discuss the effects of phase fluctuations on the superconducting state of this system. We will not analyse here the magnetic orderings which can develop in a definite range of $U>0$, $J>0$ and n at $T=0$, and compete with superconductivity. Our analysis is based on the (broken symmetry) HFA and the Kosterlitz–Thouless (K–T) theory for $d=2$ superfluid [5,7–10].

For $\vec{A}=0$ the free energy of the Superconducting (S) phase F_{S} is calculated to be:

$$\frac{F_{\mathrm{S}}}{N} = \mu\,(n-1) + \frac{4}{z}Jp^2 + (-U+J_0)\,x_{\mathrm{s}}^2 - \frac{2}{\beta N}\sum_k \ln\left[2\cosh\left(\frac{\beta E_k}{2}\right)\right] \quad (2)$$

and the superconducting order parameter $x_{\mathrm{s}} = 1/N\sum_i \langle c_{i\downarrow}c_{i\uparrow}\rangle$, the Fock term $p = 1/4N\,\sum_{k\sigma}\gamma_k\left\langle c^+_{k\sigma}c_{k\sigma}\right\rangle$ and μ are determined by the equations

$$\frac{\partial F_{\mathrm{S}}}{\partial x_{\mathrm{s}}} = 0,\ \frac{\partial F_{\mathrm{S}}}{\partial p} = 0,\ \frac{\partial F_{\mathrm{S}}}{\partial \mu} = 0\,, \quad (3)$$

where $E_k = \sqrt{\bar{\varepsilon}_k^2 + \Delta^2}$, $\bar{\varepsilon}_k = \varepsilon_k - \mu$, $\Delta = (-U + J_0)x_\mathrm{s}$, $J_0 = zJ$, $\varepsilon_k = -\widetilde{t}\,\gamma_k$, $\widetilde{t} = t + 2pJ/z$, $\gamma_k = 2\sum_\alpha \cos k_\alpha$, $\alpha = x, y, \ldots$, z is the number of nearest neighbours ($z = 4$ for SQ lattice) $\beta = 1/k_\mathrm{B}T$.

From Eqs (3) one can calculate the HFA transition temperature T_p at which the gap amplitude vanishes ($\Delta \to 0$) and which gives the estimation of the pair-formation temperature [8].

Due to fluctuation effects the superconducting phase transition will occur at the critical temperature T_c being lower than T_p. For d = 2 lattice the T_c can be derived within the K–T theory [7,9], using the K–T relation for the universal jump of the superfluid stiffness ρ_s at T_c

$$\frac{2}{\pi} k_\mathrm{B} T_\mathrm{c} = \rho_\mathrm{s}^-(T_\mathrm{c})\,. \tag{4}$$

The superfluid stiffness (helicity modulus) ρ_s, being directly related to the London penetration depth λ, calculated within HFA–RPA scheme, is given by

$$\begin{aligned} \rho_\mathrm{s}(T) &= \frac{\hbar^2 c^2}{16\pi e^2}\lambda^{-2} \\ &= -\frac{1}{2N}\sum_k |t| \left[1 - \frac{\bar{\varepsilon}_k}{E_k}\tanh\left(\frac{\beta E_k}{2}\right)\right]\cos(k_\alpha) + 2\frac{J_0}{z}x_\mathrm{s}^2 \\ &\quad -\frac{1}{2N}t^2 \sum_k \frac{\sin^2 k_x}{k_\mathrm{B}T\cosh^2\left(\frac{\beta E_k}{2}\right)}\,. \end{aligned} \tag{5}$$

2. Results and discussion

We have performed a quite extensive (analytical and numerical) analysis of the thermodynamic and electromagnetic properties of the superconducting phase of the model (1) for d-dimensional hypercubic lattices ($d \geq 2$) and arbitrary electron concentration ($0 < n < 2$) [10]. For SQ lattice examples of the evolution of T_c and T_p with a change of interaction parameters for fixed n are shown in Figs 1 and 2, whereas Fig. 3 shows the plots of transition temperatures as a function of n.

Except of the weak coupling regime there is a strong influence of the phase fluctuations on the superconducting pairing and the results show a clear separation of the energy scales for the pair formation ($\sim k_\mathrm{B}T_\mathrm{p}$) and the phase coherence ($\sim k_\mathrm{B}T_\mathrm{c}$). The K–T transition temperature T_c can be much lower than T_p, and for $U \leq 0$, $J_0 > 0$ the highest reduction is observed at small electron concentrations (*cf. e.g.* Fig. 3(a) and Ref. [5]). Notice also that the difference between T_p and T_c strongly increases with the increase of on-site attraction $U < 0$ (*cf.* Fig. 1).

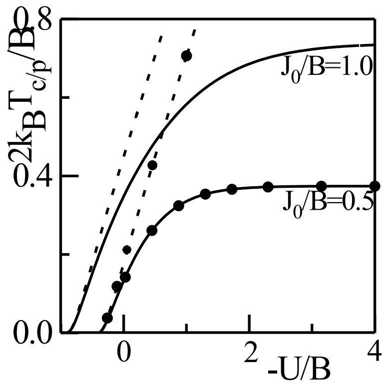

Fig. 1. Transition temperatures for the Penson–Kolb–Hubbard (PKH) model plotted as a function of U/B for $n = 0.75$ and several fixed values of $J_0/B = 0.5$; 1.0. Solid and dashed lines denote $T_{\rm c}$ and $T_{\rm p}$, respectively. SQ lattice, $B = 8t$ is the bandwidth.

In the region between $T_{\rm p}$ and $T_{\rm c}$ one has a state of incoherent s-wave pairs. In this state the pseudo-gap in the quasiparticle energy spectrum will open up and the system will exhibit non-Fermi liquid properties.

In Fig. 2 we have compared the plots of $T_{\rm c}$ and $T_{\rm p}$ *vs* interaction for the PK ($U = 0$, $J > 0$) (Fig. 2(b)) and AH ($U < 0$, $J = 0$) (Fig. 2(a)) models. Except for the weak coupling limit the interaction dependences of $T_{\rm c}$ are very different in these two models. This is due to the nonlocal pairing mechanism (intersite charge exchange) which makes the dynamics of electron pairs in the PK model to be qualitatively different from that in the AH model [1,5,6] and results in different thermodynamic and electrodynamic properties of both models. In the AH model with increasing $|U|$ the $T_{\rm c}$ increases exponentially

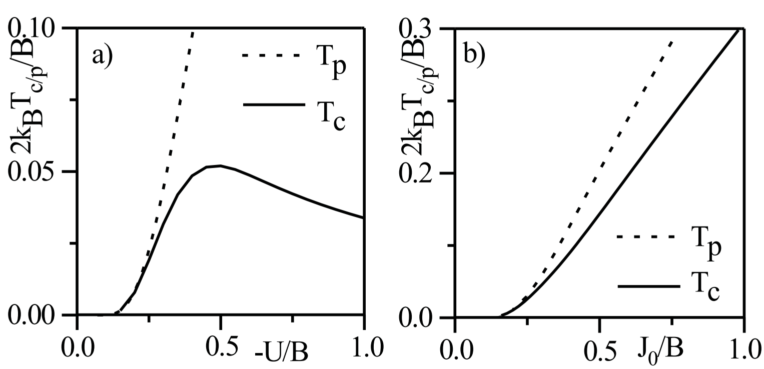

Fig. 2. Transition temperatures as a function of increasing interactions for (a) the AH model ($U < 0$, $J_0 = 0$) and (b) the PK model ($J_0 > 0$, $U = 0$) plotted for SQ lattice and $n = 0.5$. Denotations as in Fig. 1.

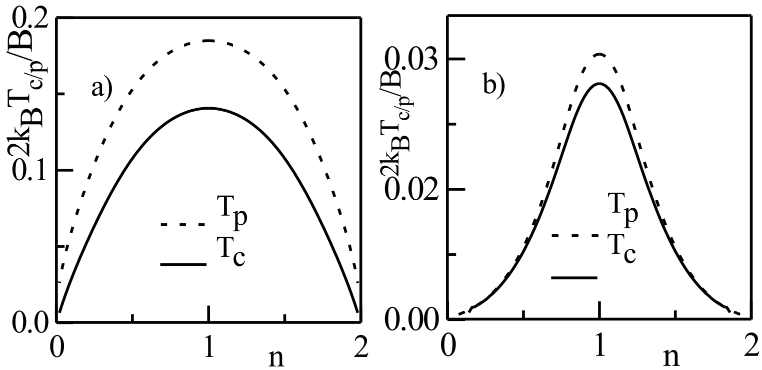

Fig. 3. Transition temperatures for the PKH model plotted as a function of n for $J_0/B = 0.5$ and (a) $U/B = 0$, (b) $U/B = 0.3$. SQ lattice, $B = 8t$ is the bandwidth.

for small $|U|$, then it goes through a round maximum and it *decreases* as $t^2/|U|$ for large coupling (*cf.* Fig. 2(a)). Analogous behavior is found for the thermodynamic critical field $H_c(0)$ [6,8]. On the contrary, in the PK model there is no maximum of T_c and $H_c^2(0)$ at intermediate J/t and both these quantities *increase* linearly with J for large coupling (*cf.* Fig. 2(b) and Refs [1,5]).

Within the K–T scenario we have also derived the Uemura-type plots for the superconducting phase of the model, and examples of the T_c *vs* $1/\lambda^2$ plots with controlling variable n (fixed J_0/B, $U = 0$) are shown in Fig. 4. Similar plots have been recently deduced for the AH model [8] and the

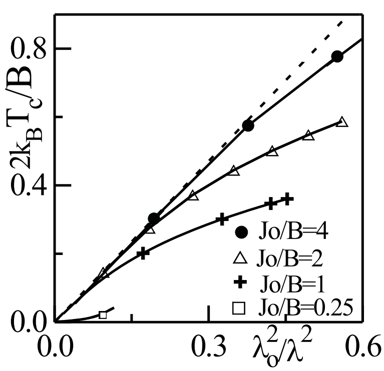

Fig. 4. The Uemura-type plots: $2k_BT_c/B$ vs λ_0^2/λ^2, with the controlling variable n, for $U = 0$ and several fixed values of J_0/B. The straight dashed line gives an upper bound for the phase ordering temperature $\pi\rho_s(0)/2$. $\lambda_0^2/\lambda^2 = 4\rho_s/B$, $\lambda_0^2 = (\hbar c/e)^2/(4\pi B)$.

extended Hubbard model with intersite attraction [11,12]. Except for weak coupling limit the T_c *vs* $1/\lambda^2$ curves have a shape similar to the experimental Uemura's plots [13,14] obtained for various classes of the short-coherence length ("exotic") superconductors, including the cuprates, bismuthates and the organic materials, and for small n the points follow the universal $\pi\rho_s(0)/2$ line. One should stress that analogous plots with T_p cannot account for the scaling [5,8,11,12].

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