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SUPERCONDUCTING CHARACTERISTICS OF THE PENSON–KOLB MODEL

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We study superconducting properties of the Penson–Kolb model, i.e. the tight-binding model with the pair-hopping (intersite charge exchange) interaction J. The evolution of the critical fields, the coherence length, the Ginzburg ratio, and the London penetration depth with particle concentration n and pairing strength are determined. The results are compared with those found earlier for the attractive Hubbard model.

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1. General formulation

The Penson–Kolb (PK) model is one of the conceptually simplest phenomenological models for studying superconductivity in systems with short-range, almost unretarded pairing [1, 2]. It 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. Thus, the superconducting properties can be essentially different in these two models [2]. In the paper we focus on the PK model with arbitrary particle concentration and discuss its superfluid characteristics which have not been considered up to now. In the analysis we have used a linear response theory [3, 4] and the electromagnetic kernel has been evaluated within HFA–RPA scheme. The model Hamiltonian has the following form:

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

where t is the single electron hopping integral, J is the pair hopping (intersite charge exchange) interaction, the limit $\langle ij\rangle$ restricts the sum to nearest neighbors (nn). The Peierls factors in (1) account for the coupling of electrons to the magnetic field via its vector potential $\boldsymbol{A}(\boldsymbol{r})$: $\Phi_{ij} = (-e/\hbar c) \int_{R_i}^{R_j} \mathrm{d}\boldsymbol{r}\boldsymbol{A}(\boldsymbol{r})$, and e is the electron charge.

From the linear response theory [3, 4] the expectation value of the Fourier transform of the *total current operator* is

$$J_\alpha(\boldsymbol{q},\omega)=N\frac{c}{4\pi}\sum_\beta\left[\delta_{\alpha\beta}K_\alpha^{\rm dia}+K_{\alpha\beta}^{\rm para}(\boldsymbol{q},\omega)\right]A_\beta(\boldsymbol{q},\omega).$$

The *diamagnetic part of kernel* evaluated within HFA has the following form:

$$K_\alpha^{\rm dia}=\frac{8\pi e^2|t|}{\hbar^2c^2a}\frac{1}{N}\sum_k\left[1-\frac{\bar{\epsilon}_k}{E_k}\tanh\left(\frac{\beta E_k}{2}\right)\right]\cos(k_\alpha)-\frac{32\pi e^2}{\hbar^2c^2a}\frac{J_0}{z}x_s^2,\qquad(2)$$

where $\bar{\epsilon}_k=\epsilon_k-\mu$, $E_k=\sqrt{\bar{\epsilon}_k^2+\Delta^2}$, $\Delta=J_0x_s$, $J_0=zJ$, $\epsilon_k=-2\tilde{t}\gamma_k$, $\tilde{t}=t+2pJ/z$, μ is the chemical potential, a is the lattice constant, $\gamma_k=\sum_\alpha\cos k_\alpha$, $\alpha=x,y,\ldots$, and z is the number of nn. The superconducting order parameter $x_s=(1/N)\sum_i\langle c_{i\downarrow}c_{i\uparrow}\rangle$, the Fock term $p=(1/4N)\sum_{k\sigma}\gamma_k\langle c_{k\sigma}^+c_{k\sigma}\rangle$ and μ are determined by the equations $\partial F_{\rm S}/\partial x_s=0$, $\partial F_{\rm S}/\partial p=0$, $\partial F_{\rm S}/\partial\mu=0$, with $F_{\rm S}$ being the free energy of the superconducting (S) phase

$$\frac{F_{\rm S}}{N}=\mu(n-1)+\frac{4}{z}Jp^2+J_0x_s^2-\frac{2}{\beta N}\sum_k\ln\left[2\cosh\left(\frac{\beta E_k}{2}\right)\right].\qquad(3)$$

In the static limit and $q\to0$ for the transverse part of the paramagnetic kernel we obtain

$$K_{xx}^{\rm para}(\omega=0)=\frac{8\pi e^2t^2}{\hbar^2c^2a}\frac{1}{N}\sum_{\boldsymbol{k}}\frac{\sin^2k_x}{k_{\rm B}T\cosh^2(\beta E_k/2)}.\qquad(4)$$

In the local approximation (London limit) *the magnetic penetration depth* is determined in terms of the transverse part of the total kernel as $\lambda=[-K_x^{\rm dia}-K_{xx}^{\rm para}(\omega=0)]^{-1/2}$. Using the value of λ and the difference of the free energy between the normal (N) and S phases one is able to determine the thermodynamic critical field $H_{\rm c}$ and the Ginzburg–London correlation length $\xi_{\rm GL}$ as $H_{\rm c}^2(T)/8\pi=[F_{\rm N}(T)-F_{\rm S}(T)]/Na^3$, $\xi_{\rm GL}=\Phi_0/2\pi\sqrt{2}\lambda H_{\rm c}$, where $\Phi_0=hc/2e$, and to obtain the estimations for the critical fields $H_{\rm c1}\simeq(\ln\kappa/\kappa)H_{\rm c}$ and $H_{\rm c2}=\Phi_0/(2\pi\xi_{\rm GL}^2)$, where $\kappa=\lambda/\xi_{\rm GL}$.

2. Results of numerical solutions and discussion

Examples of the evolution of the penetration depth (its inverse square value $1/\lambda^2$), the critical field $H_{\rm c}$, the coherence length $\xi_{\rm GL}$ and the Ginzburg ratio $\kappa=\lambda/\xi_{\rm GL}$ with n are shown in Fig. 1, for $d=2$ SQ lattice and a fixed value of J_0/B, whereas Fig. 2 shows the plots of $H_{\rm c}^2$ (for $d=2$ SQ lattice), $1/\lambda^2$ and $\xi_{\rm GL}$ (for $d=2$ SQ and $d=3$ SC lattices) as a function of J_0/B for $n=1$. As J increases the $1/\lambda^2$ evolves smoothly between the limit of weakly interacting single-particle carriers (with λ^{-2} being proportional to the bandwidth B) and that of tightly bound pairs (with $\lambda^{-2}\sim J$). Notice the increase in λ^{-2} as a function of J_0 (cf. Fig. 2), i.e. the behavior being qualitatively different than that found for the AH model, where λ^{-2} continuously decreases with increasing $|U|/B$ [4, 5]. One also finds that in the low density limit $\lambda^{-2}\sim n$ for arbitrary J_0/B (cf. Fig. 1), whereas for $J_0/B\gg1$: $\lambda^{-2}\sim n(2-n)$ for any n. With increasing J the $H_{\rm c}^2$

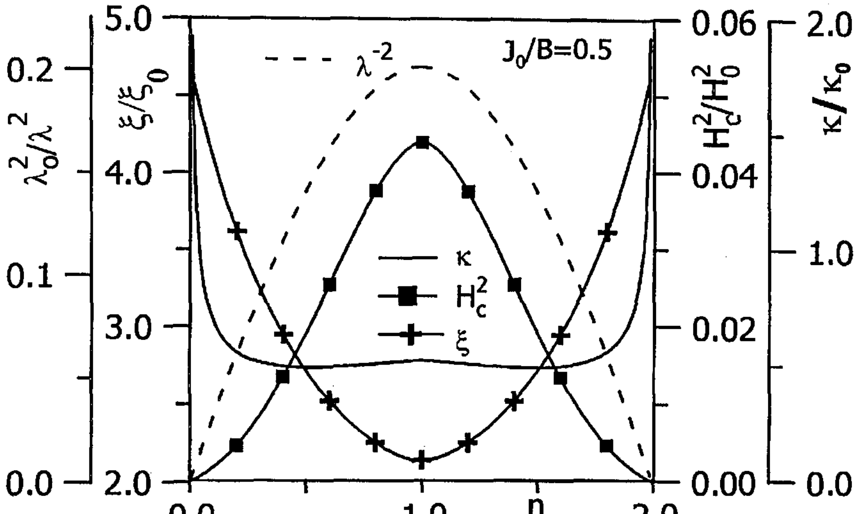

Fig. 1. Concentration dependences of $1/\lambda^2$, H_c^2, ξ_{GL}, and $\kappa = \lambda/\xi_{GL}$ at $T = 0$ for $d = 2$ square (SQ) lattice and $J_0/B = 0.5$ ($B = 2zt$). $\lambda_0 = (\hbar c/e)\sqrt{a^{d-2}/4\pi B}$, $H_0^2 = 4\pi B/a^d$, $\xi_0 = a/2\sqrt{2}$, $\kappa_0 = (\hbar c/e)\sqrt{2/\pi B a^{4-d}}$.

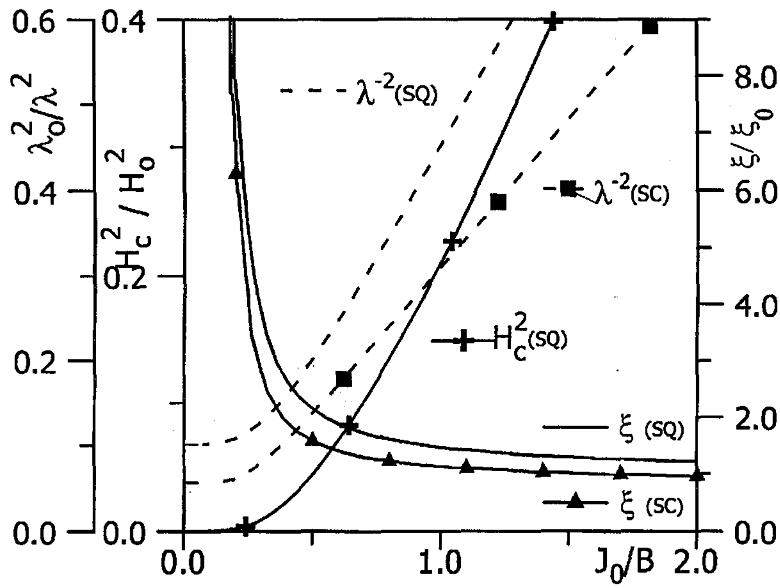

Fig. 2. The plots of H_c^2, for $d = 2$ SQ lattice, and $1/\lambda^2$, ξ_{GL}, for $d = 2$ (SQ) and $d = 3$ (SC) lattices, as a function of J_0/B for $n = 1$. The units as in Fig. 1.

increases exponentially at small J and becomes proportional to J_0 in the strong coupling (Fig. 2).

The ξ_{GL} rapidly decreases at small J ($\xi_{GL} \sim \exp(-2J_0/B)$, for $J_0 \ll B$) and tends to a constant value $\xi_\infty = a/\sqrt{2z}$, the same for all n, at large J. Note a substantial variation of $\xi_{\rm GL}$ with n in the weak-to-intermediate coupling regime (cf. Fig. 2), where $\xi_{\rm GL}$ attains the minimal value at half-filling. This feature is largely due to the strong n dependence of H_c^2, which in weak coupling is proportional to $\Delta^2 D(\overline{\mu})$, where $D(\varepsilon)$ is the density of states (DOS) function.

As it follows the analysis of limiting cases the increase in the Ginzburg ratio $\kappa = \lambda/\xi_{\rm GL}$ with J is exponential in the weak coupling limit $[\kappa \sim \exp(-B/J_0)]$, whereas in the opposite limit κ becomes proportional to $\sqrt{1/J}$. A crossover between these two types of behavior takes place for intermediate values of J $(1 < J_0/B < 2)$. In definite limits one finds universal κ vs. n dependences: (i) $\kappa \sim [n(2-n)]^{-1/2}$, for $J_0/B \gg 1$ (arbitrary n, any lattice) and (ii) $\kappa \sim 1/\sqrt{n}$, for $n \ll 1$ (arbitrary J_0/B, SQ lattice), being analogous to those obtained for the attractive Hubbard model [4]. Beyond these limits $\kappa(n)$ is not universal and strongly depends on the details of $D(\varepsilon)$. In particular, the local maximum of κ at $n = 1$ seen in Fig. 1 results from the van Hove singularity in $D(\varepsilon)$ for SQ lattice.

3. Final comment

Let us stress that due to the nonlocal pairing mechanism (intersite charge exchange) the dynamics of electron pairs in the PK model is qualitatively different from that in the attractive Hubbard model [2]. It results in different thermodynamic and electrodynamic properties of both models, especially in the strong coupling limit.

In the latter model with increasing $|U|$ the T_c and H_c^2 increase exponentially for small $|U|$, then they go through a round maximum and they *decrease* as $t^2/|U|$ for large coupling [4, 5]. On the contrary, in the PK model there is no maximum of H_c^2 and T_c at intermediate J/t and both these quantities *increase* linearly with J for large coupling (cf. Fig. 2 and Ref. [2]). Also the behavior of the penetration depth λ is different. In particular, for $t \to 0$: λ *decreases* with J in the PK model $(\lambda^2 \sim 1/J)$, while it *increases* with $|U|$ in the AH model $(\lambda^2 \sim |U|/t^2$ [4]).

In this report we have concentrated on the electromagnetic properties of the model at $T = 0$. A detailed study of the finite temperature behavior, taking into account the effects of phase fluctuations in $d = 2$ system (within the framework of Kosterlitz–Thouless scenario) and providing a rigorous solution in the case of $d = \infty$ system will be given elsewhere.

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