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Magnetic field induced phase branches of the superconducting transition in two-dimensional square π-loop arrays*

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Based on the results of explicit forms of free energy density for each possible arrangement of magnetization fluxes in large-scale two-dimensional (2D) square π-loop arrays given by Li *et al* [2007 *Chin. Phys.* **16** 1450], the field-cooled superconducting phase transition is further investigated by analysing the free energy of the arrays with a simplified symmetrical model. Our analytical result is exactly the same as that obtained in Li's paper by means of numerical calculations. It is shown that the phase transition splits into two branches with either ferromagnetic or anti-ferromagnetic flux ordering, which depends periodically on the strength of external magnetic flux ϕ_e through each loop and monotonically on the screen parameter β of the loops in the arrays. In principle, the diagram of the phase branches is similar to that of its one-dimensional counterpart. The influence of thermal fluctuation on the flux ordering during the transition from normal to superconducting states of the π-loop arrays is also discussed.

Keywords: Josephson junctions, π-loop arrays, phase branches
PACC: 7450, 7510H

1. Introduction

The phase dependent Josephson current for junctions between two d-wave superconductors has been extensively investigated.[1−3] By imposing symmetry requirements on the tetragonal lattice, Walker and Luettmer-Strathmann[3] have obtained a general expression for the angular dependent Josephson current. Their results show that the Ginzburg–Landau free energy of Josephson coupling, as well as the Josephson current, changes sign when either θ_i or θ_j, the angles of the crystallographic axes of the two connected superconductors with respect to their junction interface, undergoes a $\pi/2$ rotation. With the sign change a π-junction is defined, which can be equally described as having either a negative critical current or an additional phase shift of π. It has been suggested by several authors[1,2,4−8] that the ground state of a superconducting loop containing an odd number of π-junctions, the so-called π-loop, has a spontaneous magnetization with a flux close to half a flux quantum for a large $\beta{=}2\pi LI_c/\Phi_0$ ($\Phi_0 = h/2e$ is the quantum flux) in the absence of an external magnetic field.

After the discovery of high T_c d-wave superconductors, more and more attention has been paid to π-loops and π-loop arrays due to their potential applications in, for example, phase sensitive pairing symmetry tests[9,10] and Josephson flux-qubit designs.[11−14]

Recently, Hilgenkamp *et al* have reported the realization of large-scale coupled π-loop arrays based on $YBa_2Cu_3O_7$–Au–Nb Josephson contacts.[15,16] Their experimental results as well as the analysis given by other authors[8,17,18] showed a robust anti-ferromagnetic ordering of spontaneous magnetization in both square and triangular π-loop arrays and predominant anti-ferromagnetic nearest-neighbour coupling of half-flux quanta in hexagonal π-loop arrays in the absence of an external field. Very recently, the free energy densities in possible flux states of two-dimensional square π-loop arrays in an external magnetic field were given analytically and compared numerically by Li *et al.*[19] To complete the theory, in this paper an analytical treatment for the comparison of the free energy densities is provided with the same

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model described in Refs.[19] and [8]. Based on the comparison, a phase branch diagram is obtained; the branch formation shows a similar behaviour to that in one-dimensional arrays.[20] In addition, we will briefly discuss the effect of thermal fluctuation on branch formation during the superconducting transition.

2. Free energy densities in the possible flux states of a symmetrical square π-loop array

Generally, in large-scale π-loop arrays the edge effects on global properties can be neglected. For simplicity, we take an infinitely large two-dimensional (2D) array consisting of identical square π-loops as our model, as shown in Fig.1. This has been described in Refs.[19] and [8]. We also restrict ourselves to the symmetrical case, in which the loops have the same inductance L and the junctions have the same critical current amplitude I_c. The square π-loops in the array are arranged in such a way that each pair of neighbouring loops has a common Josephson junction,

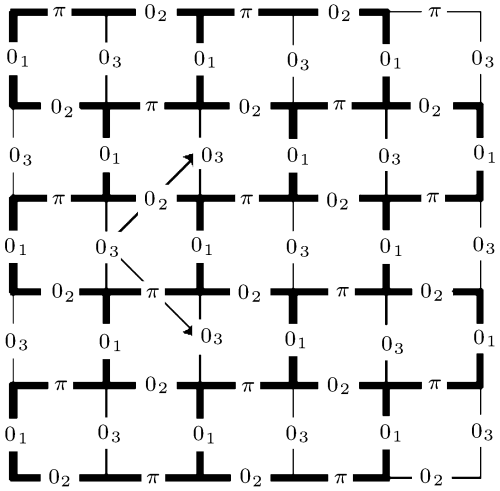


Fig.1. Schematic of a 2D square π-loop array, where zero- and π-junctions are indicated by 0 and π respectively. The 'primitive cells' are denoted by highlighted blocks. The two arrows in the diagram stand for two 'basis vectors'.

either zero- or π-junction, connected on their common side, and each junction is shared by a pair of neighbouring loops. Without loss of generality, all π-junctions are alternately set with the zero-junctions along the horizontal direction of the array. Namely, each square loop in the array has three zero-junctions and one π-junction to compose a π-loop. Therefore, the arrays have crystal-like periodic structure with a pair of horizontal (or vertical in the other equivalent way) neighbouring loops as a "primitive cell", as shown in Fig.1. According to translational periodicity, we know that there are only three kinds of zero-junctions and one kind of π-junction in the array. By imposing the symmetry on the array, there are only four possible magnetization flux arrangements of the loops: [19] anti-ferromagnetic ordering, alternating strip line flux ordering and ferromagnetic ordering with magnetization fluxes either parallel or anti-parallel to the external flux Φ_e, as shown in Figs.2(a), 2(b), 2(c) and 2(d), respectively.

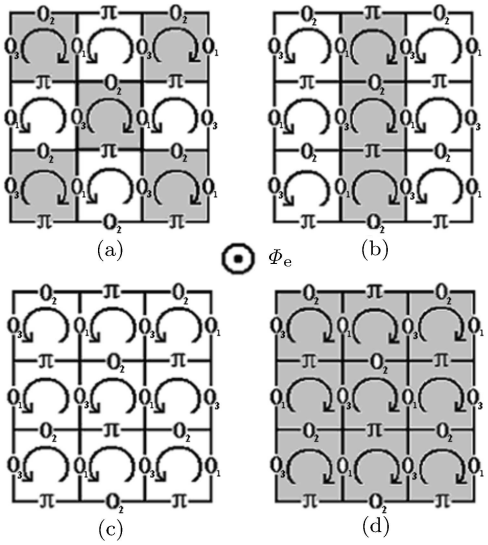


Fig.2. Schematic of four possible flux arrangements in a large-scale symmetrical 2D square π-loop array: anti-ferromagnetic ordering (a); alternating strip line ordering (b); ferromagnetic ordering with magnetization fluxes parallel (c) and anti-parallel (d) to the external flux Φ_e. The π-loops with downward and upward fluxes are denoted by clockwise and anticlockwise arrows for the circulating currents I_s, as well as shaded and non-shaded blocks, respectively.

Considering the fact that each junction in the array is shared by two neighbouring loops, we can write down the free energy per cell as

$$U = \frac{1}{2}(LI_l^2 + LI_r^2) - \frac{\Phi_0 I_c^0}{2\pi}\sum_{j=1}^{3}\cos(\gamma_j^0) - \frac{\Phi_0 I_c^\pi}{2\pi}\cos(\gamma^\pi), \qquad (1)$$

where I_l and I_r are the respective circulating currents in the left and right loops of a cell, γ_j^0 (j=1, 2, 3) and γ^π are the respective gauge-invariant phase differences of the three kinds of zero-junctions and the π-junction, and I_c^0 and I_c^π denote the respective critical currents of the zero-junctions and π-junction, namely I_c^0=I_c

and $I_c^{\pi} = -I_c$. The phase differences of the four junctions in a loop and the total flux through the loop are restricted by the flux quantization condition

$$\sum_{j=1}^{3}\gamma_j^0 + \gamma^{\pi} + \frac{2\pi}{\Phi_0}(\Phi_e + \Phi_m) = 2\pi n, \quad (n = 0, \pm1, \pm2\cdots), \tag{2}$$

where Φ_m is the magnetization flux related to the circulating current and n is an integer describing the fluxon states of the loop.

The condition (2) has periodic properties with respect to the normalized external magnetic flux $\phi_e = \Phi_e/\Phi_0$, namely ϕ_e and $\phi_e + n$ with any integer n give equivalent solutions of the problem. Without loss of generality, we take the quantized flux state n=0. Moreover, the space reflection symmetry of the array will further allow us to deal with the problem in the interval of $0 \le \phi_e \le 1/2$. Once it has been solved in the above region, the whole solution can be obtained by symmetrical and periodical extensions.

As is well known, the critical currents of and phase differences of either zero- or π-junctions satisfy the Josephson relation

$$I_J = I_c^{0,\pi}\sin(\gamma^{0,\pi}), \tag{3}$$

where I_J is the Josephson current through the junction and is the difference between the circulating currents in the two loops sharing the junction.

Considering the above Eqs.(1), (2) and (3), Li *et al* [19] have derived the different explicit forms of the free energy per cell for each possible arrangement of magnetization flux. The anti-ferromagnetic state (see Fig.2(a)) free energy per cell can be expressed as a function of ϕ_e and β

$$U_1 = U_0[2(\pi - 4\Gamma_1)^2 + 8\pi^2\phi_e^2 - 8\beta\cos(\Gamma_1)], \tag{4}$$

where $U_0 = \phi_0^2/8\pi^2 L$; Γ_1 is the gauge-invariant phase difference of the zero-junctions in the arrays (in this case $\gamma_1^0 = \gamma_2^0 = \gamma_3^0 = \Gamma_1$), and can be determined by β from the following equation

$$\beta\sin(\Gamma_1) + 8\Gamma_1 = 2\pi. \tag{5}$$

There is one-to-one correspondence between Γ_1 and β. Equation (5) tells us that Γ_1 is in the range of $0 < \Gamma_1 \le \pi/4$ for $\beta > 0$.

By introducing the normalized free energy density $u_1 = U_1/U_0$, Eq.(4) becomes

$$u_1 = 2(\pi - 4\Gamma_1)^2 + 8\pi^2\phi_e^2 - 8\beta\cos(\Gamma_1). \tag{6}$$

For the alternating strip line flux state (see Fig.2(b)), the normalized free energy density given in Ref.[19] is

$$u_2 = 2(\pi - 2\Gamma_2)^2 + 8\pi^2\phi_e^2 - 4\beta - 4\beta\cos(\Gamma_2). \tag{7}$$

This is slightly different from the anti-ferromagnetic situation. Here Γ_2 is the phase difference of the zero-junctions on the vertical sides (in this case $\gamma_1^0 = \gamma_3^0 = \Gamma_2$, $\gamma_2^0 = 0$), and satisfies the relation

$$\beta\sin(\Gamma_2) + 4\Gamma_2 = 2\pi, \tag{8}$$

thus we have $0 < \Gamma_2 \le \pi/2$.

According to Ref.[19], there are two states with magnetization fluxes parallel (Fig.2(c)) and anti-parallel (Fig.2(d)) to the external flux in the ferromagnetic ordering. And their normalized free energy densities can be written as

$$u_3 = 8\pi^2\left(\frac{1}{2} - \phi_e\right)^2 - 8\beta \tag{9}$$

and

$$u_4 = 8\pi^2\left(\frac{1}{2} + \phi_e\right)^2 - 8\beta, \tag{10}$$

respectively.

3. Phase branches

Now let us compare the normalized free energy densities u_1, u_2, u_3 and u_4 expressed by Eqs.(6), (7), (9) and (10), respectively.

From Eqs.(6) and (7), we know that both u_1 and u_2 are functions of β and ϕ_e. From Ref.[7] we know that the anti-ferromagnetic state has the lowest free energy in the absence of an external magnetic field, namely $u_1 < u_2$ at $\phi_e = 0$. Moreover, we can easily see that $\partial u_1/\partial\phi_e = \partial u_2/\partial\phi_e = 16\pi^2\phi_e$ in the whole range of $0 \le \phi_e \le 1/2$, therefore for all the values of parameters β and ϕ_e we obtain $u_1 < u_2$. In other words, the anti-ferromagnetic state is more stable than the state with alternating strip line flux ordering.

On the other hand, from Eqs.(9) and (10) we can have $u_3 \le u_4$ in the region of $0 \le \phi_e \le 1/2$; namely, the ferromagnetic state is more stable when the magnetization flux is parallel to the external flux than when it is anti-parallel.

In the following, let us compare $u_1(\phi_e)$ with $u_3(\phi_e)$ in the region of $0 \le \phi_e \le 1/2$.

(a) At $\phi_e = 0$, from Eqs.(6) and (9) we have

$$u_1(0) = 2(\pi - 4\Gamma_1)^2 - 8\beta\cos(\Gamma_1) \tag{11}$$

and

$$u_3(0) = 2\pi^2 - 8\beta. \tag{12}$$

As mentioned above, in Eq.(11) Γ_1 and β are not independent of each other. Their relation is given by Eq.(5) and depicted in Fig.3.

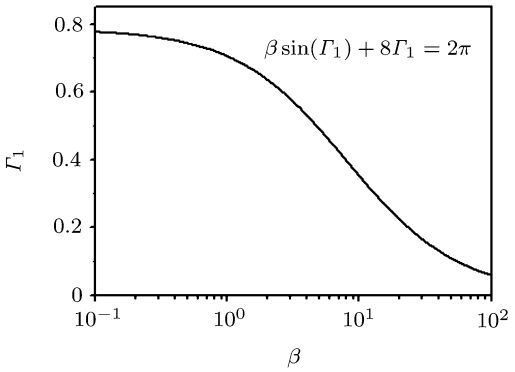


Fig.3. Phase parameter Γ_1 in the anti-ferromagnetic state as a function of screen parameter β.

At present, we regard $u_1(0)$ as a function of Γ_1 only. Obviously, from Eqs.(11) and (12) we have

$$u_1(0, \Gamma_1 = 0) = u_3(0) \tag{13}$$

and

$$\left.\frac{\partial u_1(0,\Gamma_1)}{\partial \Gamma_1}\right|_{\Gamma_1=0} = -16\pi < 0. \tag{14}$$

This means that $u_1(0, \Gamma_1) < u_3(0)$ is tenable for some Γ_1 in the region of $0 < \Gamma_1 \leq \pi/4$. Moreover, we have

$$\frac{\partial^2 u_1(0,\Gamma_1)}{\partial \Gamma_1^2} = 64 + 8\beta\cos(\Gamma_1) > 0. \tag{15}$$

Equations (14) and (15) show that $u_1(0, \Gamma_1)$ has one and only one minimum in the region $0 < \Gamma_1 \leq \pi/4$, and the corresponding Γ_1 is determined by

$$\frac{\partial u_1(0,\Gamma_1)}{\partial \Gamma_1} = -16(\pi - 4\Gamma_1) + 8\beta\sin(\Gamma_1) = 0, \tag{16}$$

which is none other than Eq.(5). Namely, $u_1(0, \Gamma_1)$ determined by Eqs.(11) and (5) is smaller than $u_3(0)$, i.e.

$$u_1(0) < u_3(0). \tag{17}$$

(b) At ϕ_e=1/2, from Eqs.(6) and (9) we can immediately obtain

$$u_1\left(\frac{1}{2}\right) > u_3\left(\frac{1}{2}\right). \tag{18}$$

Moreover, from Eqs.(6) and (9) we know that u_1 increases and u_3 decreases monotonically with increasing ϕ_e in the interval $0 \leq \phi_e \leq 1/2$, as depicted in Fig.4. Therefore, there must be a cross-over point ϕ_e^c in the region $0 \leq \phi_e \leq 1/2$. Namely, the anti-ferromagnetic state is more stable in $0 \leq \phi_e \leq \phi_e^c$, while the ferromagnetic state is more stable in $\phi_e^c \leq \phi_e \leq 1/2$. The cross-over flux ϕ_e^c can be determined by

$$u_1(\phi_e^c) = u_3(\phi_e^c). \tag{19}$$

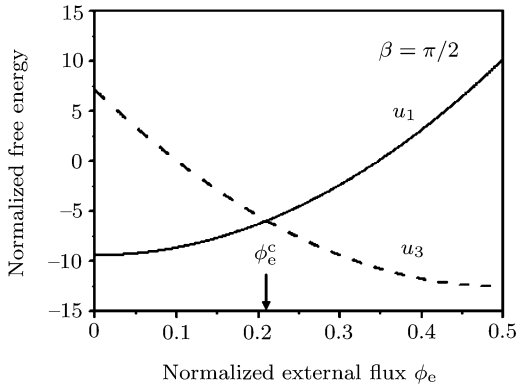


Fig.4. Typical normalized free energies per 'primitive cell' in 2D square π-loop arrays with anti-ferromagnetic (u_1) and ferromagnetic (u_3) orderings of the magnetization flux for $\beta = \pi/2$. For this β the two curves intersect each other at $\phi_e^c = 0.21$.

From Eqs.(6), (9) and (19), the solution of ϕ_e^c can be expressed as

$$\phi_e^c = (2\pi\Gamma_1 - 4\Gamma_1^2 + \beta\cos(\Gamma_1) - \beta)/\pi^2. \tag{20}$$

The ϕ_e^c–β relation can be calculated from Eqs.(5) and (20) in the range of $0 \leq \phi_e \leq 1/2$. In particular,

$$\phi_e^c = \begin{cases} 1/4 & \text{when} \quad \beta = 0; \\ 0 & \text{when} \quad \beta \to \infty. \end{cases} \tag{21}$$

Based on the periodicity of flux quantization condition and the reflection symmetry, we can extend the region of $\phi_e^c(\beta)$ from $0 \leq \phi_e \leq 1/2$ to the whole real axis. Consequently, we obtain the phase diagram shown in Fig.5. The anti-ferromagnetic and ferromagnetic branches are separated periodically with a period of $\Delta\phi_e$=1.

From Fig.5, we can see that the π-loop array must be in the ferromagnetic state in the flux range of $|\phi_e - (n+1/2)| < 1/4$, while for $|\phi_e - n| < 1/4$ the array can be in either ferromagnetic or anti-ferromagnetic state depending on the value of β.

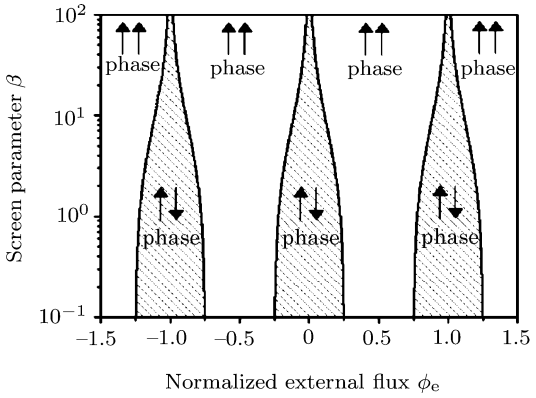


Fig.5. Phase branch diagram of magnetization flux ordering in $\beta - \phi_e$ space. The anti-ferromagnetic and ferromagnetic states with magnetization fluxes parallel to the external flux are indicated by the symbols $\uparrow\downarrow$ and $\uparrow\uparrow$, respectively.

4. Discussion and conclusion

It should be emphasized that the above results are correct only when the field-cooling condition is satisfied. Otherwise, when we change the external flux back and forth after the system has been cooled down, the ordering of the loop magnetizations becomes very complicated. Generally speaking, in the latter scenario, hysteresis among differently quantized flux states in the π-loop array occurs.

Moreover, the above results are obtained at T=0K. At finite temperatures, thermal fluctuation effects exist, so every evolution of the array from normal to either ferromagnetic or anti-ferromagnetic state is a stochastic process. When the system is cooled down near T_c, the influence of thermal fluctuation can be much larger than the Josephson effect and there exists actually no clear phase branch boundary. When the temperature is reduced further to the cross-over temperature T_{cross}, where the Josephson energy has increased and is comparable to the thermal fluctuation energy and $\beta_{cross} \approx 4\pi^2 L k_B T_{cross}/\Phi_0^2$, mutual creep of thermally activated states back and forth across the branch boundaries is still possible, making the boundaries indistinct. At temperatures much lower than T_{cross} the fluctuation effect is reduced dramatically and β becomes much larger than β_{cross}. Then at very low temperatures where β approaches to $\beta(T = 0)$, the thermal fluctuation is negligibly small and the boundaries between ferromagnetic and anti-ferromagnetic branches become clear.

The derivation leading to similar results for two-dimensional triangular π-loop arrays can be done straightforwardly in the same way. However, in hexagonal π-loop arrays the anti-ferromagnetic state does not exist.[8] Although ferromagnetic states do exist in the neighbourhood of $\phi_e = n + 1/2$, the mathematical treatment to provide a flux structure in the vicinity of $\phi_e = n$ is difficult. The predominant anti-ferromagnetic nearest-neighbour coupling can be described by the bond-order parameter σ,[15,17,21,22] which equals to –1/3 at zero temperature.

In conclusion, we have investigated the magnetization flux ordering of large-scale 2D square π-loop arrays using an infinitely large array model by analysing the free energy of the arrays and obtained exactly the same results as those in Ref.[19]. It is shown that there are two branches, ferromagnetic and anti-ferromagnetic branches, in the superconducting phase. The phase branch diagram in $\beta - \phi_e$ space calculated analytically in the thermal fluctuation-free regime is periodic with respect to ϕ_e.

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