

Self-generated magnetic flux in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ grain boundaries

R. G. Mints and Ilya Papiashvili

School of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 69978, Israel

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Grain boundaries in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ superconducting films are considered as Josephson junctions with a critical current density $j_c(x)$ alternating along the junction. A self-generated magnetic flux is treated both analytically and numerically for an almost periodic distribution of $j_c(x)$. We obtained a magnetic flux-pattern similar to the one which was recently observed experimentally.

I. INTRODUCTION

Grain boundaries in high- T_c cuprates are interesting and important for both fundamental physics and applications of high-temperature superconductivity.¹⁻³ Conventional models of strongly coupled Josephson junctions are applicable to describe electromagnetic properties of grain boundaries in thin films of high- T_c superconductors.^{4,5} A remarkable exception of this rule is the [001]-tilt boundary in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ films with a misorientation angle close to 45° .⁶⁻¹⁰ Indeed, these grain boundaries have an anomalous dependence of the critical current I_c on an applied magnetic field H_a . Contrary to a usual Fraunhofer-type dependence $I_c(H_a)$ with a major central peak at $H_a=0$ and minor symmetric side-peaks the asymmetric 45° [001]-tilt grain boundaries demonstrate a pattern without a central dominant peak. Instead two symmetric major side peaks appear at certain applied magnetic fields $H_a = \pm H_{sp} \neq 0$.⁶⁻¹¹

Several mechanisms have been suggested to explain this phenomena.^{8,9,11} The anomalous dependence $I_c(H_a)$ with symmetric major side peaks is obviously a result of a specific heterogeneity of electrical properties of the asymmetric 45° [001]-tilt grain boundaries. Two fundamental experimental observations in conjunction explain this heterogeneity in a natural way.^{9,10} *First*, a fine scale faceting of grain boundaries was discovered in experiments using the transmission electron microscopy (TEM) technique.^{3,12-15} These facets have a typical length scale l of the order of 10–100 nm and a wide variety of orientations relative to the axis of symmetry of the superconductor. *Second*, quite a few of recent experiments provide an evidence of a predominant $d_{x^2-y^2}$ wave symmetry of the order parameter in many of the high- T_c cuprates. In some experimental studies the symmetry of the order parameter is more complicated and is shown to be a certain mixture of the $d_{x^2-y^2}$ and s wave components.^{2,16-22}

These two fundamental experimental observations indicate the existence of two contributions to the phase difference of the order parameter across the grain boundary. Indeed, consider a meandering grain boundary in a film of a superconductor with the $d_{x^2-y^2}$ wave symmetry of the order parameter and assume that there is a certain magnetic flux inside the grain boundary. In this case there is a phase difference φ caused by the magnetic flux and at the same time there is an additional phase difference α caused by the mis-

alignment of the anisotropic $d_{x^2-y^2}$ wave superconductors. Therefore, the tunneling current density j_c is defined by the total phase difference $\Delta = \varphi - \alpha$. A model describing this Josephson current density $j(x)$ results from an assumption that $j(x) \propto \sin[\varphi(x) - \alpha(x)]$, where x is along the grain-boundary line.¹⁰ The local values of the phase difference $\alpha(x)$ depend on the relative orientation of neighboring facets. In the case of an asymmetric 45° grain boundary we have $\alpha(x) = 0$ or π , and therefore $j(x) \propto \sin \varphi(x) \cos \alpha(x)$.¹⁰ In other words in the framework of a model relating $j(x)$ to the orientation of the facets we arrive at $j(x) = j_c(x) \sin \varphi(x)$ with an alternating critical current density $j_c(x) \propto \cos \alpha(x)$. The dependence $j_c(x)$ is imposed by the sequence of facets along a grain-boundary line. If this sequence is periodic or almost periodic then the function $j_c(x)$ is a periodic or almost periodic alternating function. The typical length scale for $j_c(x)$ is of the same order as the length of the facets l , i.e., this length scale is of 10–100 nm.

Variation of orientation of facets along a meandering grain boundary leads to formation of local superconducting current loops even in the absence of an applied magnetic field if the total phase difference $\Delta \neq 0$. It was predicted, in particular, that these current loops can generate a certain magnetic flux at a contact of two facets with $\alpha = 0$ and $\alpha = \pi$.⁹

Self-generated randomly distributed magnetic flux was discovered in asymmetric 45° [001]-tilt grain boundaries in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ superconducting films in the absence of an applied external magnetic field.²³ This flux $\phi_s(x)$ changes its sign randomly and has an amplitude of variations less than the flux quantum ϕ_0 . The average value of $\phi_s(x)$ along the grain boundary is nearly zero. Noticeable, that this disordered nonquantized magnetic flux was observed only for the samples exhibiting the anomalous dependence of the critical current $I_c(H_a)$ on magnetic field with the two symmetric major side peaks.

It was shown analytically that under certain conditions a stationary state with a self-generated flux exists for a Josephson junction with a periodically alternating critical current density $j_c(x)$.²⁴ The same spatial distributions of $j_c(x)$ result in an anomalous dependence of the critical current $I_c(H_a)$ on the applied magnetic field.¹¹ Numerical calculations show that two symmetric major side peaks appear for a periodically alternating $j_c(x)$. The randomness of the critical current density $j_c(x)$ smears these peaks but leaves their posi-

tion in place at weak randomness. We therefore conclude that the experimental observation of the well pronounced major side peaks on the curve $I_c(H_a)$ (Refs. 6–10) means that the alternating critical current density is a periodic or almost periodic function of x . A noticeable randomness of $j_c(x)$ would smear out the dominant side peaks.¹¹

In this paper we calculate both analytically and numerically the self-generated flux ϕ_s in a Josephson junction with an almost periodically alternating critical current density $j_c(x)$. The paper is organized as follows. First, we review briefly the case when $j_c(x)$ is a periodic alternating function.²⁴ We derive the main equations of the two-scale perturbation theory and apply these equations to analyze the nonquantized self-generated flux. This approach forms a basis for the following analytical calculations. Next, we treat the self-generated flux for the case of an almost periodic alternating critical density $j_c(x)$ and start with a qualitative approach to the problem. We review then the results of our numerical simulations which verify the qualitative consideration and exhibit a magnetic flux-pattern which is similar to the one that was recently observed experimentally.²³

II. MAIN EQUATIONS

It is convenient for the following analyses to write the function $j_c(x)$ in the form

$$j_c = \langle j_c \rangle [1 + g(x)], \quad (1)$$

where $\langle j_c \rangle$ is the average value of the critical current density $j_c(x)$ over an interval with a length $L \gg l$

$$\langle j_c \rangle = \frac{1}{L} \int_0^L j_c(x) dx. \quad (2)$$

The function $g(x)$ introduced in Eq. (1) alternates on a typical length scale of l . Note that by definition the average value of $g(x)$ is zero, i.e., $\langle g(x) \rangle = 0$. The maximum value of $|g(x)|$ varies from $|g(x)|_{\max} \geq 1$ to $|g(x)|_{\max} \gg 1$. We assume also that $\lambda \ll l \ll \Lambda_J$, where λ is the London penetration depth and

$$\Lambda_J^2 = \frac{c \phi_0}{16 \pi^2 \lambda \langle j_c \rangle} \quad (3)$$

is an effective Josephson penetration depth. It is worth mentioning that in the case of an alternating current density this effective penetration depth is not a local characteristics of a tunnel junction. It is rather an effective quantity defined on the same typical length scale as $\langle j_c \rangle$.

The phase difference $\varphi(x)$ satisfies the equation

$$\Lambda_J^2 \varphi'' - [1 + g(x)] \sin \varphi = 0. \quad (4)$$

In the limiting case $l \ll \Lambda_J$ it is convenient to write a solution of this equation as a sum of a certain smooth function $\psi(x)$ with a length scale of order Λ_J and a rapidly oscillating function $\xi(x)$ with a length scale of order l (Ref. 24)

$$\varphi(x) = \psi(x) + \xi(x). \quad (5)$$

We assume also that $|\xi(x)| \ll |\psi(x)|$. After substituting Eq. (5) into Eq. (4) and keeping the terms up to the first order in $\xi(x)$ we obtain

$$\Lambda_J^2 \psi'' + \Lambda_J^2 \xi'' - [1 + g(x)] [\sin \psi + \xi \cos \psi] = 0. \quad (6)$$

Note, that experimentally²³ the self-generated flux was observed by a superconducting quantum interference device (SQUID) pickup loop with a size of several $\Lambda_J \gg l$. It means that this method is averaging out the fast alternating flux defined by the phase $\xi(x)$ and measures the spatially smooth flux defined by $\psi(x)$.

Next we consider briefly the case of a *periodically* alternating critical current density $j_c(x)$ which forms the basis of the following analysis of a general case with $j_c(x)$ being a randomly alternating function.

III. PERIODICALLY ALTERNATING CRITICAL CURRENT DENSITY

A. Two-scale perturbation theory

If the critical current density $j_c(x)$ is a periodic function, then $g(x)$ also is a periodic function. In this case an approximate solution of Eq. (6) can be obtained based on a two-scale perturbation theory.²⁵ As a first step in order to apply this approach to Eq. (6) we separate the fast alternating terms with a typical length scale l and the smooth terms varying with a typical length scale Λ_J

$$(\Lambda_J^2 \psi'' - \sin \psi - g \xi \cos \psi) + (\Lambda_J^2 \xi'' - g \sin \psi) = 0. \quad (7)$$

In Eq. (7) we omitted two out of three fast alternating terms of Eq. (6) since they are proportional to $\xi(x)$ and therefore are smaller than the term proportional to $g(x)$. Next, we note that the terms included into the first pair of brackets in Eq. (7) cancel each other independently on the terms included into the second pair of brackets in Eq. (7) as these two type of terms have very different length scales l and Λ_J and $l \ll \Lambda_J$.²⁵ The same reasoning is applicable to the terms included into the second pair of brackets in Eq. (7). As a result we obtain the following two equations for $\xi(x)$ and $\psi(x)$ (Ref. 24)

$$\Lambda_J^2 \xi'' = g(x) \sin \psi, \quad (8)$$

$$\Lambda_J^2 \psi'' - \sin \psi - \langle g(x) \xi(x) \rangle \cos \psi = 0. \quad (9)$$

It is worth noting that we obtain the *two* functions $\psi(x)$ and $\xi(x)$ from *one* equation (7) as only two type of terms with different typical length scales l and Λ_J appear in Eq. (6). If $g(x)$ would have a wide range of typical length scales the above separation would not be possible.

Introducing the Fourier transform of $g(x)$ as

$$g(x) = \sum_{-\infty}^{\infty} g_k e^{ikx}, \quad (10)$$

we find the solution of Eq. (8) in the form

$$\xi(x) = -\frac{\sin \psi}{\Lambda_J^2} \sum_{-\infty}^{\infty} \frac{g_k e^{ikx}}{k^2} = -\xi_g(x) \sin \psi, \quad (11)$$

where the sums in Eqs. (10) and (11) are over the wave vectors $k = 2\pi n / \mathcal{L}$, \mathcal{L} is the length of the junction, and n is an integer. It is worth mentioning that the function $\xi_g(x)$ is defined only by the alternating components of the critical

current density $j_c(x)$. Also while deriving Eq. (11) we ignored the spatial dependence of $\sin \psi$. This can be done since on the length-scale l the variation of the smooth function $\sin \psi(x)$ is of order $l/\Lambda_J \ll 1$. The alternating part of the critical current density has the typical wave numbers $k \sim 1/l$. Therefore, using Eq. (11) we estimate $\xi(x)$ as

$$\xi(x) \sim -\sin \psi \frac{l^2}{\Lambda_J^2} g(x). \quad (12)$$

It follows from this estimate that the typical values of the phase difference $\xi(x)$ are small ($\langle |\xi(x)| \rangle \ll 1$) if

$$\langle |g(x)| \rangle \ll \frac{\Lambda_J^2}{l^2}. \quad (13)$$

Next, using Eq. (11) we rewrite Eq. (9) for the smooth phase shift $\psi(x)$ in the form

$$\Lambda_J^2 \psi'' - \sin \psi + \gamma \sin \psi \cos \psi = 0, \quad (14)$$

where

$$\gamma = \langle g(x) \xi_g(x) \rangle = -\frac{1}{\sin \psi} \langle g(x) \xi(x) \rangle \quad (15)$$

is a constant. A similar derivation for the current density across the tunnel junction results in

$$j(x) = \langle j_c \rangle \sin \psi (1 - \gamma \cos \psi). \quad (16)$$

The magnetic field $B_s(x)$ generated by the alternating component of the critical current $\langle j_c \rangle g(x)$ is given by

$$B_s = \frac{4\pi}{c} \langle j_c \rangle \int g(x) dx = -\frac{\phi_0}{4\pi\lambda} \frac{d\xi_g}{dx} \quad (17)$$

and the averaged field $\langle B_s(x) \rangle = 0$. The alternating magnetic flux ϕ_s produced by the field B_s is equal to

$$\phi_s = -\frac{\phi_0}{2\pi} \xi_g. \quad (18)$$

Combining Eqs. (15) and (17) we find for γ the formula

$$\gamma = \frac{c\lambda}{\phi_0 \langle j_c \rangle} \langle B_s^2 \rangle = \frac{\langle B_s^2 \rangle}{\langle B_J^2 \rangle}, \quad (19)$$

where we introduce a characteristic magnetic field

$$B_J = \frac{4\pi}{c} \langle j_c \rangle \Lambda_J. \quad (20)$$

It follows from Eq. (19) that γ is a positive constant which can be estimated as

$$\gamma \sim \frac{l^2}{\Lambda_J^2} \langle g^2 \rangle. \quad (21)$$

The energy of a Josephson junction \mathcal{E} takes the form²⁶ $\mathcal{E} = \mathcal{E}_0 + \mathcal{E}_\varphi$, where \mathcal{E}_0 is independent of $\varphi(x)$ and

$$\mathcal{E}_\varphi = \frac{\langle j_c \rangle}{2e} \int dx \left\{ \frac{1}{2} \Lambda_J^2 \varphi'^2 - [1 + g(x)] \cos \varphi \right\}. \quad (22)$$

Using Eqs. (8), (11), and the definition of γ , we obtain the energy \mathcal{E}_φ in terms of the smooth phase shift $\psi(x)$

$$\mathcal{E}_\varphi = \frac{\hbar \langle j_c \rangle}{4e} \int dx \{ \Lambda_J^2 \psi'^2 - 2 \cos \psi - \gamma \sin^2 \psi \}. \quad (23)$$

Note, that solutions $\psi(x)$ of Eq. (14) correspond to the minima and to the maxima of the energy functional (23).

B. Nonquantized self-generated flux

Let us apply Eqs. (8), (9), and (15) to a consideration of the stationary states of a Josephson junction with a certain length $\mathcal{L} \gg \Lambda_J$ in an absence of applied magnetic field. In this case the average flux inside the junction is zero and thus an alternating self-generated flux $\phi_s(x)$ appears simultaneously with a certain phase $\psi = \text{const}$ as it follows from Eqs. (11) and (18).

In the stationary state with $\psi = \text{const}$ the values of ψ are determined by Eq. (14) which takes the form

$$\sin \psi (1 - \gamma \cos \psi) = 0. \quad (24)$$

Note, that this equation means also that the current density $j(x)$ across the tunnel junction is equal to zero.

In the case where $\gamma < 1$, Eq. (24) has two solutions, namely, $\psi = 0$ and $\psi = \pi$ and thus, as follows from Eq. (11), there is no self-generated flux. It is also worth mentioning that the energy of a Josephson junction \mathcal{E} has a minimum for $\psi = 0$ and maximum for $\psi = \pi$.

In the case where $\gamma \geq 1$ there are four solutions of Eq. (24), namely, $\psi = -\psi_\gamma, 0, \psi_\gamma, \pi$, where

$$\psi_\gamma = \arccos(1/\gamma). \quad (25)$$

The energy $\mathcal{E}[\psi(x)]$ has a minimum for $\psi = \pm \psi_\gamma$ and a maximum for $\psi = 0, \pi$. The self-generated flux

$$\phi_s = -\frac{\phi_0 \xi}{2\pi} = -\frac{\phi_0 \xi_g}{2\pi} \sin \psi_\gamma = \mp \phi_0 \frac{\xi_g}{2\pi} \frac{\sqrt{\gamma^2 - 1}}{\gamma} \quad (26)$$

arises in the two stationary states with $\psi = \pm \psi_\gamma$, each of these states corresponds to a minimum energy \mathcal{E} . The assumption $\langle \xi(x) \rangle \ll 1$ restricts the value of γ . However, it follows from Eqs. (13) and (21) that $\langle \xi(x) \rangle \ll 1$ and $\gamma > 1$ hold simultaneously only if

$$\frac{\Lambda_J}{l} \langle |g(x)| \rangle \ll \frac{\Lambda_J^2}{l^2}. \quad (27)$$

Inequalities (27) describe the applicability domain of the above analytical approach. In particular, Eq. (27) restricts the amount of the local critical current density variation. Indeed, the value of $\langle |g(x)| \rangle$ can be estimated as $\langle |g(x)| \rangle \sim j_c^{\text{max}}/\langle j_c \rangle$, where j_c^{max} is the maximum value of the alternating critical current density ($j_c^{\text{max}} \gg \langle j_c \rangle$). It follows then from Eq. (27) that the developed analytical approach is valid provided

$$j_c^{\text{max}} > \langle j_c \rangle \sqrt{\frac{c\phi_0}{\lambda l^2 \langle j_c \rangle}}, \quad (28)$$

and

$$j_c^{\max} \ll \langle j_c \rangle \frac{c \phi_0}{\lambda l^2 \langle j_c \rangle}, \quad (29)$$

i.e., the variation of the critical current density should be large Eq. (28); still it should not exceed the limit (29).

Using Eqs. (12) and (26) we estimate $|\phi_s(x)|$ as

$$|\phi_s(x)| \sim \phi_0 \frac{\sqrt{\gamma^2 - 1}}{\gamma} \frac{l^2}{\Lambda_J^2} |g(x)| \ll \phi_0. \quad (30)$$

The above results hold only for a periodic critical current density $j_c(x)$ and the predicted self-generated flux $\phi_s(x)$ has a typical amplitude of variations which is much less than the one observed experimentally.²³

IV. NONPERIODIC ALTERNATING CRITICAL CURRENT DENSITY

The above analytical approach to the problem of a self-generated flux in a nonuniform Josephson junction is based on an assumption that the critical current density $j_c(x)$ is an alternating periodic function. This model allows for analytical calculation and provides a reasonable preliminary insight into the properties of an idealized Josephson junction with an alternating $j_c(x)$. At the same time this simple model fails for a quantitative description of any real system with a certain randomness of the spatial distribution of Josephson critical current density $j_c(x)$. In this section we generalize the above approach assuming that the alternating critical current density $j_c(x)$ is almost periodic, i.e., we assume that there is a typical length of interchange of sign of $j_c(x)$ which is distributed randomly near some mean value l .

In the case of an almost periodic $j_c(x)$ we cannot apply the two-scale perturbation theory in the same way as we did it in the previous section. Indeed, an arbitrary solution of Eq. (8) takes the form

$$\xi(x) = \frac{\sin \psi}{\Lambda_J^2} G(x), \quad (31)$$

where

$$G(x) = \int_a^x dx' \int_{a'}^{x'} dx'' g(x''), \quad (32)$$

and the integration constants a and a' are defined by the boundary conditions. The random function $G(x)$ increases with an increase of the integration interval. In general, the value of $|G(x)|$ can become arbitrarily large if the length of the tunnel junction \mathcal{L} becomes large enough. This is in contradiction with our main assumption that the phase $\xi(x)$ is a small and fast varying component of the total phase difference $\varphi(x)$. To solve this contradiction we write $\xi(x)$ as

$$\xi(x) = \frac{\sin \psi}{\Lambda_J^2} [G(x) - G_a(x)]. \quad (33)$$

The function $G_a(x)$ is a smoothing average of $G(x)$ over an interval with a certain length \mathcal{L}_a , where $l < \mathcal{L}_a \ll \mathcal{L}$.

The procedure of filtering out the smooth part of $G(x)$ is especially evident if we use Fourier series for $g(x)$ and $G(x)$. Introducing the Fourier transform for $g(x)$ as

$$g(x) = \sum_{-\infty}^{\infty} g_k e^{ikx} \quad (34)$$

we find the Fourier series for the function $G(x)$ in the form

$$G(x) = - \sum_{-\infty}^{\infty} \frac{g_k}{k^2} e^{ikx}, \quad (35)$$

where the sums in Eqs. (34) and (35) are over the wave vectors $k = 2\pi n/\mathcal{L}$ and n is an integer. The smooth part of the function $G(x)$ can be obtained by extracting the fast-Fourier harmonics, i.e., by extracting from the sum (35) terms with wave vectors $|k| > k_a \sim 2\pi/\mathcal{L}_a$. As a result we find for $G_a(x)$ and $\xi(x)$ the series

$$G_a(x) = - \sum_{-k_a}^{k_a} \frac{g_k}{k^2} e^{ikx}, \quad (36)$$

$$\xi(x) = \frac{\sin \psi}{\Lambda_J^2} \left(\sum_{-\infty}^{-k_a} + \sum_{k_a}^{\infty} \right) \left[\frac{g_k}{k^2} e^{ikx} \right]. \quad (37)$$

The small and fast alternating part $\xi(x)$ of the phase difference $\varphi(x)$ is thus defined by Eq. (33). This equation is a straightforward generalization of the two-scale perturbation theory approach to a real case of an almost periodic $g(x)$.

Next, we use Eq. (33) to derive an equation for the smooth part $\psi(x)$ of the phase $\varphi(x)$. *First*, combining Eqs. (33), (7), and (32) we arrive at the relation

$$\Lambda_J^2 \psi'' - [1 + G_a''(x)] \sin \psi - g(x) \xi(x) \sin \psi = 0. \quad (38)$$

Second, we average Eq. (38) over an interval with a certain length L assuming that $l \ll L \ll \mathcal{L}_a$. This averaging results in an equation describing the phase $\psi(x)$

$$\Lambda_J^2 \psi'' - [1 + G_a''(x)] \sin \psi + \gamma(x) \sin \psi \cos \psi = 0, \quad (39)$$

where $\gamma(x)$ is defined by Eq. (15). It is worth mentioning that Eq. (39) differs from the analogues Eq. (9) by an additional term $G_a''(x)$ in the coefficient before $\sin \psi$ and by the fact that the parameter $\gamma = \gamma(x)$ is a function of the coordinate x along the junction.

The coefficient $1 + G_a''(x)$ is defined by magnetic field $B_c(x)$ which would be generated by a current with the density $j_c(x)$. Indeed, using Eqs. (1), (32), and Maxwell's equation $dB_c/dx = 4\pi j_c/c$ we obtain for $G(x)$

$$\begin{aligned} G(x) &= \frac{c}{4\pi \langle j_c \rangle} \int dx' [B_c(x') - B_a(x')] \\ &= \frac{2\pi \Lambda_J^2}{\phi_0} [\phi_c(x) - \phi_a(x)], \end{aligned} \quad (40)$$

where the magnetic field $B_a(x)$ would be generated by a constant current density $\langle j_c \rangle$, i.e., $dB_a/dx = 4\pi \langle j_c \rangle/c$, and $\phi_c(x)$ and $\phi_a(x)$ are the fluxes of the fields $B_c(x)$ and $B_a(x)$. It follows now from Eq. (40) that

$$1 + G_a''(x) = \frac{2\pi \Lambda_J^2}{\phi_0} \langle \phi_c(x) \rangle''. \quad (41)$$

As shown above the value of the parameter γ is determining the existence or absence of the self-generated flux. Using Eq. (8) and the definition of $\gamma(x)$ given by Eq. (15) we obtain for $\gamma(x)$ an expression

$$\gamma(x) = -\frac{\Lambda_J^2}{\sin^2 \psi} \langle \xi'' \xi \rangle = \frac{\Lambda_J^2}{\sin^2 \psi} \langle \xi'^2 \rangle > 0 \quad (42)$$

demonstrating that the condition $\gamma(x) > 0$ holds also in the case of an almost periodic critical current density.

A. Self-generated flux in a stationary state

Let us now consider stationary solutions for the smooth part $\psi(x)$ of the phase difference $\varphi(x)$ qualitatively. Assume *first* that there are sufficiently large intervals with lengths $L_i \gg \Lambda_J$, where the function $\psi(x)$ is constant or varies with a typical space scale of order $\mathcal{L}_i \gg \Lambda_J$. In this case Eq. (39) reduces to

$$[1 + G_a''(x) - \gamma(x) \cos \psi] \sin \psi = 0. \quad (43)$$

This equation is similar to Eq. (24) which we derived for the case of a periodic critical current density $j_c(x)$ and has different solutions depending on the value of the parameter

$$\gamma_r(x) = \frac{\gamma(x)}{1 + G_a''(x)}. \quad (44)$$

In the regions with $\gamma_r(x) < 1$, Eq. (43) has two solutions $\psi = 0$ and $\psi = \pi$ and therefore as it follows from Eq. (31) there is no self-generated flux in these regions.

The energy of a Josephson junction \mathcal{E}_φ given by Eq. (22) can be written in terms of the smooth part of the phase difference $\psi(x)$. In the case of an almost periodic critical current density $j_c(x)$ this equation reads

$$\mathcal{E}_\varphi = \frac{\hbar \langle j_c \rangle}{4e} \int dx \{ \Lambda_J^2 \psi'^2 - 2 \cos \psi [1 + G_a''(x)] - \gamma(x) \sin^2 \psi \} \quad (45)$$

and if $\gamma_r(x) < 1$, then the energy \mathcal{E}_φ has a minimum for $\psi = 0$ and a maximum for $\psi = \pi$.

In the regions where the function $\gamma_r(x) > 1$, Eq. (43) has four solutions $\psi = -\psi_\gamma(x)$, 0 , $\psi_\gamma(x)$, π , with

$$\psi_\gamma(x) = \arccos \left[\frac{1}{\gamma_r(x)} \right] = \arccos \left[\frac{1 + G_a''(x)}{\gamma(x)} \right]. \quad (46)$$

The energy \mathcal{E}_φ has a minimum for $\psi = \pm \psi_\gamma(x)$ and a maximum for $\psi = 0, \pi$. The self-generated flux is thus nonzero in the regions with $\gamma_r > 1$. This flux has a fast and a smoothly varying parts defined by $\xi(x)$ and $\psi_\gamma(x)$.

The randomness of the function $g(x)$ causes variation of $\gamma_r(x)$ along the junction. As a result of this variation intervals with $\gamma_r(x) > 1$ are interlaced with intervals with $\gamma_r(x) \leq 1$. As it was mentioned above, in the case of $\gamma_r > 1$ the energy of the Josephson junction \mathcal{E}_φ has a minimum for $\psi = \pm \psi_\gamma(x)$ and a maximum for $\psi = 0, \pi$. When the value of

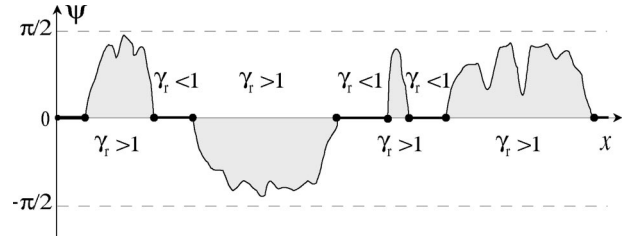


FIG. 1. Scheme of the smooth phase spatial distribution $\psi(x)$ as an alternation of two types of solutions corresponding to different values of the parameter γ_r .

$\gamma_r(x)$ changes from $\gamma_r(x) > 1$ to $\gamma_r(x) \leq 1$ the energy \mathcal{E}_φ still has a maximum if $\psi = \pi$, but a state with $\psi = 0$ becomes a state with a minimum energy.

The above results provide a qualitative description of experimentally observable flux distribution along a Josephson junction with an almost periodic alternating critical current density. This flux distribution spatially averaged by the measurement tools is defined by the function $\psi(x)$ (see Fig. 1). Inside the intervals with $\gamma_r(x) > 1$ the phase $\psi(x)$ tends to one of the solutions $\pm \psi_\gamma(x)$. The profile of the function $\psi(x)$ correlates with the profile of $\psi_\gamma(x)$, though does not coincide with it exactly because the solution $\psi(x) = \psi_\gamma(x)$ was obtained under assumption $\psi'' = 0$, which does not hold exactly for the intervals $\gamma_r(x) > 1$. The smooth part of the phase difference inside the intervals with $\gamma_r(x) \leq 1$ is $\psi = 0$ which is consistent with the assumption $\psi'' = 0$.

The value of ψ_γ increases quite fast with an increase of the parameter γ (see Fig. 2). In particular, for $\gamma = 2$ the value of ψ_γ is already about 0.75 of its maximum value $\pi/2$. This means that for most of the experimentally observable peaks of the self-generated flux the values of ψ will be close to $\pi/2$ which corresponds to a magnetic flux $\phi_0/4$. In some places of the junction the phase ψ changes from $-\psi_\gamma$ to ψ_γ . The flux localized in this area of the junction will be close to $\phi_0/2$.

V. NUMERICAL SIMULATIONS

A. The finite difference scheme

To study the self-generation of magnetic flux in a tunnel junction with an alternating critical current density numeri-

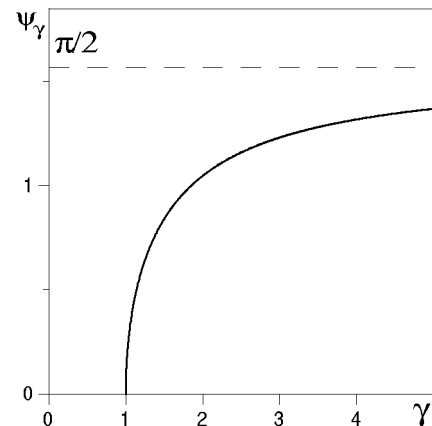


FIG. 2. Dependence of the smooth phase ψ_γ on the parameter γ .

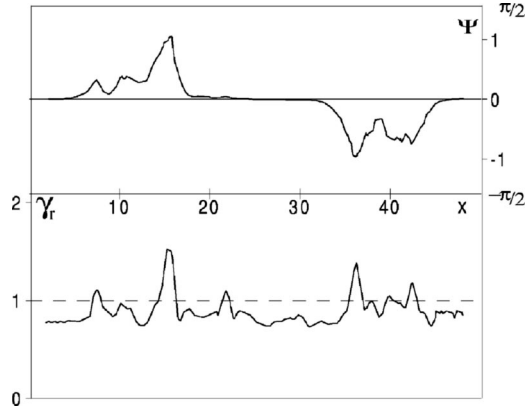


FIG. 3. Spatial distributions of the parameter $\gamma_r(x)$ and the corresponding smooth phase $\psi(x)$.

cally we introduced time dependence into the main equation (4)

$$\ddot{\varphi} + \alpha \dot{\varphi} - \Lambda_J^2 \psi'' + [1 + g(x)] \sin \varphi = 0, \quad (47)$$

where $\alpha \sim 1$ is a decay constant. This approach allows us to study both dynamics and statics of the system.

The term $\alpha \dot{\varphi}$ introduces dissipation. As a result of this dissipation the relaxation of the system ends up in one of the stable stationary states described by a certain solution of the static equation (4). Moreover, for a given distribution of the critical current density $j_c(x)$ we obtained different static solutions when we start the numeric simulation from different initial states. We compare and classify these solutions based on the features of the function $j_c(x)$. Indeed, this function essentially describes the pinning properties of the junction. Therefore, a variety of initial conditions can converge to a similar flux-pinning pattern.

To solve Eq. (47) numerically we use the finite difference scheme.²⁷ We adapted this method to our case and checked the stability and convergency of the obtained solutions. As a result we arrived at the following scheme:

$$\varphi \rightarrow \frac{\varphi_{m+1}^n + \varphi_{m-1}^n}{2} \equiv \tilde{\varphi}_m^n, \quad (48)$$

$$\dot{\varphi} \rightarrow \frac{\tilde{\varphi}_m^n - \varphi_m^{n-1}}{\tau}, \quad (49)$$

$$\ddot{\varphi} \rightarrow \frac{\varphi_{m+1}^{n+1} + \varphi_{m-1}^{n+1} - 2\tilde{\varphi}_m^n}{\tau^2}, \quad (50)$$

$$\varphi'' \rightarrow \frac{\varphi_{m+1}^n + \varphi_{m-1}^n - 2\varphi_m^n}{h^2}, \quad (51)$$

where $f_m^n = f(x_m, t_n)$, τ and h are steps along t and x correspondingly. Next, we choose units providing $\Lambda_J = 1$ and set $h = \tau$. As a result we arrive at the following finite difference scheme:

$$\varphi_m^{n+1} = -(1 - \alpha\tau)\varphi_m^{n-1} + (2 - \alpha\tau)\tilde{\varphi}_m^n - \tau^2(1 - g_m)\sin \tilde{\varphi}_m^n. \quad (52)$$

B. Stationary solutions

Initially a certain random function $g(x)$ is generated for an interval with a length L with a given values of l and δl [a typical length scale of the function $g(x)$ and its dispersion], g and δg [amplitude of the function $g(x)$ and its dispersion]. This allows us to calculate the function $\gamma_r(x)$ for the whole interval. An initial state $\varphi_0(x)$ is prepared as a random or some specific function. Finally, the dynamical rules (52) are applied to the initial state iteratively until a stationary state is established.

In Fig. 3 we show one of the stationary solutions obtained by a numerical simulation and the function $\gamma_r(x)$ calculated for this solution. It is clearly seen from Fig. 3 that $\varphi(x)$ arises at the places where $\gamma_r(x)$ exceeds 1. Heights of the peaks are less than $\pi/2$, and thus the corresponding magnetic flux amplitudes are less than $\phi_0/4$.

In general a different initial state of the same sample, i.e., for the same function $\gamma_r(x)$, generates a different stationary state. Our numerical simulations show that these different states differ only by the sign of some peaks of $\varphi(x)$, but the shapes and locations stay unchanged.

We have compared our results with the experimental data.²³ The typical amplitude of the flux variations measured by a SQUID pickup loop with a size of several Λ_J is about 0.25 of ϕ_0 with rare narrow picks with an amplitude about $0.5\phi_0$ which is in good agreement with our calculations.

VI. SUMMARY

We treated a Josephson junction with an alternating critical current density $j_c(x)$ as a model for considering electromagnetic properties of grain boundaries in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ superconducting films. The study is mainly focused on a specific case of an almost periodically alternating function $j_c(x)$. We demonstrated both analytically and numerically that under certain conditions a self-generated flux pattern arises for this type of spatial distribution of the critical current density $j_c(x)$. The obtained flux pattern with two types of interlacing flux domains is similar to the one which was recently observed experimentally in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ superconducting films in the absence of an external magnetic field. The typical amplitude for the magnetic flux peaks is of order $\phi_0/4$ and $\phi_0/2$ and the typical distance between the peaks depends on the spatial distribution of $j_c(x)$.

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