New ideas for long Josephson junctions realistic devices simulation

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Abstract. In the paper, we consider the problem of numerical simulation of long Josephson Junction (JJ) devices. Our interest to the problem is motivated by need of effective parameters calculation of Flux Flow Oscillator (FFO). Practical FFOs have complicated structures and traditional model in form of simple perturbed sine-Gordon equation is inadequate because it doesn’t capture important physical details. In this work, we evaluate variable coefficient 1D sine-Gordon equation and boundary conditions for this 1D equation starting from full 2D model of junction and 3D magnetic field problem for bias and control line currents. Then this 1D problem is solved numerically using implicit time stepping numerical procedure. As result program FFOSIM was developed. It is a general tool that allow calculations of critical current, I-V curves and other values. We present results of calculations of junctions inside microstrips where boundary conditions were evaluated using 3D magnetic field calculation program 3D-MLSI.

1. Introduction

Long distributed Josephson Flux Flow Oscillators (FFO) presently are successfully implemented in superconductive microwave devices. The problem of design of practical microwave devices requires accurate and reliable numerical models of FFO and adequate simulation tools. Conventional mathematical model of long FFO is one-dimensional perturbed sine-Gordon equation. Unfortunately classical ideal form of this equation with constant coefficients does not contain important physical effects and is not accurate enough. Thus the focus of simulation needs is moving now to more practical features that conventional model doesn’t take into account. In the paper we re-evaluate more general one-dimensional static and dynamic sine-Gordon equations with variable coefficients using full two-dimensional equations and solve one-dimensional problem numerically using accurate and stable numerical procedure. This numerical procedure was implemented in our code FFOSIM that was specially developed for engineering simulations of FFO and other long JJ devices. This program can calculate variable width junctions, p - junctions, idle regions and unbiased tails. Bias current as well as control line current can be non-homogeneous and can contain delta functions. For correct device modeling realistic bias current and control line currents are necessary. We calculate these currents using our three-dimensional simulation tool 3D-MLSI and import results into FFOSIM. I-V curves and critical currents can be calculated as well as dynamics of fluxons. Results of calculations of
critical current for inline sin-like JJ inside rectangular microstrip and one practical FFO design [1] are presented in the paper.

2. Problem formulation

2.1. 3D problem for overlap JJ

The problem we consider schematically is presented on Fig. 1. Superconducting sheets form double layer overlapping microstrip structure. Josephson junction $A^I$ occupy whole or a part of overlapping region. The device is driven by two currents, bias current $I_b(t)$ that pass from one sheet to another across JJ and controlling current $I_d(t)$ that flow on top or bottom sheet. Sheets thickness is assumed to be thin to compare with London penetration depth. $w_1(x)$ is width of JJ area $A^I$ and $w_2(x)$ is the width of overlapping area where $L$ is the length overlapping region and $0 \leq x \leq L$. Both functions $w_1(x)$ and $w_2(x)$ are non-negative and can be stepped.

In [2] it is shown that using shortening principle the problem for current flow can be approximately splitted on two separate problems. First problem is 3D task for sheet current evaluation when double layer structure is combined to single layer structure by filling dielectrics between superconductor sheets by superconductor thus resulting in single sheet of variable thickness. When first problem is solved and current in joint sheet is evaluated, normalized current component normal to boundary of overlap region $A^{II}$ should be taken as result of calculations. On certain part $C^-$ of boundary of $A^{II}$, $C = C^+ \cup C^-$ (see Fig. 1), normal component should be inverted. Thus the answer for first problem are two functions $M_b(r)$ and $M_d(r)$ given on the boundary of the overlapping region $C$ and normal to this boundary current $j_n(r,t)$:

$$ j_n(r,t) = M_b(r) \cdot I_b(t) + M_d(r) \cdot I_d(t). $$

and

$$ \int_C M_b(r)dl = 1, \quad \int_C M_d(r)dl = 0. $$

Figure 1. 2D overlap JJ, top view. $A^I$ - junction, $A^{II}$ - microstrip overlapping layers, $A^{III}$ - single layer structure needed for 3D magnetic field and currents calculations.
Second problem is boundary value problem in overlapping region \( A^I \cup A^{II} \) for JJ dynamics when boundary current \( j_n(r, t) \) is given.

The accuracy of this approach depends on importance of stray field effects for buried JJ. If stray field is small then these two problems can be accurately decoupled. The problem of stray field for FFO was investigated in [4]. It was found that for typical long JJ FFO stray field effects can be neglected. In our work we assume that decoupling approach is valid.

2.2. 2D problem for JJ

Two-dimensional problem for JJ are well-known [2]. Let \( L_{\square} = \mu_0 d(r) \) be per-square inductance, \( d(r) \) -effective magnetic gap, \( \varphi(r, t) \) - phase difference between layers. Solution domain is presented on Fig. 3. Then current conservation law gives

\[
\nabla \left( \frac{\Phi_0}{2\pi L_{\square}(r)} \nabla (\varphi(r, t) + \beta \dot{\varphi}(r, t)) \right) = J_z(r).
\]

(3)

For brevity we assume that current density across JJ has simple resistive form [2, 3]

\[
J_z(r, t) = C_{\square}(r) \dot{v}(r, t) + \begin{cases} \dot{I}_c \dot{\varphi}(r, t) \sin(\varphi) + v(r, t)/R_{\square}(r) & r \in A^I, \\ 0 & r \in A^{II}. \end{cases}
\]

(4)

where \( C_{\square} \) is area capacitance, \( v(r, t) = \frac{\hbar}{2\pi} \dot{\varphi}(r, t) \) - voltage. We use non-dimensional function \( \dot{I}_c(r) \) for definition of non-uniform critical current density. In computer program, we have several different models for normal and superconductive currents across JJ [2].

Boundary conditions for (3) are

\[
\frac{\Phi_0}{2\pi L_{\square}(r)} \frac{\partial}{\partial n}(\varphi(r, t) + \beta \dot{\varphi}(r, t)) = j_n(r, t), \quad r \in C.
\]

(5)

where \( j_n(r, t) \) is calculated using (1).

In general (3) is wave equation. Typically JJ per-square capacitance in JJ domain \( A^I \) is much larger then in microstrip domain \( A^{II} \). Then capacitance in \( A^{II} \) can be neglected. In this case equation (3) differential-algebraic from respect to \( t \).

![Figure 2. 2D problem in \( A^I \cup A^{II} \).](image-url)
2.3. 1D problem for long JJ

The problem (3), (5) still can be simplified if microstrip with JJ is sufficiently long. Let \( \lambda_J^2 = \Phi_0/(2\pi L \square L_c) \). If \( w_2(x), w_1(x) \ll \lambda_J \ll L \), then one-dimensional equation for mean value function

\[
\varphi(x) = \frac{1}{w_2(x)} \int_{y_{\min}(x)}^{y_{\max}(x)} \varphi(x, y) dy
\]

can be evaluated [2]. For brevity, we take everywhere below \( \beta = 0 \).

Consider standard notations

\[
L\square = \mu_0 \cdot (\lambda_1 + \lambda_2),
\]

\[
W(x) = w_1(x) \frac{L\square}{LII(x)} + (w_2(x) - w_1(x)) \frac{L\square}{LII(x)},
\]

\[
C\square = \frac{\varepsilon_1 \varepsilon_0}{d_1},
\]

\[
C(x) = w_1(x) \frac{\varepsilon_1 \varepsilon_0}{d_1(x)} + (w_2(x) - w_1(x)) \frac{\varepsilon_2 \varepsilon_0}{d_2(x)}.
\]

\( LII(x) \) and \( LII(x) \) are inductances in \( A' \) and \( A'' \), \( d_1(x) \) and \( d_2(x) \) are dielectric gaps, \( \varepsilon_1 \) and \( \varepsilon_2 \) are dielectric permittivities, \( \lambda_1 \) and \( \lambda_2 \) are London penetration depths in bottom and top sheets, see Fig. 2. Then averaging (3) over \([y_{\min}(x), y_{\max}(x)]\) the next problem for \( \varphi(x, t) \) can be obtained:

\[
\frac{\partial}{\partial x} \left( \frac{\Phi_0 W(x)}{2\pi L\square} \frac{\partial \varphi(x, t)}{\partial x} \right) = \frac{\hbar}{2e} C(x) \frac{\partial^2 \varphi}{\partial t^2} + w_1(x) \left( \bar{I}_c(x) I_c \sin(\varphi) + \frac{\hbar}{2e R\square} \frac{1}{\partial t} \frac{\partial \varphi}{\partial t} \right) - j(x, t),
\]

\( j(x, t) = I_b(t) \cdot \bar{I}_b(x) + I_{cl}(t) \cdot \bar{I}_{cl}(x), \)

\[
\frac{\Phi_0 W(0)}{2\pi L\square} \frac{\partial \varphi}{\partial x}(0, t) = I_0(t),
\]

\[
\frac{\Phi_0 W(L)}{2\pi L\square} \frac{\partial \varphi}{\partial x}(L, t) = I_L(t).
\]

From (1) we also obtain

\[
\bar{I}_b(x) = M_b(x, y_{\max}(x)) + M_b(x, y_{\min}(x)) + \sum_k p_k \delta(x_k),
\]

\[
\bar{I}_{cl}(x) = M_{cl}(x, y_{\max}(x)) + M_{cl}(x, y_{\min}(x)) + \sum_k q_k \delta(x_k)
\]

\[
I_0(t) = M_{bL}^0 I_b(t) + M_{clL}^0 I_{cl}(t),
\]

\[
I_L(t) = M_{bL}^L I_b(t) + M_{clL}^L I_{cl}(t)
\]

where \( K \) is the number of vertical segments of boundary, see Fig. 2, \( p_k, q_k \) are coefficients, \( \delta(x_k) \) are delta-functions.

The procedure of evaluation of 1D equations starting from 2D problem is a known technique [2]. We only pay attention that stepped boundary gives stepped functions \( W(x) \) and delta-function terms in \( j(x, t) \).

When the 1D problem is formulated, we can introduce additional terms in the equations. We allow any lumped values of capacitance \( C \), normal resistance \( R \) and critical current density
\( I_s(x) \) in the equation. For boundary conditions we can introduce external \( RC \) loads as it was done in [5].

Before the solution, the problem should be presented in non-dimensional form. Standard procedure is implemented. Taking values \( \lambda^2 = \frac{\varphi_0}{2\pi L_\square I_c}, \omega_\varphi^2 = \frac{2eL_c}{RC}, \omega_c = \frac{2eL_c R_c}{\hbar}, \alpha = \frac{\varphi}{\omega_c} \) and \( x = \lambda_J \xi \quad 0 \leq \xi \leq L/\lambda_J = l, \theta = \omega_p t, \) and measuring length in microns we obtain equation

\[
(W(\xi) \varphi_\xi)_\xi = \kappa(\xi) \ddot{\varphi} + \alpha(\xi) \dot{\varphi} + w_1(\xi) \bar{I}_c(\xi) \sin(\varphi) - \frac{j(\xi, \theta)}{I_c},
\]

\[
\kappa(\xi) = \frac{C(\xi)}{C_\square}, \quad \alpha(\xi) = \frac{\omega_p w_1(\xi)}{\omega_c R_c(\xi)}.
\]

Boundary conditions are

\[
W(0) \varphi_\xi(0, \theta) = \frac{I_0}{L_\square \lambda_J} = \Gamma_0(\theta), \quad W(L) \varphi_\xi(L, \theta) = \frac{I_L}{L_\square \lambda_J} = \Gamma_L(\theta)
\]

or more complicated expressions accounting external circuits currents. Thus weakly non-linear wave equation with variable coefficients is obtained. This equation should be solved numerically.

3. Outline of numerical technique

3.1. Goals of calculations

Two problems are most interesting for numerical calculation. First problem is calculation of sequence of I-V curves in form of a table for voltage \( V(I_\text{cl}, I_\text{b}) \). Second problem is calculation of critical bias current when voltage reach small threshold value. Thus for given threshold the table for function \( I_\text{cl}(I_\text{b}) \) should be calculated. In both cases the key problem is voltage calculation.

We can calculate voltage if we can calculate solutions of (11), (20) [6].

Let \( \langle \varphi(x, t) \rangle \) be the mean value of \( \varphi(x, t) \) on \([0, L]\). Then voltage \( V \) is the limit of values \( V_n \) when \( n \) tends to infinity and suitable sufficiently large averaging window size \( T \) is given:

\[
V_n = \frac{1}{T} \int_{T/(n-1)}^{T-n} \langle \varphi_t(x, t) \rangle dt = \frac{1}{T} (\langle \varphi(x, T \cdot n) \rangle - \langle \varphi(x, T \cdot (n - 1)) \rangle).
\]

Our main task is to solve (11), (20) numerically on a large time interval. Thus it is important to pay some attention on stability and accuracy of numerical technique. In other case systematic errors can make solution noisy and results doubtful.

3.2. Approximation in space

The right numerical algorithm should express physical conservation laws. For 1D problem space approximation of the solution can be evaluated using Finite Volume method that express current balance. For that purpose we rewrite the equation

\[
(W(\xi) \varphi_\xi)_\xi = \Phi(\xi), \quad \Phi(\xi) = F(\varphi, \xi, \theta) + \kappa(\xi) \ddot{\varphi} + \alpha(\xi) \dot{\varphi}.
\]

Then we introduce numerical mesh \( \{\xi_i\}, \quad i = 0, \ldots, N, \xi_0 = 0, \xi_N = l \) and write numerical approximation for the left part

\[
(W(\xi) \varphi_\xi)_\xi(\xi_i) \approx (L_n \varphi)_i = \frac{1}{h_i} (W_{i+1/2} \frac{\varphi_{i+1} - \varphi_i}{h_{i+1}} - W_{i-1/2} \frac{\varphi_i - \varphi_{i-1}}{h_i}),
\]

\( h_i \) is the mean value of \( \varphi \) in the equation. For boundary conditions we can introduce external \( RC \) loads as it was done in [5].
where $h_i = 0.5 * (h_{i+1} - h_i)$, $h_i = \xi_i - \xi_{i-1}$ are steps of non-uniform mesh. Special care should be taken for boundary points $i = 0$ and $i = N$. After simple evaluation we obtain result:

$$\kappa(\xi_i)\dot{\varphi}_i + \alpha(\xi_i)\dot{\varphi}_i = (L_h\varphi)_i - F_i, \quad i = 1, \ldots, N - 1; \quad (24)$$

$$\kappa(\xi_0)\dot{\varphi}_0 + \alpha(\xi_0)\dot{\varphi}_0 = 2W_{0.5}\frac{\varphi_1(\theta) - \varphi_0(\theta)}{h_1^2} - \frac{2\Gamma_0(\theta)}{h_1} - F_0(\theta), \quad (25)$$

$$\kappa(\xi_N)\dot{\varphi}_N + \alpha(\xi_N)\dot{\varphi}_N = -2W_{N-0.5}\frac{\varphi_N(\theta) - \varphi_{N-1}(\theta)}{h_N^2} + \frac{2\Gamma_N(\theta)}{h_N} - F_N(\theta). \quad (26)$$

This finite differences or finite volumes technique is well known. The only thing one should mention is to have all points of discontinuity and delta-functions points as mesh points. This simple approximation has second order of accuracy in space and doesn’t introduce any non-physical current sources because simply express current conservation law on the mesh.

### 3.3. Approximation in time

Next step is constructing time stepping procedure. For this purpose we rewrite the equations in matrix form $C\ddot{\varphi}_i + G\dot{\varphi}_i + K\varphi_i = g_i$, $i = 0, \ldots, N$. Here $C$ and $G$ are diagonal matrices and $K = -L_h$ is tridiagonal matrix. Matrix $C$ can contain zeros or highly different non-zero values on main diagonal. It dictates the choice of implicit time stepping procedure. Let $\tau$ be time step, then we apply well-known symmetric Newmark implicit scheme

$$\frac{\varphi^{n+1} - 2\varphi^n + \varphi^{n-1}}{\tau^2} + \frac{G(\varphi^{n+1} - \varphi^{n-1})}{2\tau} + \frac{1}{4}K(\varphi^{n+1} + 2\varphi^n + \varphi^{n-1}) = \frac{1}{4}(g^{n+1} + 2g^n + g^{n-1}) \quad (27)$$

To resolve non-linearity, in the area of JJ $A^{II}$ we make one step using explicit scheme and calculate $g^{n+1}$. For linear problems without losses (27) is energy preserving.

On every time step the system of linear equations with well-defined tridiagonal matrix $C + 0.5\tau G + 0.25\tau^2K$ should be solved. It is very simple and fast procedure. The implicit time stepping algorithm is nearly equal in CPU time to explicit time stepping procedure but allow larger time step.

On practice we take space and time steps in the way that fluxons were correctly approximated with sufficient number of nodes. The accuracy of this method is $O(\tau^2 + (\max(h_i))^2)$.

### 3.4. FFOSIM

The described numerical algorithm was implemented in our program FFOSIM. It can calculate I-V curves, critical currents and dynamics of junction. The input for this program is ASCII text file where in simple form non-homogenous data including steps and delta-functions can be easily presented. Typically numerical technique parameters are not very interested for user. The program can evaluate these parameters automatically from physical input data. Nevertheless manual tuning of tolerances, accuracy and relaxation time is also possible. Bias and control line currents can be calculated and imported from our program 3D-MLSI [7] as well as the geometry of junction.

### 4. Results of calculations

#### 4.1. Inline JJ with idle regions

One of the non-trivial problems with known solution is the inline junction with sin-like junction inside rectangular microstrip, Fig. 3. The measurements for this device were presented in [8]. Calculations of critical current were performed in [9]. Problem definition, the necessary parameters values and results of these calculations can be also found in [2]; we reiterated these calculations using FFOSIM. The results are presented on Fig. 3. We see that good agreement between calculations and measurements is obtained.
4.2. FFO critical current calculations

Other example is calculation of critical current of one sample of FFO family described in [1]. The rough draft of the device is the Fig. 1. Using 3D code [7] we calculate $M_b(r)$ and $M_d(r)$ (1) and pass this data as well as junction geometry to FFOSIM. FFOSIM build 1D model with realistically mixed overlap-inline current supply. Then we define the necessary material parameters (critical current density and others) and calculate critical current. The results are on Fig. 4.

It is seen that we obtain qualitative agreement with measurements but our critical current profile is more narrow then measured. The possible reason of this deviation is low accuracy of our 3D magnetic field calculation tool [7]. Really code [7] for this problem operates over it’s limit of reliability.

5. Conclusions

We evaluated modeling technique and software FFOSIM for long JJ simulation. The program support realistic geometry of the devices and can import boundary conditions from 3D magnetic field calculation program [7]. The distinction feature of FFOSIM is the ability to handle irregular data including stepped and delta functions. The program can easily simulate stepped width junctions as well as different $\pi$-junctions. For simulation of dynamics different JJ models [2], [3]: resistive, non-linear resistive and adiabatic, can be used.

The calculations we performed show that for accurate quantitative comparison with measurements some improvements are necessary. The accuracy and ability to solve large size problems of companion program 3D-MLSI [7] should be improved. As it was shown in [10] and [5], for accurate I-V curves calculation more accurate models then resistive and non-linear resistive models of JJ current are necessary. Thus we plan to improve 3D magnetic field calculations and investigate the accuracy of more complicated models for JJ current. Other features we plan to implement are annular geometry and coupling with external loading circuit.
Acknowledgments

We would like to thank V. P. Koshelets, E. B. Goldobin and A. S. Sobolev for fruitful discussions. The work was supported by ISTC project 3174 and Russian Fund for Basic Research (grants # 08-02-90105-mol-a, # 07-02-00918-a).

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