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Numerical Study of Josephson Nanostructures Using Parallel Computing

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Abstract. We investigate the phase dynamics of the stack of long JJs, the length of which exceeds the Josephson penetration depth λ_J , taking into account the inductive and capacitive couplings between junctions and diffusion current. Numerical simulation of current-voltage characteristics of the stack is based on numerical solution of a system of nonlinear partial differential equations by the fourth order Runge-Kutta method and finite-difference approximation. The calculations are performed using the MPI technique for parallel implementation. The methodical calculations on multi-processor cluster (LIT JINR) with a different number of parallel MPI-processes are carried out. We have shown that the developed parallel algorithm provides about 7 time acceleration in comparison with serial simulation.

Keywords: Josephson junction, inductive coupling, capacitive coupling

1. Introduction

The layered high-Tc superconducting materials such as $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) can be considered as a stack of coupled Josephson junctions (JJs) [1]. The interest to the investigation of this system is caused by its rich nonlinear properties. The JJs stack demonstrates a series of interesting properties such as parametric resonance [2,3,4], chaotic features [5] and in this system the fluxons [6,7,8,9] and collective excitations [4,10,11] can arise. Also, this system is one of the promising objects of superconducting electronics [12,13]. Coherent terahertz electromagnetic radiation from this system provides wide possibilities for various applications [14]. The possibility of branching of the current–voltage characteristic in the region of zero field step was demonstrated [15], which is associated with different numbers of fluxons in each Josephson junctions. In Ref.[16] we showed the coexistence of the charge traveling wave and fluxon states. This state considered as a new collective excitation in the system of coupled Josephson junctions. It was demonstrated that the observed collective excitation leads to the decrease of radiation power from the system.

So, the stack of coupled JJs can be considered as a laboratory for studying nonlinear phenomena in superconducting nanostructures. Therefore, the construction of a model that ensures an adequate description of the properties of the coupled JJs in the high temperature superconductors is one of the topical tasks of modern physics of superconductivity. Also, an actual problem is the construction of effective numerical algorithms for simulation of the phase

dynamics of the stack of JJ.

To describe the JJs stack in Ref. [17] a model with inductive coupling between JJs was proposed. Later, Machida and Sakai proposed the model which takes into account both inductive and capacitive couplings [18]. In Ref. [4], we generalized this model with the additional diffusion current [19], whose significance was emphasized.

In this paper, we investigate the effectiveness of a parallel numerical approach for simulation of phase dynamics of stacked JJs taking into account the inductive and capacitive couplings [17,18] and the diffusion current [20]. Simulation is based on a numerical solution of a system of nonlinear partial differential equations by the fourth order Runge-Kutta method, a finite-difference approximation, and the MPI technique for parallel implementation. The effectiveness of the MPI/C++ code is confirmed by calculations on the multi-processor cluster (LIT JINR, Dubna). Contributions, which report significant and original research results in different areas of physics, are welcomed.

2. Theoretical model and numerical approach

Let us consider the layered structure with $N+1$ superconducting and interjacent insulating layers. The x-and y-axes are directed along the length of JJ L and along the width of superconducting layers W, respectively. The z-axis is perpendicular to the superconducting layers. The length of JJ $L > \lambda_J$ and the width $W << \lambda_J$. Each superconducting layer with number l is described by the Ginzburg-Landau order parameter $\Delta_l = |\Delta_0| \exp(i\theta_l)$, where θ_l is the phase of the order parameter. The l-th and $l-1$-th superconducting layers form the l-th JJ and it is described by the gauge-invariant phase difference (1) of the Ginsburg-Landau order parameter [18].

$$\varphi_l = \theta_l - \theta_{l-1} - \frac{2e}{\hbar c}\int_{z_{l-1}}^{z_l} A_z dz \tag{1}$$

where e - the electrical charge, $\hbar$ - the Plank constant, c - the speed of light in vacuum and A_z is the vector potential. In the framework of this model, due to the presence of capacitive coupling, the AC Josephson relation is generalized and can be written as

$$\frac{\hbar}{2e}\frac{\partial \varphi_l}{\partial t} = D_c V_l + s_c V_{l+1} + s_c V_{l-1}, \tag{2}$$

where $D_c = 1 + (2\lambda_e / d_I)\coth(d_s / \lambda_e)$ is the effective electrical thickness of JJ normalized to the insulating layer thickness d_I, $s_c = -\lambda_e / [d_I \sinh(d_s / \lambda_e)]$ is the capacitive coupling parameter, V_l is the voltage on the l-th JJ, d_s is the thickness of superconducting layer, and λ_e is is Debye screening length. The derivative of phase difference φ_l of lth with respect to the coordinate depends on the magnetic field of the l-th JJ and neighbor $l+1$-th and $l-1$-th junctions.

$$\frac{\hbar c}{2eD_{£}}\frac{\partial\varphi_l}{\partial x}=B_l+SB_{l+1}+SB_{l-1}, \tag{3}$$

where $S=s_{£}/D_{£}$ is the inductive coupling parameter, $s_{£}=-\lambda_L/\sinh(d_s/\lambda_L)$, $D_{£}=d_I+2\lambda_L\coth(d_s/\lambda_L)$ is the effective magnetic thickness of JJ, and λ_L is the London penetration depth. The valid values of the inductive coupling parameter S are in the range $S\in(-0.5,0]$. The system of equations, which describes the phase dynamics of the coupled long JJs stack in the normalized quantities, can be written as follows:

$$\begin{cases}\dfrac{\partial\varphi_l}{\partial t}=D_C V_l+s_C V_{l+1}+s_C V_{l-1},\\ \dfrac{\partial V_l}{\partial t}=\displaystyle\sum_{k=1}^{N}£_{lk}^{-1}\frac{\partial^2\varphi_k}{\partial x^2}-\sin\varphi_l+\beta\frac{\partial\varphi_l}{\partial t}+I,\end{cases} \tag{4}$$

In this system of equations the voltage is normalized to $V_0=\hbar\omega_p/(2e)$, where $\omega_p=\sqrt{8\pi d_I e j_c/(\hbar\varepsilon)}$ is the plasma frequency of JJ, j_c is the critical current of JJ, and ε is the dielectric constant of the insulating layer. The time t and coordinate x are normalized to ω_p and λ_J, respectively. Here $\beta=\sigma V_0/(d_I j_c)$ is the dissipation parameter, σ is the conductance of JJ, and I is the bias current normalized to the critical current j_c. The matrix of inductive coupling $£$ has the form

$$\hat{£}=\begin{pmatrix}1 & S & 0 & \dots & & & S\\ & & & & \dots & & \\ \dots & 0 & S & 1 & S & 0 & \dots\\ & & & & & & \\ S & & & & 0 & S & 1\end{pmatrix},$$

The initial conditions for the system of equations (4) are $\varphi_l(x,0)=0$ and $V_l(x,0)=0$. The boundary conditions in the x direction given by the external magnetic field $(\hbar c)/(2eD_{£})\partial\varphi_l/\partial x|_{x=0,L}=B_{ext}$. In the z direction we use the periodic boundary condition: in the case $l=N$ $\varphi_{l+1}=\varphi_1$, $V_{l+1}=V_1$; in the case $l=1$ $\varphi_{l-1}=\varphi_N$, $V_{l-1}=V_N$.

3. Simulation of current-voltage characteristic

One of the main electromagnetic properties of the system is current--voltage characteristics (CVC). In order to calculate CVC, we first of all solve numerically the system of partial differential equations (4) for the fixed value of bias current I and obtain the spatiotemporal distribution of the phase difference $\varphi(x,t)$ and voltage $V(x,t)$ of JJs. The details of numerical

solution of differential equations are considered in the next section, and here we confine ourselves just to the consideration of the algorithm calculation of CVC. Next, we have averaged the obtained $V_l(x,t)$ with respect to the coordinate x using

$$\overline{V_l}(t) = \frac{1}{L}\int_0^L V_l(x,t)dx \tag{5}$$

and with respect to the time t with expression

$$\langle V_l \rangle = \frac{1}{T_{\max} - T_{\min}} \int_{T_{\min}}^{T_{\max}} \overline{V_l}(t)dt\,, \tag{6}$$

where $T_{\min}$ is the beginning of the averaging interval. The total voltage of the JJs stack can be calculated using $\langle V \rangle = \sum_{l=1}^{N} \langle V_l \rangle$. Integrals (5) and (6) are calculated using the Simpson method and the rectangles method, respectively. Then we change the bias current value by ΔI and repeat the above procedure. In our calculations the bias current increases from the starting value $I = 0.01$ to $I = I_{\max}$ and then decreases to $I = 0$.

4. Numerical scheme

In order to solve the system of eq.(4), we introduce the uniform mesh with the step size Δx in the coordinate x along JJ and the step size Δt in time (Fig.1).

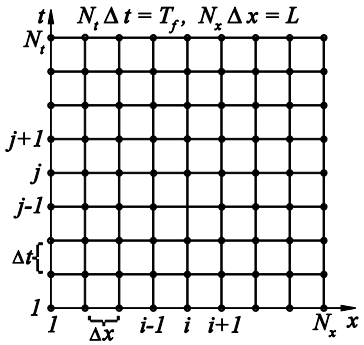

Figure 1. The uniform spatiotemporal mesh scheme

We denote the discrete coordinate by $x_i = \Delta x \times (i-1)$, where $i = 1,\ldots,N_x$ and $N_x = L/\Delta x + 1$ - the number of coordinate nodes. The discrete time is denoted by $t_j = \Delta t \times (j-1)$, where $j = 1,2,\ldots N_t$. The $x = 0$ corresponds to x_1; and $x = L$, to x_{N_x}. In the same way, $t = 0$ corresponds to t_1; and $t = T_{\max}$, to t_{N_t}, where $T_{\max}$ is the end of the time domain. We employ the standard second order finite difference approximation in the spatial coordinate x

$$\frac{\partial^2\varphi_l^1}{\partial x^2}=\frac{2(\varphi_l^2-\varphi_l^1)}{\Delta x^2}-\frac{2B_{\text{ext}}}{\Delta x},\qquad \frac{\partial^2\varphi_l^{N_x}}{\partial x^2}=\frac{2(\varphi_l^{N_x-1}-\varphi_l^{N_x})}{\Delta x^2}+\frac{2B_{\text{ext}}}{\Delta x},$$

$$\frac{\partial^2\varphi_l^i}{\partial x^2}=\frac{\varphi_l^{i+1}-2\varphi_l^i+\varphi_l^{i-1}}{\Delta x^2}.$$

Then we solve numerically the resulting system of ordinary differential equations for a fixed value of current I by the 4th-order Runge-Kutta (RK) algorithm (here l is the JJ number) in the interval $[0,L]$ by the coordinate and $[0,T_{\max}]$ by time and obtain the $\varphi_l(x,t)$ and $V_l(x,t)$ as functions of x and t. We put $\Delta t=\Delta x/5$ in accordance with the Courant-Friedrichs-Lewy condition in order to provide stability of the numerical scheme.

In order to investigate the collective excitations in the JJs stack like the longitudinal plasma wave[21] or charge traveling wave[22], we need to calculate the electric charge-time dependence in the superconducting layers. In this case, we calculate the electric charge normalized to $Q_0=\varepsilon V_0/4\pi d_s d_I$ as a function of x and t using the expression $Q_l(x,t)=V_l(x,t)-V_{l-1}(x,t)$ [4]. Then we average the value of $Q_l(x,t)$ with respect to the coordinate x using the Simpson method. For the external current value corresponding to the fluxon states we calculate the magnetic field \$B\$ in the JJs using the expression $B_l=\sum_{k=1}^{N}£_{lk}^{-1}(\partial\varphi_k/\partial x)$. The magnetic field is normalized to $B_0=\hbar c/2eD_L\lambda_J$.

5. Parallel implementation

The parallel algorithm is based on the distribution of calculations in the coordinate nodes x_i between the group of P_m parallel MPI-processes, where $m=0,1\ldots,M$. At each time step t_j, each process P_m calculates the RK coefficients and $V_l(x_i,t_j)$, $\phi_l(x_i,t_j)$ in the nodes $i_{\min}\le i<i_{\max}$, where $i_{\min}=m\times L_x/M$ and $i_{\max}=(m+1)\times L_x/M$. At each t_j the exchange between neighbor processes is arranged: each process P_m $(m<M-1)$ sends the RK coefficients and values of V and φ at $i=i_{\max}-1$-th point to the P_{m+1}-process; each P_m process $(m>0)$ sends the RK coefficients and solutions at $i=i_{\min}$ to the P_{m-1}-process. In order to calculate the average value V_l, the parallel calculation of the integral (5) is performed at each time-step t_j. Each P_m-process calculates the partial sum of elements $V_l(x_i,t_j)$ at each JJ with number l, in accordance with the Simpson quadrature formula. Then the resulting summation is performed in the process P_0. In the P_0-process V_l is averaged in time and in JJs number, and the resulting value is saved to the file. For some values of I the solutions $V_l(x_i,t_j)$ and $\phi_l(t_i,t_j)$ are collected in the process P_0 where they are saved to the file together with the respective physical characteristics.

6. Results and discussion

Let us discuss the effectiveness of the parallel algorithm. The calculations have been performed on the multi-processor cluster (LIT JINR) with a different number of parallel MPI-processes. For these calculations we put the number of JJs $N=10$ and $N=5$, the JJ length $L=5$ and $L=10$; $\Delta x=0.05$; $\Delta I=0.0001$. Figure 2 shows the calculation time (in minutes) of the CVC vs number of parallel processes for the following cases: $N=10$, $L=5$; $N=5$, $L=10$ and $N=10$, $L=5$. For all cases the minimal calculation time is achieved in the case of 12 processes. The ratio of the calculation time of 1 process and 12 processes for the case of $L=5$ and $N=10$ (line 1 in Fig.2) is equal to 5.38. The same ratio for the case of $L=10$ and $N=5$ (line 2 in Fig.2) is equal to 6.1. In the case $L=10$, $N=5$ the speedup is equal to 6.97 (line 3 in Fig.2).

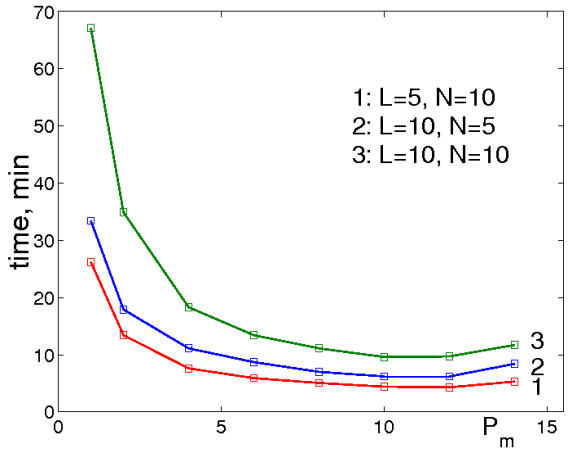

Figure 2. The dependence of calculation time on the number of processes.

One can see that the developed parallel algorithm provides 5-7 times acceleration (depending on the values of N and L) in comparison with the serial simulation. We should like to note that the good speed up of calculations can be obtained for the cases of big values of JJ length. In order to demonstrate efficient of IV-curve simulation using MPI technique we have calculated coefficient of acceleration of simulation depending on process numbers and this results are presented in Table 1.

Table 1. Acceleration of IV-curve simulation for stack with $N=10$ JJ and length $L=10$. The calculation are performed using MPI technique with coordinate step size $\Delta x=0.05$.

Process number	1	2	3	4	5
Acceleration coefficient	1.000	1.647	2.355	2.991	3.482
Process number	6	7	8	9	10
Acceleration coefficient	4.099	4.370	4.879	5.311	5.523
Process number	11	12	13	14	15
Acceleration coefficient	6.070	5.593	6.256	6.526	6.734

7. Conclusions

In this paper, we have presented the method of numerical simulation of the phase dynamics of the stacked JJs taking into account the inductive and capacitive couplings between junctions and diffusion current. In our investigation, we used the parallel and serial calculations of CVC. The parallel implementation is based on the MPI technique. We showed that the parallel algorithm provides about 7 time acceleration in comparison with the serial one.

Conflict of Interest

There are no conflicts of interest.

Author Contributions

The statement of the problem and derivation of model equations and preliminary serial numerical calculations have been done by I.R.Rahmonov and Yu.M. Shukrinov. The development of parallel simulation algorithm and parallel calculations are performed by E.V. Zemlyanaya, M.V. Bashashin and P.Atanasova. The results presented in Table 1 is obtained by A. R. Rahmonova. All authors are participated in the writing of the text.

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