Theory and Simulation of Electromagnetic Wave Emission from Intrinsic Josephson Junctions

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Abstract. Concerning the spontaneous THz electromagnetic wave emission from intrinsic Josephson junctions, we revisit the theory for intrinsic Josephson effects from standpoints of the couplings between stacked junctions and consequent superconducting phase dynamics. After reviewing the previous simulation works based on the theory, we present recent multi-physics simulation studies suggested by authors to systematically reproduce the emission experiments. Some typical simulation results are exhibited and the future perspective of the simulation is also given.

1. Introduction

The discovery of THz emission from layered High-\textit{T}_c cuprate Bi\textsubscript{2}Sr\textsubscript{2}CaCu\textsubscript{2}O\textsubscript{8+\textdelta} \cite{1} has significantly renewed our research style on intrinsic Josephson effects, because the experimental stage generating the large emission was rather different from the previous idea \cite{2, 3, 4, 5, 6, 7, 8}. The employed sample size was much beyond our expectation size fully guaranteeing sample uniformity. Indeed, the size belongs to a long junction class, but the whole sample surprisingly behaves just as a cavity. The other surprise was the zero magnetic-field condition for the strong spontaneous emission. Since the transverse excitation is required to generate the electromagnetic wave, a key factor for large spontaneous emission has been believed to be the application of the magnetic field. Consequently, the most of the previous works concentrated on the Josephson vortex flow \cite{2, 3, 4, 5, 6, 7, 8}. However, the large emission was observed with no magnetic field \cite{1}, i.e., the transverse component is spontaneously excited without any external induction.

Since the seminal observation of the strong emission \cite{1, 9, 10, 11}, the central interest in the community studying intrinsic Josephson effects has been focused on mechanism of the strong emission and technique to practically enhance the emission power. The mechanism has been intensively pursued by successive experimental efforts. Now, it is well-known that when AC Josephson oscillation resonates with the cavity mode the strong spontaneous emission occurs \cite{1}. Recently, a non-equilibrium heated range of \textit{I-V} characteristics \cite{12} has been also newly added to the strong emission stage, and the internal excitation pattern was found to be not fixed but rather controllable by dynamics of hot spot induced close to the electrode \cite{10}. On the other hand, the technical advancement to enhance the emission power has been experimentally and
theoretically examined. Consequently, not a situation attached on a large crystal substrate but a simply suspended one is suggested as one of the most promising one [13].

The first aim of the present paper is to revisit the theoretical framework to approach the emission mechanism in intrinsic Josephson junctions. Next, we review theoretical important concepts, i.e., the couplings between neighboring stacked junctions and the other dynamical issues [14]. The basic framework has been still kept and used after the observation of the strong emission. The essence of the emission is believed to be inside the framework. Finally, we briefly touch the phase dynamics resonating with the cavity excitation numerically examined within the framework [13]. We suggest the so-called “multi-physics simulation” to directly simulate the electromagnetic wave emission and exhibit its typical simulation results.

2. Theoretical Framework on Intrinsic Josephson Junction

In this section, we begin with a microscopic Euclidean action, which is created by Bardeen-Cooper-Schrieffer (BCS) microscopic Hamiltonian for layered High-$T_c$ superconductors [14]. By integrating out the fermion degree of freedom on the action [15], we have an effective action, which describes the superconducting phase dynamics in intrinsic Josephson junctions as shown in Fig. 1. We also have the equations of motion of both the superconducting phase and the charge density from the effective action. In the equations, an approximation, in which the charge screening length goes to zero, reduces to the coupled sine-Gordon equation derived by Sakai et al. [16] and Bulaevskii et al. [17], and another assumption, in which the in-plane variation is negligible, leads to the equation of motion suggested by Machida et al. [14]. Finally, the equation arrives at the simplest Koyama-Tachiki model [18] if the diffusion current via the capacitive coupling is dropped. The assumption is fully valid in under-damped junctions. These equations have been numerically and analytically examined by several authors to study the intrinsic Josephson effects repeatedly [4, 5, 6, 19, 20, 21, 22, 23, 24, 25, 26]. We briefly touch the typical results.

![Figure 1. A schematic picture for an intrinsic Josephson junction.](image)

2.1. Modeling and Effective Action

Let us start with a microscopic description for the stacked Josephson junction schematically depicted in Fig. 1. We confine ourselves a case, where the current is biased parallel to the layer stacking direction and the magnetic field is applied only parallel to the junction plane as shown in Fig. 1, i.e., the magnetic field piercing the junction plane creating pancake vortices are not taken into account.

Employing the BCS model for each single superconducting tunneling-junction and extending the model into stacked junction systems, the system’s grand partition function is given by the
following imaginary-time functional integral over the Grassmann fields, \( \hat{\psi}_{\sigma \ell}, \psi_{\sigma \ell} \), for electrons, the gauge field, \( \varphi_{\ell}, A_{\ell}^{\pm} \), and the auxiliary field corresponding to the superconducting order parameter, \( \Delta_{\ell} \), where \( \ell \) is the layer index and the \( z \)-component of the vector potential is defined on the link as \( A_{\ell+1,\ell}^{z} = \int_{\ell}^{\ell+1} dz A_{z}^{\ell} \).

\[
Z = \prod_{\ell} \int D\tilde{\psi}_{\sigma \ell} D\psi_{\sigma \ell} DA_{\ell} D\varphi_{\ell} D\Delta_{\ell} e^{-\frac{1}{\hbar} S[\psi_{\sigma \ell}, \psi_{\sigma \ell}, A_{\ell}^{\pm}, A_{\ell+1,\ell}^{\pm}, \varphi_{\ell}, \Delta_{\ell}]}.
\]  

(1)

In Eq. (1), \( S \) is the Euclidean action defined as \( S = S_{\text{matter}} + S_{\text{field}} \), where

\[
S_{\text{matter}} = \sum_{\ell} \int_{0}^{\beta_{\ell}} d\tau \int d\mathbf{r} \left\{ \frac{|\Delta_{\ell}|^{2}}{g} + \bar{\psi}_{\sigma \ell}(\mathbf{r}, \tau)(\hbar \partial_{\tau} + ie\varphi_{\ell})\psi_{\sigma \ell}(\mathbf{r}, \tau) + \bar{\Delta}_{\ell}\psi_{1}(\mathbf{r}, \tau) + \Delta_{\ell}\bar{\psi}_{1}(\mathbf{r}, \tau) - \bar{\psi}_{\sigma \ell}(\mathbf{r}, \tau) \left[ \frac{\hbar^{2}}{2m} \left( \nabla - i\frac{e}{\hbar c} A_{\ell}^{y} \right)^{2} + \mu_{\ell} \right] \psi_{\sigma \ell}(\mathbf{r}, \tau) + (T_{\ell+1,\ell} A_{\ell+1,\ell}^{s} \psi_{\sigma \ell+1} \psi_{\sigma \ell} + c.c.) \right\},
\]

(2)

and

\[
S_{\text{field}} = \sum_{\ell} \int_{0}^{\beta_{\ell}} d\tau \int d\mathbf{r} \frac{D}{8\pi} \left[ \epsilon_{c}(E_{\ell+1,\ell}^{z})^{2} + (B_{\ell+1,\ell}^{x})^{2} + (B_{\ell+1,\ell}^{y})^{2} \right],
\]

(3)

where, \( T_{\ell+1,\ell} \) is the tunneling matrix element between \( \ell \)th and \( (\ell+1) \)th superconducting layers, \( E_{\ell+1,\ell}^{z} \) is the electric field \( \equiv (1/cD)\partial_{\tau} A_{\ell+1,\ell}^{z} - (\varphi_{\ell+1} - \varphi_{\ell})/D \) along the \( z \)-axis, \( \epsilon_{c} \) is the dielectric constant of the insulating barriers, and \( B_{\ell+1,\ell}^{x} \equiv (1/D)\partial_{y} A_{\ell+1,\ell}^{x} - (A_{\ell+1}^{y} - A_{\ell}^{y})/D \) and \( B_{\ell+1,\ell}^{y} \equiv (A_{\ell+1}^{x} - A_{\ell}^{x})/D - (1/D)\partial_{x} A_{\ell+1,\ell}^{y} \) are the components of the magnetic field parallel to the junctions.

Following the standard technique to integrating out the fermion degree of freedom \cite{15}, we have the following effective action for the gauge invariant superconducting phase difference with electromagnetic fields,

\[
S_{\text{eff}} = \sum_{\ell} \int_{0}^{\beta_{\ell}} d\tau \int d\mathbf{r} \left\{ \frac{D}{8\pi} \left[ \epsilon_{c}(E_{\ell+1,\ell}^{z})^{2} + (B_{\ell+1,\ell}^{x})^{2} + (B_{\ell+1,\ell}^{y})^{2} \right] + m_{s}v_{s} \right\}^{2} + s \left\{ \frac{\phi_{0}}{2\pi c} \frac{\partial \theta_{\ell}}{\partial \tau} + \varphi_{\ell} \right\}^{2} + J \cos P_{\ell+1,\ell}(\tau, r_{\|}) + \sum_{\ell} \int_{0}^{\beta_{\ell}} d\tau \int_{0}^{\beta_{\ell}} d\tau' \int d\mathbf{r}_{\perp} \left[ -\alpha(\tau - \tau') \cos \frac{P_{\ell+1,\ell}(\tau, r_{\|}) - P_{\ell+1,\ell}(\tau', r_{\|})}{2} \right].
\]

(4)

where \( \mu_{f} = \sqrt{\lambda_{\text{TF}}^{2}/4\pi\epsilon} \) is a constant related to the Thomas-Fermi screening length \( \lambda_{\text{TF}} \), \( s \) is the thickness of the superconducting layers, \( n_{s} \) is the superfluid density, and \( P_{\ell+1,\ell} \) and \( v_{s} \) are, respectively, the gauge-invariant phase difference and the in-plane superfluid velocity defined as \( P_{\ell+1,\ell} \equiv \theta_{\ell+1} - \theta_{\ell} - (2\pi/\phi_{0})A_{\ell+1,\ell}^{y} \) and \( v_{s} \) as \( (h/2m)[\nabla_{\|} \theta_{\ell} - (2\pi/\phi_{0})A_{\ell}^{y}] \). In obtaining Eq. (4), we utilize a local approximation for the integral kernels coming from the intra-layer current, charge density, and Cooper pair tunneling current, i.e. \( m_{s}n_{s}, 2/8\pi\mu_{f}^{2}, \) and \( J \) are given as local coefficients \cite{27, 28}. These approximations are valid for the low energy phenomena, with which the tunneling process is relevant. The integral kernels \( \alpha(\tau - \tau') \) in Eq. (4) describes the frequency-dependent quasi-particle tunneling, whose explicit formula is given in Ref. \cite{15} for example. It should be noted that \( \alpha(\tau) \) contributes to the phase dynamics as Ohmic dissipation discussed in the Caldera-Leggett type model \cite{29}.
2.2. Dynamical Equations and Couplings between Junctions

From the action, Eq. (4), one can get the following coupled equations for the gauge-invariant phase difference and the charge density,

\[ \frac{\epsilon_c \phi_0}{2 \pi c^2 D} \frac{\partial^2 P_{\ell+1,\ell}}{\partial t^2} + \frac{4 \pi}{c D} (\epsilon_c \mu_f^2 - \lambda_{ab}^2) \left( \frac{\partial \rho_{\ell+1}}{\partial t} - \frac{\partial P_{\ell+1,\ell}}{\partial t} \right) - \frac{\phi_0}{2 \pi D} \frac{\partial^2 P_{\ell+1,\ell}}{\partial x^2} + \frac{4 \pi}{c} (\sin P_{\ell+1,\ell} + \beta \frac{dP_{\ell+1,\ell}}{dt} - \frac{4 \pi \lambda_{ab}^2}{c s D} (\sin P_{\ell+2,\ell+1} + \sin P_{\ell,\ell-1} - 2 \sin P_{\ell+1,\ell})) \]

\[ - \frac{4 \pi \lambda_{ab}^2}{c s D} \beta \left( \frac{dP_{\ell+2,\ell+1}}{dt} + \frac{dP_{\ell,\ell-1}}{dt} - 2 \frac{dP_{\ell+1,\ell}}{dt} \right) = 0, \]  

(5)

\[ \frac{\phi_0}{2 \pi c D} \frac{\partial P_{\ell+1,\ell}}{\partial t} - \frac{\partial P_{\ell,\ell-1}}{\partial t} + \frac{4 \pi \epsilon_c \mu_f^2}{D} (\rho_{\ell+1} + \rho_{\ell-1} - 2 \rho_{\ell}) = 4 \pi s \rho_{\ell}, \]  

(6)

In deriving Eqs. (5) and (6), one uses the modified Josephson relations,

\[ \frac{\phi_0}{2 \pi c} \frac{\partial P_{\ell+1,\ell}}{\partial t} = -4 \pi \mu_f^2 (\rho_{\ell+1} - \rho_{\ell}) + D E_{\ell+1,\ell}^2, \]  

(7)

\[ \frac{\phi_0}{2 \pi} \frac{\partial P_{\ell+1,\ell}}{\partial x} = \frac{4 \pi \lambda_{ab}^2}{c} \left( j_{\ell+1}^x - j_{\ell}^x \right) + D B_{\ell+1,\ell}. \]  

(8)

It is noted that Eq. (7) and (8) contain two parameters, \( \mu_f \) and \( \lambda_{ab} \), which differ extremely in their length-scales, i.e., \( \mu_f \ll \lambda_{ab} \). The terms with the coefficient \( \lambda_{ab} \) originate from the inductive coupling between junctions \([16, 17]\), while the capacitive coupling between junctions, which arises from the incomplete charge-screening along the stacking direction, yields the terms with the coefficient \( \mu_f \) \([18, 30]\). The difference between these two couplings can be understood by linearizing the sinusoidal function and taking a continuum limit on the discretized difference terms. The approximated equations corresponds to the extended versions of the London equations for anisotropic superconductors, which clarify characteristic lengths of both the couplings. Since \( \epsilon_c \mu_f^2 \ll \lambda_{ab}^2 \), one finds that the inductive coupling is overwhelmingly dominant in the presence of the parallel magnetic field. However, only from this fact, one cannot conclude that the capacitive coupling between junctions can be always neglected in intrinsic Josephson junctions systems, since the inductive coupling vanishes in the absence of Josephson vortices. This is just the case, in which the electromagnetic wave emission is experimentally observed.

3. Numerical Simulations and Superconducting-Phase Dynamics

In the previous section, we derived the general equations describing both the inductive and capacitive couplings. In this section, we revisit the intrinsic Josephson effects based on each coupling by separating out the other couplings. First, we begin with the simplest situation, in which the spatial variation of the superconducting phase along the junction plane is dropped and only the superconducting phase dynamics relevant to the capacitive coupling is taken into account. We also touch recent theoretical advancement on the superconducting phase dynamics. Next, we turn to the case of the so-called stacked long-junctions, in which the inductive coupling is a dominant coupling and the vortex dynamics play a key role.

3.1. Koyama-Tachiki Model and Multiple Branches in I-V Characteristics

Under the assumption of uniformity of the superconducting phase along the junction plane, the terms originated from the inductive coupling diminish in Eq. (5) and (6), and a simple equation appears as follows,

\[ \frac{d^2}{dt^2} P_{\ell+1,\ell} + \gamma \frac{d}{dt} P_{\ell+1,\ell} + \sin P_{\ell+1,\ell} = \frac{I}{j_c} + \frac{\epsilon_c \mu_f^2}{s D} \left[ \sin P_{\ell+2,\ell+1} - 2 \sin P_{\ell+1,\ell} + \sin P_{\ell,\ell-1} \right] \]

\[ + \frac{\epsilon_c \mu_f^2}{s D} \gamma \left[ \frac{dP_{\ell+2,\ell+1}}{dt} - 2 \frac{dP_{\ell+1,\ell}}{dt'} + \frac{dP_{\ell,\ell-1}}{dt} \right], \]  

(9)

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where \( t' = \omega_p t \) and \( \omega_p \) is the Josephson-plasma frequency, \( \omega_p = \sqrt{8 \pi^2 c D j_c / \epsilon_c \phi_0} \). This equation was firstly derived by Machida et al. [14], through the microscopic treatment as briefly described above. We immediately notice that if one drops the third term in the right-hand side, then Eq. (9) coincides with Koyama-Tachiki model [18] derived by their phenomenological treatment. The model has been extensively investigated initially by Machida et al. [30], and recently by Shukrinov et al. [25, 26]. The main physics of the model is the existence of the localized rotating mode, which has been intensively studied in nonlinear physics community motivated by a counter-intuitive concept, in which fully stable localized excitations emerge even on non-integrable discrete lattices like solitonic excitations. The experimental confirmation of such localized excitations has been long an important issue for the nonlinear physics community [32, 33]. Machida et al. [31] argued that intrinsic Josephson junction is an excellent reality of the localized excitation.

![Figure 2](image_url) A typical numerical simulation result (I-V characteristics) of the Koyama-Tachiki model. \( \alpha = 0.10, \gamma = 0.10 \) in Eq. (9). The number of the stacked junctions, \( N = 4 \).

Here, let us display a typical example of the simulation studies on Koyama-Tachiki model. Fig. 2 is typical I-V characteristics obtained by ramping up/down the current. The I-V characteristics clearly show the branching behaviors, which are always measured in well-fabricated small samples. The numerical simulation reveals that the branching arises from the varietical excitation nature of the localized rotating mode. On the other hand, the instability of the AC Josephson oscillation due to the resonance with the longitudinal plasma mode has been recently examined through numerical studies done by Shukrinov et al. [25]. The instability is called “breakpoint”, which is a unique feature characteristic to capacitively coupled intrinsic Josephson junctions. This can be assigned as a cavity resonance of AC Josephson oscillation along the longitudinal stacked direction. The breakpoint phenomenon is dual to the electromagnetic wave emission, in which AC Josephson oscillation resonates with a cavity mode excited along the in-plane direction. Shukrinov et al. [26] also revealed that the longitudinal resonance brings about charge-density oscillation dynamics as a consequence of the resonant instability. The experimental confirmation has been challenged by some experimental groups. However, it still remains unexplored fully.

### 3.2. Coupled sine-Gordon Equation and Resonant Vortex Dynamics

By eliminating the constraint of the uniformity along the in-plane direction and taking into account of only the inductive coupling in Eqs. (7) and (8), we have the coupled sine-Gordon equation derived by Sakai et al. [16] and, Bulaevskii et al. [17] as follows.

\[
\frac{\partial^2 P_{\ell+1,\ell}}{\partial x'^2} = -\frac{\lambda_{ab}^2}{sD} \left( \frac{\partial^2 P_{\ell+2,\ell+1}}{\partial t'^2} + \frac{\partial^2 P_{\ell,\ell-1}}{\partial t'^2} - 2 \frac{\partial^2 P_{\ell+1,\ell}}{\partial t'^2} \right) - \frac{\lambda_{ab}^2}{sD} (\sin P_{\ell+1,\ell} + \sin P_{\ell,\ell-1} - 2 \sin P_{\ell+1,\ell})
\]
\[- \frac{\lambda_{ab}^2}{sD} \gamma (\frac{\partial P_{\ell+2,\ell+1}}{\partial t'} + \frac{\partial P_{\ell,\ell-1}}{\partial t'} - 2 \frac{\partial P_{\ell+1,\ell}}{\partial t'}) + \sin P_{\ell+1,\ell} + \gamma \frac{\partial P_{\ell+1,\ell}}{\partial t'} + \frac{\partial^2 P_{\ell+1,\ell}}{\partial t'^2}, \] (10)

where \( x' = x/\lambda_c \) with \( \lambda_c = \sqrt{c\phi_0/8\pi^2D_J c} \). This equation was initially examined by Sakai et al., \[16\] in their analytical way, while a pioneering simulation on the Josephson vortex dynamics was made by Kleiner \[20\]. The main issues of the equation are the existence of the multiple plasma excitation modes propagating mainly along the in-plane direction, called the transverse plasma, and the resonant vortex dynamics with the multiple plasma modes. The latter issue has been numerically investigated by several groups repeatedly. To our knowledge, the most surprising physics is the emergence of the in-phase locked flux flow as shown in Fig. 3 due to the resonance between the in-phase like propagating mode and flowing vortex lattice. This flow state was expected to emerge in a high-bias voltage range because the resonating mode frequency is the highest among all the transverse modes, and the predicted stability was numerically confirmed by Ustinov et al.\[21\] and Machida et al.\[14\]. Afterwards, several experiments have been made on the equivalent situations, and indirect evidence has been actually obtained \[7, 8\]. However, since the application of the magnetic field, whose magnitude is an order of Tesla, complicates the experimental setups, the advancement speed is slow compared to the recent zero-field radiation.

**Figure 3.** A typical numerical result of the coupled sine-Gordon equation, Eq. (10). In the high voltage region III, which is pointed by the pink color, the in-phase locked flux flow state emerges.

4. Multi-physics Modeling for Electromagnetic Wave Emission

In this section, we briefly present our recent theoretical and numerical works to understand the mechanism of the strong spontaneous electromagnetic-wave emission in the zero field application \[13\]. Our strategy of the simulation work is as follows. Since the emission is sensitively dependent on the experimental setups, a full consideration on the experimental situations is of importance to understand the mechanism and investigate device design including further power enhancement. Thus, we take account of the external vacuum, attached electrodes, superconducting or normal substrate as well as internal capacitively and inductively coupled junctions. Initially, we made two-dimensional frameworks, so-called \( x'y' \)- and \( xz \)-models, which assume uniformity in \( z \)-(c-axis) and \( y' \)-(an in-plane) axis directions, respectively, to avoid an enormous computational degree of freedoms in three-dimensional direct cases. At the present, we also start to perform three-dimensional full simulations by parallelizing the simulation code.
and employing a multi-scale technique to save the computational degree of freedom through consideration of the scale difference between the internal junction and external vacuum regions.

4.1. Two-dimensional $xy$-model Simulation

Here, we concentrate on only $xy$-model due to the space limitation. For $xz$-model, see Ref. [13]. Figure 4 shows typical simulation results for the excited magnetic field inside and outside the junction. The central regions dominated by red arrows are intrinsic Josephson junctions, and the surrounded ones are the external vacuum. The emitted electromagnetic wave passes through the edges of the external vacuum and does not reflect at all. For no reflection, we put a specific region called “perfect matched layer” at the edges. See Refs. [13, 34] for the details of the perfect matched layer.

The Maxwell equations inside the junction region for the $xy$-model are given as [13]

$$\frac{1}{c} \frac{\partial \epsilon E_z}{\partial t} = \frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y} - \frac{4\pi}{c} j_c \sin \phi - \sigma E_z,$$

(11)

$$\frac{1}{c} \frac{\partial B_x}{\partial t} = -\frac{\partial E_z}{\partial y}, \quad \frac{1}{c} \frac{\partial B_y}{\partial t} = \frac{\partial E_x}{\partial x},$$

(12)

where $\sigma$ is the quasi-particle conductivity, $j_c$ is the critical Josephson current density, and $\phi$ is the gauge-invariant phase difference. The external $c$-axis current is introduced by the Ampere’s law. The external vacuum region outside the junction obeys the Maxwell equations, which coincides with $\sigma = j_c = 0$, and $\epsilon = \epsilon_0$ in Eq.(11) and (12). Typical simulation results are displayed in Fig. 4, where the snapshots of the spatial distribution of the inductive field are displayed. Through this kind of simulation, we can obtain the angle dependence of the power of the emitted electromagnetic wave with $I$-$V$ characteristics. The spatial pattern depends on the sample shape and size and the internal excitation pattern varying with the voltage. For more details of the results and their analysis, see Ref. [13].

![Figure 4](image-url)

**Figure 4.** Spatial distributions of emitted magnetic fields depending on the applied voltage. The junction regions are drawn by red arrows.

5. Summary

We reviewed the theoretical framework for the intrinsic Josephson junction systems. We started with the microscopic model and derived the general equations of the superconducting phase and the charge density. The obtained equations were reduced to the Koyama-Tachiki model only for the capacitive coupling and the coupled sine-Gordon equation describing only the most dominant inductive coupling, and typical intrinsic Josephson effects were presented. Finally,
we introduced our recent numerical works on the strong electromagnetic wave emission. The used framework is basically the same as the previous works, but the device reality including the external vacuum, attached electrodes, and substrates is taken into account. With further advancement of supercomputers, the employed simulation style, i.e., multi-physics simulation will have an more important role in the future development of intrinsic Josephson junctions as a THz light source.

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