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Collective Phase Frustration and Time Reversal Symmetry Broken on Single Long Josephson Junction Based on MgB_2 Superconductor

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Abstract: *In the present work, a system of perturbed sine Gordon equations has been derived for a superconductor-insulator-superconductor (SIS) long Josephson junction, following the long route of path integral formalism. The system of equations has been solved numerically by the discretization of the equations using finite difference approximation and applied to the MgB$_2$ superconductor with SiO$_2$ as the junction material. The solution of unperturbed sine-Gordon equation has been considered as the initial profile for the simulation. It is observed that the perturbation terms play the role to deform the profile as time goes on. It is also observed that, the perturbation terms play the role for alternative phase frustration leading the time reversal symmetry broken. The competitive inter-band and intra-band phase frustrations occur faster for high tunneling potential.*

Key Words: *Long Josephson junction, Hubbard-Stratonovich transformation, sine-Gordon equation, phase frustration, Goldston mode*

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I. Introduction

Among the known metallic compounds, MgB_2 has the highest critical temperature of about $T_c = 39$ K [1], It has two three-dimensional and two two-dimensional bands [2]. Due to such type of band structure the MgB_2 has two energy gap and hence is called two-gap superconductor with energies $\approx$ 7.2 meV associated to σ-band and $\approx$ 2.3 meV associated to π-band [3]. Since there are two weakly coupled s-wave order parameters $\Psi_1 = \Delta_1 e^{i\theta_1}$ and $\Psi_2 = \Delta_2 e^{i\theta_2}$, the internal degree of freedom is the inter-band phase differences $\theta(\vec{r},t) = \theta_1 - \theta_2$. When the two superconducting layers are brought together to form a Josephson junction, spontaneous super-current flows from one superconductor to the other due to the existence of phase difference between the layers as well as bands [4]. There are four channels available for cooper pair tunneling in a two-gap superconducting junction [5].

In the present work, first of all, the Hamiltonian of the system is defined. A phenomenological path integral formalism has been proceeded up to the derivation Lagrangian density of the system. Using the Euler-Lagrange equation of motion, a system of generalized equations of motion for gauge invariant phase differences in the stack of long Josephson junctions has been derived. The system of phase equations is numerically solved for the case of single junction system for MgB_2 superconductor with SiO_2 as junction material. The phase differences correspond long Josephson to each channel are plotted in space-time domain. The ground state is obtained by minimizing the Josephson energy and observed the variation of minimum Josephson energy with time.

II. Theoretical Formulation

The total Hamiltonian of the system comprises the free Hamiltonian (H_{free}), pairing Hamiltonian (H_{pair}) and tunneling Hamiltonian (H_T) i.e.

$$H = H_{free} + H_{pair} + H_T \qquad (1)$$

Where

$$H_{free} = \sum_{l,i,\sigma} \int d^3 r a^{\dagger}_{li\sigma} \left[\frac{1}{2m} \left(i\hbar\nabla + e^* \vec{A}^i_l \right)^2 + e^* A^{0i}_l \right] a_{li\sigma} \} \tag{2}$$

$$H_{pair} = \sum_{L,l',i,i'} \int d^3 r V^{i,i'}_{l,l'} a^{\dagger}_{li\uparrow} a^{\dagger}_{li\downarrow} a_{l'i'\downarrow} a_{l'i'\uparrow} \tag{3}$$

$$H_T = \sum_{l,i,i',\sigma} \int d^3 r \left[T^{i,i'}_{l,l+1} a^{\dagger}_{li\sigma} a_{l+1,i',\sigma} + T^{*i'i}_{l+1} a^{\dagger}_{l+1,i',\sigma} a_{l,i,\sigma} \right] \tag{4}$$

Here, $a^{\dagger}_{\sigma}(a_{\sigma})$ is the creation(annihilation) operator for fermion with spin $\sigma = (\uparrow \text{ or } \downarrow)$. These operators are the function of spatial coordinate $\vec{r}$ and imaginary time $\tau = -it$. $a^{\dagger}_{\sigma}(\vec{r},\tau)$ creates a fermion with spin σ at the given site $(\vec{r},\tau)$ and $a_{\sigma}(\vec{r},\tau)$ destroy the fermion from there. These are with dimension of inverse square root of volume. $\vec{A}_l$ and A^0_l are the magnetic vector potential and electric scalar potential respectively. $e^* = 2e$ and e is the electronic charge and m is the mass of a fermion. The operator $-i\hbar\nabla - e^*\vec{A}_l$ is called the canonical momentum operator. $V^{ii'}_{ll'}$ is the coupling constant and $T^{ii'}_{l,l+1}$ is tunneling matrix elements.

Using the special techniques of path integral formalism [6–8], first the action functional has been defined and then quantum mechanical partition function can be obtained. Then the procedure has been followed by Hubbard-Stratonovich transformation, Grassman integration, Matsubara sum, saddle point approximation, Goldston mode etc. As a result of which Lagrangian density can be obtained. The Lagrangian density has been minimized using Euler-Lagrange equation of motion. A system of equations for the phase dynamic for a typical single long Josephson junction has been obtained as

$$\frac{\partial^2 \varphi}{\partial \bar{t}^2} - \frac{\partial^2 \varphi}{\partial \bar{x}^2} + (\mathrm{P}_0)^{-1} \mathrm{P}_F (\bar{j} \sin\varphi) = 0 \tag{5}$$

with

$$\mathrm{P}_0 = \begin{pmatrix} \beta_0 & 0 & 2\varepsilon^2_{rb} & 0 \\ 0 & \beta_0 & 0 & 2\varepsilon^2_{rb} \\ 2\varepsilon^2_{rb} & 0 & \beta_0 & 0 \\ 0 & 2\varepsilon^2_{rb} & 0 & \beta_0 \end{pmatrix}, \ \mathrm{P}_F = \begin{pmatrix} \beta_1 & -2\varepsilon^2_{rb} & \beta_2 & 0 \\ -2\varepsilon^2_{rb} & \beta_1 & 0 & \beta_2 \\ \beta_2 & 0 & \beta_1 & -2\varepsilon^2_{rb} \\ 0 & \beta_2 & -2\varepsilon^2_{rb} & \beta_1 \end{pmatrix}, \ \beta_0 = \frac{\varepsilon_{rb} bd}{\lambda^2_F} + 2\varepsilon^2_{rb},$$

$$\beta_1 = \frac{b^2 d^2}{\lambda^2_L \lambda^2_{TF}} + 2\varepsilon_{rb} bd \left(\frac{1}{\lambda^2_{TF}} + \frac{1}{\lambda^2_L} \right) + 4\varepsilon^2_{rb}, \ \beta_2 = 2\varepsilon_{rb} bd \left(\frac{1}{\lambda^2_{TF}} + \frac{1}{\lambda^2_L} \right) + 6\varepsilon^2_{rb}$$

$\bar{j} = \frac{j}{J_0}$, i.e. the current densities are measured in the dimension of $J_0 = \frac{\varepsilon_0 dc^2\hbar}{\lambda^2_{TF}\lambda^2_L e^*}$, λ_{TF} and λ_L are the Thomas-Fermi screening length an London penetration depth respectively. $\varphi = \left(\varphi^{ss}_{12}, \varphi^{sd}_{12}, \varphi^{ds}_{12}, \varphi^{dd}_{12}\right)^T$ is the column vector with elements as the phase differences and $\bar{j}$ is a diagonal matrix with $\bar{j}^{ss}_{12}$, $\bar{j}^{sd}_{12}$, $\bar{j}^{ds}_{12}$, $\bar{j}^{dd}_{12}$ as the diagonal elements. d is the thickness of the superconducting layer and b is that of for the junction material. ε_{rb} is the dielectric constant of the junction material. The Josephson tunneling coupling constant i.e. current density is

$$j^{ii'}_{l,l+1} = \frac{2e^* dT^{ii'}_{l,l+1} T^{i'i}_{l+1,l} N(0) \Delta_{0li} \Delta_{0,l+1,i'}}{\hbar\left(\Delta^2_{0,l+1,i'} - \Delta^2_{0li}\right)} \ln\left(\frac{\Delta_{0,l+1,i'}}{\Delta_{0li}}\right) \backslash\backslash + \frac{e^* d}{\hbar} \Delta^*_{0li} \left(V^{-1}\right)^{ii'}_{l,l+1} \Delta_{0,l+1,i'} \tag{2}$$

The gauge invariant phase difference $\varphi^{ii'}_{l,l+1}$ has been introduced as

$$\varphi_{l,l+1}^{ii'} = \theta_{l+1}^{i'} - \theta_l^i - \frac{be^*}{\hbar} A_{l,l+1}^{zii'} \tag{7}$$

The Josephson energy of the system is

$$E_J = \frac{\hbar}{e^*} J_{11}^{ss} + \frac{\hbar}{e^*} J_{11}^{dd} + \frac{\hbar}{e^*} J_{22}^{ss} + \frac{\hbar}{e^*} J_{22}^{dd} + 2\frac{\hbar}{e^*} J_{11}^{sd} \cos\left(\varphi_{12}^{ds} - \varphi_{12}^{ss}\right) + 2\frac{\hbar}{e^*} J_{22}^{sd} \cos\left(\varphi_{12}^{sd} - \varphi_{12}^{ss}\right)$$
$$- \frac{\hbar}{e^*} j_{12}^{ss} \cos\varphi_{12}^{ss} - \frac{\hbar}{e^*} j_{12}^{sd} \cos\varphi_{12}^{sd} - \frac{\hbar}{e^*} j_{12}^{ds} \cos\varphi_{12}^{ds} - \frac{\hbar}{e^*} j_{12}^{dd} \cos\varphi_{12}^{dd} \tag{8}$$

The Josephson energy of the system is

III. Numerical Computation

The finite difference technique has been implemented for solving the Equation **Error! Reference source not found.**. For this purpose the equation has been discretized in the space-time domain. The discretized system of equations are numerically solved for the different time steps. The solution of unperturbed sine-Gordon equation i.e. $\varphi = 4\tan^{-1}\exp(\bar{x})$ is considered as the initial profile [9]. The boundary condition at the left end is maintained as $\varphi(-L) = 0$ and that of at the right end is maintained as $\varphi(L) = 2\pi$. The computation has been done for MgB_2. The simulations have been performed for the typical junction system of MgB_2 as shown in **Figure 1** with superconducting layer thickness of 4 $\AA$ and SiO_2 junction thickness of 3 $\AA$ as suggested by Abrikosov [10]. The dielectric constant of SiO_2 is taken as 3.7 and Fermi velocity of MgB_2 is taken as 4.7×10^5 m/s [11]. The Josephson energies have been computed at every space and time step and the minimum of the energy is extracted at every time step. At the same time step the intra-band and inter-band phase differences are computed. The plots of minimum energy versus time and corresponding phases versus time have been displayed on the respective graphs.

IV. Result and Discussion

Figure 2 and **Figure 3** show that the phase differences φ_{12}^{ss} and φ_{12}^{sd} vary with same manner in the space-time region. Similarly, the phase differences φ_{12}^{ds} and φ_{12}^{dd} also show the same behavior. This means one inter-band and one intra-band phase differences are in collective phase fluctuation. **Figure 4** and **Figure 6** show the plots of minimum Josephson energy and the corresponding phase differences vs time for the tunnel voltage of 0.08V. According to this figure, the energy minimization occurs with the phase differences 0 to π up to time 7 units. Within this limit the phase difference is found to be gauge invariant. Above the time of about 7 units, energy minimization occurs only for the phase difference greater than π. If the energy is minimum for the phase difference does not belong to the range from 0 to π, then the phase frustration is said to be occurred [4,5,12,13]. The phase frustration has been obtained at about 5 units of time for the tunnel voltage of 0.12V as shown in **Figure 5** and **Figure 7** . This phase frustration leads the time reversal symmetry broken for the Josephson energy of the system.

Among four phase differences φ_{12}^{ss}, φ_{12}^{sd}, φ_{12}^{ds}, and φ_{12}^{dd}, when two of them (φ_{12}^{ss} and φ_{12}^{sd}) are in phase frustration, the remaining two (φ_{12}^{ds} and φ_{12}^{dd}) are not and vice-versa. The time for starting the phase frustration decreases with increase in tunnel voltage. The transferring of the phase frustration situation occurs alternatively between the two sets { φ_{12}^{ss}, φ_{12}^{sd} } and { φ_{12}^{dss}, φ_{12}^{dd} } as time goes on. During the transferring of the phase frustration between the two sets of phase differences, the minimum of Josephson energy abruptly increases and decreases immediately as the transferring ends. The collision of fluxon and anti-fluxon which appears during Cooper pairs tunneling through the various channels may cause the phase frustration. The fluxon or anti-fluxon may flow along the junction either in phase or out of phase during this process which leading the appearance and disappearance of phase frustration as time goes on. More simulation for higher tunnel voltages have also been performed, but not shown here, and found that the phase frustration is quicker as the tunnel voltage is increased. The results conclude that the collision of fluxon and anti-fluxon as well as in- or out-phase of collective motion is more active for higher tunnel voltage.

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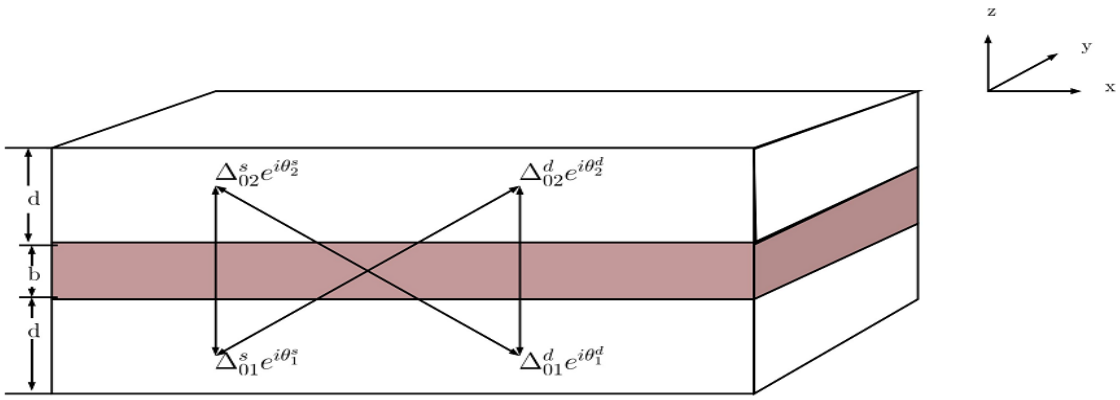

Figure 1: *A typical single long Josephson junction system*

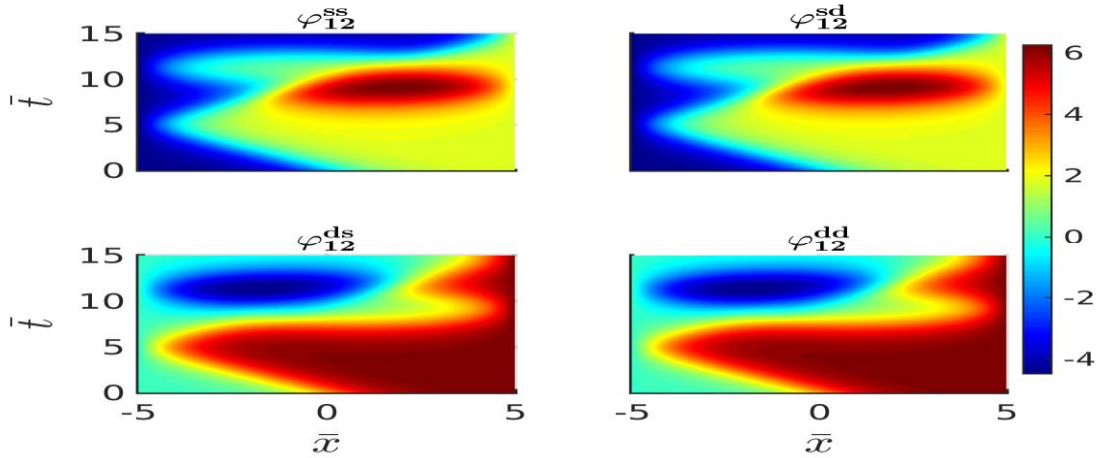

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Figure 2: *(color online) The plot of phase differences on space-time domain for tunnel voltage of 0.08 V. The red color represents the maximum value and blue represents the minimum value of phase differences. The time is taken in the unit of* λ_F / c *and position is taken in the unit of* λ_F

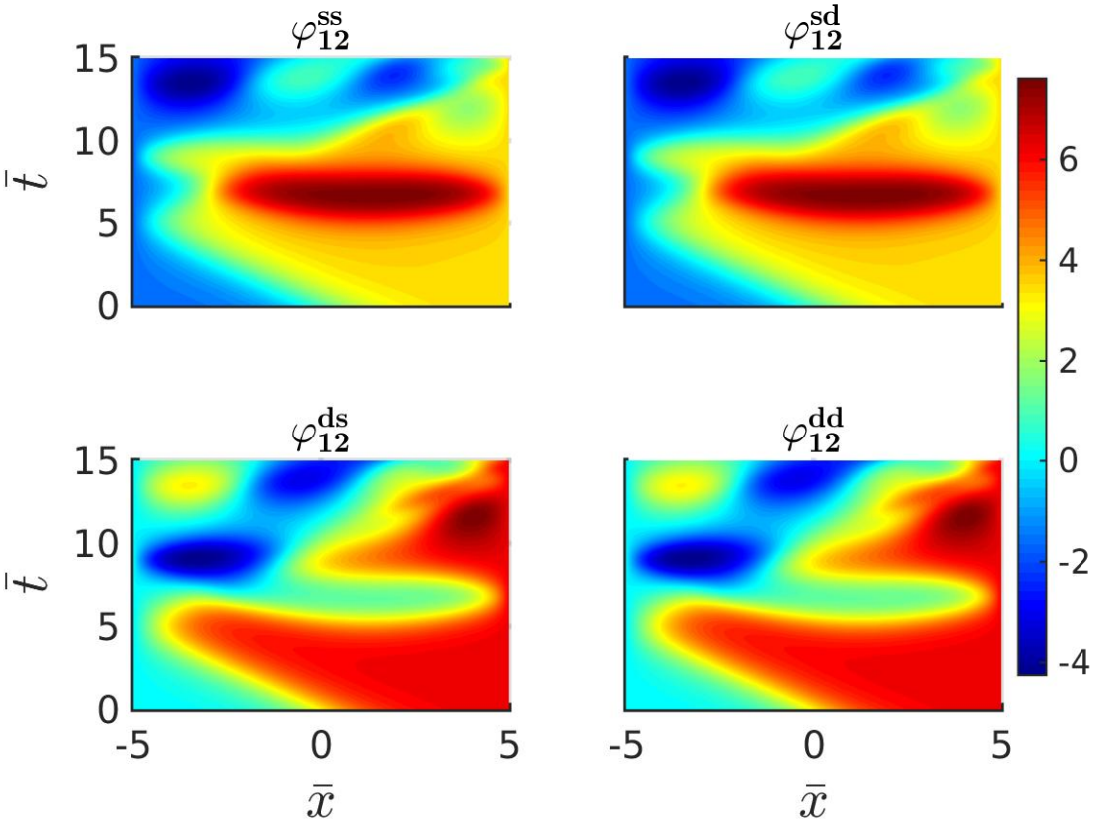

Figure 3: *(color online) The plot of phase differences on space-time domain for tunnel voltage of 0.12 V. The red color represents the maximum value and blue represents the minimum value of phase differences. The time is taken in the unit of* λ_F / c *and position is taken in the unit of* λ_F

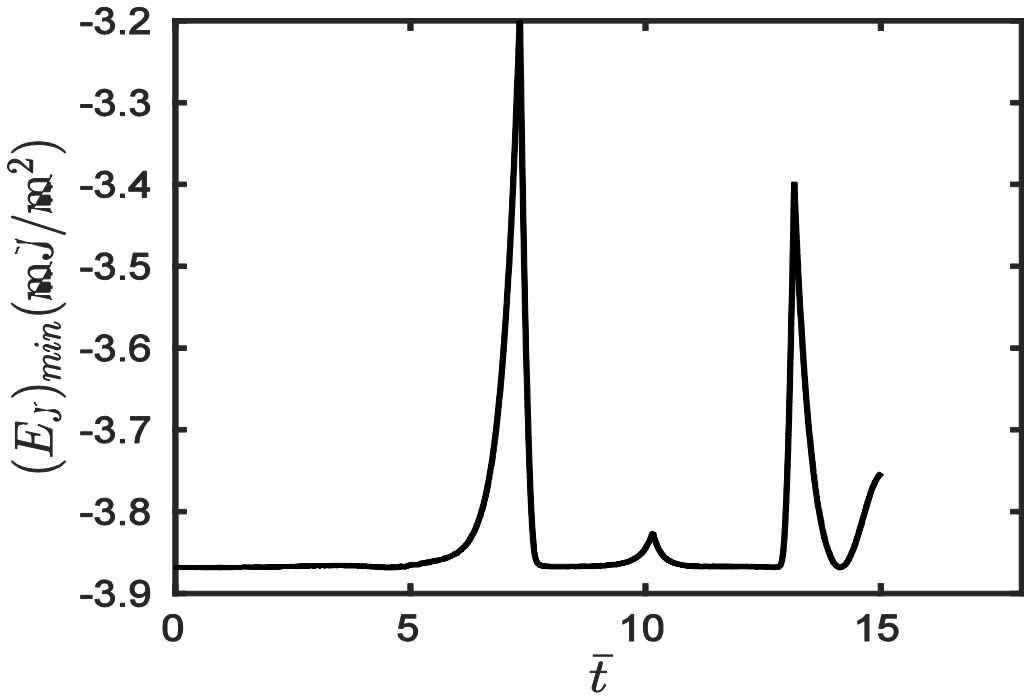

Figure 4: *The plot of minimum Josephson energy versus time taken in the unit of λ_F / c for tunnel voltage of 0.08 V. The peaks reflect the transferring the phase frustration situation between the two set of intra and inter-band phase differences.*

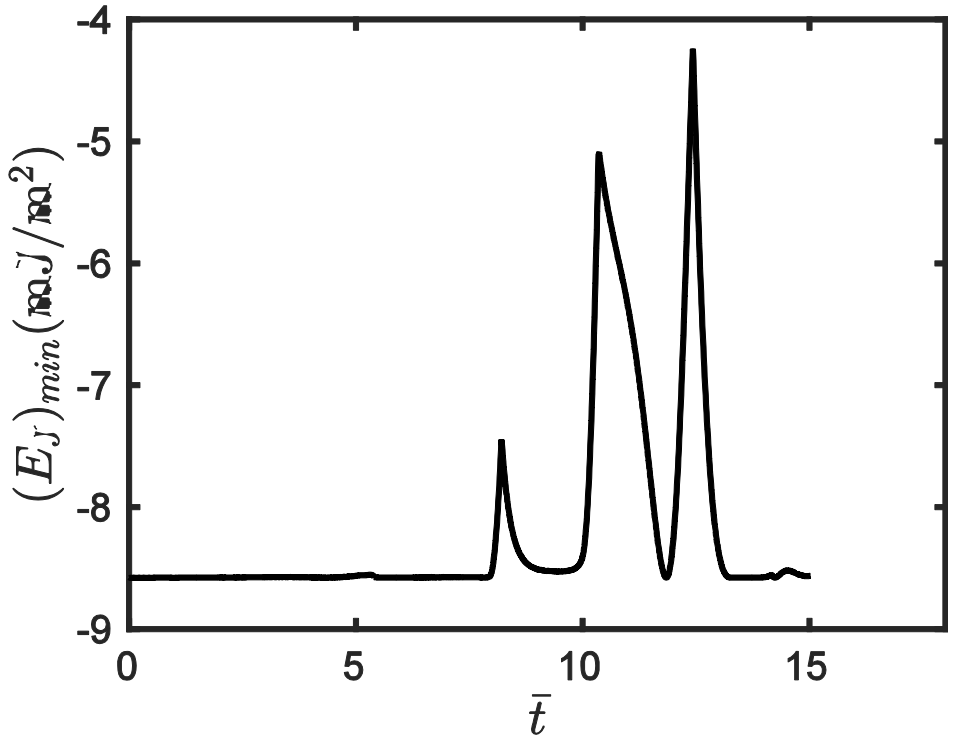

Figure 5: *The plot of minimum Josephson energy versus time taken in the unit of λ_F / c for tunnel voltage of 0.12 V. The peaks reflect the transferring the phase frustration situation between the two set of intra and inter-band phase differences.*

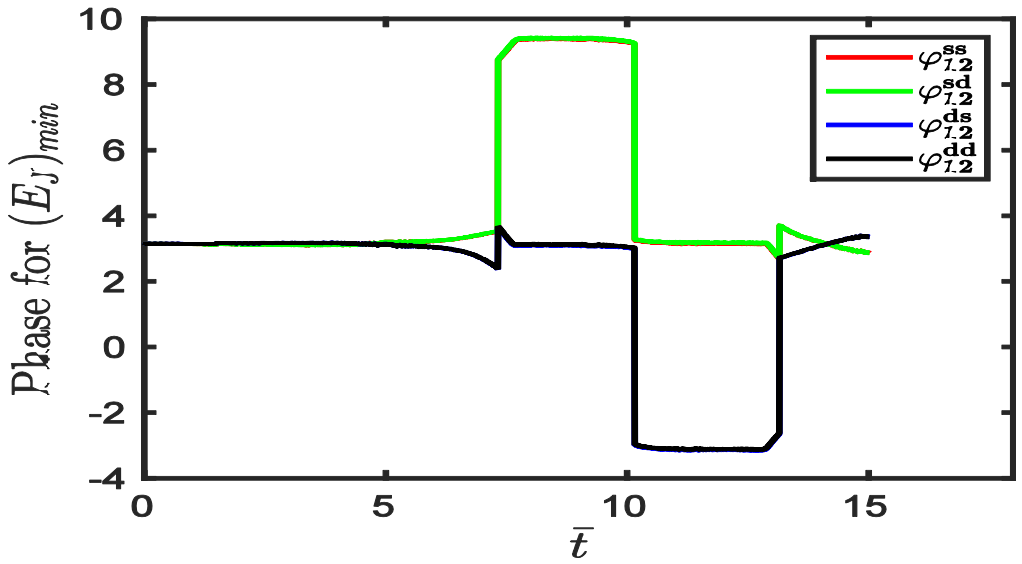

Figure 6: *The plot of phase differences corresponds to minimum Josephson energy versus time taken in the unit of* λ_F / c *for tunnel voltage of 0.08 V. The phase frustration approximately starts at about 7 time units.*

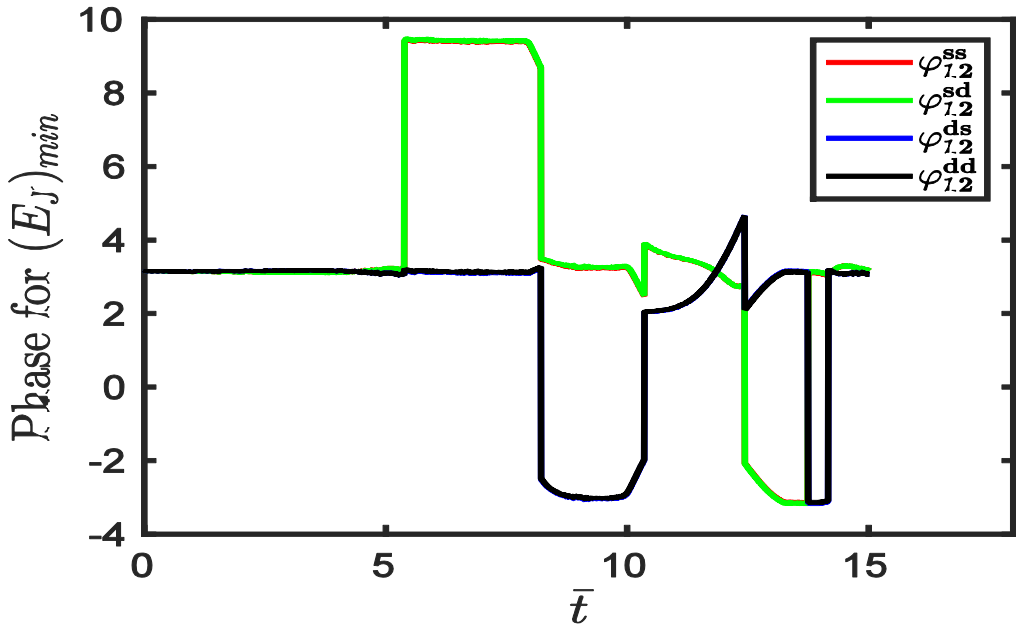

Figure 7: *The plot of phase differences corresponds to minimum Josephson energy versus time taken in the unit of* λ_F / c *for tunnel voltage of 0.08 V. The phase frustration approximately starts at about 7 time units.*