

1 Introduction

The interaction between the quantum system and its environment is one of the active research topics in the condensed matter physics. Historically, the Kondo model successfully describes the resistivity minimum due to the magnetic impurity in the metallic environment [6], and spin-boson model has been the basic theoretical platform for the light-matter-coupled system [11]. The Anderson impurity model also plays the central role in the dynamical mean-field theory as an auxiliary system for the self-consistent solutions [7].

One another famous example of the system-environment coupled systems is *resistively shunted Josephson junction* (RSJJ). RSJJ is a circuit system consisting of a single JJ connected to an RC resonator which acts as a circuit resistance [Fig.3]. Several studies have reported that the RSJJ reveals a phase transition line that depends on the coupling strength between the Junction and the circuit resistance[1,2,17] Such early predictions render RSJJ a prototypical model for the quantum phase transition, especially for the Schmid quantum dissipative transition. Particularly in the latest study [Fig.2], novel reentrant behavior of quantum phase transition was predicted.

On the other hand, it has been known that the quantum phase transition has genuine impacts on the *finite-temperature* behavior of the system. Emanating from the quantum critical point at zero temperature like fan-shape form in the temperature-(nonthermal) parameter plane [19], the various experimentally measurable response functions can show peculiar nature for wide range of temperatures. The strange metallicity in the heavy fermion system is a representative example of such paradigm of the quantum phase transition.

However, the finite-temperature nature of the QPT in the RSJJ has not been thoroughly investigated. So, in this thesis, we study the finite-temperature nature of possible underlying QPT using the strong-coupling expansions. By employing the framework of strong-coupling expansions, we expect a concrete description of the phase transition in the RSJJ, which is an ongoing debate. The precise nature of this transition is to be addressed through the analysis of the quantum state of electrons.

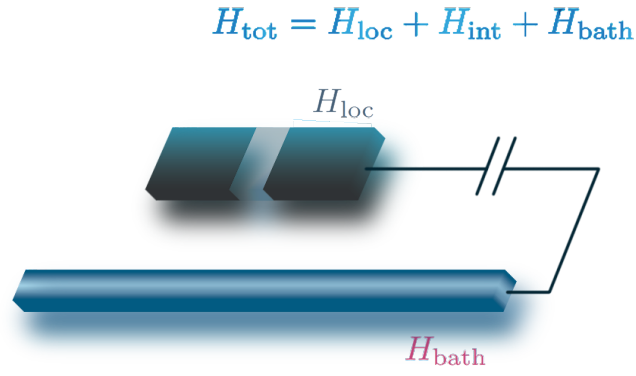


Figure 1: Brief Image of Resistivity shunted Josephson junction

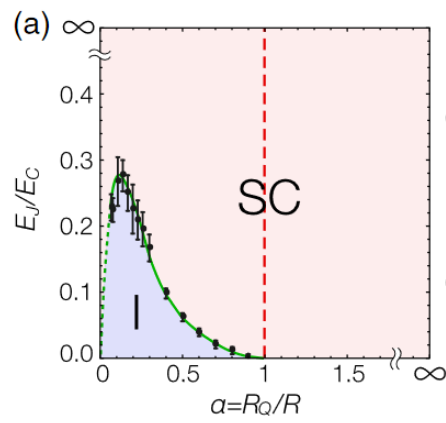


Figure 2: Zero temperature phase diagram with reentrant phase transition[2]

2 Theoretical method

2.1 Field operator and Green's function

This chapter will briefly summarize the theoretical framework of Green's function, circuit, and expansion methods. In quantum many-body theory, the physical system is depicted over the frame of the fermionic (bosonic) creation and annihilation operator, and $\hat{a}(\hat{a}^\dagger)$ as an annihilation (creation) operator, it satisfies the following commutation relations:

$$\begin{aligned} [\hat{a}_i, \hat{a}_j] &= \{\hat{a}_i, \hat{a}_j\} = 0 \\ [\hat{a}_i^\dagger, \hat{a}_j^\dagger] &= \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0 \\ [\hat{a}_i, \hat{a}_j^\dagger] &= \delta_{ij} \quad (\text{bosonic case}) \\ \{\hat{a}_i, \hat{a}_j^\dagger\} &= \delta_{ij} \quad (\text{fermionic case}) \end{aligned} \tag{2.1}$$

The symbol δ_{ij} is the Kronecker-delta function. In the following discussion, we will drop the lower indices of the field operator, assuming it can indicate any arbitrary quantum state. If we consider that the Hamiltonian system can be split into two parts, for the local system and the interaction, we can write the total Hamiltonian H :

$$H = H_0 + H_{\text{int}} \tag{2.2}$$

Here, H_0 is the local (Free) Hamiltonian, and H_{int} is the Hamiltonian for interaction (external potential). To express the dynamics of a given operator in Matsubara formalism, we depict the time dependency of the operator in the interaction picture :

$$\begin{aligned} \hat{a}(\tau) &= e^{H_0\tau} \hat{a} e^{-H_0\tau} \\ \hat{a}^\dagger(\tau) &= e^{-H_0\tau} \hat{a}^\dagger e^{H_0\tau} \end{aligned} \tag{2.3}$$

With the above time dependency, we can define the Green's function as follows :

$$G_0(\tau, \tau') = \langle \mathcal{T} \hat{a}(\tau) \hat{a}^\dagger(\tau') \rangle = \begin{cases} \langle \hat{a}^\dagger(\tau') \hat{a}(\tau) \rangle & (\tau > \tau') \\ \pm \langle \hat{a}^\dagger(\tau) \hat{a}(\tau') \rangle & (\tau < \tau') \end{cases} \tag{2.4}$$

Here, the symbol \mathcal{T} is the time ordering operator. One of the features of Green's function is that it satisfies the given equation of motion :

$$-\partial_\tau \mathcal{G}(\tau, \tau') = \delta(\tau - \tau') + \langle \mathcal{T}_\tau ([H, \hat{a}](\tau) \hat{a}^\dagger(\tau')) \rangle \tag{2.5}$$

2.2 Circuit model

Hamiltonian of resistivity shunted Josephson junction

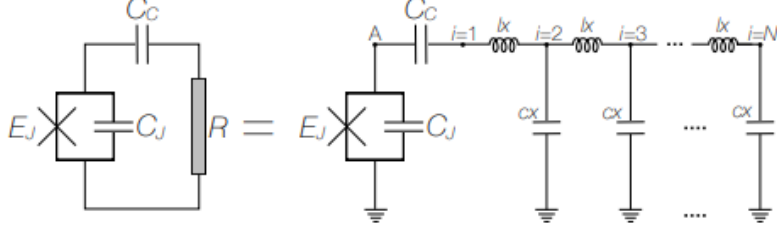


Figure 3: Picture of resistivity shunted Josephson junction connected with exterior transmission line.[18]

We introduce the impurity model for the resistivity shunted Josephson junction (RSJJ) circuit. Specific Hamiltonians and physical parameters are based on the [2]. The circuit is composed of a single Josephson junction connected to the transmission line, which acts as the resistance of the total circuit system. Each circuit component is mapped onto each composition of the total Hamiltonian. The given circuit Hamiltonian form is represented as follows :

$$H_{\text{sys}} = (E_C \hat{N}^2 - E_J \cos \phi) - \hat{N} \sum_{0 < k \leq K} \hbar g_k (\hat{b}_k^\dagger + \hat{b}_k) + \sum_{0 < k \leq K} \hbar \omega_k \hat{b}_k^\dagger \hat{b}_k, \quad (2.6)$$

where $\hat{N} = i\partial/\partial\phi$ is the charge operator, \hat{b}_k (\hat{b}_k^\dagger) is the bosonic annihilation (creation) operator of k -th mode, coupled to the charge of JJ of coupling energy scale $\hbar g_k$. Equation (2.6) can be divided into three parts:

$$H_{\text{sys}} = H_{\text{loc}} + H_{\text{int}} + H_{\text{bath}}, \quad (2.7)$$

each of which represents the local JJ, the bath bosons, and coupling between them;

$$\begin{aligned} H_{\text{loc}} &= E_C \hat{N}^2 - E_J \cos \phi \\ H_{\text{bath}} &= \sum_{0 < k \leq K} \hbar \omega_k \hat{b}_k^\dagger \hat{b}_k \\ H_{\text{int}} &= -\hat{N} \sum_{0 < k \leq K} \hbar g_k (\hat{b}_k^\dagger + \hat{b}_k) \end{aligned} \quad (2.8)$$

The detailed description of basic symbols is summarized in Table 1.

Both in the local JJ and the bosonic bath, degrees of freedom satisfy the fundamental commutation relation: the phase of JJ and its conjugate charge operator in the local Hamiltonian and annihilation and creation operators for the bath Hamiltonian.

$$\begin{aligned} [\hat{\phi}, \hat{N}] &= i\hbar, \\ [\hat{b}_k, \hat{b}_{k'}^\dagger] &= \delta_{kk'}. \end{aligned} \quad (2.9)$$

Symbols	Formula	Physical quantities
ϕ		Phase of Josephson junction
\hat{N}	$-i \frac{\partial}{\partial \phi}$	Charge operator
ω_k	$vk = \frac{vm\pi}{L}$	Bath frequency
$\hat{b}_k^\dagger, \hat{b}_k$		Bosonic creation, annihilation operator
R_Q	$\frac{h}{4e^2}$	Quantum resistance of junction
R		Resistance of bath
E_C	$\frac{(2e)^2}{2C_J}$	Josephson junction charging energy
E_J		Josephson coupling energy
g_k	$\sqrt{\frac{2\pi v}{\alpha L} \frac{\omega_k}{1+(\frac{v\omega_k}{W})^2}}$	Coupling with bath in mode k
ν	$\frac{\pi}{\alpha \epsilon_C}$	
ϵ_C	$\frac{E_C}{\hbar W}$	

Table 1: Basic symbols used for describing Hamiltonian.

The coupling between the JJ and the k -th mode boson is denoted by g_k , and $\alpha = \frac{R_Q}{R}$ controls the global coupling strength for all bosonic modes. On the other hand, the competition between the Josephson coupling E_J and the charge energy scale E_C is controlled by $\gamma = \frac{E_J}{E_C}$ in the local part. α and γ will be our basic control parameters. We've set E_C as an energy unit.

H_{loc} in Josephson phase basis

To adjust the expansion method to the RSJJ Hamiltonian model, We represent the local system Hamiltonian in matrix formulation using the basis of the Josephson wave function. We adopt the macroscopic point of view to observe the superconducting effect expected in our junction system. The free-particle wavefunction in the 2π -periodic JJ phase (ϕ) space can be written in the exponential form:

$$|\psi_{JJ}\rangle = \sum_{-\infty}^{\infty} c_m \frac{e^{im\phi}}{\sqrt{2\pi}}, \quad (2.10)$$

where, $e^{im\phi}/\sqrt{2\pi}$ constitutes the complete basis with wavenumber m . In trigonometric form,

$$|\psi_{JJ}\rangle = \frac{a_0}{\sqrt{2\pi}} + \frac{1}{\sqrt{\pi}} \sum_{m=1}^{\infty} (a_m \cos m\phi + b_m \sin m\phi). \quad (2.11)$$

Since the local Hamiltonian doesn't mix the even and odd sectors, one can safely write down the even and odd eigenvectors separately:

$$|\text{even}_k\rangle = \frac{a_0^{(k)}}{\sqrt{2\pi}} + \sum_{n=1}^{\infty} \frac{a_n^{(k)}}{\sqrt{\pi}} \cos n\phi, \quad (2.12)$$

$$|\text{odd}_k\rangle = \sum_{m=1}^{\infty} \frac{b_m^{(k)}}{\sqrt{\pi}} \sin m\phi. \quad (2.13)$$

Here, k is the eigenstate index.

Considering the differential form of local system Hamiltonian in the trigonometric basis,

$$H_{\text{loc}} = -\frac{\partial^2}{\partial \phi^2} - \gamma \cos \phi \quad (2.14)$$

the Hamiltonian can be written as follows.

$$H_{\text{loc even}} = \begin{pmatrix} 0 & -\frac{\gamma}{\sqrt{2}} & 0 & \cdots \\ -\frac{\gamma}{\sqrt{2}} & 1 & -\frac{\gamma}{2} & 0 & \cdots \\ 0 & -\frac{\gamma}{2} & 4 & & \\ \vdots & & & \ddots & \end{pmatrix} \quad (m = 0, 1, 2, \dots), \quad (2.15)$$

$$H_{\text{loc odd}} = \begin{pmatrix} 1 & -\frac{\gamma}{2} & 0 & \cdots \\ -\frac{\gamma}{2} & 4 & -\frac{\gamma}{2} & 0 & \cdots \\ 0 & -\frac{\gamma}{2} & 9 & & \\ \vdots & & & \ddots & \end{pmatrix} \quad (m = 1, 2, \dots). \quad (2.16)$$

One can numerically diagonalize H_{loc} . Because the difference between the energy levels becomes more significant as m increases, we truncate the local Hilbert space for computationally manageable subsets of low-lying states.

Matrix form of \hat{N} in local eigen basis

3-level case

Now, we can span the charge operator in eigenvectors of $H_{\text{loc even}}$ and $H_{\text{loc odd}}$. In the 2-level case, we can use the total lowest three states as the basis vector,

$$\begin{aligned} |\text{gs}\rangle &= \frac{a_0^{(0)}}{\sqrt{2\pi}} + \sum_{n=1} \frac{a_n^{(0)}}{\sqrt{\pi}} \cos n\phi = \frac{a_0}{\sqrt{2\pi}} + \frac{a_1}{\sqrt{\pi}} \cos \phi + \frac{a_2}{\sqrt{\pi}} \cos 2\phi + \cdots, \\ |\text{1st}\rangle &= \sum_{m=1} \frac{b_m^{(1)}}{\sqrt{\pi}} \sin m\phi = \frac{b_1}{\sqrt{\pi}} \sin \phi + \frac{b_2}{\sqrt{\pi}} \sin 2\phi + \cdots, \\ |\text{2nd}\rangle &= \frac{a_0^{(1)}}{\sqrt{2\pi}} + \sum_{n=1} \frac{a_n^{(1)}}{\sqrt{\pi}} \cos n\phi = \frac{a'_0}{\sqrt{2\pi}} + \frac{a'_1}{\sqrt{\pi}} \cos \phi + \frac{a'_2}{\sqrt{\pi}} \cos 2\phi + \cdots. \end{aligned} \quad (2.17)$$

Here, we note the upper indices with a round brace to indicate the energy excitation of the local system. The matrix form of \hat{N} becomes :

$$\begin{aligned} \hat{N} &= \begin{pmatrix} \langle \text{gs} | -i \frac{\partial}{\partial \phi} | \text{gs} \rangle & \langle \text{gs} | -i \frac{\partial}{\partial \phi} | \text{1st} \rangle & \langle \text{gs} | -i \frac{\partial}{\partial \phi} | \text{2nd} \rangle \\ \langle \text{1st} | -i \frac{\partial}{\partial \phi} | \text{gs} \rangle & \langle \text{1st} | -i \frac{\partial}{\partial \phi} | \text{1st} \rangle & \langle \text{1st} | -i \frac{\partial}{\partial \phi} | \text{2nd} \rangle \\ \langle \text{2nd} | -i \frac{\partial}{\partial \phi} | \text{gs} \rangle & \langle \text{2nd} | -i \frac{\partial}{\partial \phi} | \text{1st} \rangle & \langle \text{2nd} | -i \frac{\partial}{\partial \phi} | \text{2nd} \rangle \end{pmatrix}, \\ &= i \begin{pmatrix} 0 & \sum_{n=1} n a_n^{(0)} b_n^{(1)} & 0 \\ -\sum_{n=1} n a_n^{(0)} b_n^{(1)} & 0 & -\sum_{n=1} n a_n^{(1)} b_n^{(1)} \\ 0 & \sum_{n=1} n a_n^{(1)} b_n^{(1)} & 0 \end{pmatrix}. \end{aligned} \quad (2.18)$$

Multilevel case

For the higher-level case, one can easily generalize the matrix expression of \hat{N} . Now, based on the above discussion, the extended form of charge operator in higher dimension is :

$$\begin{aligned} \hat{N} &= \begin{pmatrix} \langle \text{gs} | -i \frac{\partial}{\partial \phi} | \text{gs} \rangle & \langle \text{gs} | -i \frac{\partial}{\partial \phi} | \text{1st} \rangle & \cdots \\ \langle \text{1st} | -i \frac{\partial}{\partial \phi} | \text{gs} \rangle & \ddots & \vdots \\ \vdots & \cdots & \langle \text{nth} | -i \frac{\partial}{\partial \phi} | \text{nth} \rangle \end{pmatrix} \\ &= i \begin{pmatrix} 0 & \sum_{n=1} n a_n^{(0)} b_n^{(1)} & \cdots \\ -\sum_{n=1} n a_n^{(0)} b_n^{(1)} & \ddots & \\ \vdots & \sum_{n=1} n a_n^{(n-1)} b_n^{(n)} & -\sum_{n=1} n a_n^{(n-1)} b_n^{(n)} \end{pmatrix} \end{aligned} \quad (2.19)$$

In this case, the maximum dimension of \hat{N} is $2n + 1$.

Matrix Form of $\hat{\cos} \phi$

The physical observable $\hat{\cos} \phi$ represents the phase coherence of the currents flowing at both ends of the Josephson junction. If the junction exhibits superconducting properties, the value of $\hat{\cos} \phi$ will be greater than 0, while it will be close to 0 if it exhibits insulating properties. The expectation of $\hat{\cos} \phi$ can be calculated in following formula:

$$\langle \cos \phi \rangle = \frac{\text{Tr}[\hat{\cos} \phi e^{-\beta H}]}{\text{Tr}[e^{-\beta H}]} \quad (2.20)$$

3-level case

Since we aim to understand the system from the perspective of which represents the Josephson junction with three energy levels, we intend to expand order parameter $\cos \phi$ in a similar procedure by calculating \hat{N} matrix. Adopting the form of Fourier basis in the case of 3-level in the representing \hat{N} matrix, $\cos \phi$ can be rewritten as a matrix operator, and

$$\hat{\cos} \phi = \begin{pmatrix} \langle \text{gs} | \cos \phi | \text{gs} \rangle & \langle \text{gs} | \cos \phi | \text{1st} \rangle & \langle \text{gs} | \cos \phi | \text{2nd} \rangle \\ \langle \text{1st} | \cos \phi | \text{gs} \rangle & \langle \text{1st} | \cos \phi | \text{1st} \rangle & \langle \text{1st} | \cos \phi | \text{2nd} \rangle \\ \langle \text{2nd} | \cos \phi | \text{gs} \rangle & \langle \text{2nd} | \cos \phi | \text{1st} \rangle & \langle \text{2nd} | \cos \phi | \text{2nd} \rangle \end{pmatrix} \quad (2.21)$$

When obtaining eigenvectors for the 3-level truncated 3*3 H_{loc} matrix, the matrix form of $\cos \phi$ is expressed as follows.

$$\hat{\cos} \phi = \begin{pmatrix} \frac{2}{\sqrt{2}} a_0 a_1 + a_1 a_2 & 0 & \frac{1}{\sqrt{2}} (a_1 a'_0 + a_0 a'_1) + \frac{1}{2} (a_1 a'_2 + a_2 a'_1) \\ 0 & b_1 b_2 & 0 \\ \frac{1}{\sqrt{2}} (a_1 a'_0 + a_0 a'_1) + \frac{1}{2} (a_1 a'_2 + a_2 a'_1) & 0 & \frac{2}{\sqrt{2}} a'_0 a'_1 + a'_1 a'_2 \end{pmatrix} \quad (2.22)$$

Multilevel case

When including more than three levels, expressing the order parameter in matrix form for the Hamiltonian H_{loc} involves the following steps. First, the calculation of the even function form of the order parameter $\cos \phi$ is as follows:

$$\cos \phi | \text{even}_k \rangle = \frac{a_0^{(k)}}{\sqrt{2\pi}} \cos \phi + \sum_{n=1} \frac{a^{(k)}}{\sqrt{\pi}} \cos \phi \cos n\phi \quad (2.23)$$

The final inner product result is:

$$\langle \text{even}_l | \cos \phi | \text{even}_k \rangle = \int_0^{2\pi} \left(\frac{a_0^{(m)}}{\sqrt{2\pi}} + \sum_{m=1} \frac{a^{(m)}}{\sqrt{\pi}} \cos m\phi \right) \left(\frac{a_0^{(n)}}{\sqrt{2\pi}} \cos \phi + \sum_{n=1} \frac{a^{(n)}}{\sqrt{\pi}} \cos \phi \cos n\phi \right) \quad (2.24)$$

The calculation for the odd function form is as follows:

$$|\text{odd}\rangle = \sum_{n=1} \frac{b_n^{(k)}}{\sqrt{\pi}} \sin n\phi \quad , \quad \cos \phi |\text{odd}\rangle = \sum_{n=1} \frac{b_n^{(k)}}{\sqrt{\pi}} \cos \phi \sin n\phi \quad (2.25)$$

Similar to the case of even state eigenvector, the inner product result is:

$$\begin{aligned} \langle \text{odd}_l | \cos \phi | \text{odd}_k \rangle &= \sum_{n,m=1} \int_0^{2\pi} d\phi \left(\frac{b_n^{(k)} b_m^{(l)}}{\pi} \cos \phi \sin n\phi \sin m\phi \right) \\ &= \begin{cases} \text{if } k < l : & \sum_{n=1}^N \left(\frac{\hat{b}_n^{(k)} \hat{b}_{n-1}^{(l)}}{2} + \frac{\hat{b}_n^{(k)} \hat{b}_{n+1}^{(l)}}{2} \right) \\ \text{if } k > l : & \sum_{n=1}^N \left(\frac{\hat{b}_{n-1}^{(k)} \hat{b}_n^{(l)}}{2} + \frac{\hat{b}_{n+1}^{(k)} \hat{b}_n^{(l)}}{2} \right) \end{cases} \end{aligned} \quad (2.26)$$

Therefore, when the entire $\cos \phi$ is expressed in matrix form, it takes the following form:

$$\cos \hat{\phi} = \begin{pmatrix} \ddots & & & \vdots & & \\ & \langle \text{even}_k | \cos \phi | \text{even}_k \rangle & 0 & \langle \text{even}_k | \cos \phi | \text{even}_{k+1} \rangle & \dots & \\ & 0 & \langle \text{odd}_k | \cos \phi | \text{odd}_k \rangle & 0 & \langle \text{odd}_k | \cos \phi | \text{odd}_{k+1} \rangle & \\ & \langle \text{even}_{k+1} | \cos \phi | \text{even}_k \rangle & 0 & \langle \text{even}_{k+1} | \cos \phi | \text{even}_{k+1} \rangle & & \\ & & \vdots & & \ddots & \end{pmatrix} \quad (2.27)$$

2.3 Diagrammatic method

Diagrammatic expansion of Green's function

Single Green's function corresponding with one specific imaginary time interval can be represented diagrammatic, which is the basic formulation of the diagrammatic method. We can draw a line from τ' to τ ,

$$\hat{a}(\tau') \longrightarrow \hat{a}^\dagger(\tau) \qquad \hat{a}(\tau') \longleftarrow \hat{a}^\dagger(\tau)$$

Figure 4: Diagram of single Green's function. The direction of arrow corresponds with the direction of time flow.

In equilibrium statistical mechanics, the expectation value of the physical observable is characterized by the partition function that satisfies the given restricted energy condition in phase space. Based on these concepts, on the grand canonical ensemble, the statistical structure of counting Green's function becomes :

$$G_0(\tau, \tau') = \frac{\text{Tr}[e^{-\beta H_0} \hat{a}^\dagger(\tau) \hat{a}(\tau')]}{\text{Tr}[e^{-\beta H_0}]} = \frac{\text{Tr}[e^{-\beta H_0} e^{iH_0\tau} \hat{a}^\dagger e^{-H_0(\tau-\tau')} \hat{a} e^{-iH_0\tau'}]}{\text{Tr}[e^{-\beta H_0}]} \quad (2.28)$$

This is the basic form of Green's function in imaginary time corresponding to the diagram structure. Similar case with the creation and annihilation operator, the time dependency of external potential term Hamiltonian:

$$H'(\tau) = e^{H_0\tau} H e^{-H_0\tau} \quad (2.29)$$

If we consider the effect of interaction, we can adopt full Green's function includes the interaction operator $U(\tau)$,

$$G(\tau, \tau') = \frac{\text{Tr}[e^{-\beta H_0} U(\beta) \hat{a}^\dagger(\tau) \hat{a}(\tau')]}{\text{Tr}[e^{-\beta H_0} U(\beta)]} = \frac{\text{Tr}[e^{-\beta H} U(\tau) \hat{a}^\dagger U(\tau' - \tau) \hat{a} U(\tau')]}{\text{Tr}[e^{-\beta H}]} \quad (2.30)$$

Where the interaction operator is:

$$U(\tau) = \mathcal{T} e^{-\int_0^\tau d\tau' H_{\text{int}}(\tau')} \quad (2.31)$$

In the imaginary time interval $[\tau, 0]$, full Green's function in the expectation form can be represented,

$$G(\tau, 0) = \frac{\text{Tr}[e^{-\beta H_0} U(\beta) \hat{a}^\dagger(\tau) \hat{a}]}{\text{Tr}[e^{-\beta H_0} U(\beta)]} = \frac{\langle U(\beta) \hat{a}^\dagger(\tau) \hat{a} \rangle_0}{\langle U(\beta) \rangle_0} \quad (2.32)$$

The under index 0 of the angled bracket indicates its expectation value was calculated in H_{loc} frame. If the interaction Hamiltonian is in the form of the multiplication of a pair of annihilation-creation operator \hat{a}^\dagger and \hat{a} , we can adjust Wick's theorem to expand each of the expectation values in denominator and numerator into a multiplication of Green's functions in each time interval. A brief discussion of Wick's theorem will be introduced in the Appendix.

Diagrammatic expansion in strong coupling case

The Hamiltonian system can be divided into three parts as a general case of the time-dependent impurity model with a bosonic bath:

$$H_{sys} = H_{loc} + H_{int} + H_{bath} \quad (2.33)$$

In the second quantized form, This can be rewritten:

$$H(t) = H_{loc}(t) + \underbrace{\sum_n \epsilon_n \hat{b}_n^\dagger \hat{b}_n}_{\text{bath}} + \underbrace{\sum_{m,n} [V_{m,n}(t) c_m^\dagger b_n + \text{H.c.}]}_{\text{interaction}} \quad (2.34)$$

The operator $\hat{b}(\hat{b}^\dagger)$ indicates bosonic annihilation(creation) operator, $\hat{c}(\hat{c}^\dagger)$ is fermionic annihilation(creation) operator. Based on this structure, the expansion method was constructed. Continue, from the Hamiltonian, the action of the entire system can be written into :

$$S = \int_0^\beta d\tau H_{loc}(\tau) + \int_0^\beta d\tau d\tau' P(\tau) \mathcal{W}(\tau - \tau') P(\tau') \quad (2.35)$$

Here, H_{loc} is the Hamiltonian of the local system, indicating the impurity we want to focus on. The terms P and \mathcal{W} correspond with the Hermitian operator and the interaction term. While considering the interaction process, the term \mathcal{W} includes the scalar factor to represent the effect of the bosonic bath. With a similar procedure to the diagram expansion, We can calculate the expectation value of the observable using the partition function Z ,

$$Z = \text{tr} \left[T_\tau e^{-S} \right] \quad (2.36)$$

This result takes the form of Dyson's equation in quantum mechanics, which can be represented in the diagram structure. If we define full \mathcal{G} as :

$$\mathcal{G} = \langle \psi_a(\tau) \psi_b^\dagger(\tau') \rangle = \frac{\text{Tr}[e^{-\beta H} \psi_a(\tau) \psi_b^\dagger(\tau')]}{\text{Tr}[e^{-\beta H}]} \quad (2.37)$$

Then the diagram of the Dyson equation is shown in Figure 4.



Figure 5: Diagram for Dyson equation with self energy

This form of equation satisfies the integral-differential form agrees with the equation of motion in the quantum mechanical aspect.

$$[-\partial_\tau - H_{loc} + \lambda] \mathcal{G}(\tau) - \int_0^\tau d\tau_1 \Sigma(\tau - \tau_1) \mathcal{G}(\tau_1) = 0 \quad , \quad (\tau > 0) \quad (2.38)$$

Evaluation of correlation function

The Correlation function for green's function is defined as follows:

$$\chi_{sp}(\tau) = \frac{1}{Z} \text{Tr}[e^{-S} P(\tau) P(0)] \quad (2.39)$$

where S is an action of the system. The corresponding topological diagram is:

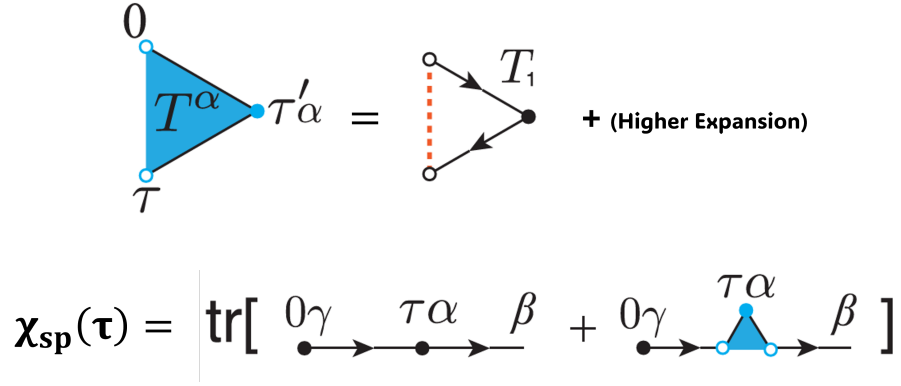


Figure 6: Specific diagram for T matrix[4].

2.4 Applying to circuit hamiltonian model

This section will introduce how we adjust the expansion method to our circuit model. The basic notation and mathematical structure follows the reference[4,5]. In our study, we consider that the total system is a thermal equilibrium state; thus, a methodology using Matsubara's method is available. To begin, we assume that each operator from RSJJ Hamiltonian mapped toward the general impurity model: More specifically, each parameter

Hamiltonian	RSJJ	Impurity
H_{bath}	$\sum_k \hbar\omega_k \hat{b}_k^\dagger \hat{b}_k$	$\sum_n \epsilon_n \hat{b}_n^\dagger \hat{b}_n$
H_{int}	$\sum_k g_k \hat{N}(\hat{b}_k^\dagger + \hat{b}_k)$	$\sum_{m,n} [V_{m,n}(t) c_m^\dagger b_n + \text{H.c.}]$

Table 2: Comparison with term from Circuit hamiltonian and impurity solver

has corresponding relations,

$$\begin{aligned}
\hbar\omega_k &\rightarrow \epsilon_n \\
g_k &\rightarrow V_{m,n} \\
\hat{N} &\rightarrow \hat{c}_m^\dagger (\hat{c}_m) \\
\hat{b}_k^\dagger (\hat{b}_k) &\rightarrow \hat{b}_n^\dagger (\hat{b}_n)
\end{aligned} \tag{2.40}$$

Using the relations, we can calculate the system's partition function as we dealt with in the eqn(2.44). Notice that instead of the fermion operator $\hat{c}^\dagger(\hat{c})$, the operator \hat{N} is written in the vector space spanned through the eigenstates of the Josephson junction.

Calculation of bosonic action

To focus our attention on the local system where we are interested, we calculate the expectation value of partition function in the aspects of the bath, which separates the effects of the bath by evaluating the system dynamics from bath points of view:

$$\begin{aligned}
Z &= Z_{\text{bath}} \text{Tr}_{JJ} \left[\frac{\text{Tr}[e^{-\beta H_{\text{bath}}} U_{\text{sys}}(\tau)]}{\text{Tr}[e^{-\beta H_{\text{bath}}}] } \right] \\
&= Z_{\text{bath}} \text{Tr}_{JJ} [\langle \mathcal{T}_\tau e^{-\int_0^\beta H_{\text{loc}}(\tau) + H_{\text{bath}} + H_{\text{int}}} \rangle_{\text{b}}]
\end{aligned} \tag{2.41}$$

Here the term JJ means tracing out the effect of local system, in our case, Josephson junction system, and term is tracing out the effect of bosonic effect, which is $\langle n_b | \mathcal{O} | n_b \rangle$, n_b is number operator for bosonic field operator, \mathcal{O} is physical quantity to calculate. To expand the interaction term, we can rewrite the equation into :

$$Z = Z_{\text{bath}} \text{Tr}_{JJ} [\langle \mathcal{T}_\tau e^{-\int_0^\beta H_{\text{loc}}(\tau) + H_{\text{bath}}} \sum_l Z_l \rangle_{\text{b}}] \tag{2.42}$$

Here, l corresponds with the number of the highest order of perturbative expansion. The derivation of Term Z_k begins from

$$\mathcal{T}_\tau e^{-\int_0^\beta H_{\text{int}}(\tau)} \approx 1 - \int_0^\beta H_{\text{int}}(\tau) d\tau + \frac{1}{2} \int_0^\beta H_{\text{int}}(\tau_1) H_{\text{int}}(\tau_2) d\tau_1 d\tau_2 + \dots \quad (2.43)$$

Following the reference[4], we can rewrite the formula into:

$$\begin{aligned} Z_l = & \sum_{k_1 \dots k_l} \sum_{k'_1 \dots k'_l} g_{k_1} g_{k'_1} g_{k_2} g_{k'_2} \dots g_{k_l} g_{k'_l} \int_0^\beta d\tau_1 \int_{\tau_1}^\beta d\tau_2 \dots \int_{\tau_{l-1}}^\beta d\tau_l \int_0^\beta d\tau'_1 \int_{\tau'_1}^\beta d\tau'_2 \dots \int_{\tau'_{l-1}}^\beta d\tau'_l \\ & \times \hat{N}(\tau_1) \hat{b}_{k_1}^\dagger(\tau_1) \hat{N}(\tau'_1) \hat{b}_{k'_1}^\dagger(\tau'_1) \hat{N}(\tau_2) \hat{b}_{k_2}^\dagger(\tau_2) \hat{N}(\tau'_2) \hat{b}_{k'_2}^\dagger(\tau'_2) \dots \hat{N}(\tau_l) \hat{b}_{k_l}^\dagger(\tau_l) \hat{N}(\tau'_l) \hat{b}_{k'_l}^\dagger(\tau'_l) \end{aligned} \quad (2.44)$$

Here, the lower index k_i indicates the oscillation mode of the i th harmonic oscillator from the bath, represented by a pair of bosonic creation and annihilation operators. The number $\frac{1}{k_l!}$ was eliminated due to considering all permutations during ordering time. Using $L(V)$ as a notation for linear operator space for vector space V , we should consider that,

1. $k_i = k'_j$ for all (i, j)
2. $\hat{N} = \{\hat{N} \in L(V_{JJ}) \mid V_{JJ} \text{ is span of } \{|\psi\rangle_{JJ}\}\}$
 $\hat{b}_k^\dagger(\hat{b}_k) = \{\hat{b}_k^\dagger(\hat{b}_k) \in L(V_{\text{bath}}) \mid V_{\text{bath}} \text{ is span of LC resonator bosonic basis}\}$ (Appendix A.)

Thus $[\hat{N}, \hat{b}^\dagger(\hat{b})] = 0$. We can adjust Z_l as follows:

$$\begin{aligned} Z_l = & \sum_{k_1 \dots k_l} (g_{k_1} g_{k_2} \dots g_{k_l})^2 \int_0^\beta d\tau_1 \int_{\tau_1}^\beta d\tau_2 \dots \int_{\tau_{k_l-1}}^\beta d\tau_{k_l} \int_0^\beta d\tau'_1 \int_{\tau'_1}^\beta d\tau'_2 \dots \int_{\tau'_{k_l-1}}^\beta d\tau'_{k_l} \\ & \times \hat{N}(\tau_1) \hat{b}_{k_1}^\dagger(\tau_1) \hat{b}_{k_1}(\tau'_1) \hat{N}(\tau'_1) \hat{N}(\tau_2) \hat{b}_{k_2}^\dagger(\tau_2) \hat{b}_{k_2}(\tau'_2) \hat{N}(\tau'_2) \dots \hat{N}(\tau_{k_l}) \hat{b}_{k_l}^\dagger(\tau_{k_l}) \hat{b}_{k_l}(\tau'_{k_l}) \hat{N}(\tau'_{k_l}) \end{aligned} \quad (2.45)$$

To calculate the effect of bath, the form of the equation turns out:

$$\begin{aligned} & \langle \mathcal{T}_\tau e^{-\int_0^\beta H_{\text{loc}}(\tau) + H_{\text{bath}}} \sum_l Z_l \rangle_{\text{b}} \\ & = \mathcal{T}_\tau e^{-\int_0^\beta H_{\text{loc}}} \langle \mathcal{T}_\tau e^{-\int_0^\beta H_{\text{bath}}} \sum_l Z_l \rangle_{\text{b}} \\ & = \mathcal{T}_\tau e^{-\int_0^\beta H_{\text{loc}}} \langle \mathcal{T}_\tau e^{-\int_0^\beta H_{\text{bath}}} \sum_l (\text{bosonic terms}) \rangle_{\text{b}} \\ & \times \int_0^\beta d\tau_1 \int_{\tau_1}^\beta d\tau_2 \dots \int_{\tau_{k_l-1}}^\beta d\tau_{k_l} \int_0^\beta d\tau'_1 \int_{\tau'_1}^\beta d\tau'_2 \dots \int_{\tau'_{k_l-1}}^\beta d\tau'_{k_l} \hat{N}(\tau_1) \hat{N}(\tau'_1) \hat{N}(\tau_2) \hat{N}(\tau'_2) \dots \hat{N}(\tau_{k_l}) \hat{N}(\tau'_{k_l}) \end{aligned} \quad (2.46)$$

Here, each bosonic term contains a calculation of form $\langle \hat{b}_{k_1}^\dagger(\tau_1) \hat{b}_{k_1}(\tau'_1) \hat{b}_{k_2}^\dagger(\tau_2) \hat{b}_{k_2}(\tau'_2) \dots \hat{b}_{k_l}^\dagger(\tau_l) \hat{b}_{k_l}(\tau'_l) \rangle_{\text{b}}$, where Wick's theorem is available. Before applying Wick's theorem to a given equation, notice that harmonic oscillators

in the bath do not interact with each other, leading to only one available property for contraction,

$$\begin{aligned}
& \langle \hat{b}_{k_1}^\dagger(\tau_1) \hat{b}_{k_1}(\tau'_1) \hat{b}_{k_2}^\dagger(\tau_2) \hat{b}_{k_2}(\tau'_2) \cdots \hat{b}_{k_l}^\dagger(\tau_l) \hat{b}_{k_l}(\tau'_l) \rangle_b \\
&= \langle \hat{b}_{k_1}^\dagger(\tau_1) \hat{b}_{k_1}(\tau'_1) \rangle_b \langle \hat{b}_{k_2}^\dagger(\tau_2) \hat{b}_{k_2}(\tau'_2) \rangle_b \cdots \langle \hat{b}_{k_l}^\dagger(\tau_l) \hat{b}_{k_l}(\tau'_l) \rangle_b \\
&+ \langle \hat{b}_{k_1}(\tau'_1) \hat{b}_{k_1}^\dagger(\tau_1) \rangle_b \langle \hat{b}_{k_2}(\tau'_2) \hat{b}_{k_2}^\dagger(\tau_2) \rangle_b \cdots \langle \hat{b}_{k_l}(\tau'_l) \hat{b}_{k_l}^\dagger(\tau_l) \rangle_b
\end{aligned} \tag{2.47}$$

which is a full bosonic term that turns out to be the sum of the multiplication of a single bosonic Green's function. It is known that when the ensemble Hamiltonian, aimed at observing a certain physical quantity, takes the form of a harmonic oscillator, it can be expressed as $\hat{a}^\dagger(\tau) = e^{E\tau}$, $\hat{a}(\tau) = e^{-E\tau} \hat{a}$ where E is a eigenvalue of Hamiltonian.[7] Using this formula, each single Green's function can be calculated as:

$$\begin{aligned}
& \langle e^{-\omega_k \tau} \hat{b}_k^\dagger e^{-\omega_k \tau'} \hat{b}_k \rangle_b = \langle e^{\omega_k(\tau-\tau')} \hat{b}_k^\dagger \hat{b}_k \rangle_b = e^{\omega_k \tau} n_B(\omega_k) \quad (\tau > \tau') \\
& \langle e^{-\omega_k \tau} \hat{b}_k e^{-\omega_k \tau'} \hat{b}_k^\dagger \rangle_b = \langle e^{\omega_k(\tau-\tau')} \hat{b}_k \hat{b}_k^\dagger \rangle_b = \langle e^{\omega_k(\tau-\tau')} (1 + \hat{b}_k^\dagger \hat{b}_k) \rangle_b = e^{\omega_k(\tau-\tau')} (1 + n_B(\omega_k)) \quad (\tau < \tau')
\end{aligned} \tag{2.48}$$

By multiplying the corresponding coupling parameter g_k^2 in mode k , the full equation becomes :

$$\begin{aligned}
& \langle \mathcal{T}_\tau e^{-\int_0^\beta H_{\text{bath}} Z_l} \rangle_b = g_{k_1}^2 (e^{\omega_{k_1}(\tau_1-\tau'_1)} (\theta(\tau_1 - \tau'_1) n_B(\omega_{k_1}) + \theta(\tau'_1 - \tau_1) [1 + n_B(\omega_{k_1})])) \\
& \times g_{k_2}^2 (e^{\omega_{k_2}(\tau_2-\tau'_2)} (\theta(\tau_2 - \tau'_2) n_B(\omega_{k_2}) + \theta(\tau'_2 - \tau_2) [1 + n_B(\omega_{k_2})])) \\
& \vdots \\
& \times g_{k_l}^2 (e^{\omega_{k_l}(\tau_l-\tau'_l)} (\theta(\tau_l - \tau'_l) n_B(\omega_{k_l}) + \theta(\tau'_l - \tau_l) [1 + n_B(\omega_{k_l})]))
\end{aligned} \tag{2.49}$$

In the general approach, the term that corresponds to bosonic action from a pseudo-particle solver can be expressed as follows:

$$\mathcal{W}(\tau) = \begin{cases} \sum_k |g_k|^2 e^{\omega_k \tau} n_B(\omega_k) & (\tau > 0) \\ \sum_k |g_k|^2 e^{\omega_k \tau} (1 + n_B(\omega_k)) & (\tau < 0) \end{cases} \tag{2.50}$$

We use notation $V_k(\tau)$ to representing simultaneously for retarded and advanced cases,

$$V_k(\tau) = e^{-\omega_k \tau} \theta(-\tau) n_B(\omega_k \beta) + e^{-\omega_k \tau} \theta(\tau) (1 + n_B(\omega_k \beta)) \tag{2.51}$$

In which we can rewrite as the form of:

$$V_k(\tau) = e^{-\omega_k \tau} \frac{\cosh \frac{\omega_k}{2}}{\sinh \frac{\omega_k}{2}} \tag{2.52}$$

Calculation of Propagator

Now, after calculating the bosonic action, we can calculate the structure of the propagator. To begin, the result of equation (2.44) after calculating $V_k(\tau)$ turns out to be:

$$Z = Z_{\text{bath}} \text{Tr}_{JJ} [\mathcal{T}_\tau e^{-\int_0^\beta d\tau H_{\text{loc}}(\tau)} \langle \mathcal{T}_\tau e^{-\int_0^\beta d\tau H_{\text{bath}}(\tau)} \sum_l Z_l \rangle_{\text{b}}] \quad (2.53)$$

Where Z_l is :

$$Z_l = \sum_{\mathcal{P} \in S} \sum_{k_1 \dots k_l} \int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_{k_l} \int_0^\beta d\tau'_1 \dots \int_0^\beta d\tau'_{k_l} V_k \cdot \hat{N}(\tau_{k_1}) \hat{N}(\tau'_{k_1}) \hat{N}(\tau_{k_2}) \hat{N}(\tau'_{k_2}) \dots \hat{N}(\tau_{k_l}) \hat{N}(\tau'_{k_l}) \quad (2.54)$$

Here \mathcal{P} indicates the possible permutation which $\mathcal{P} \in S$ for $\{S \mid \text{All possible permutation satisfying condition}\}$.

The trace for Josephson junction turns out to be:

$$\text{Tr}_{JJ} \left[\sum_l \sum_{\mathcal{P} \in S} \sum_{k_1 \dots k_l} \int_0^\beta d\tau_{k_1} \dots \int_0^\beta d\tau'_{k_l} V_k \cdot \mathcal{T}_\tau e^{-\int_0^\beta d\tau H_{\text{loc}}(\tau)} \hat{N}(\tau_{k_1}) \hat{N}(\tau'_{k_1}) \dots \hat{N}(\tau_{k_l}) \hat{N}(\tau'_{k_l}) \right] \quad (2.55)$$

Based on the above form, we can define self-energy in the above formula using the different l values.

$$l = 1 \quad , \quad \text{Tr}_{JJ} \left[\sum_{\mathcal{P} \in S} \sum_{(\text{mode})} \int_0^\beta d\tau_{k_1} \int_0^\beta d\tau'_{k_1} V_k \cdot \underbrace{\mathcal{T}_\tau e^{-\int_0^\beta d\tau H_{\text{loc}}(\tau)} \hat{N}(\tau_{k_1}) \hat{N}(\tau'_{k_1})}_{\mathcal{G}(\beta - \tau_{k_1}) \cdot V_k \cdot \hat{N} \mathcal{G}(\tau_{k_1} - \tau'_{k_1}) \hat{N} \mathcal{G}(\tau'_{k_1})} \right] \quad (2.56)$$

$= \Sigma^{(1)}$

$$l = 2 \quad , \quad \text{Tr}_{JJ} \left[\sum_{\mathcal{P} \in S} \sum_{(\text{mode})} \int_0^\beta d\tau_{k_1} \int_0^\beta d\tau'_{k_1} \int_0^\beta d\tau_{k_2} \int_0^\beta d\tau'_{k_2} V_k \cdot \underbrace{\mathcal{T}_\tau e^{-\int_0^\beta d\tau H_{\text{loc}}(\tau)} \hat{N}(\tau_{k_1}) \hat{N}(\tau'_{k_1}) \hat{N}(\tau_{k_2}) \hat{N}(\tau'_{k_2})}_{\mathcal{G}(\beta - \tau_{k_1}) \cdot V_k \cdot \hat{N} \mathcal{G}(\tau_{k_1} - \tau'_{k_1}) \hat{N} \mathcal{G}(\tau'_{k_1} - \tau_{k_2}) \hat{N} \mathcal{G}(\tau_{k_2} - \tau'_{k_2}) \hat{N} \mathcal{G}(\tau'_{k_2})} \right] \quad (2.57)$$

$= \Sigma^{(2)}$

For instance, if we consider only the first-order self-energy expansion, the result coincides with the well-known Non-crossing approximation method. Here, the ordering of the time index dominated through pre-decided V_k for arbitrary τ_i . In the order $l = 1$, the diagram structure corresponds with a Non-crossing approximation. The case $l = 2$ corresponds with a One-crossing approximation. Getting more diagrams corresponding with a higher-order expansion, such as TOA, can be achievable by increasing the maximum value of the l index.

Calculating correlation function

After calculating the action in the above section and the remaining terms again for the Josephson junction, we can obtain terms of the form of equation (2.60). Through calculating the correlation function as in equation (2.50)

using the obtained form, we additionally introduced an operator λ_1 defined as follows:

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (2.58)$$

This operator was introduced to investigate the degree of mixing between the ground state and the first excited state among the energy states of the junction. By applying the operator, the final expression for calculating the correlation function in the RSJJ Hamiltonian model can be written as follows:

$$\begin{aligned} \chi_{sp}(\tau) = & \text{Tr}[\mathcal{G}(\beta - \tau)\lambda_1\mathcal{G}(\tau)\lambda_1] \\ & + \int \int \text{Tr}[V(\tau_2 - \tau_1)\mathcal{G}(\beta - \tau_1)\hat{N}\mathcal{G}(\tau_1 - \tau_2)\lambda_1\mathcal{G}(\tau_2 - \tau)\hat{N}\mathcal{G}(\tau)\lambda_1] \\ & + \dots \end{aligned} \quad (2.59)$$

$$\sum_{\text{OCA}} = \text{Diagram 1} + \text{Diagram 2}$$

Diagram 1: A horizontal double line with a wavy line loop above it labeled w and a black triangle on the double line labeled \mathcal{G} .

Diagram 2: A horizontal double line with two wavy line loops above it and two black triangles on the double line.

$$\Sigma_{\text{TOA}} = \text{[Diagram 1]} + \text{[Diagram 2]}$$

18