Heat transport via a local two-state system

Masanari Kato[1], Takeo Kato[1] and Keiji Saito

[1] IOP Publishing, Temple Circus, Temple Way, Bristol BS1 6HG, UK

E-mail: kato@issp.u-tokyo.ac.jp

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Abstract. test

1. Introduction

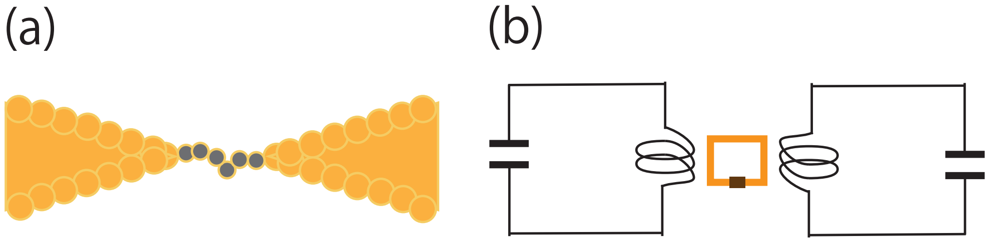

Figure 1. (a)molecular junction, (b)Josephson junction in the super conducting circuit

2. Model and Exact Formula

In this section, we explain the model which describes the heat transport via a local two-state system. Then, we derive the exact formula of liner heat conductance in this system by using the Keldysh formalism.

When we discuss the heat transport via a zero-dimensional object, we should consider the system where a local oscillator is localized between two phonon baths. Now, we adopt the double well potential as the local oscillator because this potential can denote the boson interaction caused by nonlinearity. In reality, this system can be implemented as the molecular junction or the Josephson junction in the super conducting circuit[**?**](Fig. 1). At low temperature, when the potential barrier is infinitely higher than the energy level difference from the ground state to the first excited state, the local oscillator can be regarded as the two-state system described by the ground state where the system is localized at the right or left well. Then, we can relate the two-state system to the pseudo-spin system. Then, the Hamiltonian of local oscillator is described by the Pauli matrix $\sigma_i(i : x, y, z)$ as

$$H = \frac{\hbar\Delta}{2}\sigma_x + \frac{\hbar\epsilon}{2}\sigma_z, \tag{1}$$

where Δ is the tunneling amplitude and ϵ is the bias of the system, i.e., the difference in the ground-state energies of the local two states. In this study, we assume the symmetric double well, i.e., $\epsilon = 0$. Then, the local two-state system coupling to two phononic baths is described by the spin-boson Hamiltonian:

$$H = \frac{\hbar\Delta}{2}\sigma_x + \sum_{\nu=L,R}\sum_{\nu k}\hbar\omega_{\nu k}b^\dagger_{\nu k}b_{\nu k} + \frac{\sigma_z}{2}\sum_{\nu=L,R}\sum_{\nu k}\hbar\lambda_{\nu k}(b_{\nu k} + b^\dagger_{\nu k}), \tag{2}$$

where $\omega_{\nu k}$, $b_{\nu k}$ is the frequency and annihilation operator of phonon with the wavenumber k in the νth bath, and $\lambda_{\nu k}$ is the coupling strength between the local two-state system and phonons in two phononic baths. (Fig. 2) is the image? of this system. The spectral function defined as

$$I_\nu(\omega) \equiv \sum_{\nu k}\lambda^2_{\nu k}\delta(\omega - \omega_{\nu k}) \tag{3}$$

characterizes the behavior of heat transport under the spin-boson model. We assume that the spectral function takes the form of power law:

$$I_\nu(\omega) = \alpha_\nu\tilde{I}_\nu(\omega), \tag{4}$$

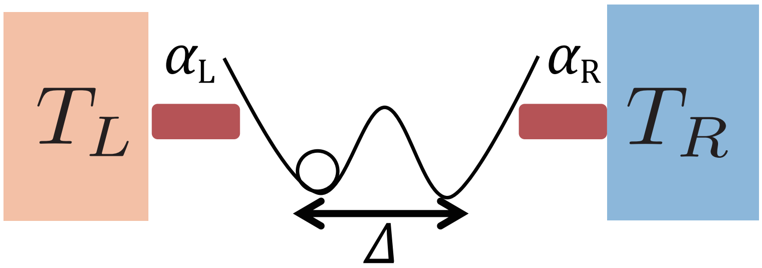

Figure 2. The two-state system coupling to two phononic baths. If the temperature of two baths is slightly different, phonon can be transported from one bath to another.

$$\tilde{I}_\nu(\omega) = 2\omega_c^{1-s}\omega^s f(\omega/\omega_c), \tag{5}$$

where α_ν is the dimensionless coupling strength between the local two-state system and the νth heat bath, ω_c is the cutoff frequency satisfying $\omega_c \gg \Delta, \epsilon$, and $f(\omega/\omega_c)$ is the cutoff function in the range [0,1]. For simplicity, we assume the cutoff function $f(\omega/\omega_c)$ takes the form of step function $\theta(\omega_c - \omega)$. The case of $s = 1$ is called "ohmic" and the ohmic case is studied in detail as we discussed in the section 1. The case of $s > 1$ and $s < 1$ is called "super-ohmic" and "sub-ohmic", respectively, and these non-ohmic case is our main interest. Starting with this setup, we derive the exact formula of thermal conductance under the spin-boson model by using Keldysh formalism.

First, we define the operator of the heat current flowing from the νth bath into the local two-state system as

$$J_\nu \equiv \frac{dH_{\mathrm{bath},\nu}}{dt}, \tag{6}$$

where the Hamiltonian of the νth bath is defined as $H_{\mathrm{bath},\nu} \equiv \sum_k \hbar\omega_{\nu k} b_{\nu k}^\dagger b_{\nu k}$. This operator follows the Heisenberg's equation of motion, then

$$J_\nu = -\frac{i}{\hbar}[H_{\mathrm{bath},\nu}, H] \tag{7}$$

$$= -i\sum_k \frac{\lambda_{\nu k}}{2}\hbar\omega_{\nu k}\sigma_z(-b_{\nu k} + b_{\nu k}^\dagger). \tag{8}$$

The ensemble average of heat current $\langle J_\nu(t)\rangle = \mathrm{Tr}[\rho J_\nu(t)]$, where ρ is the density matrix of initial state, is calculated as

$$\langle J_\nu(t)\rangle = \mathrm{Re}\left[\sum_k \frac{\hbar^2\omega_{\nu k}\lambda_{\nu k}}{2} G^<_{\sigma_z, b^\dagger_{\nu k}}(t_1, t_2)\right]\Bigg|_{t_1=t_2=t}, \tag{9}$$

where the lesser Green's function is defined as

$$G^<_{\sigma_z, b^\dagger_{\nu k}}(t_1, t_2) \equiv -\frac{i}{\hbar}\langle b^\dagger_{\nu k}(t_2)\sigma_z(t_1)\rangle. \tag{10}$$

Then, by using Keldysh formalism, we can derive the heat current at the steady state[13]:

$$\langle J_\nu\rangle = \frac{\hbar}{4}\int_0^\infty d\omega\, \hbar\omega \left[\mathrm{Im}[G^r_{\sigma_z,\sigma_z}(\omega)]I_\nu(\omega)n_\nu(\hbar\omega) - iG^<_{\sigma_z,\sigma_z}(\omega)\frac{I_\nu(\omega)}{2}\right], \tag{11}$$

where $n_\nu(\hbar\omega)$ means the Bose-Einstein distribution function and the retarded Green's function is defined as

$$G^r_{A,B}(t_1,t_2) \equiv -\frac{i}{\hbar}\theta(t_1-t_2)\langle[A(t_1),B(t_2)]\rangle. \tag{12}$$

Here, we introduce the quantity γ_ν which denotes the symmetry of coupling to the two baths:

$$\gamma_\nu = \frac{\int_0^\infty d\omega\,\hbar\omega G^<_{\sigma_z,\sigma_z}(\omega)I_\nu(\omega)}{\sum_{\nu'=L,R}\int_0^\infty d\omega\,\hbar\omega G^<_{\sigma_z,\sigma_z}(\omega)I_{\nu'}(\omega)}. \tag{13}$$

Remarking the conservation law of the particle number $\langle J_L\rangle + \langle J_R\rangle = 0$, $\langle J_L\rangle$ can be denoted as follows by γ_ν

$$\langle J_L\rangle = \gamma_R\langle J_L\rangle - \gamma_L\langle J_R\rangle \tag{14}$$

$$= \frac{1}{4}\int_0^\infty d(\hbar\omega)\,\hbar\omega \mathrm{Im}[G^r_{\sigma_z,\sigma_z}(\omega)]\left[\gamma_R I_L(\omega)n_L(\hbar\omega) - \gamma_L I_R(\omega)n_R(\hbar\omega)\right] \tag{15}$$

Here, we assume $\tilde{I}_L(\omega) = \tilde{I}_R(\omega) = \tilde{I}(\omega)$, then $\langle J_L\rangle$ is

$$\langle J_L\rangle = \frac{\alpha_L\alpha_R}{4(\alpha_L+\alpha_R)}\int_0^\infty d(\hbar\omega)\hbar\omega\mathrm{Im}[G^r_{\sigma_z,\sigma_z}(\omega)]\tilde{I}(\omega)\left[n_L(\hbar\omega) - n_R(\hbar\omega)\right]. \tag{16}$$

In the linear response regime, thermal conductance is defined as

$$\kappa \equiv \lim_{\Delta T\to 0}\frac{\langle J_L\rangle}{\Delta T}. \tag{17}$$

Finally, we can get the exact formula of thermal conductance:

$$\kappa = \frac{k_B\alpha\omega_c^{1-s}}{4}\int_0^\infty d(\hbar\omega)\mathrm{Im}[\chi(\omega)]\omega^s\left[\frac{\beta\hbar\omega/2}{\sinh(\beta\hbar\omega/2)}\right]^2, \tag{18}$$

where we assumed the symmetric coupling strength $\alpha = \alpha_L = \alpha_R$ and substituted the response function $\chi(\omega)$ for $G^r_{\sigma_z,\sigma_z}(\omega)$ by considering the linear response theory. Eq. (18) is the main result in this section. When we evaluate the value of conductance (18), we have to calculate the response function $\mathrm{Im}[\chi(\omega)]$. But, except the special case like "Toulouse limit" ($\alpha = 1/2$ in the ohmic case), it is difficult to analytically calculate $\mathrm{Im}[\chi(\omega)]$. Here, in this study, we numerically evaluate $\mathrm{Im}[\chi(\omega)]$ by the Monte Carlo method. Although we explain how to numerically calculate $\mathrm{Im}[\chi(\omega)]$ in section 4 in detail, in the next section, we derive the approximate formulas of thermal conductance (18) in three different situations.

3. Approximate Formulas

3.1. sequential tunneling

consider $T \simeq \mathit{\Delta}_{\rm eff}$
then the spectral function

$$S(\omega) \equiv \frac{\mathrm{Im}[\chi(\omega)]}{\omega} \tag{19}$$

$$S(\omega) = \frac{\Delta}{\pi}\left[\delta(\omega - \Delta) + \delta(\omega + \Delta)\right] \tag{20}$$

is approximated as

$$S(\omega) \simeq A\delta(\omega - \mathit{\Delta}_{\rm eff}) + \delta(\omega + \mathit{\Delta}_{\rm eff}) \tag{21}$$

where $\delta(x)$ is delta function. then we apply Kramers-Kronig relation

$$\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega S(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega \frac{\mathrm{Im}[\chi(\omega)]}{\omega} \tag{22}$$

$$= \mathrm{Re}[\chi(0)] \tag{23}$$

$$\chi_m \equiv \lim_{\epsilon \to 0} \frac{\langle \sigma_z \rangle}{\epsilon} \tag{24}$$

in the super ohmic and ohmic case $\chi_m = 2\mathrm{tanh}(\beta\mathit{\Delta}_{\rm eff}/2)/\mathit{\Delta}_{\rm eff}$. then (18) is

$$\kappa \simeq \frac{\pi\alpha\omega_c^{1-s}}{4}\frac{\Delta_{\rm eff}^s}{2n(\Delta_{\rm eff})+1}\left[\frac{\beta\Delta_{\rm eff}/2}{\sinh(\beta\Delta_{\rm eff}/2)}\right]^2 \tag{25}$$

3.2. cotunneling

consider lowtemperature $T \ll \mathit{\Delta}_{\rm eff}$, where $\mathit{\Delta}_{\rm eff}$is abatically renormalized tunnneling rate.
generalized Shiba's relation

$$\lim_{\omega \to 0+} \frac{\mathrm{Im}[\chi(\omega)]}{\omega^s} = 2\pi\alpha\left(\frac{\chi_m}{2}\right)^2 \tag{26}$$

where χ_m is susceptibility
then (18) is

$$\kappa \simeq \frac{\pi\omega_c^{s-1}\chi_m^2}{8}\int_0^{\omega_c} d\omega I_L(\omega) I_R(\omega)\left[\frac{\beta\omega/2}{\sinh(\beta\omega/2)}\right]^2 \tag{27}$$

$$\kappa \simeq \frac{\pi\omega_c^{1-s}}{8}\left(\alpha\chi_m\right)^2 F(s) T^{2s+1}, \tag{28}$$

$$F(s) = \int_0^{\beta\omega_c} dx x^{2s}\left[\frac{x/2}{\sinh(x/2)}\right]^2 \tag{29}$$

3.3. incoherent tunneling

consider $T \gg \Gamma$. master eq.

$$\frac{dP_+(t)}{dt} = \Gamma P_-(t) - \Gamma P_+(t) \tag{30}$$

Fermi's golden rule

$$\Gamma = \left(\frac{\Delta}{2}\right)^2 \int_{-\infty}^{\infty} dt\; e^{-Q(t)}, \tag{31}$$

$$Q(t) = \int_0^\infty d\omega \frac{I(\omega)}{\omega^2} \left\{\coth\left(\frac{\beta\omega}{2}\right)[1-\cos(\omega \mathrm{t})] + i\,\sin(\omega t)\right\} \tag{32}$$

$$\langle \sigma_z(t)\rangle = \frac{P_+ - P_-}{P_+ + P_-} = e^{-2\Gamma t} \tag{33}$$

$$C(t) = \langle \sigma_z(t)\sigma_z(0)\rangle = e^{-2\Gamma|t|} \tag{34}$$

$$C(t) \equiv \langle \sigma_z(t)\sigma_z(0) + \sigma_z(0)\sigma_z(t)\rangle/2 \tag{35}$$

$$= \langle \sigma_z(t)\sigma_z(0)\rangle \tag{36}$$

$$= e^{-2\Gamma|t|} \tag{37}$$

Fourier transformation

$$C(\omega) = \frac{4\Gamma}{\omega^2 + 4\Gamma^2} \tag{38}$$

fluctuation-dissipation theorem

$$C(\omega) = \coth\left(\frac{\beta\omega}{2}\right)\mathrm{Im}[\chi(\omega)] \tag{39}$$

$T \gg \Delta$

$$C(\omega) \simeq 2\frac{\mathrm{Im}[\chi(\omega)]}{\beta\omega} = 2TS(\omega) \tag{40}$$

then the spectral function is

$$S(\omega) = \frac{2\Gamma/T}{\omega^2 + 4\Gamma^2} \simeq \frac{2\Gamma}{\omega^2 T} \tag{41}$$

then (18) is

$$\kappa \simeq \frac{\alpha\omega_c^{1-s}}{4}\int_0^{\omega_c} d\omega \frac{2\Gamma}{T}\omega^{s-1}\left[\frac{\beta\omega/2}{\sinh(\beta\omega/2)}\right]^2 \tag{42}$$

$$= \frac{\alpha\omega_c^{1-s}}{2}G(s)\Gamma T^{s-1} \tag{43}$$

$$G(s) = \int_0^{\beta\omega_c} dx\, x^{s-1}\left[\frac{x/2}{\sinh(x/2)}\right]^2 \tag{44}$$

ohmic case

$$\kappa \simeq \frac{\sqrt{\pi}\Gamma(\alpha)}{4\Gamma(\alpha+1/2)}\frac{\Delta^2}{\omega_c}\left(\frac{\pi T}{\omega_c}\right)^{2\alpha-1} \tag{45}$$

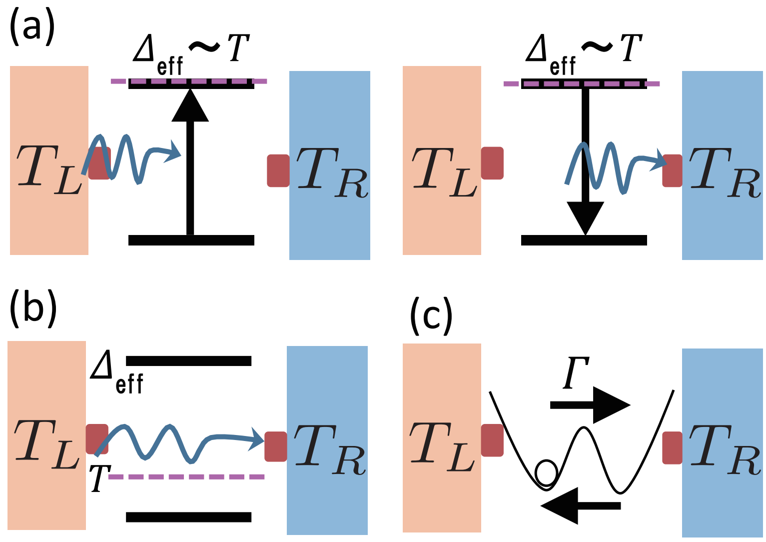

Figure 3. mechanism

sub ohmic case

$$\kappa \simeq \frac{\alpha\omega_c^{1-s}}{2}G(s)\frac{\Delta^2}{4}e^{-\frac{\beta\Lambda_1}{4}}\sqrt{\frac{\pi\beta}{\Lambda_2}}T^{s-1} \tag{46}$$

where

$$\Gamma \;=\frac{\Delta^2}{4}e^{-\frac{\beta\Lambda_1}{4}}\sqrt{\frac{\pi\beta}{\Lambda_2}}, \tag{47}$$

$$\Lambda_1 = 8T\alpha\Gamma(s-1) + 16T\alpha\Gamma(s-1)\left(\frac{T}{\omega_c}\right)^{s-1}(2-2^{s-1})\zeta(s-1), \tag{48}$$

$$\Lambda_2 = T\left(\frac{T}{\omega_c}\right)^{s-1}2\alpha(2^{s+1}-1)\Gamma(s+1)\zeta(s+1) \tag{49}$$

4. Monte Carlo method

In this section, we map the spin-boson model to the Ising model with long-range interactions on the imaginary axis by deriving the partition function of the spin-boson model in the imaginary time form. And, we explain how to numerically calculate the response function $\mathrm{Im}[\chi(\omega)]$ by Monte Carlo method to the long-range Ising model.

First, we divide the spin-boson hamiltonian (**??**) into two parts:

$$H = \frac{\Delta\sigma_x}{2} + H_z, \tag{50}$$

$$H_z = \sum_{\nu=L,R}\sum_k \omega_{\nu k} b_{\nu k}^\dagger b_{\nu k} + \sum_{\nu=L,R}\sum_k \frac{\sigma_z}{2}\lambda_{\nu k}(b_{\nu k} + b_{\nu k}^\dagger). \tag{51}$$

Then, the partition function $Z = \mathrm{Tr}[e^{-\beta H}]$ can be described as

$$Z = Z_+ + Z_-, \tag{52}$$

$$Z_\pm = \langle\pm|\,\mathrm{Tr}_{\mathrm{boson}}[e^{-\beta H}]\,|\pm\rangle\,, \tag{53}$$

where $|\pm\rangle$ means the eigen state of σ_z, i.e., $\sigma_z|\pm\rangle = \pm 1|\pm\rangle$, and $\mathrm{Tr}_{\mathrm{boson}}$ means the trace for the boson's degree of freedom. Here, we introduce $\tilde{\sigma}_x(u)$ defined as $\tilde{\sigma}_x(u) \equiv e^{iH_z u}\sigma_x e^{-iH_z u}$, then we can expand Z_+ into

$$Z_+ = \mathrm{Tr}_{\mathrm{boson}}\left[\langle +|\, e^{-\beta H_z} e^{-\int_0^\beta du \Delta\tilde{\sigma}_x(u)/2}\,|+\rangle\right] \tag{54}$$

$$= \sum_{n=0}^{\infty}\mathrm{Tr}_{\mathrm{boson}}\left[\langle +|\, e^{-\beta H_z}\int_0^\beta d\tau_1 \ldots \int_0^{\tau_{2n-1}-\tau_c} d\tau_{2n}\left(\frac{\Delta}{2}\right)^{2n}\tilde{\sigma}_x(\tau_1)\ldots\tilde{\sigma}_x(\tau_{2n})\,|+\rangle\right] \tag{55}$$

where τ_c is the cutoff on the imaginary time axis and it is given by $\tau_c = 1/\omega_c$. By calculating the trace for the boson's degree of freedom, we can derive the instanton-like partition function with n-kink pairs? [5, 6]:

$$Z_+ = Z_0\sum_{n=0}^{\infty}\left(\frac{\Delta\tau_c}{2}\right)^{2n}\int_0^\beta \frac{d\tau_1}{\tau_c}\ldots\int_0^{\tau_{2n-1}-\tau_c}\frac{d\tau_{2n}}{\tau_c}\exp\left[\sum_{j>i}^{2n}(-1)^{i+j}W(\tau_j-\tau_i)\right], \tag{56}$$

where Z_0 is the partition function of bosons in the heat bath, and $W(\tau)$ is given by

$$W(\tau) = \int_0^\infty d\omega\frac{I(\omega)}{\omega^2}\frac{\cosh(\beta\omega/2) - \cosh(\beta\omega/2-\tau)}{\sinh(\beta\omega/2)}. \tag{57}$$

We can calculate Z_- in the same way. If we regard $\tilde{\sigma}_x(\tau_j)$ as a kink charge, Eq. (56) can be regarded as the "kink" representation of the one-dimensional Ising model with the system states distinguished by the kink-degree of freedom $\{\tilde{\sigma}_x(\tau_i)\}$. Now, we consider rewriting it to the "spin" representation. Generally, the partition function of the one-dimensional Ising model with long-range interactions with the lattice constant a is written in the kink representation as

$$Z_{\mathrm{ising}} = \sum_{n=0}^{\infty} y^{2n}\int_0^\beta \frac{d\tau_1}{a}\ldots\int_0^{\tau_{2n-1}-a}\frac{d\tau_{2n}}{a}\exp\left[\sum_{j>i}^{2n}(-1)^{i+j}4U\left(\frac{\tau_j-\tau_i}{a}\right)\right] \tag{58}$$

where $U(\tau)$ is the kink-kink interaction, and y is the chemical potential which satisfies $y = e^{2U(0)}$. According to [6, 7], we can calculate the spin-spin interaction $V(n)$ from the

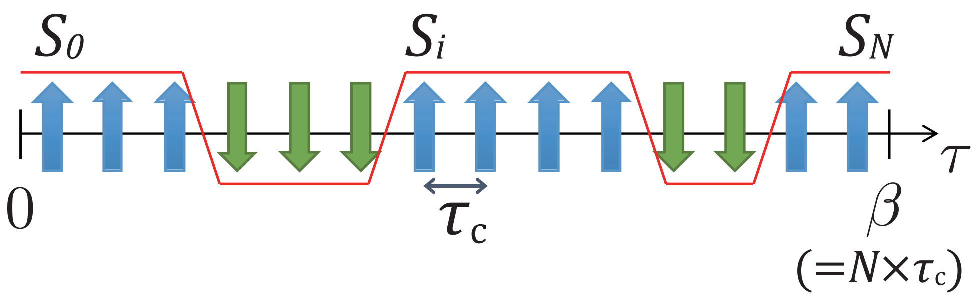

Figure 4. the one-dimensional Ising model with long-range interactions on the imaginary τ-axis.

kink-kink interaction $U(n)$ by the following recurrence relation:

$$V(n) = U(n+1) - 2U(n) + U(n-1), \ (n : \text{integer} > 0), \tag{59}$$

then, Eq. (58) is described by $V(n)$ as

$$Z_{\text{ising}} = \sum_{S_1 \ldots S_N} \exp\left[-\sum_{j>i} V(j-i) S_i S_j\right], \tag{60}$$

where $S_i, (i : \text{integer})$ is the spin of the ith site, N is the total number of sites, and S_i satisfies the boundary condition $S_i = S_{i+N}$ (Fig. 4). In this study, we divide β in length on the τ-axis into N parts, i.e., $\tau_c = \beta/N$. Then, we put Ising spins on the each sites and chose $V(n)$ as Eq. (58) becomes our desiring partition function(56). Specifically, we decide $U(n)$ from $W(\tau)$, and calculate $V(n)$ by Eq. (59). Actually, we can derive $V(n) \propto n^{-(s+1)}$ for the large enough total number of sites N, i.e., $n/N \ll 1$. In this way, we can map the spin-boson model to the one-dimensional Ising model with long-range interactions.

Now, we remark the algebraic relation between the response function $\chi(\omega)$ and the spin-correlation function $C(\tau)$:

$$\chi(\omega) \quad = C(i\omega_n \to \omega + i\delta), \tag{61}$$

$$C(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} C(\tau), \tag{62}$$

$$C(\tau) \quad = \langle \sigma_z(\tau)\sigma_z(0)\rangle, \tag{63}$$

where Eq. (62) means the analytic continuation. These relations means we can derive $\text{Im}[\chi(\omega)]$ by calculating $C(\tau)$. And, we can derive $C(\tau)$ by calculating the spin correlation $\langle S_i S_0\rangle$ of the long-range Ising model because they satisfies $\langle \sigma_z(\tau_i)\sigma_z(0)\rangle \simeq \langle S_i S_0\rangle$. In this study, we use the Monte Carlo method to calculate $C(\tau)$ of the Ising model derived from Eq. (60). But, it takes very long time to numerically calculate $C(\tau)$ because the Ising model derived from Eq. (60) has $r^{-(s+1)}$ long-range interactions. Especially, this problem notably appears in the low temperature. It is known that if you use the single flip method [8], the relaxation time of the system diverges near the critical temperature (called "critical slowing down"). This problem can be solved by the cluster-flip method like the Wolff algorithm[14]. In this study, we use an efficient Monte

Carlo method based on the Wolff algorithm developed by E.Luijten [15]. The Luijten's algorithm utilizes the cumulative frequency distribution and in this algorithm we need not look at all spins in order to build a cluster but calculate the site at which the spin to add into a cluster first appears. Actually, we can realize more efficient implementation by making use of the bisection method to calculate the site. In this way, we adopt the Wolff method utilizing the cumulative frequency distribution to calculate the spin correlation $\langle S_i S_0 \rangle$.

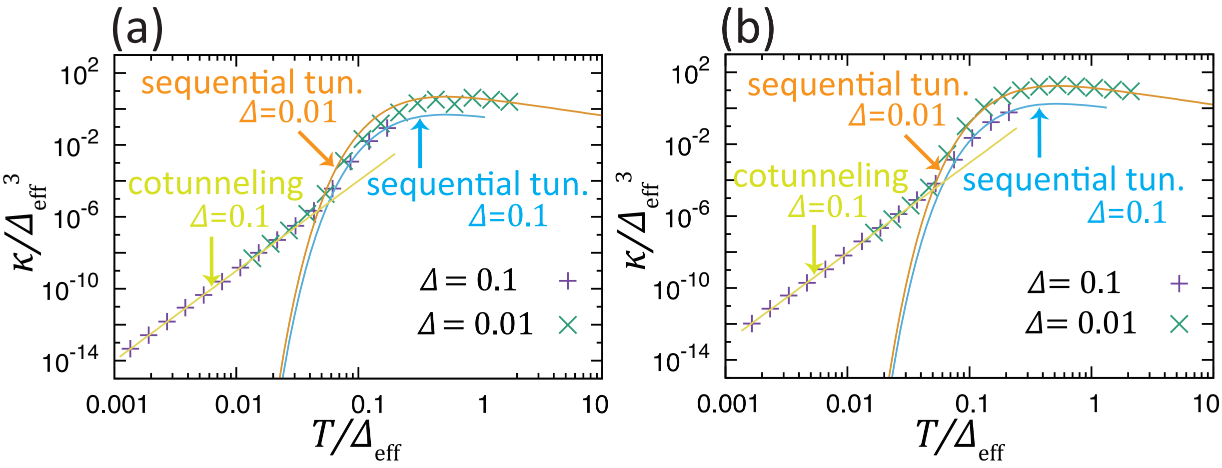

Figure 5.

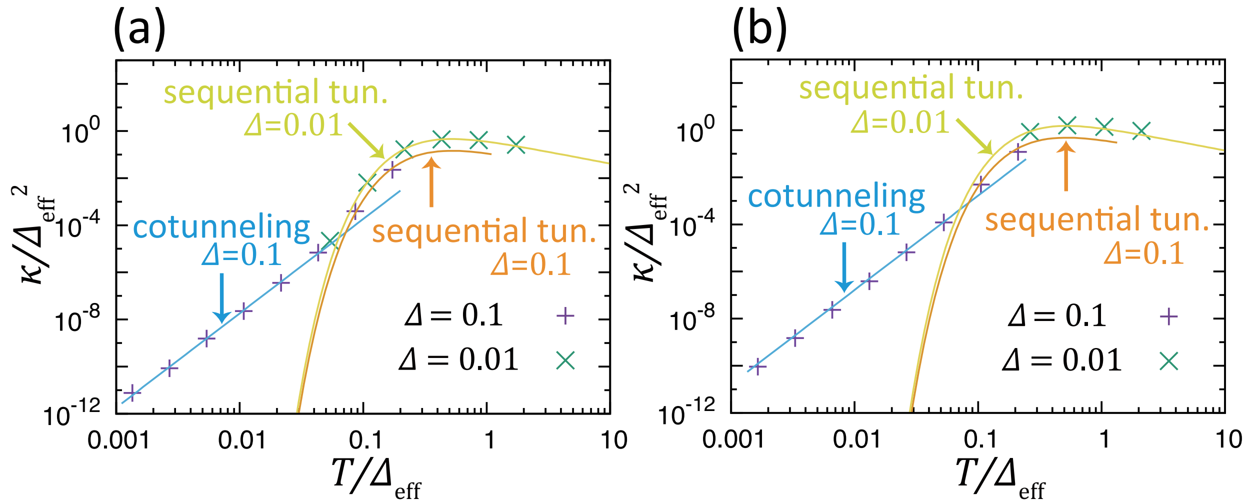

Figure 6.

5. Numerical result

5.1. Super ohmic

The results for s=2.0

The results for s=1.5

5.2. Ohmic

The results for s=1

$\alpha \geq 1$

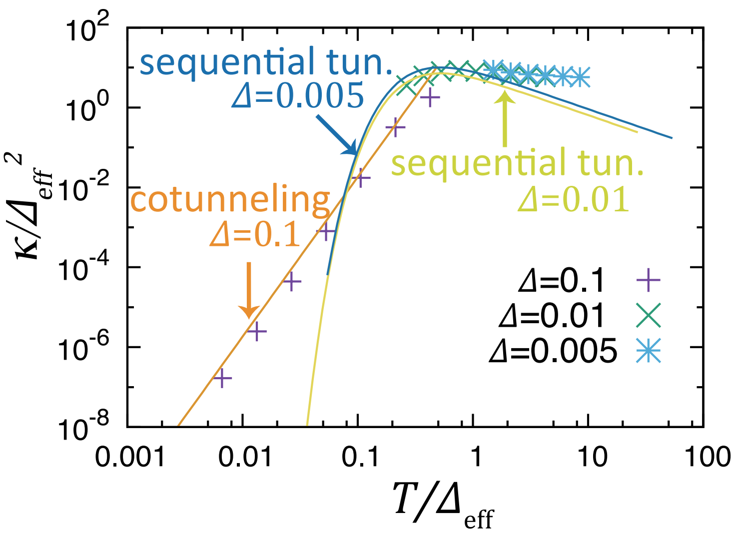

Figure 7.

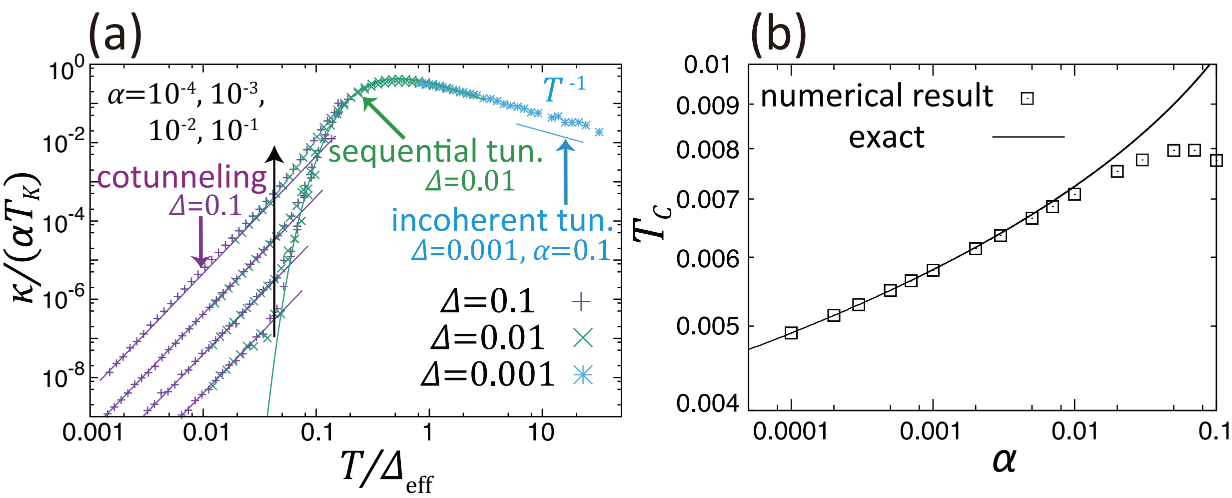

Figure 8.

5.3. Sub ohmic

The results for s=0.9

The results for s=0.6

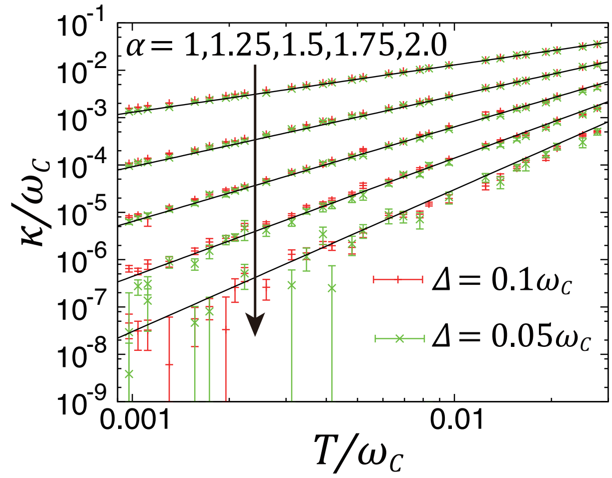

Figure 9.

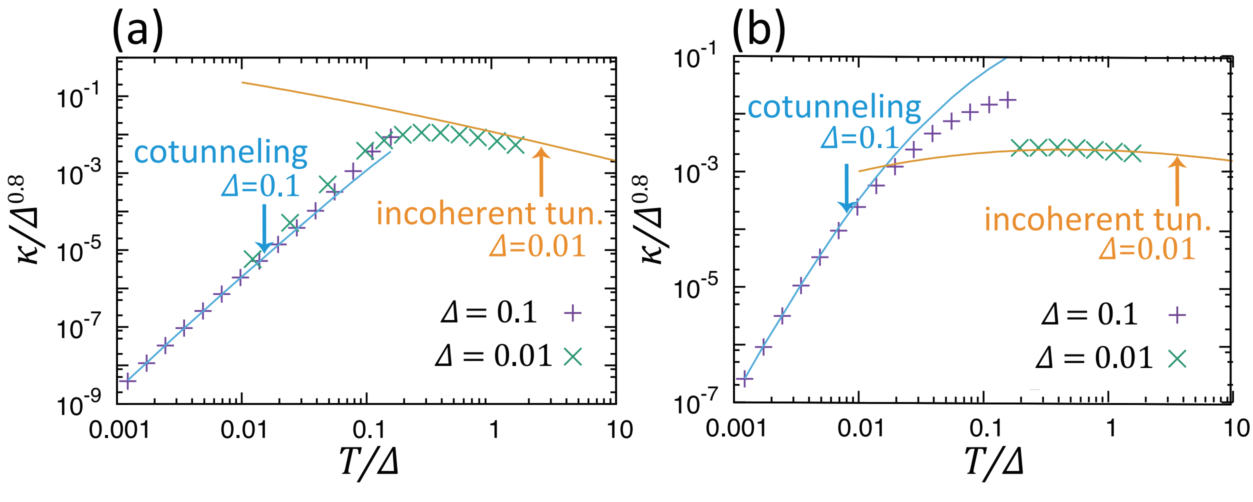

Figure 10.

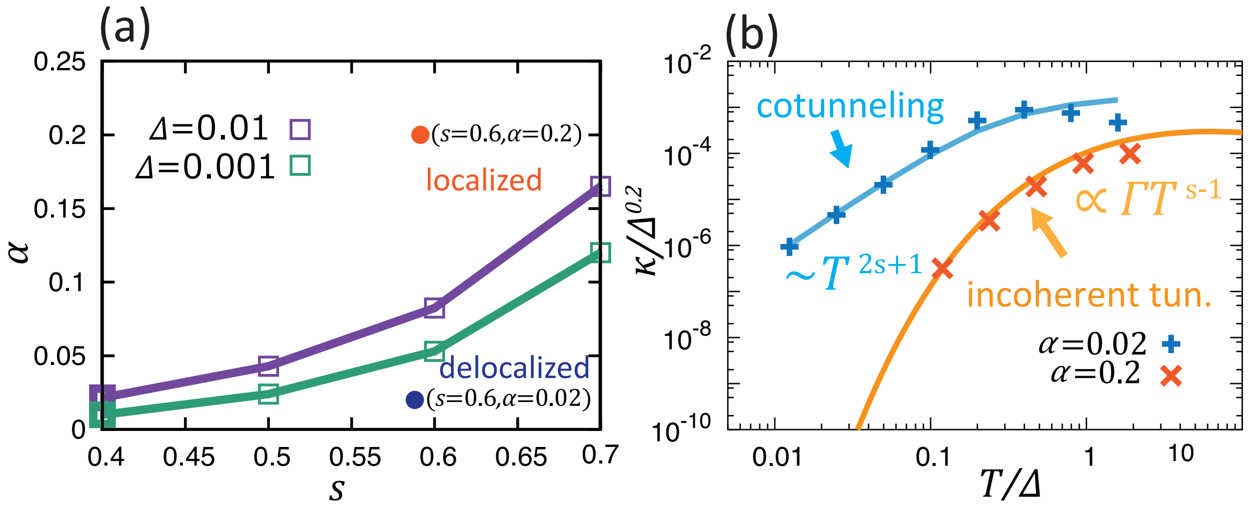

Figure 11.

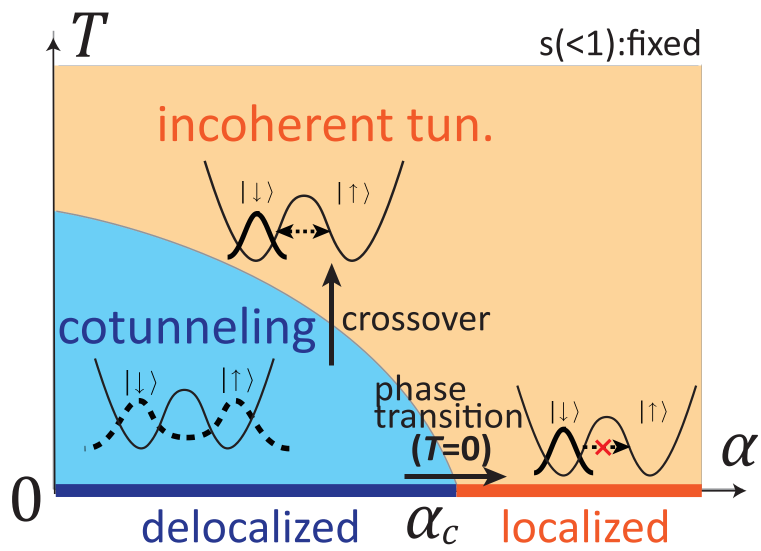

Figure 12.

6. Summary

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