Quantum heat transport through a spin-boson nanojunction

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Quantum heat transport through a two-level system is investigated by a spin-boson model with two heat baths kept in different temperatures. The Nonequilibrium Green's Function (NEGF) method is used to calculate the heat current in a perturbative manner. To cope with spin-spin correlators, the Majorana fermion representation of spin operators is exploited, which allows us to make use of the Wick's Theorem for standard diagrammatic techniques. A formula of heat current is obtained, and some numerical results are presented in comparison with other methods, and two kinds of transport mechanisms are identified. In particular, an anomalous inhibition of heat current by increasing the coupling strength between the baths and the intermediate system is confirmed, which is possibly due to the Quantum Zeno effect (QZE) on the transition rate.

I. Model

The Hamiltonian is of a standard spin-boson model with two heat baths. The coupling term includes only transverse component:

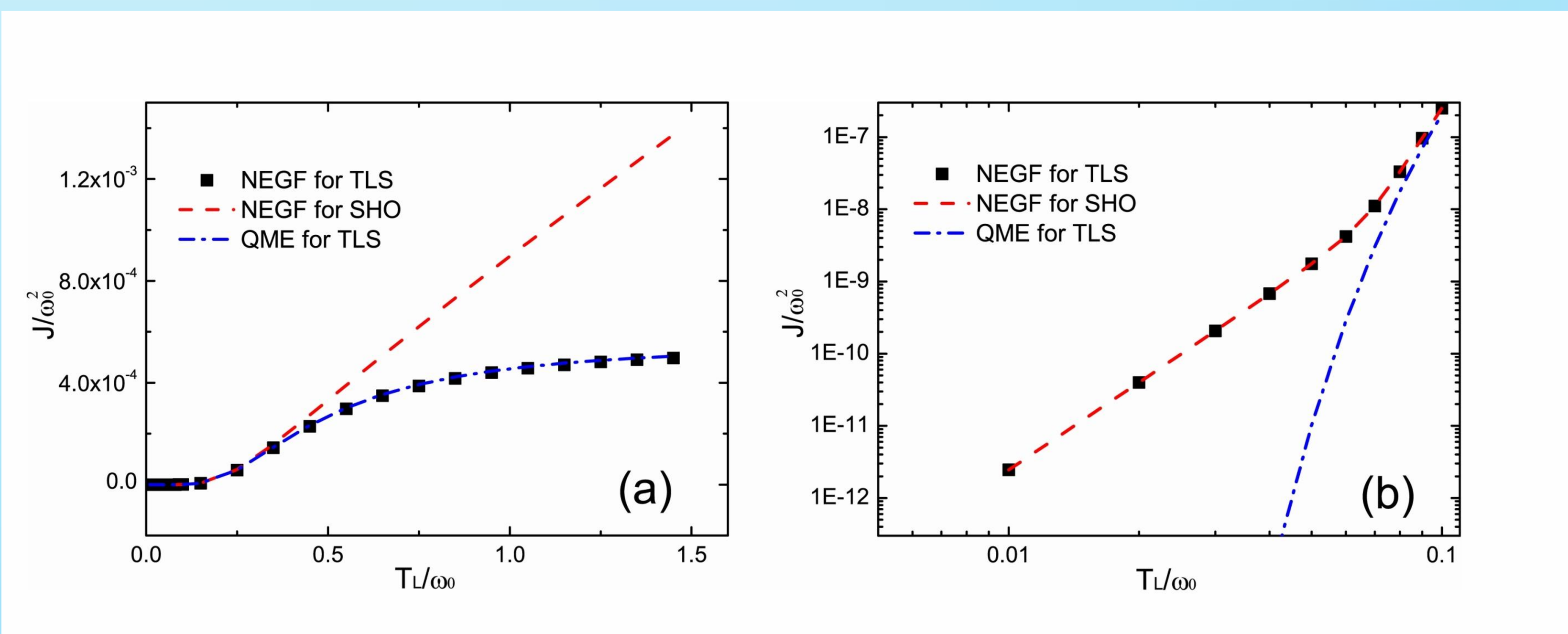
$$H = H_L + H_R + H_S + H_C,$$

$$H_S = \frac{1}{2}\Delta\sigma_z + \frac{1}{2}\varepsilon\sigma_x,\ H_{L/R} = \sum_{j\in L/R}\omega_j\left(a_j^\dagger a_j + \frac{1}{2}\right),\ H_C = \sigma_z\sum_{j\in L,R} g_j\left(a_j^\dagger + a_j\right).$$

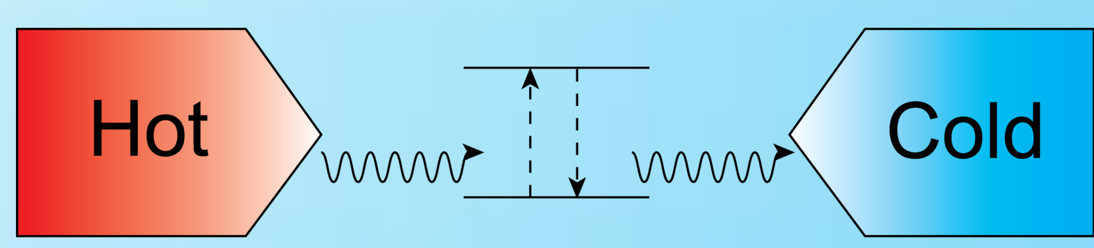
II. Heat current formula

The heat current formula is calculated by a standard Meir-Wingreen approach, with the help of the Majorana fermion representation of spin correlators. The one-loop diagram approximation is adopted when calculating the Green's functions. The figures below shows the heat currents under high and low temperatures respectively.

$$J = \frac{2}{\pi}\int_0^\infty d\omega \frac{\omega\Gamma_L(\omega)\Gamma_R(\omega)\omega_0^2}{\left(\omega^2-\omega_0^2\right)^2 + \omega^2\left[\Gamma_L(\omega)\coth\left(\frac{\beta_L\omega}{2}\right) + \Gamma_R(\omega)\coth\left(\frac{\beta_R\omega}{2}\right)\right]^2}\left[n_L(\omega) - n_R(\omega)\right].$$

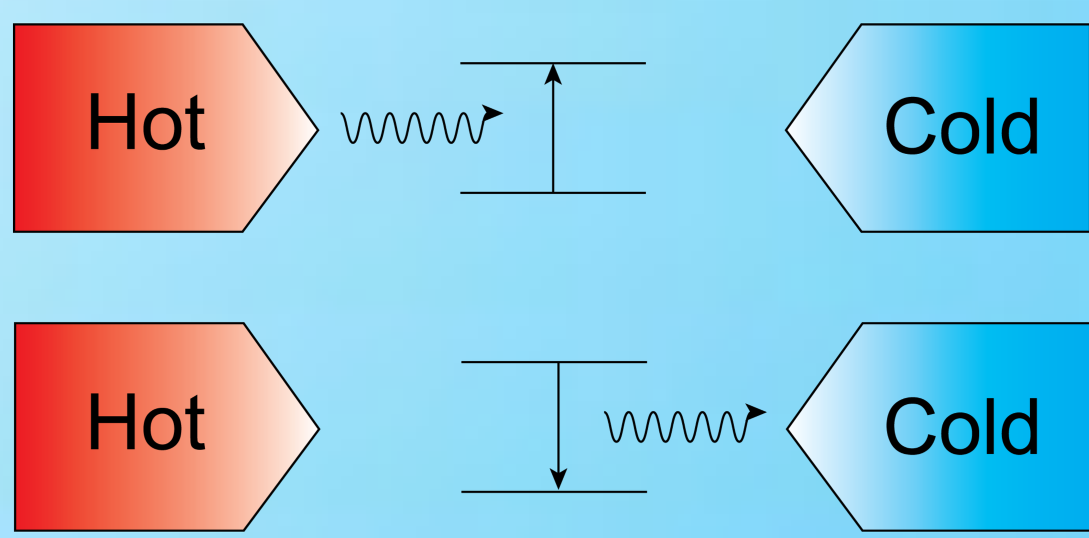


(a)



Schematic diagram of "cotunneling" transport process. The energy fluctuation of the hot bath is not strong enough to excite the intermediate system to its higher energy level. But heat can be transported to the cold bath by a virtual excitation-relaxation process of the intermediate system.

(b)



Schematic diagram of "sequential" transport process. The energy fluctuation of the hot bath is strong enough to excite the intermediate system to its higher energy level. The system then releases its energy to the cold bath through relaxation process.

III. Two mechanisms of heat transport

In low temperatures, heat transport is dominated by the coherent "cotunneling" process: (See the Fig.(a) above.)

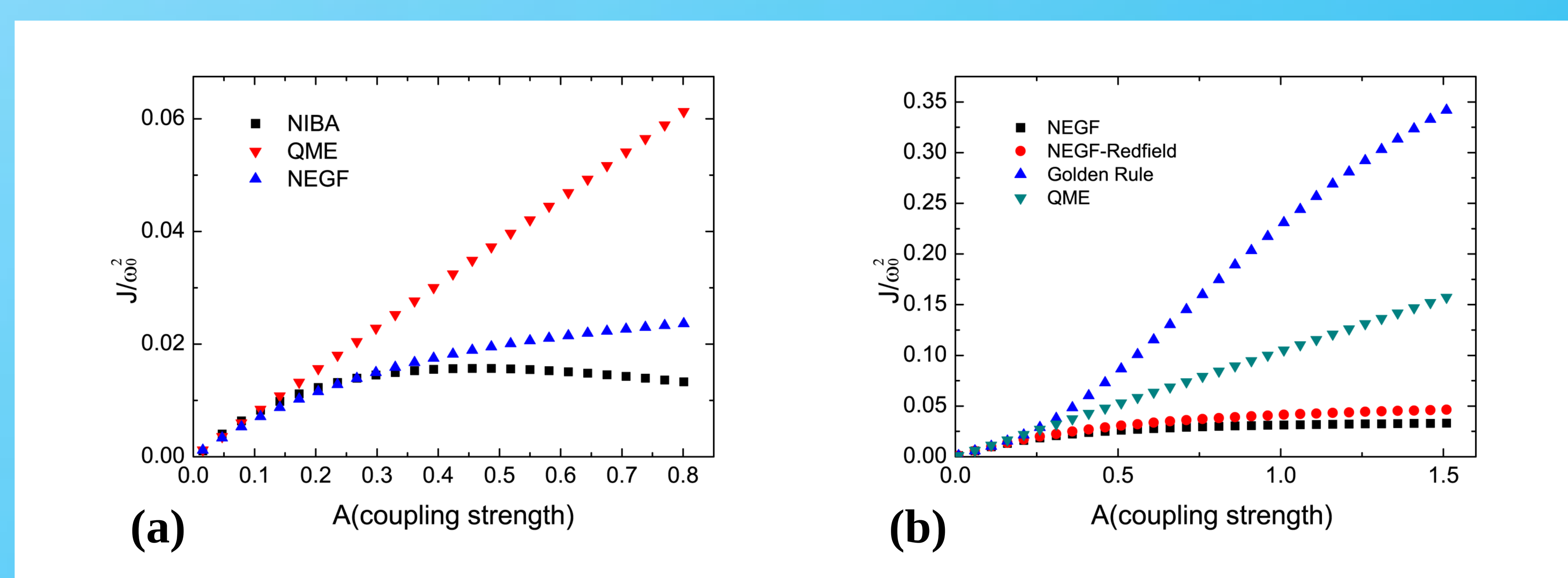
$$J = \frac{2}{\pi\omega_0^2}\int\Gamma_L(\omega)\Gamma_R(\omega)\left[n_L(\omega) - n_R(\omega)\right]\omega d\omega$$

In high temperatures, heat transport is dominated by the incoherent "sequential" process: (See the Fig.(b) above.)

$$J = \omega_0\frac{\Gamma_L(\omega_0)\Gamma_R(\omega_0)\left[n_L(\omega_0) - n_R(\omega_0)\right]}{\Gamma_L(\omega_0)\left[2n_L(\omega_0)+1\right] + \Gamma_R(\omega_0)\left[2n_R(\omega_0)+1\right]}$$

IV. The role of coupling strength

The heat current under a fixed temperature bias does not increase linearly with the coupling strength. In the strong coupling region, the heat current goes up very slowly when coupling strength increases. This is much more similar to the result of the noninteracting blip approximation equations (NIBA), which shows a "turn-over" of the heat current when coupling strength increases. See Fig.(a) on the left. Fig.(b) shows a comparison of the coupling-current curves by a variet of methods.



V. Conclusion

We have studied heat transport through a spin-boson system under nonquilibrium steady state (NESS), both in high and low temperatures. The NEGF plus Majorana representation method which we exploited was proved to be effective in a highly anharmonic system like TLS, without enforcing Redfield approximation in the theory. The numerical results show that at least two mechanisms are involved in the heat transport process, low temperatures and the sequential tunneling case in high temperatures, respectively. The transitional region is quite smooth, so we believe our theory can deliver a good description of the crossover between high temperature region and low temperature region. To verify the applicability of our method in a variety of parametric regions, experimental results are needed. Possible experiments include a superconducting flux qubit coupling to two linear circuits. Moreover, it is possible to extend this method to the case of a TLS chain, so that heat transport properties of molecular chains, such as polymer, DNA and polypeptide, can be investigated.