Electron-hole pair excitation and energy transport in hybrid electron-boson junctions

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We show that a current-carrying coherent conductor can be treated as bosonic energy baths involving different types of electron-hole pair excitation. Hybrid energy transport between the nonequilibrium electrons and bosons can be described by a Landauer-Büttiker formula at the lowest order in their coupling. This allows for simple, unified account of a variety of heat transport problems in hybrid electron-boson systems, including non-reciprocal heat transport, thermoelectrical current from a cold-spot and radiative cooling.

The celebrated Landauer-Büttiker formalism has been widely used in the study of particle and energy transport in meso- and nano-scale conductors, carried by quasiparticles following different statistics, including electrons[], photons[1], and phonons[2–8]. The energy current between two baths ($i = 1, 2$) can be written as the following general form

$$J = \int_0^{+\infty} \frac{d\omega}{2\pi} \hbar\omega T(\omega)[n(\omega, \mu_1, T_1) - n(\omega, \mu_2, T_2)]. \quad (1)$$

Here, the transmission coefficient $T(\omega)$ describes the transmission probability of particle with energy $\hbar\omega$ from bath 1 to 2 and vice versa. The two baths are assumed to be in thermal equilibrium, and the corresponding distribution function $n(\omega, \mu_\alpha, T_\alpha)$ of each bath is determined by the particle statistics. It is the Fermi-Dirac distribution for fermions, and Bose-Einstein distribution for bosons. A difference in the distribution drives an energy current flow between the two thermal baths. This driving force for energy transport could be a chemical potential or temperature bias for fermions. However, for bosons we have $\mu = 0$ in thermal equilibrium, following the textbook argument that bosons without number conservation have zero chemical potential. Thus, for bosonic energy transport the only driving force is temperature.

However, there are a large class of energy transport processes that can not be directly handled by Eq. 1. Hybrid energy transport between fermions and bosons is one case, and baths under nonequilibrium state is another. These kinds of processes are ubiquitous in the study of energy transport in nano-junctions. Examples include electrical-current-driven light emission, Joule heating, current-induced cooling and so on.

In this work, we show that to the second order in their coupling energy transport between steady-state nonequilibrium electrons and bosons can be well described by a Landauer-Büttiker formula between bosonic baths with non-zero chemical potentials. The key observation is that, the electronic system can be treated as bosonic electron-hole pair (EHP) baths with possibly non-zero chemical potential. Energy transport between electrons and bosons is always accompanied by the generation or annhilation of different kinds of EHPs. Our theory thus gives a unified account of different physical processes and generalizes the Landauer-Büttiker formalism to hybrid energy transport between nonequilibrium baths.

Model.– We consider a model system schematically shown in Fig. 1 (a). The *system* composed of an independent set of bosonic degrees of freedom (DOF) taken as a set of harmonic oscillators. The system couples to two kinds of baths. One is an equilibrium boson bath (ph-bath), modeled by an infinite number of harmonic oscillators. The other is an electronic bath (e-bath), which itself includes a central part and two electrodes (L and R). The e-bath may be driven into a nonequilibrium steady state by a voltage bias applied between electrodes L and R. Without loss of generality, we assume that the system couples only to the central region of the e-bath. Energy transport between e-bath and ph-bath takes place through their simultaneous coupling to the system.

Within the picture of Landauer-Büttiker formalism, we treat the electrons as non-interacting. But they may be driven into nonequilibrium by applying voltage or temperature bias between L and R electrodes. The electrons couples to the 'displacement' of the system harmonic oscillator

$$H_{es} = \sum_{i,j,k} M_{ij}^k c_i^\dagger c_j u_k. \quad (2)$$

Here, M_{ij}^k describes the coupling of the system mode k to the electronic transition between electron states i and j, and u_k is the 'displacement' operator of the system mode k. We consider the weak coupling case so that we only need to take into account the interaction up to the second order in M. The coupling of system to the ph-bath is linear between harmonic oscillators and can be treated exactly.

Electron-hole pair excitation.– Our key observation is that the interaction between the system and electron bath can be modeled by different kinds of reactions between EHPs in the e-bath and the bosonic modes in the system. The creation and annihilation of the bosonic mode is always accompanied by the recombination and creation of EHPs. These processes can be expressed in

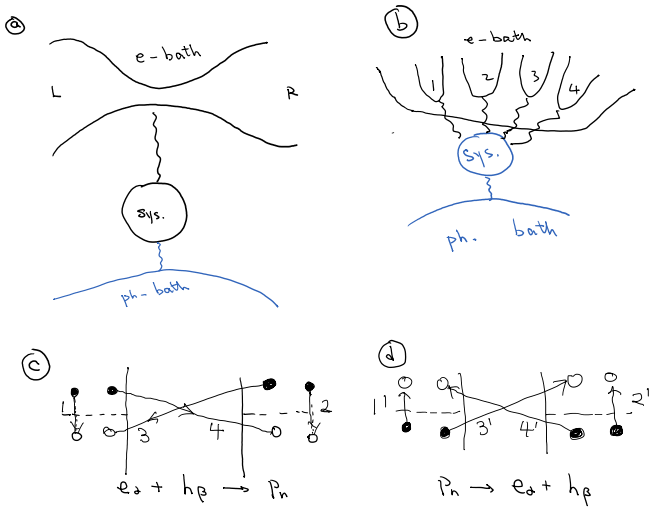

FIG. 1. (a) Schematics of the model we consider. The system consists a set of independent bosonic modes. It couples to an electron bath (e-bath), which is modeled as a conductor including a left (L) and a right (R) electrode, with temperature T_e and chemical potential μ_L and μ_R, respectively. The system further couples to an external thermal bath (ph-bath) at temperature T_{ph}. (b) The electron bath can be treated as four different kinds of electron-hole pair (EHP) baths (1-4), shown in (c). (c-d) Four kinds of EHP recombination (c) and excitation (d) processes. The EHPs are classified according to the spatial location of the electron (e_α) and the hole (h_β). (1,1') Both are at electrode L, (2,2') Both are at electrode R, (3,3') The electron at electrode R and a hole at electrode L. (4,4') The electron at electrode L and a hole at electrode R.

the form of reactions

$$e_\alpha + h_\beta \rightleftharpoons p_n, \tag{3}$$

where e_α, h_β and p represent electron in electrode α, hole in electrode β and bosonic mode n in the system. It is equivalent to the more obvious form

$$e_\alpha \rightleftharpoons e_\beta + p_n, \tag{4}$$

representing inelastic electronic transition from electrode α to β, accompanied by emission (forward) and absorption (backward) of bosonic mode n.

There are four types of EHPs which we label by the spatial location of the electron (α) and hole (β) state. They are schematically shown in Fig. 1 (c), and termed EHP-i, with $i = 1, 2, 3, 4$. They are further divided into two groups, where 1, 2 are intra-electrode type (LL, RR), and 3, 4 are inter-electrode type (RL, LR). In additional to energy transfer between e-bath and the system, the generation and recombination of inter-electrode EHPs ($\alpha \neq \beta$) also involves electron transport across the system. We take the energy of mode p_n $\varepsilon_n = \hbar\omega_n$ and that of the EHPs to be positive.

The key quantity to describe the EHPs is the coupling-weighted EHP power spectrum. It can be written as

$$\Lambda^{\alpha\beta}_{mn}(\omega) = \hbar\omega \left(n_B(\hbar\omega - \mu_{\alpha\beta}, T_e) + \frac{1}{2} \right) \Gamma^{\alpha\beta}_{mn}(\omega), \tag{5}$$

with the coupling weighted density of states (DOS)

$$\begin{aligned}\Gamma^{\alpha\beta}_{mn}(\omega) = &- \sum_{i_\alpha, f_\beta} \langle \psi_{i_\alpha}(\varepsilon_i) | M^m | \psi_{f_\beta}(\varepsilon_f) \rangle \qquad (6)\\ &\times \langle \psi_{f_\beta}(\varepsilon_f) | M^n | \psi_{i_\alpha}(\varepsilon_i) \rangle \delta(\varepsilon_i - \varepsilon_f - \hbar\omega)\\ &\times (n_F(\varepsilon_\alpha - \mu_\alpha, T_\alpha) - n_F(\varepsilon_\beta - \mu_\beta, T_\beta))(\hbar\omega)^{-1}\\ = &- \int \frac{d\varepsilon_\alpha}{2\pi} \mathrm{tr}[M^m A_\beta(\varepsilon - \hbar\omega) M^n A_\alpha(\varepsilon_\alpha)]\\ &\times (n_F(\varepsilon_\alpha - \mu_\alpha, T_\alpha) - n_F(\varepsilon_\beta - \mu_\beta, T_\beta))(\hbar\omega)^{-1} \qquad (7)\end{aligned}$$

Here, n_F and n_B are the Fermi-Dirac and the Bose-Einstein distributions, respectively,

$$n_{F/B}(\varepsilon, T) = \frac{1}{\exp(\beta_B \varepsilon) \pm 1}, \tag{8}$$

and $\beta_B = (k_B T)^{-1}$, $\mu_{\alpha\beta} = \mu_\alpha - \mu_\beta$. They are fixed by the e-bath temperature T_e and the chemical potentials of the two electrodes.

Equation 5 follows the normal form of fluctuation-dissipation relation for an equilibrium boson bath, albeit with a possibly non-zero chemical potential. The intra-electrode EHPs (i=1,2) are always in equilibrium with $\mu_{\alpha\alpha} = 0$ and temperature T_e. But the two inter-electrode EHPs (i=3, 4) have opposite chemical potential $mu_{RL} = -\mu_{LR}$. They are nonzero when there is a voltage bias applied. This effective model is shown in Fig. 1 (b). Thus, we have shown that the *nonequilibrium* e-bath can be divided into four *equilibrium* EHP baths with different chemical potentials.

Detailed balance and effective temperature.– We now proceed to show that, a slightly modified detailed balance relation applies to each of the EHP baths. To simplify the analysis, we consider one bosonic mode with angular frequency Ω. A simple rate equation for the mode population N can be established by considering the forward and backward reaction processes

$$\dot{N} = B(N + 1) - AN, \tag{9}$$

where B and A are the reaction rates for the emission and absorption of bosonic quanta, respectively. They can be calculated by summing over the individual rates $B = \sum_{\alpha\beta} B_{\alpha\beta}$, $A = \sum_{\alpha\beta} A_{\alpha\beta}$. The reaction rates of each EHP bath follows a generalized detailed balance relation

$$\frac{A_{\alpha\beta}}{B_{\alpha\beta}} = \exp(\beta_B(\hbar\Omega - \mu_{\alpha\beta})). \tag{10}$$

with a possibly nonzero chemical potential $\mu_{\alpha\beta} = \mu_\alpha - \mu_\beta$, as required by the equilibrium condition for reaction 3.

The bosonic mode reaches steady state when $\dot{N} = 0$, with

$$N = \frac{1}{A/B - 1}. \tag{11}$$

In equilibrium ($\mu_\alpha = \mu_\beta$), we have $A/B = \exp(\beta_B \hbar\Omega)$. When there is voltage bias applied, the final distribution can not be written as a simple form. Normally, an effective temperature is defined by assuming N follows the Bose-Einstein distribution with zero chemical potential

$$k_B T_{eff} = \frac{\hbar\Omega}{\ln(1 + N^{-1})}. \tag{12}$$

According to previous discussion, we can equivalently defined an effective chemical potential by assuming N follows the Bose-Einstein distribution at T_e

$$\mu_{eff} = \hbar\Omega - k_B T \ln(1 + N^{-1}). \tag{13}$$

These two effective parameters are related through

$$T_{eff} = \frac{T_e}{1 - \mu_{eff}/(\hbar\Omega)}. \tag{14}$$

Energy transport.– Within the effective EHP model in Fig. 1 (b), hybrid energy transport between the electrons and the system bosons can be treated as bosonic transport. To the lowest order approximation, we arrive at a Landauer-Büttiker formula for the energy transport from e-bath to the system as a summation of contributions from all the EHP baths

$$J = \sum_{\alpha,\beta} \int_0^{+\infty} \frac{d\omega}{2\pi} \hbar\omega \; \mathcal{T}^{\alpha\beta}(\omega) \times [n_B(\omega - \mu_{\alpha\beta}, T_e) - n_B(\omega, T_{ph})] \tag{15}$$

where

$$\mathcal{T}^{\alpha\beta}(\omega) = \mathrm{Tr}[\Gamma^{\alpha\beta}(\omega)\mathcal{A}_{ph}(\omega)], \tag{16}$$

is the transmission between the EHP bath and the ph-bath. Here, T_e and T_{ph} are the temperature of the e-bath and ph-bath, respectively. The trace Tr is over system DOF, with $\mathcal{A}_{ph} = D^r \Gamma_{ph} D^a$ the spectral function of the system due to coupling to the ph-bath. The summation over $\alpha\beta$ includes contributions from all the four types of EHPs. Each of them contributes to an energy transport channel. In the following we show several applications of this central result.

Non-reciprocal heat flow.– Firstly, we consider the situation where the e-bath and ph-bath are in their own thermal equilibrium with two different temperature T_e and T_{ph}. This indicates that $\mu_\alpha = \mu_\beta$ and $T_\alpha = T_\beta = T_e$. If we ignore the energy dependence of A in Eq. (7), the EHP DOS becomes a constant,

$$\Gamma_{mn} = \mathrm{tr}[M^m A M^n A], \tag{17}$$

with $A = A_L + A_R$. Consequently, the transmission $\sum_{\alpha\beta} \mathcal{T}^{\alpha\beta}$ does not depend on T_e. Equation (15) reduces to the Landauer formula for heat transport between two harmonic thermal baths. Thus, the EHPs behave as linear harmonic oscillator thermal baths.

On the other hand, if we consider the energy dependence of $A(\varepsilon)$, $\Gamma(\omega)$, $\mathcal{T}^{\alpha\beta}$ will depend on T_e. Energy transport becomes nonlinear. In this case, non-reciprocal heat transport is possible, i.e., $J(\Delta T) \neq J(-\Delta T)$, with $\Delta T = T_e - T_{ph}$. We thus find a necessary condition for non-reciprocal heat transport in a hybrid electron-boson system: the electron DOS in the thermal window near the chemical potential has to be energy dependent[9, 10]. For normal metal electrode, the energy scale of electrons is much larger than thermal energy, leading to a flat DOS within the thermal window. The energy dependence of A can be engineered by changing the electronic states of the central part. For example, discrete energy levels of a molecular junction or quantum dot can be used. Figure 2 shows two limiting cases. We have two electronic levels which couple to the left and right electrodes, respectively. The left level lies below μ_L and the right level lies above μ_R. Depending on their relative positions, one of the inter-electrode EHPs couples strongest to the bosonic system. This setup has been studied in Ref. 11.

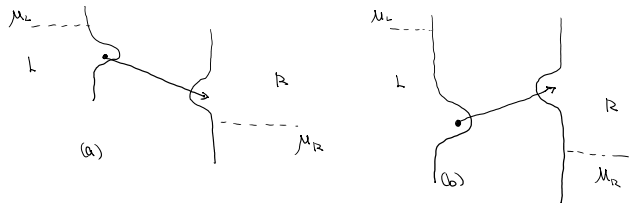

FIG. 2. Two limiting cases of electronic heating (a) and cooling (b). For the e-bath, we have a filled electronic level that couples to the left electrode with chemical potential μ_L, and an empty level that couples to the right electrode. Electron transport between the two states is mediated by the bosonic mode in the system. (a) Heating of bosonic mode due to resonant recombination of EHPs. (b) Cooling of bosonic mode due to resonant generation of EHPs.

Electrical current from a cold-spot.– Another problem we can look at is the thermoelectric transport. When $T_{ph} \neq T_e$, in addition to the heat transport between system and e-bath, an electrical current may also be induced between left and right electrodes[12, 13]. In our EHP picture, this is realized through coupling of the bosonic mode with two inter-electrode EHPs. Since they contribute to two electrical current with opposite directions, in order to get a non-zero electrical current, these two channels should not get canceled. Here, we consider the case where $T_{ph} < T_e$ and $\mu_L = \mu_R$. The temperature difference between e-bath and ph-bath generates a heat current flow from the e-bath to the ph-bath. At a re-

sult of the heat transport, electron transport between L and R electrode takes place. Previously, electrical current generated from a phonon hot-spot ($T_{ph} > T_e$) has been considered[12]. The situation we consider here is somewhat counter-intuitive, since the electrical current is generated by a cold-spot. This demonstrates the decoupling of heat and charge transport as an advantage of thermoelectricity in hybrid nano-junctions.

Electronic cooling of bosonic mode.– The presence of voltage bias between the two electrodes changes the initial and final electron states of the EHP excitation. Thus, the EHP DOS can be tuned by voltage bias. More importantly, the inter-electrode EHPs acquire a non-zero chemical potential, determined by the electrochemical potential difference between the two electrodes. We assume $\mu_L > \mu_R$ without loss of generality. The EHP-4 has a chemical potential of $eV = \mu_L - \mu_R > 0$, while EHP-3 gets a chemical potential with opposite value $-eV$. Change of the chemical potential breaks the equilibrium in the reaction, and drives the energy transport between e-bath and the system. If we assume $T_e = T_{ph}$, the energy transport is through the two inter-electrode EHP channels. Direction of energy flow depends on the relative magnitude of two fluxes. It can be engineered by tuning the electronic band structure, or more specifically, the transition probability. Figure 2 shows two limiting cases. In Fig. 2 (a), process 4 is enhanced due to resonant inelastic electron tunneling when the separation between the two DOS peaks is resonant with energy of the bosonic mode. Consequently, energy flows from e-bath to the system. In Fig. 2 (b), the reverse of process 3 is resonantly enhanced, resulting in energy flow in the opposite direction. Electronic cooling becomes possible using this resonantly enhanced process. Very recently, experimental demonstration of near field radiative cooling using a reversely-biased p-n junction has been demonstrated [14]. This serves as the minimum model to understand the experimental results.

In summary, we have shown that a normal two-probe electron conductor can be effectively viewed as EHP baths with chemical potential determined by the applied voltage bias. Properties of the EHP baths can be engineered through tuning the parameters of the conductor. This bath engineering provides an efficient way of tuning hybrid energy and thermoelectric transport in electron-boson junctions.

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