Interplay of charge and heat transport in a nano-junction in the out-of-equilibrium cotunneling regime

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Abstract

We study the charge transport and heat transfer through a nano-junction composed of a small metallic grain weakly coupled to two metallic leads. We focus on the cotunneling regime out-of-equilibrium, where the bias voltage and the temperature gradient between the leads strongly drive electron and phonon degrees of freedom in the grain, which in turn have a strong feedback on the transport through the grain. We derive and solve the heat balance equation for electron and phonon degrees of freedom in the grain and self-consistently find the current–voltage characteristics. We demonstrate that the transport in the nano-junction is very sensitive to the spectrum of the bosonic modes in the grain.

1. Introduction

Quantum composite materials are the subject of current intense research activity [1–3]. A typical quantum composite material (QCM) is a granular conductor, where the grains are so small that the typical charging energy of one electron, $E_C$, is the largest energy scale, in particular it is larger than temperature and voltage.

The equilibrium properties of granular conductors are well understood [1]. However, much less is known about the transport properties of quantum composite conductors out-of-equilibrium, e.g., at large bias or at large enough temperature gradients, when linear response theory is not valid.

There are several transport channels for electron propagation though the granular QCM. At weak coupling between the grains and not very high temperatures, cotunneling is the main mechanism of electron transport [4]. It provides a conduction channel at low applied biases and temperatures, where otherwise the Coulomb blockade arising from the electron–electron repulsion would suppress the current flow. The essence of a cotunneling process is that an electron tunnels via virtual states, thus bypassing the large Coulomb barrier [5]. Here we focus on the out-of-equilibrium cotunneling through a single grain, see figure 1(a), the building block of a quantum composite material, attached to two bulk leads. Voltage and/or temperature differences between the leads strongly drive electron and phonon degrees of freedom in the grain. The solution of the transport problem implies a self-consistent calculation, which takes into account the mutual feedback of highly excited degrees of freedom in the grain on the cotunneling electrons and vice versa.

Inelastic cotunneling of electrons from one lead to the other through a grain is accompanied by the creation of electron–hole pairs in the granule. Those pairs are heating the grain when they decay. On the other hand, electrons in the grain exchange energy with phonons. Thus, the electron temperature in the granule depends on

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balance between heating by electron–hole pairs and cooling by phonons. Recently, heating effects in a single grain and a chain of grains due to inelastic cotunneling have been discussed in several papers [7–10]. However, our consideration [7, 8] was in the linear response regime, i.e., valid for small gradients of voltage and temperature. Here we follow a general approach, which also holds in out-of-equilibrium. Finally, this temperature is used to obtain the current–voltage characteristics, $I(V)$.

As a main result, it turns out that the transport characteristics of these junctions are very sensitive to the temperature of the electron degrees of freedom in the grain, $T_g$. The grain temperature, $T_g(V, T_L, T_R)$, is found explicitly as a function of voltage bias $V$ and both lead temperatures from the expression for the heat fluxes in the nano-junction out-of-equilibrium. Finally, this temperature is used to obtain the current–voltage characteristics, $I(V)$.

The heat, $\dot{Q}$, generated in the grain due to inelastic electron cotunneling can be derived as follows—representing the first main result of our work:

$$\dot{Q}(T_L, T_R, V) = a |T^4_T - T^4_{g}|, \quad T^4_T = T^4_m + \frac{5}{2\pi^2} T^2_m (eV)^2 + \frac{5}{8\pi^4} (eV)^4,$$

where $T^2_m = (T^2_L + T^2_R)/2$ and $a$ is a material dependent constant, which is derived below (see equation (37)). The energy scale $T^4_T$ has the physical meaning of an effective temperature of the cotunneling electrons. It is important to note that the rhs in equation (2) can be positive or negative, indicating a heating or cooling of the grain, respectively. For equal temperatures $T_L = T_R$ and zero voltage $V = 0$ we reproduce the results of [12] from equation (2).

The heat dissipation in the granule goes through two stages. First, electron–hole pairs are excited by inelastic cotunneling processes and, second, the electron–hole pairs recombine and release their excess energy to the phonon bath. The heat flux between phonons and electrons (electron–hole pairs) has the form [14, 15]

$$\dot{q}(T_g, T_{ph}) = (T^2_T - T^2_{ph}) \kappa,$$

where $T_{ph}$ is the temperature of the phonon bath and the parameters $\kappa$ and $\alpha$ depend on the particular model of electron–phonon interaction; typically $\alpha = 4, 5$ or 6.

In order to obtain the grain temperature, we have to solve the heat balance equation in the grain

$$\dot{Q}(T_g, T_{ph}) = \dot{Q}(T_L, T_R, V),$$

where $\dot{Q}(T_L, T_R, V)$ is given in equation (2).
It is useful to express all temperatures\(^7\) and voltages (more precisely \(eV\)) in terms of the charging energy \(E_c\), which we will denote by a tilde, e.g., \(T_{\text{eff}} = \tilde{T}_{\text{eff}}/E_c\) or \(V = eV/E_c\).

Introducing the dimensionless parameter \(b = aE_c^{d-\nu}/\kappa\), equation (5) can be written as

\[
\tilde{T}_g^4 - \tilde{T}_{\text{ph}}^4 = b(\tilde{T}_{\text{ph}}^4 - \tilde{T}_g^4). \tag{6}
\]

For \(\alpha = 4\), equation (6) can be solved analytically:

\[
\tilde{T}_g(\tilde{V}) = \left(\tilde{T}_{\text{ph}}^4 + b\tilde{T}_{\text{eff}}^4\right)/(1 + b). \tag{7}
\]

Using equation (7) for the grain temperature \(T_g\), we can finally calculate the current–voltage characteristics due to inelastic cotunneling

\[
f^{(\text{inel})}(V) = \frac{1}{12\pi^3} \frac{R_g^2 eE_c}{R_L R_R \hbar} \left(V^2 + 2\pi^2(\tilde{T}_m^2 + \tilde{T}_g^2)\right) V, \tag{8}
\]

which is the second main result of this paper. At small voltages this \(I-V\) characteristics is determined by a linear behavior with a coefficient which is temperature dependent and also weakly voltage dependent via \(T_{\text{eff}}\). In figure 2 graphs of \(f^{(\text{inel})}(V)\) are shown for different exponents \(\alpha\) and different \(T_m\), i.e., different lead temperatures.

When deriving equations (2)–(7), we neglected the contribution from sequential electron tunneling. The latter is exponentially suppressed in the Coulomb blockade regime if the temperature and voltage are below the characteristic single-electron charging energy in the grain, \(eV, T < E_c\) with \(E_c \sim e^2/C_\Sigma\), where \(C_\Sigma = C_L + C_R + C_g\) is the total capacitance, see figure 1(b). Furthermore, the leads are assumed to be in equilibrium at similar temperatures, and energy relaxation processes within the grain are fast enough such that we can use a local-equilibrium description.

In the following section we present the general out-of-equilibrium description of the heat and charge transport through the junction, which yields the derivation of equations (2)–(7) and eventually results in equation (8).

7 We use the units \(\hbar = 1\) and \(e\) variables refer to energy quantities.

3. Cotunneling transport

We start with the most general expression for the current–voltage characteristics due to inelastic electron cotunneling.

3.1. Inelastic cotunneling rate

The inelastic cotunneling rate for an electron transfer from the left to the right lead has the following form [13]:

\[
\tilde{T}^{(\text{inel})} = \frac{1}{2\pi^3 R_L R_R \hbar} \int d\epsilon_1 d\epsilon_2 d\epsilon_3 f_1^{(L)}(\epsilon_1) \times \left[1 - f_2^{(\theta)}(\epsilon_2)\right] f_3^{(\theta)}(\epsilon_3) \left[1 - f_4^{(R)}(\epsilon_4)\right] \times \frac{1}{\epsilon_2 - \epsilon_1 + \Delta F_L^+(n)} + \frac{1}{\epsilon_4 - \epsilon_3 + \Delta F_R^-(n)} \right]^2 \times \delta(\epsilon V + \epsilon_1 - \epsilon_2 + \epsilon_3 - \epsilon_4), \tag{9}
\]

where \(V\) is the bias voltage between the left and right leads. The distribution functions \(f_1^{(L,R)}(\epsilon)\) describe electrons within the left and right leads, respectively.

If the temperature of the left (right) lead is \(T_{L(R)}\) then \(f_{L(R)}^{(\nu)}(\epsilon) = f_\nu(\epsilon, T_{L(R)})\), with \(f_\nu(\epsilon, T) = 1/\left[\exp(\epsilon/T) + 1\right]\) being the Fermi–Dirac distribution function. Function \(f_\theta^{(\nu)}(\epsilon)\) in equation (9) is the electron distribution in the grain. The functions \(\Delta F_{L(R)}^\pm(n)\) denote the change of the charging energy when an electron tunnels from the left (right) lead onto the island with excess charge \(n e\), while \(\Delta F_{L(R)}^\pm(n)\) denotes the change of the charging energy when an electron tunnels out of the island with excess charge \(n e\) to the left (right) lead

\[
\Delta F_L^\pm = \frac{e^2}{C_\Sigma} \left[\frac{1}{2} \pm \left(\frac{C_L V g}{e}\right)\right] \pm \left[\frac{C_R + C_g/2}{e}\right], \tag{10}
\]

\[
\Delta F_R^\pm = \frac{e^2}{C_\Sigma} \left[\frac{1}{2} \pm \left(\frac{C_R V g}{e}\right)\right] \pm \left[\frac{C_L + C_g/2}{e}\right], \tag{11}
\]

where all the capacitances are defined in figure 1(b) and \(C_\Sigma\) is the total capacitance introduced below equation (8). The number of excess electrons on the grain is determined by the
condition that \( n \) results in the minimal electrostatic energy: \( \Delta F_L^\text{el}(n) > 0 \) and \( \Delta F_R^\text{el}(n) > 0 \), \[\text{[13]}\].

The inelastic electron cotunneling rate \( \Gamma^\text{inel} \) from the right to the left lead can be found using equation (9) with proper substitutions: \( V \rightarrow -V \) in the \( \delta \)-function and interchange between the left and the right leads, ‘L’ \( \equiv \) ‘R’.

3.2. Cotunneling current

To write the total cotunneling current we also take into account elastic electron cotunneling rates, \( \Gamma^\text{el} \), which can be written similarly to equation (9), i.e.,

\[
I(V) = e(\Gamma^\text{inel} - \Gamma^\text{el} + \Gamma^\text{ph} - \Gamma^\text{el}).
\]

Here we stress that the rates and the current in equation (12) strongly depend on the electron distribution function \( f^\text{inel} \) in the grain. This distribution can be approximated by an equilibrium distribution with phonon bath temperature, \( T^\text{ph} \), only for small voltage and temperature gradients across the junction \[\text{[13]}\]. In this paper we consider the current–voltage characteristics beyond the equilibrium approximation. We write the kinetic equation governing the behavior of function \( f^\text{inel} \) and find the dependence of grain temperature \( T \) on the bias voltage \( V \), lead temperatures \( T_L, T_R \), and the phonon temperature, \( T^\text{ph} \).

In the following we concentrate on the inelastic component of the cotunneling current \( I^\text{inel}(V) \), which heats the grain in contrast to the elastic part, see appendix B.2.

4. Kinetic equation for \( f^\text{inel} \)

To calculate the current–voltage characteristics, \( I(V) \), in equation (12) we need to know the electron distribution function \( f^\text{inel} \) in the grain. This distribution function satisfies the kinetic equation

\[
\frac{d}{d\tau} f^\text{inel}(\tau, t) = \mathcal{I}^\text{inel}(\tau) + \mathcal{I}^\text{ph}(\tau) + \mathcal{I}^\text{el}(\tau),
\]

where \( \tau \) is the mean level spacing in the grain. The left hand side of this equation describes the change of the electron distribution function with time \( \tau \). The right hand side is the sum of collision integrals, with \( \mathcal{I}^\text{inel}(\tau) \) are the scattering integral due to cotunneling processes, while \( \mathcal{I}^\text{ph}(\tau) \) and \( \mathcal{I}^\text{el}(\tau) \) being the electron–phonon and electron–electron scattering integrals, respectively. We write the scattering integral \( \mathcal{I}^\text{inel}(\tau) \) explicitly in appendix A.

We emphasize that only inelastic cotunneling contributes to the scattering integral \( \mathcal{I}^\text{inel}(\tau) \) in equation (13). It satisfies the particle conservation law

\[
\int \mathcal{I}^\text{inel}(\tau) d\tau \equiv 0.
\]

This property does not contradict the current flow through the junction since the grain can be considered as a virtual haven for tunneling electrons during the cotunneling processes. However, the scattering integral \( \mathcal{I}^\text{inel}(\tau) \) does not conserve energy, since each inelastic cotunneling process leaves an excited electron–hole pair behind in the grain. The heat dissipation rate into the grain is

\[
\dot{Q} = \int \epsilon \mathcal{I}^\text{inel}(\tau) d\tau.
\]

Here the energy \( \epsilon \) in the electron grain distribution function \( f^\text{inel}(\tau) \) is counted from the local electrochemical potential.

4.1. Local-equilibrium approximation

To solve the kinetic equation (13) we use a local-equilibrium approximation. This approximation is valid because for small grains the electron–electron (Coulomb) interaction is strong. Therefore the effective electron–electron scattering time, \( \tau^\text{el} \), corresponding to the scattering integral \( \mathcal{I}^\text{el}(\tau) \) in equation (13), is shorter than the inelastic cotunneling scattering time, \( \tau^\text{inel} \), and the electron–phonon scattering time, \( \tau^\text{ph} \),

\[
\tau^\text{el} \ll \min(\tau^\text{inel}, \tau^\text{ph}).
\]

In addition, the scattering integral \( \mathcal{I}^\text{el}(\tau) \) in equation (13) conserves the energy and the particle number. Therefore we can find the solution of the kinetic equation (13) using the local-equilibrium approximation,

\[
f^\text{inel}(\tau) \approx f^\text{eq}(\tau, T^\text{el}).
\]

This expression substituted into the scattering integral \( \mathcal{I}^\text{el}(\tau) \) in equation (13) lets it vanish. Using the particle conservation law, equation (14), the correction to the effective electrochemical potential in the grain in the local-equilibrium approximation can be neglected. Therefore in this approximation there is only one unknown parameter, the grain temperature \( T^\text{el} \).

4.2. Heat balance equation

The heat rate between electrons and phonons,

\[
\dot{q} = \int \epsilon \mathcal{I}^\text{ph}(\tau) d\tau,
\]

in the local-equilibrium approximation, equation (17), is given by equation (4). Therefore the problem of finding the grain temperature \( T^\text{el} \) in the local equilibrium approximation, equation (17), reduces to the solution of the heat balance equation that follows from equation (13)

\[
\dot{q}(T^\text{el}, T^\text{ph}) = \dot{Q}(T^\text{el}, T_L, T_R, V)
\]

Solving equation (19) we find the grain temperature \( T^\text{el}(T_L, T_R, V, T^\text{ph}) \) as a function of lead temperatures \( T_L, T_R \), the bias voltage \( V \), and the phonon temperature \( T^\text{ph} \). Using the result for grain temperature \( T^\text{el}(T_L, T_R, V, T^\text{ph}) \) we find the current–voltage characteristics in equation (12). Below we proceed with this program, focusing on the analytical solution of equations (12) and (19).
5. Bosonic representation of charge and heat rates

Here we consider the expressions for the inelastic cotunneling rate \( \Gamma^\text{(inel)} \) in equation (9) and for the heat dissipation rate \( \dot{Q} \) in equation (15) in more detail.

For small grains the electrostatic energies, \( \Delta F_L^+(n) \) and \( \Delta F_R^-(n) \) in equation (9), are much larger than all other characteristic energy scales in the problem, including temperature and voltage. Therefore we can neglect in the denominators of equations (9), (A.1), and (A.3) the energy \( \epsilon \) and \( \epsilon_i \), \( i = 1, \ldots, 4 \). This limit allows an analytical solution of the heat balance equation (19) in order to calculate the grain temperature \( T_g \). In addition, we show that it is more convenient to rewrite all transport characteristics in terms of electron–hole (dipole) excitations to find the current–voltage characteristics in equation (12).

First, we perform the substitution \( \epsilon_i \to \epsilon_i - eV/2 \) and \( \epsilon_i \to \epsilon_i + eV/2 \) in equation (9), which moves the voltage dependence into the distribution functions and in particular implies that \( f_{LR}(\epsilon) = f_{LR}(\epsilon + eV/2, T_{LR}) \).

After the energy-integration, we obtain the following expression for the inelastic cotunneling rate (see appendix B) (see footnote 1) (see equation (5))

\[
\Gamma^\text{(inel)} = \frac{1}{2\pi} \frac{R_L^2}{R_L R_R \hbar} \int_0^\infty d\omega \frac{\omega^2}{E_c^2} \left[ n_{\omega} (N_{\omega} + 1) + 1 + \tilde{n}_{\omega}^{(\text{LR})} \right].
\]

(20)

where we used the notation

\[
\frac{1}{E_c} = \frac{1}{\Delta F_L^+(n)} + \frac{1}{\Delta F_R^-(n)}.
\]

(21)

For the heat dissipation rate in the grain we obtain, using equations (A.2)–(A.3):

\[
\dot{Q} = \frac{1}{\pi} \frac{R_L^2}{R_L R_R \hbar E_c^2} \int_0^\infty d\omega \left\{ n_{\omega} (N_{\omega} + 1) - 1 + \tilde{n}_{\omega}^{(\text{LR})} \right\}.
\]

(22)

Here we introduce the following form-factors, see figure 3, to describe the nonequilibrium electron–hole pairs\(^8\)

\[
\tilde{n}_{\omega}^{(\text{LR})} = \frac{1}{\omega} \int_0^\infty d\epsilon f^{(L)}(\epsilon_+) [1 - f^{(R)}(\epsilon_-)],
\]

(23)

\[
n_{\omega}^{(\text{RL})} = \frac{1}{\omega} \int_{-\infty}^0 d\epsilon f^{(R)}(\epsilon_+) [1 - f^{(L)}(\epsilon_-)],
\]

(24)

\[
1 + \tilde{n}_{\omega}^{(\text{LR})} = -n_{\omega}^{(\text{LR})},
\]

(25)

\[
1 + \tilde{n}_{\omega}^{(\text{RL})} = -n_{\omega}^{(\text{RL})},
\]

(26)

where \( \epsilon_{\pm} = \epsilon \pm \omega/2 \). General identities coupling the bosonic form-factors with and without tilde (see proof in

\(8\) If we defined the form-factors differently: \( n_{\omega}^{(\text{LR})} = \frac{1}{\omega} \int_0^\infty d\epsilon f^{(L)}(\epsilon_+) [1 - f^{(R)}(\epsilon_-)], \) and similarly, \( n_{\omega}^{(\text{RL})} = \frac{1}{\omega} \int_0^\infty d\epsilon f^{(R)}(\epsilon_+) [1 - f^{(L)}(\epsilon_-)], \) then we would get: \( n_{\omega}^{(\text{LR})} = \tilde{n}_{\omega}^{(\text{RL})} \) and \( n_{\omega}^{(\text{RL})} = \tilde{n}_{\omega}^{(\text{LR})} \). However, then the factors \( \omega \pm V \) would appear explicitly in the expressions for \( \dot{I} \) and \( \dot{Q} \) renormalizing the boson–boson interaction vertices.

Figure 3. The form-factor \( \tilde{n}_{\omega}^{(\text{LR})} (\tilde{n}_{\omega}^{(\text{RL})}) \) can be interpreted as the distribution function of electron–hole pairs, where the electron sits at the first lead while the hole is on the second lead. The form-factor \( n_{\omega}^{(\text{LR})} (n_{\omega}^{(\text{RL})}) \) corresponds to the opposite situation.

appendix B.3) are given by:

\[
n_{\omega}^{(\text{LR})} - n_{\omega}^{(\text{RL})} = \frac{eV}{\omega},
\]

(27)

\[
n_{\omega}^{(\text{RL})} - n_{\omega}^{(\text{LR})} = -\frac{eV}{\omega}.
\]

(28)

Finally we define the form-factors \( n_{\omega} \) and \( N_{\omega} \) in equations (5)

\[
n_{\omega} = \frac{1}{\omega} \left\{ n_{\omega}^{(\text{LR})} + n_{\omega}^{(\text{RL})} \right\},
\]

(29)

\[
N_{\omega} = \frac{1}{\omega} \int_{-\infty}^{\infty} d\epsilon f^{(g)}(\epsilon_+) [1 - f^{(g)}(\epsilon_-)].
\]

(30)

The functions \( n_{\omega} \) and \( N_{\omega} \) satisfy the basic property of the Bose function \( N_{\omega}(\omega, T) = \frac{T}{e^{\hbar \omega}/T - 1}, N_{\omega}(\omega, T) = -[1 + N_{\omega}(\omega, T)] \), e.g., \( n_{\omega} = -[1 + n_{\omega}] \). Below we refer to the distribution functions \( n_{\omega} \) and \( N_{\omega} \) of the electron–hole distribution functions in the leads and in the grain, respectively.

5.1. Physical interpretation of equations (23)–(29)

The effective electron–hole distribution function \( n_{\omega} \) in equation (29) has a direct physical meaning. It describes the concentration of electron–hole pairs where the electron is localized in the left and the hole in the right lead or vice versa [19–22].

The form-factor \( n_{\omega}^{(\text{LR})} \) in equation (23) is more specific than \( n_{\omega} \). It describes the concentration of ‘polarized’ electron–hole pairs with the electron sitting strictly in the left lead while the hole occupies the right lead, see figure 3. Therefore the annihilation of such an electron–hole pair (or the creation of the ‘RL’ electron–hole pair) leads to charge transfer from the left to the right lead.

The expression \( n_{\omega}^{(\text{LR})} [N_{\omega} + 1] \), in the rhs of equation (20), is proportional to the probability of annihilation of an electron in the left lead and a hole in the right lead and the creation of an electron–hole pair localized in the grain. The physical realization of such a process leads to a charge transfer from the left to the right lead.
The expression, \( n_{\text{in}}[N_{\omega} + 1] \), in the rhs of equation (22) is proportional to the probability for the annihilation of an electron–hole pair in the leads (electron in the left lead and a hole in the right lead and vice versa) and the creation of an electron–hole pair localized in the grain. This process increases the energy in the grain, but does not necessarily imply a charge transfer between the leads. Finally, the product \( [1 + n_{\text{in}}]N_{\omega} \) corresponds to the reverse process that cools the grain.

5.2. Cotunneling current–voltage characteristics

Using equation (20) we can write the inelastic cotunneling current in the following form

\[
f^{\text{(inel)}} = \frac{1}{2\pi^3} \frac{R^2_{\text{q}}}{R_L R_R} \frac{e}{h} \int_0^\infty d\omega \frac{\omega^2}{E_c} \left[ n^{\text{(LR)}}_{\omega} - n^{\text{(RL)}}_{\omega} \right] [N_{\omega} + 1] + \left[ n^{\text{(LR)}}_{\omega} - n^{\text{(RL)}}_{\omega} \right] N_{\omega}. \tag{31}
\]

Identities (27)–(28) allow us to simplify equation (31) and separate the grain and the lead degrees of freedom. So we get for the integral in equation (31)

\[
f^{\text{(inel)}} = \frac{1}{2\pi^3} \frac{R^2_{\text{q}}}{R_L R_R} \frac{e}{h} \int_0^\infty d\omega \frac{\omega^2}{E_c} \times \left[ n^{\text{(LR)}}_{\omega} - n^{\text{(RL)}}_{\omega} + \frac{2eV}{\omega} N_{\omega} \right]. \tag{32}
\]

The integration over the energy \( \omega \) in equation (32) leads to the final result for the inelastic cotunneling current given in equation (12), where we used equations (B.11)–(B.14) for the integration of the \( n^{\text{(LR)}}_{\omega}, n^{\text{(RL)}}_{\omega} \) parts of the integral in equation (32).

5.3. Evaluation of the heat dissipation rate \( \dot{Q} \) in the grain

Formally the heat dissipation rate into the grain \( \dot{Q} \) in equations (15) and (22) can be obtained using the effective kinetic equation for electron–hole pairs

\[
\frac{d}{d(h^{-1}E_{\text{F}})} N_{\omega} = \frac{n_{\omega}(N_{\omega} + 1) - N_{\omega}(1 + n_{\omega})}{\tau^{\text{(inel)}}(\omega)}, \tag{33}
\]

where the relaxation rate for electron–hole pairs in the grain is mediated by their interaction with cotunneling electrons

\[
\frac{1}{\tau^{\text{(inel)}}(\omega)} = \frac{1}{\pi^3} \frac{R^2_{\text{q}}}{R_L R_R} \frac{e^2}{E_c}. \tag{34}
\]

Equation (34) means that the relaxation rate of electron–hole pairs in the grain in the cotunneling channel is proportional to the second power of temperature at small temperatures, \( 1/\tau^{\text{(inel)}}(\omega) \sim T^2 \).

For very low temperatures, where electron–electron and electron–phonon interactions are frozen out and scattering due to cotunneling is the leading scattering mechanism we obtain \( N_{\omega} = n_{\omega} \) using equation (33).

However, for a small metallic grain the electron–electron interaction is the main scattering mechanism. It drives the electron–hole distribution function, \( N_{\omega} \), to the local-equilibrium form, \( N_{\omega} \approx N_{\text{B}}(\omega, T_g) \). (The last statement follows from the fact that in the local-equilibrium approximation the distribution function \( f^{\text{(B)}} \approx f_T(\epsilon, T_g) \) and therefore, according to equation (30), \( N_{\omega} \approx N_{\text{B}}(\omega, T_g) \).) In this case the effective grain temperature \( T_g \) is determined by the heat balance equation (19).

To evaluate the heat dissipation rate in the grain, \( \dot{Q} \) in equation (22), we need to know the integral

\[
\dot{Q} = \frac{1}{\pi^3} \frac{R^2_{\text{q}}}{R_L R_R} \frac{1}{hE_c} \int_0^\infty d\omega \frac{\omega^3}{4} (n_{\omega} - N_{\omega}) d\omega. \tag{35}
\]

Using equations (29), (B.11)–(B.14) (see appendix B) for the first term in this integral we obtain \( \int_0^\infty d\omega \omega^3 n_{\omega} d\omega = T_{\text{eff}}^4 \pi^4/15 \), where

\[
T_{\text{eff}} = T_m^4 + \frac{5}{2\pi^2} T_m^2 (eV)^2 + \frac{5}{8\pi^4} (eV)^4, \tag{36}
\]

\( T_{\text{eff}} \) being the effective temperature. The second contribution to the integral in equation (35) leads accordingly to \( \int_0^\infty d\omega \omega^3 n_{\omega} d\omega = T_{\text{eff}}^2 \pi^4/15 \). Thus we obtain our main result, equation (2), with parameter \( a \) given by the expression

\[
a = \frac{\pi}{15} \frac{R^2_{\text{q}}}{R_L R_R} \frac{1}{hE_c}. \tag{37}
\]

Here we stress that the effective temperature \( T_{\text{eff}} \) in equation (36) follows the limit, \( \lim_{\omega_0 \rightarrow 0} n_{\omega_0} d\omega = 2\pi^{3/2} \coth \frac{\sqrt{eV}}{2T_m} \), only for small bias voltages, \( eV \lesssim T_m \).

6. Discussion

6.1. Behavior of the grain temperature \( T_g \) as functions of \( T_{\text{eff}} \)

The behavior of the grain temperature \( T_g \) in equation (7) as a function of \( T_{\text{eff}} \) and \( T_{\text{ph}} \) for different \( a \) and values of parameter \( b = 0.01, 1, 10, 100 \) is presented in figure 4. These curves are quite universal since, e.g., the effect of (slightly) different lead temperatures or finite voltages is captured by a change of \( T_{\text{eff}} \) only (see equation (36)). Remarkably, the graphs for \( T_g(T_{\text{ph}}) \) and \( T_g(T_{\text{eff}}) \) show an intersection point (if the other parameter is kept constant), marked in figure 4. This is a manifestation of the Vollhardt invariance, a phenomenon specific to strongly correlated systems [16–18].

6.2. Quasi-equilibrium limit of the current–voltage characteristics

For equal lead and grain temperatures, \( T_L = T_R = T_g \), we reproduce the known result for the cotunneling current, [1, 13]. However, in the general case, the inelastic current \( f^{\text{(inel)}} \) in equations (31) and (8) strongly depends on both the grain and the lead temperatures.

6.3. Heat dissipation rate and total power

The total power of the junction, given by the product of current and bias voltage, \( IV \), and the heat dissipated into the
**Figure 4.** (Top, left) Behavior of the grain temperature \( T_g \) as a function of \( T_{\text{eff}} \). The blue curves are for \( \alpha = 4 \), red for \( \alpha = 5 \), and green for \( \alpha = 6 \). The solid line are for \( T_{\text{th}} = 0.1 \), the dashed line for \( T_{\text{ph}} = 0.2 \), and the dotted thick lines for \( T_{\text{ph}} = 0.3 \). In all curves the dimensionless parameter is fixed to \( b = 0.5 \) (see text). (Top, right) Behavior of \( T_g \) as a function of \( T_{\text{th}} \) with same parameters as above (the role of \( T_{\text{th}} \) and \( T_{\text{eff}} \) is just reversed). (Bottom) Behavior of \( T_g \) as a function of \( T_\text{eff} \) for \( \alpha = 4 \), \( T_{\text{th}} = 0.1 \), and different \( b \). The solid curve is for \( b = 0.01 \), dashed for \( b = 1 \), dotted for \( b = 10 \), and dash-dotted for \( b = 100 \). The dependence of \( T_g \) on \( T_{\text{ph}} \) for fixed \( T_{\text{th}} \) looks similar if \( b \) is replaced by \( b^{-1} \) (exactly the same for \( \alpha = 4 \)). In all plots the intersection of the curves with either \( T_{\text{th}} \) or \( T_{\text{eff}} \) being constant is marked by a gray dot (see text for explanation).

Equation (39) has transparent physical meaning—half of the energy in the cotunneling process is spent in generating electron–hole pairs in the grain and the other half in injecting the nonequilibrium electrons into the leads that finally equilibrate in the bulk of the leads. Remarkably, the ratio \( \dot{Q}/(f^{\text{inel}} V) \) is universal and does not depend on temperature \( T \) and voltage \( V \).

6.4. Transport in a semiconducting nano-junction and spectrum of bosonic modes in the grain

Calculating the current and the heat we implicitly assume that the grain is metallic, meaning that electron–hole pairs with an arbitrary small energy \( \omega \) can be created during the inelastic cotunneling process. However, if the grain is made of a semiconducting material then the spectrum of electron–hole pairs would have a gap \( \Delta \). In this case the lower limit of integration over the energy \( \omega \) in equation (31) would be \( \Delta \) and a smooth weight function \( \rho(\omega) \) would appear under the integral, renormalizing the interaction vertex of electron–hole pairs with the cotunneling electrons. Therefore in this case the current would be exponentially suppressed for voltages \( V \) and temperatures \( T = T_L = T_R = T_g \) smaller than the gap \( \Delta \), \( f^{\text{inel}}(V) \sim V \exp(-\Delta/T) \). This shows that the current–voltage characteristics is very sensitive to the spectrum of the grain.

...
7. Conclusions

We studied the charge transport and the heat transfer through a small metallic grain weakly coupled to two metallic leads. We focused on the cotunneling regime out-of-equilibrium, when the bias voltage and the temperature gradient between the leads strongly drive electron and phonon degrees of freedom in the grain, which in turn have a strong feedback on transport through the grain. We derived and solved the coupled kinetic equations for electron and phonon degrees of freedom in the grain, found the heat fluxes between cotunneling electrons, bosonic electron–hole excitations in the grain, and phonons, and self-consistently obtained the current–voltage characteristics. We demonstrated that the transport in the nano-junction is very sensitive to the spectrum of the bosonic modes in the grain.

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Appendix A. Scattering integral due to cotunneling

Here we present the scattering integral \( \Sigma^{(\text{inel})}(\epsilon) \) induced by cotunneling processes

\[
\Sigma^{(\text{inel})}(\epsilon) = \frac{1}{2\pi^3} \frac{R_q^2}{R_L R_R} \frac{1}{\hbar} \int d\epsilon_1 d\epsilon_3 d\epsilon_4 f^{(L)}(\epsilon_1) [1 - f^{(R)}(\epsilon_4)] \\
\times f^{(g)}(\epsilon_3) [1 - f^{(g)}(\epsilon_4)] \left\{ \frac{1}{\epsilon - \epsilon_1 + \Delta F_{\text{L}}^+(n)} + \frac{1}{\epsilon - \epsilon_3 + \Delta F_{\text{R}}^-(n)} \right\}^2 \delta(\epsilon + \epsilon_1 - \epsilon - \epsilon_3 - \epsilon_4) \\
+ \frac{R_q^2}{2\pi^3} \frac{1}{R_L R_R} \frac{1}{\hbar} \int d\epsilon_1 d\epsilon_2 d\epsilon_4 f^{(L)}(\epsilon_1) \\
\times [1 - f^{(g)}(\epsilon_2)] f^{(g)}(\epsilon_3) [1 - f^{(R)}(\epsilon_4)] \\
\times \delta(\epsilon + \epsilon_1 - \epsilon_2 + \epsilon_3 - \epsilon_4) + (L \leftrightarrow R, V \to -V),
\]  

(A.1)

where the last term in the brackets results from the contribution of the electron cotunneling rate \( \Sigma^{(\text{inel})}_{\text{el}} \) from the right to the left leads. Elastic cotunneling does not contribute to the scattering integral.

Using equation (A.1) we rewrite the heat flux dissipated into the grain in terms of the heat rates similar to equation (9):

\[
\dot{Q} = \dot{T}^c_{Q} + \dot{T}^c_{\text{Q}},
\]  

(A.2)

where the heat rate from the left to the right lead is

\[
\dot{T}^c_{Q} = \frac{1}{2\pi^3} \frac{R_q^2}{R_L R_R} \frac{1}{\hbar} \int d\epsilon_1 d\epsilon_2 d\epsilon_3 d\epsilon_4 (\epsilon_2 - \epsilon_3) f^{(L)}(\epsilon_1) \\
\times [1 - f^{(g)}(\epsilon_2)] f^{(g)}(\epsilon_3) [1 - f^{(R)}(\epsilon_4)] \\
\times \left\{ \frac{1}{\epsilon_2 - \epsilon_1 + \Delta F_{\text{L}}^+(n)} + \frac{1}{\epsilon_4 - \epsilon_3 + \Delta F_{\text{R}}^-(n)} \right\}^2 \delta(\epsilon + \epsilon_1 - \epsilon_2 + \epsilon_3 - \epsilon_4).
\]  

(A.3)

The plus sign in equation (A.2) implies that the particular direction of the cotunneling process, from the left to the right or from the right to the left, is not important for heating or freezing of the grain.

Appendix B. Bosonic representation of charge and heat rates

\subsection*{B.1. Inelastic scattering rate}

Integrating the expression for the inelastic cotunneling rate \( \dot{T}^c_{Q}^{(\text{inel})} \) in equation (9) over the \( E = (\epsilon_2 + \epsilon_3)/2 \) and introducing new variables \( \omega = \epsilon_2 - \epsilon_3 \) and \( \omega' = \epsilon_1 - \omega_4 \), we obtain

\[
\int_{\epsilon_1, \epsilon_4} f_{g}^{(L)}(\epsilon_2) [1 - f_{g}^{(R)}(\epsilon_3)] f_{g}^{(g)}(\epsilon_4) \delta(\epsilon_2 - \epsilon_3 - \epsilon_4) \\
\times \delta(\epsilon + \epsilon_1 - \epsilon_2 + \epsilon_3 - \epsilon_4) \\
= \int_{-\omega}^{\infty} d\omega \int_{-\omega}^{\infty} d\omega' \int_{-\omega}^{\infty} dE \int_{-\omega}^{\infty} dE' f_{E_+}^{(L)} f_{E_{-}}^{(R)} [1 - f_{E_+}^{(g)}] [1 - f_{E_{-}}^{(g)}] \delta(\omega + \omega')
\]  

(B.1)

where \( E_{\pm} = \pm \omega/2 \) and \( E'_{\pm} = \pm \omega'/2 \). The form-factors \( n_{\omega_{\text{LR}}} \) and \( N_{\omega} \) in equation (B.1) can be interpreted as the effective distributions of electron–hole pairs, see discussions below equations (23) and (29). This interpretation is possible for positive frequencies \( \omega > 0 \). Therefore it is convenient to transform the integral in the last line of equation (B.1) and find

\[
\int_{0}^{\infty} d\omega \omega^2 n_{\omega_{\text{LR}}} [1 + N_{\omega}] = \int_{0}^{\infty} d\omega \omega^2 n_{\omega_{\text{LR}}} [1 + N_{\omega} + [1 + N_{\omega}]].
\]  

(B.2)

This result immediately leads to equation (20) for the inelastic scattering rate \( \dot{T}^c_{Q}^{(\text{inel})} \) given in the text.

\subsection*{B.2. Elastic scattering rate}

Generalizing the results of [5, 13] we write the elastic contribution to the current far from equilibrium

\[
\dot{I}^{(el)}(V) = e \dot{T}^{(el)} - \dot{T}^{(el)},
\]  

(B.3)

where the elastic cotunneling rate from the left to the right lead is

\[
\dot{T}^{(el)} = \frac{2\pi}{\hbar} \int_{km} f_{km}^{(L,R,g)} f_{km}^{(R,L,g)} \left\{ 1 - f_{\nu k}^{(s)} \right\} \\
\times F(\epsilon_1, \epsilon_m, \epsilon_n) F(\epsilon_k, \epsilon_m, \epsilon_n) \delta(\epsilon_m - \epsilon_n + eV),
\]  

(B.4)
and

\[ F(\epsilon, \epsilon_m, \epsilon_n) = \frac{1 - f_R^{(g)}}{\Delta F_L^\prime + \epsilon - \epsilon_m} - \frac{f_R^{(g)}}{\Delta F_R^\prime - \epsilon + \epsilon_n}. \]  

(B.5)

Here \( T_{km}^{(L,g)} \) is the tunnel matrix element between the left lead and the grain. We assume the summation convention over repeated indices \( n, k, \ldots \) that label electron energy levels in the leads and in the grain.

For metallic leads we can simplify the expression for the elastic tunneling rate following [13]

\[ \Gamma_{(el)} = \frac{\lim_{\omega \rightarrow 0} \omega^3 n_0^{(LR)}}{R_{(el)}}, \]

where the elastic resistance \( R_{(el)} \) is given by the expression:

\[ \frac{1}{R_{(el)}[f_{(g)}]} = \frac{2}{meV} \int_0^\infty dt \int d^2 x_1, d^2 x_2 |F(t)|^2 g_{(L,g)}(x_1, n_1) \times g_{(R,g)}(x_2, n_2) \mathcal{P}(x_1, n_1; x_2, n_2; |f|), \]

(B.7)

where \( v_0 \) is the density of states in the grain at the Fermi level and \( F(t) \) is the Fourier transform of \( F(\epsilon, 0, 0) \). Here \( g_{(L,g)}(x_1, n_1) \) is the probability that an electron tunnels from the left lead into the grain with the direction of momentum \( n_1 \) near the point \( x_1 \) of the interface (\( f d n_1 g_{(L,g)}(x_1, n_1) \) is the conductance of the unit area). \( \mathcal{P}(x_1, n_1; x_2, n_2; |f|) \) is the quasiclassical probability for an electron to propagate through the grain from the state \( (x_1, n_1) \) at one interface to the state \( (x_2, n_2) \) at the other interface within time \( t \).

Using the notation for the effective voltage, \( \lim_{\omega \rightarrow 0} \omega n_0^{(LR)} = \nu_0^{(LR)} = eV_{(el)} \), we finally find

\[ I_{(el)}(V) = \frac{V_{(el)}^{(el)}}{R_{(el)}[f_{(g)}]}, \]

(B.8)

For equal lead temperatures, \( T_L = T_R \), one finds \( V_{(el)}^{(el)} = V \). Our nonequilibrium expression for the elastic cotunneling current, equation (B.8), reduces to the results of [13] by substituting the voltage \( V \) by the effective voltage, \( V_{(el)}^{(el)} \), and the temperature \( T \) by the grain temperature, \( T_L \). The heat does not dissipate in the grain during an elastic cotunneling process, i.e., \( Q_{(el)}^{(el)} = 0 \); all the heat, \( V_{(el)}^{(el)}(V) \), dissipates in the leads. For a typical junction with a metallic grain, the elastic cotunneling contribution to transport is suppressed compared to the inelastic one. The reasons for that are the same as described in [13].

B.3. Bosonic form-factors

To prove identities, equations (27)–(28), we rewrite equation (25),

\[ 1 + n_0^{(LR)} = \frac{1}{\omega} \int_{-\infty}^{\infty} d\epsilon [f_{(L)}(\epsilon_\cdot) - f_{(R)}(\epsilon_\cdot)] \]

\[ = \frac{1}{\omega} \int_{-\infty}^{\infty} d\epsilon [f_{(R)}(\epsilon_+) - f_{(L)}(\epsilon_-)]. \]

(B.9)

Taking the distribution functions \( f_{(L)}(\epsilon, T_1) = f_{(L)}(\epsilon - eV/2, T_1) \) and \( f_{(R)}(\epsilon, T_2) = f_{(R)}(\epsilon + eV/2, T_2) \), and using \( \int_{-\infty}^{\infty} [f_{(R)}(\epsilon, T_1) - f_{(R)}(\epsilon, T_2)] d\epsilon = 0 \), we find for the last integral:

\[ \frac{1}{\omega} \int_{-\infty}^{\infty} d\epsilon [f_{(R)}(\epsilon_+) - f_{(L)}(\epsilon_-)] \]

\[ = \omega + eV \int_{-\infty}^{\infty} d\epsilon \frac{1}{\omega} \frac{d}{d\epsilon} \left[ f_{(R)}(\epsilon) + f_{(L)}(\epsilon) \right] \]

\[ = -1 - eV/\omega. \]  

(B.10)

This proves the validity of equations (27)–(28).

Using the distribution functions \( f_{(L)}(\epsilon, T_L) = f_{(L)}(\epsilon - eV/2, T) \) and \( f_{(R)}(\epsilon, T_R) = f_{(R)}(\epsilon + eV/2, T) \) in equation (A.3), with \( T \) being the temperature of both leads, we find the explicit form of the form-factors (see footnote 2)

\[ n_0^{(LR)} = \frac{\omega - eV}{\omega} N_B(\omega - eV, T), \]

(11)

\[ n_0^{(LR)} = \frac{eV}{\omega} + \frac{eV}{\omega} N_B(\omega + eV, T), \]

(12)

\[ n_0^{(RL)} = \frac{\omega + eV}{\omega} N_B(\omega + eV, T), \]

(13)

\[ n_0^{(RL)} = -\frac{eV}{\omega} + \frac{eV}{\omega} N_B(\omega - eV, T). \]

(14)

Equations (11)–(14) are exact for equal lead temperatures only, \( T_L = T_R \). However, if the lead temperatures are different \( T_L \neq T_R \) then equations (11)–(14) still give a good approximation of the form-factors if we use the substitution, \( T \rightarrow T_m = \frac{T_L + T_R}{2} \). This is a good approximation for \( T_L, T_R \gg eV \) and for \( T_L, T_R < eV \) when \( T_L \sim T_R \). Furthermore, it reproduces \( \lim_{\omega \rightarrow 0} \omega n_0^{(LR,R)} = eV/2T_m \).

The integrals of form \( \int_0^{\infty} \omega^3 n_0^0 d\omega, a = 2, 3, \ldots \) can be calculated analytically using equations (29), (11) and (13), and expressed through the polylogarithms 9. So, for instance,

\[ \int_0^{\infty} \omega^3 n_0^0 d\omega = \{\text{Li}_3(e^{-1}) - \text{Li}_3(e^1)\}v \]

\[ + 3[\text{Li}_1(e^{-1}) - \text{Li}_1(e^1)] \]

\[ = -\frac{\pi^4}{24}B_4 - \frac{4\pi^3}{3}B_3 \left( -\frac{v}{2\pi^2} \right) \]

\[ = \frac{(\pi T)^4}{15} \left\{ 1 + \frac{5}{2\pi^2} + \frac{5}{8\pi^4} - \frac{v^2}{2\pi^2} \right\}. \]

(B.15)

where we use the notation \( v = eV/T \).

References

[1] Beloborodov I S, Lopatin A V, Vinokur V M and Efetov K B 2007 Rev. Mod. Phys. 79 469

9 More generally, integrals of this type can be expressed in terms of polylogarithms, \( \text{Li}_a(z) \), using \( \int_0^{\infty} \frac{x^a}{(e^{x}+1)} \frac{dx}{x^a} = \text{Li}_a(e^{-x}) \). The \( \text{Li}_a \) functions can be written in terms of Bernoulli polynomials, \( B_n \), using the identity, \( \text{Li}_a(z) + (-1)^a \text{Li}_a(1/z) = \frac{-2(-1)^n}{n!}B_n \frac{1}{z} + n!(-1)^{n-1} \frac{z}{2\pi i} \). The latter identity gives the result for \( n_0 \) directly.
