Scattering theory of thermocurrent in quantum dots and molecules

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In this work we theoretically study properties of electric current driven by a temperature gradient through a quantum dot/molecule coupled to the source and drain charge reservoirs. We analyze the effect of Coulomb interactions between electrons on the dot/molecule and of thermal environment on the thermocurrent. The environment is simulated by two thermal baths associated with the reservoirs and kept at different temperatures. The scattering matrix formalism is employed to compute electron transmission through the system. This approach is further developed and combined with nonequilibrium Green’s functions formalism, so that scattering probabilities are expressed in terms of relevant energies including the thermal energy, strengths of coupling between the dot/molecule and charge reservoirs and characteristic energies of electron-phonon interactions. It is shown that one may bring the considered system into regime favorable for heat-to-electric energy conversion by varying the applied bias and gate voltages.

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I. INTRODUCTION

The field of molecular electronics has been rapidly expanding during the last two decades owing to continuous improvement of techniques intended to electrically contact and control quantum dots and single molecules in transport junctions. Recent advances in heat measurements in nanoscale systems allow to study thermoelectric properties of molecular junctions and similar systems. These studies bring a deeper understanding of transport mechanisms [1–4] and additional information concerning electronic and vibrational excitation spectra of molecules [5, 6]. Also, in the recent years a new field of molecular thermoelectronics have emerged [7]. Thermal analogs of molecular transistors and heat-into-electricity converters were proposed [5, 6, 12].

Heat-to-electric power converters operate due to Seebeck effect which appears provided that thermal and electric driving forces simultaneously affect electron transport through the considered system. When a temperature gradient $\Delta T$ is applied across the system, a thermovoltage $V_{th}$ emerges under the condition of zero net current thus indicating the energy conversion. At small temperature gradients ($\Delta T \ll T_0$, $T_0$ being the temperature of the cool region) the system operates within the linear regime and $V_{th} = -S\Delta T$. Within this regime, thermopower $S$ is the decisive quantity determining the extent of energy conversion. Accordingly, the thermopower was intensively studied [3, 10, 13, 16] along with the thermoelectric figure of merit $ZT$ [13, 17, 18]. Another interesting quantity characterizing thermoelectric transport through molecular junctions and other systems of similar kind is thermocurrent $I_{th}$. The latter may be defined as a difference between the electron tunnel current flowing through a biased thermoelectric junction where the electrodes are kept at different temperatures ($T_L = T_0 + \Delta T$, $T_R = T_0$) and the current flowing in absence of temperature gradient [19]:

$$I_{th} = I(V, T_0, \Delta T) - I(V, T_0, \Delta T = 0).$$

As well as the thermovoltage, the thermocurrent is simultaneously controlled by electric and thermal driving forces. The combined effect of these forces depends of the type of charge carriers involved in transport and of the bias voltage polarity. For example, assuming that the chemical potential of the left (hot) electrode is made higher than that of the right (cold) one due to the applied bias voltage, the thermocurrent takes on negative/positive values when the charge carriers are electrons/holes, respectively. At the same time it was shown that (disregarding electron-phonon interactions) maximum efficiency of molecular heat-to-electricity converter could be reached under the condition of vanishing current $I(V, T_0, \Delta T)$. Under this condition, $I_{th} = -I(V, T_0, \Delta T = 0)$. Therefore, negative and relatively large in magnitude thermocurrent flowing through a system may indicate that the system operates in the regime favorable for energy conversion. On the contrary, positive values of $I_{th}$ show that the energy conversion does not occur [20].

Properties of the thermovoltage in molecular junctions and quantum dots were theoretically analyzed in numerous works [20–29]. As yet, less attention was paid to studies of thermocurrent in spite of the fact that $I_{th}$ is more straightforward to measure and model than $V_{th}$, as stated in the recent work [19]. However, theoretical analysis of $I_{th}$ behavior within a weakly nonlinear regime was recently suggested [25]. The purpose of the
The present work is to analyze the effect of the gate voltage, electron-electron interactions and thermal phonons on the characteristics of thermocurrent flowing through a single-molecule junction or a quantum dot.

To properly analyze thermoelectric transport through molecules/quantum dots one needs to use an approach including unified treatment of electron and phonon dynamics in the considered system. For this purpose, one may use diagrammatic technique or nonequilibrium Green’s function formalism (NEGF), as described in the review [30]. However, application of these advanced formalisms to realistic models simulating molecular junctions is extremely difficult. Several simplified approaches based on scattering theory [6] and on quantum rate equations [3, 14, 20, 31, 32] were developed and used to study thermoelectric properties of molecular junctions taking into account contributions of vibrational phonons and electron-vibron interactions. Very recently, a scattering theory based approach was suggested to analyze weakly nonlinear thermoelectric transport in mesoscopic systems [25, 27]. Nevertheless, these studies are not completed so far.

In the present work we use a scattering theory first suggested by Buttiker [33] combined with certain NRGF based results. The adopted approach allows to derive the expression for the electron transmission which remains applicable for an arbitrary value of the difference between the temperatures of the electrodes. Therefore, this expression may be employed to analyze nonlinear effects in thermoelectric properties of considered systems.

II. MODEL AND RESULTS

The schematics of the suggested model is presented in the Fig. 1. To simplify the computations we mimic the bridge linking the electrodes by a single state with the energy $E_0$. To analyze the effect of thermal phonons associated with the electrodes on the thermocurrent, we introduce two phonon baths representing thermal phonons on the electrodes. The baths are treated as reservoirs where electron could be scattered while on the bridge. In a reservoir, it undergoes inelastic scattering accompanied by phase breaking, and afterwards returns to the bridge. The intensity of these processes is characterized by scattering probabilities $\epsilon_{\beta}$ where $\beta \in L, R$ corresponds to the bath associated with the left/right electrode.

So, within the accepted model the coupling of the bridge to the leads is twofold. First, there is a conventional coupling which determines the probability of electron tunneling between the bridge and an electrode. Secondly, the electron is coupled to phonon baths associated with the electrodes. Correspondingly, the accepted model includes six transport channels, and the relations between incoming particle fluxes $J_k$ and outgoing fluxes $J'_k$ take on the form $1 \leq i \leq k \leq 6$:

$$J'_k = \sum T_{ik} J_k. \tag{2}$$

Here, the coefficients $T_{ik}$ are related to matrix elements of the scattering matrix $M$: $T_{ik} = |M_{ik}|^2$. To maintain the charge conservation in the system, zero net current should flow in the channels linking the bridge with the reservoirs:

$$J_3 + J_4 - J'_3 - J'_4 = 0,$$

$$J_5 + J_6 - J'_5 - J'_6 = 0. \tag{3}$$

Solving the equations (2), (3) one arrives at the following expression for the electron transmission [34]:

$$\tau(E) = \frac{J'_2}{J_2} = T_{21} + \sum_{m,n} K_{mn}^{(2)} (W^{-1})_{mn} K_n^{(1)}. \tag{4}$$

Within the considered model, $1 \leq m, n \leq 2$,

$$K_n^{(1)} = T_{2m+1,1} + T_{2m+2,1},$$

$$K_n^{(2)} = T_{2,2m+1} + T_{2,2m+2}, \tag{5}$$

and matrix elements of $2 \times 2$ matrix $W$ are given by

$$W_{mn} = (2 - R_{mn}) \delta_{mn} - \tilde{R}_{mn} (1 - \delta_{mn}) \tag{6}$$

where

$$R_{mn} = T_{2m+1,2m+1} + T_{2m+2,2m+2} + T_{2m+2,2m+1} + T_{2m+1,2m+2},$$

$$\tilde{R}_{mn} = T_{2m+1,2m+1} + T_{2m+1,2m+2} + T_{2m+2,2m+1} + T_{2m+2,2m+2}. \tag{7}$$

We remark that within the adopted model the phonon thermal conductance through the junction is zero. This

![FIG. 1: (Color online) Schematics of the considered system. Semicircles represent the left and right electrodes, square stands for the molecule/quantum dot sandwiched in between. Dephasing/dissipative reservoirs are associated with the electrodes and characterized by temperatures $T_L$ and $T_R$, respectively.](image)
seems a reasonable assumption for experiments give low values of phonon thermal conductance in several molecular junctions \[35, 36\]. This may be attributed to the fact that in many molecules the majority of vibrational transitions lie above the range determined by thermal energy.

Provided that relevant temperatures take on values below room temperature \[13, 37\].

The expression for the scattering matrix corresponding to the considered model was derived in the form \[38\]:

\[
M = \frac{1}{Z} \begin{pmatrix}
  r_L + a^2_L a^3_L r_R & a_L a_R r_{L2} & b_L t_L \\
  a_L a_R r_{L2} & r_R + a^2_L a^3_L r_L & b_L t_R \\
  b_L t_L & b_L t_R & a_L a_R b_{L2} t_{LR}
\end{pmatrix}
\]

(8)

Here, \( Z = 1 - a^2_L a^3_L r_{LR} \), \( a^2_L r_{LR} = 1 - \epsilon_L r_{LR} \), and transmission \((t_L, t_R)\) and reflection \((r_L, r_R)\) amplitudes characterize electron tunneling through the potential barriers separating the left/right electrode from the bridge. In the following analysis we focus on a symmetrically coupled system assuming the self-energy terms \( \Gamma^*_{L,R} \) describing coupling of an electron on the bridge (with a certain spin orientation \( \sigma \)) to the electrodes to be equal: \( \Gamma^*_{L} = \Gamma^*_{R} = \Gamma \). For such a system in the case of coherent and elastic transport, the electron transmission function may be presented as follows:

\[
\tau(E) = \frac{1}{2} \Gamma(E) \sum_{\sigma} [G^r_{\sigma}(E) - G^a_{\sigma}(E)] \equiv g^2(E)
\]

(9)

where \( G^r_{\sigma}(E) \) and \( G^a_{\sigma}(E) \) are the retarded and advanced Green’s functions associated with the molecule/quantum dot linking electrodes. Provided that the electron transport through the junction is undisturbed by electron-phonon interactions and disregarding spin-flip processes, \( G_{\sigma}^r(E) \) may be approximated as \[39\]:

\[
G^r_{\sigma}(E) = \frac{E - E_0 - \Sigma^\beta_{\sigma} - U \left(1 - \langle n_{-\sigma}\rangle \right)}{(E - E_0 - \Sigma^\alpha_{\sigma})(E - E_0 - U - \Sigma^\beta_{\sigma}) + iU \Sigma^\sigma_{\sigma}}.
\]

(10)

In this expression, \( U \) is the charging energy describing Coulomb repulsion between electrons on the bridge, and \( \langle n_{\sigma}\rangle \) are one-particle occupation numbers which could be computed by integration of the imaginary part of the lesser Green’s function \( G^r_{\sigma}(E) \) over the whole range of tunnel energy \( E \) values. Self-energy terms \( \Sigma^\alpha_{\sigma}, \Sigma^\beta_{\sigma} \) and \( \Sigma^\sigma_{\sigma} \) appear in the Eq. (10) due to the coupling of the bridge to the leads. Previously introduced coupling parameters \( \Gamma^*_{L,R} \) are closely related to \( \Sigma^\alpha_{\sigma} \), namely: \( \Sigma^\sigma_{\sigma} = \Sigma^L_{\sigma} + \Sigma^R_{\sigma}, \quad \Gamma^*_{L,R} = -2i \text{Im} \Sigma^\sigma_{\sigma} \). We remark that \( \Sigma^\sigma_{\sigma} \) and \( \Sigma^\sigma_{\sigma} \) depend on the temperatures of electrodes which is taken into account in further computations.

Provided that the dephasing reservoirs are detached from the bridge \( (\epsilon_L = \epsilon_R = 0) \) and the barriers separating the electrodes from the bridge are identical \( (t_L = t_R = t, r_L = r_R = r) \), the electron transmission determined by Eqs. (1)–(8) accepts a simple form:

\[
\tau(E) = t^4 \frac{(1 + r^2)^2}{(1 + r^2)^2}.
\]

(11)

Comparing this result with the expression \[29\], we obtain:

\[
t^2 = \frac{2g}{1 + g}.
\]

(12)

Scattering probabilities \( \epsilon_L, \epsilon_R \) may be given an explicit physical meaning by expressing them in terms of relevant energies. In the considered system, dephasing and energy dissipation originate from interactions of charge carriers with thermal phonons associated with the electrodes. So, one can approximate these parameters as follows \[40\]:

\[
\epsilon_\beta = \frac{\Gamma^\beta_{\phi}}{2(\Gamma_L + \Gamma_R) + \Gamma^\beta_{\phi}^\phi}.
\]

(13)

Here, \( \Gamma^\beta_{\phi} \) represents the self-energy term occurring due to electron interactions with thermal phonons associated with one or another electrode \( (\beta \in L, R) \). Using NEGF to compute the relevant electron and phonon Green’s functions within the self-consistent Born approximation, one may derive a relatively simple approximation for \( \Gamma^\beta_{\phi} \)

\[
\Gamma^\beta_{\phi}(E) = 2\pi \lambda^2 \int_0^\infty d\omega \rho^\beta_{\phi}(\omega) \times \left\{ N_B(\omega) [\rho_{el}(E - \hbar\omega) + \rho_{el}(E + \hbar\omega)] + \left[1 - n(E - \hbar\omega)\right] \rho_{el}(E - \hbar\omega) + n(E + \hbar\omega) \rho_{el}(E + \hbar\omega) \right\},
\]

(14)

where \( n(E) = \frac{1}{2}(f_L + f_R) \), \( f_{L,R} \) are Fermi distribution functions for the electrodes, \( \rho_{el}(E) \) is the electron density of states on the bridge level and \( \rho^\beta_{\phi}(\omega) \) is
the phonon spectral function for the reservoir associated with the electrode $\beta$. We assume that the electrodes are kept at different temperatures $T_\beta$ so, we introduce two phonon distribution functions $N_\beta(\omega) = \{ \exp [\omega/kT_\beta] - 1 \}^{-1}$, ($k$ being the Bolzmann’s constant). Finally, the constant $\lambda_\beta$ describes the coupling strength for electron interactions with thermal phonons belonging to the corresponding bath. Further we assume for simplicity that $\lambda_L = \lambda_R = \lambda$.

The phonon spectral function may be determined using molecular dynamic simulations. However, to qualitatively analyze the effect of thermal phonons on the transport characteristics, one may use the approximation [41]:

$$\rho_{ph}^\beta(\omega) = \rho_{0\beta} \frac{\omega}{\omega_c^\beta} \exp \left( - \frac{\omega}{\omega_c^\beta} \right).$$

(15)

Here, the parameters $\rho_{0\beta}$ are proportional to the electron-phonon coupling strengths, and $\omega_c^\beta$ characterize relaxation times for the thermal phonons.

As the electron density of states includes self-energy corrections appearing due to electron-phonon interactions, Eq. (14) is an integral equation for $\Gamma_{ph}$. Substituting the approximation (15) into Eq. (14) one may see that the major contribution to the integral comes from the region where $\omega \ll \omega_c$. On these grounds, one may omit the terms $\hbar \omega$ in the arguments of slowly varying functions in the integrand of Eq. (14) thus reducing this equation to the form [10]:

$$\Gamma_{ph}^\beta = \rho_{el} (E, \Gamma, \Gamma_{ph}^L, \Gamma_{ph}^R) \cdot Q(\lambda, \omega_c^\beta, T_\beta).$$

(16)

Here,

$$Q(\lambda, \omega_c^\beta, T_\beta) = \frac{4\pi \lambda}{\hbar \omega_c^\beta} (kT_\beta)^2 \zeta \left( 2; 1 + \frac{kT_\beta}{\hbar \omega_c^\beta} \right)$$

(17)

and $\zeta(\tau; q)$ is the Riemann’s $\zeta$ function.

For a considered symmetrically coupled junction, the thermocurrent is described by the following expression:

$$I_{th} = \frac{e}{\pi \hbar} \int dE \left\{ \tau(E, T_0, \Delta T) f^L(E, T_0 + \Delta T) - \tau(E, T_0, \Delta T = 0) f^L(E, T_0) + \Delta \tau f^R(E, T_0) \right\}$$

(18)

where $\Delta \tau$ is given by:

$$\Delta \tau = \tau(E, T_0, \Delta T) - \tau(E, T_0, \Delta T = 0).$$

(19)

The suggested approach allows one to analyze the effect of thermal phonons on characteristics of thermoelectric transport beyond the linear regime. Using Eqs. (14)-(17), one may compute the electron transmission function for an arbitrary value of the ratio $\Delta T/T_0$. This result may be used to calculate thermocurrent and analyze how it is affected by various characteristics of the considered junction (such as the quality of contact between the electrodes and the linker, electron-electron and electron-phonon interactions) and by external factors including the bias and gate voltage and temperature gradient.

III. DISCUSSION

The most interesting thermoelectric properties are better pronounced in weakly coupled junctions where electron transmission exhibits sharp maxima [20]. Correspondingly, in further analysis we assume that $\Gamma < kT$. Then, as shown in the Fig. 2, $\Delta \tau$ displays sharp dips at $E = E_0$ and $E = E_0 + U$, and the magnitudes of these features increase as the difference in the temperatures of electrodes enhances. Electron-phonon interactions significantly affect the transmission. As the coupling between electrons and thermal phonons strengthens, $\Delta \tau$ generally takes on greater values. However, too strong electron-phonon interactions bring partial spreading of the resonance features which is not favorable for nonlinear behavior of thermocurrent to be revealed.

Thermocurrent dependence of the applied bias voltage is illustrated in the left panel of the Fig. 3 assuming for certainty that the left (hot) electrode is kept at higher voltage and the bridge energy level $E_0$ is situated below the Fermi level for the electrodes. When the bias is small so that $E_0$ remains outside the conduction window whose width is determined by the difference between chemical potentials of electrodes $\mu_L$ and $\mu_R$, the charge flow is driven by the temperature gradient. Higher temperature of the left electrode enhances probability for an electron to tunnel there from the bridge provided that $E_0$ is rather close to the Fermi level, so that their difference is of the same order as the thermal energy $kT$. Under these conditions, $I_{th}$ takes on positive values. When the bias becomes greater, $E_0$ enters the conduction window, and the electric driving forces come into play. As a result, the thermocurrent changes its sign. It remains negative at moderate bias indicating the possibility of energy conversion in the considered system. In strongly
biased junctions, electric driving forces predominate, and $I_{th}$ approaches zero. The depth of the dip appearing on the $I_{th} - V$ curves, as well as its position, are controlled by several factors. Assuming that the charging energy $U$ and electron-phonon coupling strength $\lambda$ are fixed, it is determined by the value of $\Delta T$. The greater becomes the difference between the electrodes temperatures, the greater is the maximum magnitude of $I_{th}$.

It was recently reported [19] that thermocurrent flowing through a quantum dot may exhibit a nonlinear dependence of $\Delta T$ even at small values of the latter. As recently suggested [23], the nonlinearity appears due to renormalization of the energy $E_0$ in the presence of temperature gradient. Taking into account the suggested energy renormalization, we showed that weak nonlinearity of $I_{th}$ versus $\Delta T$ curves may be actually traced (see right panel of the Fig. 3). Presented curves demonstrate a qualitative agreement with the experimental results of Ref. [19]. However, we remark that the suggested renormalization $E_0 \rightarrow E_0 + z k \Delta T$ where $|z| < 1$ may significantly affect the thermocurrent behavior only at certain values of the bias voltage, when $E_0$ is very close to the boundary of the conduction window. In general, nonlinear behavior of $I_{th}$ develops at greater values of $\Delta T$ regardless of the bridge level energy renormalization.

Coulomb repulsion between electrons on the bridge and the electron interactions with thermal phonons may significantly influence thermoelectric transport through the junction, as demonstrated in the Fig. 4. The enhancement of charging energy narrows down the interval where $I_{th}$ accepts negative values and makes the dips in the $I_{th} - V$ curves more shallow. This may be explained by considering the role taken by Coulomb interactions. Electron-electron interactions are hindering electron flow through the system in both directions, which leads to the Coulomb blockade. These interactions could be treated as a source of an effective force opposing any predominating driving force (originating either from the bias voltage or from the temperature gradient applied across the junction). As a result, the characteristic features manifested in the shapes of $I_{th} - V$ curves become less distinctly pronounced.

Electrons interactions with thermal phonons do not change the width of the region where $I_{th}$ remains negative. However, these interactions may affect the magnitude of thermocurrent. In the right panel of the Fig. 4, we present the $I_{th}$ value at the bottom of the dip as a function of the electron-phonon coupling strength. As shown in the figure, the dip depth reduces as $\lambda$ increases. This effect is better pronounced at weak or moderate electron-phonon coupling ($\lambda \lesssim \Gamma, kT_0$), and it fades away when $\lambda$ significantly exceeds $\Gamma$.

As known, transport properties of molecular junctions and other similar systems may be controlled by varying the positions of the bridge energy levels. Practically, the levels may be shifted by a gate voltage applied to the system. Within the accepted model, the bridge in the considered junction is represented by a single energy level $E_0$. In the Fig. 5 we trace the thermocurrent dependencies of $E_0$. The presented results confirm those shown in the previous figures. Again, the thermocurrent acquires a negative sign when the bridge level moving upwards appears in the conduction window. For a symmetrically coupled system this happens at $E_0 = -\frac{1}{2} V$ assuming that the Fermi level for unbiased junction $\mu = 0$. As the bridge level moves higher, $I_{th}$ remains negative while the level is still inside the conduction window. When it leaves the window but remains near its upper boundary, the thermocurrent may change sign once more, being
influenced by electron-electron interactions and electrons coupling to the thermal phonons associated with the electrodes. However, when the bridge level moves farther away from the conduction window, both terms in the Eq. (1) approach zero, so the thermocurrent disappears.

IV. CONCLUSION

Finally, we repeat again that various aspects of energy conversion in nanoscale systems attract significant interest of the research community. The present work was inspired by this common interest. Also, the present research was motivated by recent experimental observations of nonlinear thermocurrent flowing through quantum dots. The thermocurrent defined by Eq. (1) is an important characteristic of thermoelectric transport. The sign and magnitude of thermocurrent may indicate that the corresponding system operates as an energy converter. In a nanoscale junction consisting of a quantum dot or molecule sandwiched in between two electrodes, the thermocurrent value is controlled by several factors. These include temperatures of electrodes, bias and gate voltage, charging energy characterizing electron-electron interactions on the bridge and specific energies characterizing the coupling of the bridge to the electrodes and electron-phonon interactions. To theoretically analyze possible effect of the above factors on thermocurrent we employ a single-particle scattering approach pioneered by Landauer in the context of charge transport in mesoscopic systems.

For simplicity, we simulate the bridge in the considered junction by a single orbital, and we assume that it is symmetrically coupled to the electrodes. Then the thermocurrent is expressed in terms of electron transmission functions (which depend on all above mentioned factors) and Fermi distribution functions for the electrodes. We derive the expression for the electron transmission which remains valid for an arbitrary value of the difference between the temperatures of electrodes. This makes it suitable for analysis of thermoelectric transport both within and beyond linear in temperature regime. Using this expression, we show that varying the bias and gate voltage one may create favorable conditions for heat-to-electricity conversion in a junction assuming that the most important characteristic energies $kT_0$, $U$ and $\lambda$ are fixed. Also, we analyze how electron-electron interactions on the bridge and electrons interactions with thermal phonons associated with electrodes may affect the thermoelectric properties of the considered systems. Coulomb repulsion between electrons opposes electron transport through the junction at small bias voltage. We show that this brings a partial suppression of the thermocurrent. Electron-phonon interactions assist in the increase of scattering probabilities thus destroying the coherence of electron transport and bringing additional suppression of thermocurrent, as illustrated in Figs. 4, 5.

The computational method employed in the present work may be further generalized to include the effect of molecular vibrations. Also, one may simulate the bridging molecule/quantum dot by several orbitals thus opening the way to studies of quantum interference effects. So, we believe that presented computational scheme and obtained results may be helpful for further understanding of thermoelectric properties of nanoscale systems.

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