Phonon-assisted thermoelectric effects in a two-level molecule

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Abstract

Thermoelectric properties of a two-level molecule attached to the metallic electrodes are analyzed using the equation of motion technique within the Green’s function formalism. Results show that the electrical conductance is strongly dependent on the electron and phonon temperatures and the electron-phonon coupling strength. In addition, it is observed that the thermal conductance peaks in the electron-hole symmetry points are vanished in the presence of the strong electron-phonon interaction. It is also found that the figure of merit is strongly suppressed in the strong electron-phonon interaction. The violation of the Wiedemann-Franz law is also observed coming from the Coulomb interactions.

1 Introduction

Transport phenomena through molecular devices have been attracted a lot of attention during recent two decades. Experimental and theoretical results show that the electron transport through the molecular transistors results in novel and interesting effects such as Coulomb and spin blockade effects [1, 2, 3, 4], Kondo effect [5, 6, 7], negative differential conductance [8, 9, 10], and so on. In addition, it has been predicted that the molecular devices can be efficient for conversion of heat into electric energy [11, 12]. Thermoelectric efficiency of a device is indicated by a dimensionless quantity called figure of merit, $ZT = S^2G_eT/\kappa$, where $G_e$ is the electrical conductance and $S$ is the thermopower. $\kappa$ is the thermal conductance which is the sum of the electronic contribution, $\kappa_e$, and the lattice thermal conductance, $\kappa_p$, and $T$ denotes the operating temperature. In bulky samples and according to the Wiedemann-Franz Law, the ratio of the electrical conductance to the thermal conductance is related to the operating temperature. Research shows that the strong Coulomb repulsions, discreteness of energy levels, interference effects and etc. in nanostructures result in the violation of the Wiedemann-Franz law [13, 14, 15] and as a consequence, the increase of $ZT$. For these reasons, the investigation of the thermoelectric prop-
erties of the systems composed of a single or two quantum dots has attracted a lot of attention in recent years [15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25].

Electron-phonon interaction (EPI) is an interesting and important phenomenon in the molecular devices which can significantly affect the transport characteristics of the devices. The center of mass oscillation of the molecule [26], or thermally-induced acoustic phonons [27] can be the origin of the coupling between the electronic degree of freedom and the vibrational degree of freedom. The influence of the EPI on the electronic characteristics of the molecular transistors and the carbon nanotube quantum dots has been extensively studied using both rate equation approach [28, 29, 30, 31, 32] and the Green’s function formalism [33, 34, 35, 36, 37]. However, the influence of the EPI on the thermoelectric properties of the molecular devices is an interesting issue needing more attention. Koch and co-workers [38] analyzed the thermopower in a single level molecule by means of the master equation. Furthermore, the effect of the EPI on the thermoelectric properties of a single-level quantum dot was studied in a few articles using the Green’s function formalism [39, 40, 41].

In this article, we consider a two-level molecule in which the electronic degree of freedom is coupled to the vibrational degree of freedom. Using the equation of motion technique within the Green’s function formalism and using the polaronic transformation, the density of the states of the molecule (DOS) and the thermoelectric properties of the device are analyzed. With respect to the fact that the phonon subsystem has a smaller heat capacity than the electron subsystem, it is completely probable an electron-phonon nonequilibrium thermodynamics is dominant so that the electron temperature, $T_e$, and phonon temperature, $T_p$, are different. The difference can result in the appearance of the phonon absorption sidebands in the DOS in the low electron temperatures which are not seen in the EP thermal equilibrium. The effects of the EP nonequilibrium and EP coupling strength on the thermoelectric properties of the system are analyzed in detail. In the next section, formalism is presented. Section 3 is devoted to the numerical results and in the end; some sentences are given as a summary.

2 Model and formalism

We consider a two-level molecule coupled to the normal metal electrodes. The Hamiltonian describing the system is given as

$$H = \sum_{ak\sigma} \varepsilon_{ak\sigma} c^\dagger_{ak\sigma} c_{ak\sigma} + \sum_{i=1,2\sigma} \varepsilon_{i\sigma} n_{i\sigma} + \frac{1}{2} \sum_{i j \sigma \sigma^\prime} U_{ij} n_{i\sigma} n_{j\sigma^\prime} + \sum_{i\sigma} \omega a^\dagger a + \sum_{i\sigma} \lambda n_{i\sigma} [a^\dagger a] + \sum_{ak\sigma i} [V_{i}^{\dagger} c_{ak\sigma} d_{i\sigma} + H.C.]$$

where $c^\dagger_{ak\sigma}$ creates an electron with wave vector $k$, spin $\sigma$, and energy $\varepsilon_{ak\sigma}$ in lead $\alpha$. $d^\dagger_{i\sigma}$ creates an electron in the $i$th level of the molecule with energy $\varepsilon_{i\sigma}$, while $U_{ii}$ stands for the on-site Coulomb repulsion and $U_{ij}$ ($i \neq j$) denotes the inter-level Coulomb repulsion. The energy levels of the molecule are tuned by a
gate voltage thus we set $\varepsilon_{i\sigma} = \varepsilon_{i\sigma}^0 + V_g$ so that $\varepsilon_{i\sigma}^2 = \varepsilon_{i\sigma}^0 + \Delta$ where $\Delta$ denotes the level spacing. $a^\dagger(\alpha)$ is the creation (annihilation) operator for the phonons with energy $\omega$ and $\lambda$ describes the electron-phonon coupling strength. The last term in the above equation describes the tunneling process between the electrodes and the molecule and $V_{i\alpha\kappa\sigma}^i$ is the coupling strength between the lead $\alpha$ and the $i$th energy level. $V_{i\alpha\kappa\sigma}^i$ induces a tunneling rate from the molecule to the electrode $\alpha$, $\Gamma_{i\alpha\kappa\sigma}^i = 2\pi \sum_{k\in\alpha} \rho_\alpha |V_{i\alpha\kappa\sigma}^i|^2$ where $\rho_\alpha$ is the electronic density of the lead $\alpha$.

The EPI can be eliminated using polaronic transformation [42], $\hat{H} = e^S \hat{H} e^{-S}$, where $S = \exp(\sum_{i\sigma} \lambda n_{i\sigma}|a^\dagger - a|)$. Thus, equation (1) becomes

$$\hat{H} = \sum_{\alpha k \sigma} \varepsilon_{i\alpha k\sigma} c^\dagger_{i\alpha k\sigma} c_{i\alpha k\sigma} + \sum_{i\sigma} \varepsilon_{i\sigma} n_{i\sigma} + \frac{1}{2} \sum_{ij\sigma \sigma'} \tilde{U}_{ij} n_{i\sigma} n_{j\sigma'} \omega a^\dagger a + \sum_{\alpha k \sigma} |\tilde{V}_{i\alpha k\sigma}^i| c^\dagger_{i\alpha k\sigma} d_{\sigma} + H.C. \tag{2}$$

where $\varepsilon_{i\sigma} = \varepsilon_{i\sigma} - \lambda^2/\omega$, and $\tilde{U}_{ij} = U_{ij} - 2\lambda^2/\omega$. The polaronic transformation results in the renormalization of the molecule levels and Coulomb repulsions. In addition, the tunneling amplitude is transformed into $\tilde{V}_{i\alpha k\sigma}^i = V_{i\alpha k\sigma}^i X$ where $X = \exp(-\frac{\lambda}{\omega}[a^\dagger - a])$ is the phonon operator. In the following, we replace the operator $X$ with its expectation value, $<X> = \exp(-\frac{\lambda}{\omega}(N_p + 1/2))$ where $N_p$ stands for the averaged number of phonons. This approximation is used in the localized polaron and is valid when the tunneling amplitude is smaller than the EPI, i.e. $V_{i\alpha k\sigma} << \lambda$. Hence, the tunneling rate is renormalized according to $\tilde{\Gamma}_{i\sigma}^i = \Gamma_{i\sigma}^i < X >^2$. $<X >^2$ just narrows the tunneling rate.

In order to compute the electronic current, $I_e$, and the heat flux, $I_Q$, the Green function formalism is used so that the electronic current and heat current are expressed as [43, 44]

$$I_e = -\frac{e}{h} \sum_{i\sigma} \int_{-\infty}^{\infty} d\varepsilon \frac{\Gamma_{L\sigma}^i \Gamma_{R\sigma}^i}{\Gamma_{L\sigma}^i + \Gamma_{R\sigma}^i} [f_L(\varepsilon) - f_R(\varepsilon)] \text{Im} G_{i\sigma}^i(\varepsilon) \tag{3a}$$

$$I_Q = -\frac{1}{h} \sum_{i\sigma} \int_{-\infty}^{\infty} d\varepsilon \frac{\Gamma_{L\sigma}^i \Gamma_{R\sigma}^i}{\Gamma_{L\sigma}^i + \Gamma_{R\sigma}^i} (\varepsilon - \mu)[f_L(\varepsilon) - f_R(\varepsilon)] \text{Im} G_{i\sigma}^i(\varepsilon) \tag{3b}$$

where $f_\alpha(\varepsilon) = (1 + \exp((\varepsilon - \mu_\alpha))/kT_e)^{-1}$ is the Fermi distribution function and $\mu_\alpha$, and $T_e$ are the chemical potential and electron temperature in the lead $\alpha$. It is worth noting that equation (3) is computed with respect to the tunneling part of the Hamiltonian, equation (1), so the bare tunneling rates are used. However, the influence of the EPI on the electronic and heat currents is saved in the Green function, $G_{i\sigma}^i$. $\text{Im} G_{i\sigma}^i(\varepsilon)$ is the DOS of the level $i$ composed of the phononic and electronic parts which can be computed by evaluating the phonon part of the trace by Feynman disentangling technique [42], and using the
Keldysh equations [44] for the lesser and greater Green functions, as follows [33]

\[ ImG_{i\alpha}^{r}(\varepsilon) = \sum_{\alpha=L,R} \sum_{\nu=-\infty}^{\infty} \frac{L_{\nu}}{\Gamma_{\nu}^{L} + \Gamma_{\nu}^{R}} \left[ \tilde{\Gamma}_{\alpha\nu}^{L} f_{\alpha}(\varepsilon + n\omega) Im\tilde{G}_{i\sigma}^{r}(\varepsilon + n\omega) + \tilde{\Gamma}_{\alpha\nu}^{R} (1 - f_{\alpha}(\varepsilon - n\omega)) Im\tilde{G}_{i\sigma}^{r}(\varepsilon - n\omega) \right] \]

where \( L_{\nu} \), for nonzero temperatures, is given as

\[ L_{\nu} = e^{-(\lambda/\omega)^{2}(1+2N_{ph})(N_{ph} + 1/2)} \sqrt{N_{ph}(N_{ph} + 1)} \]

where \( I_{\nu}(x) \) are the Bessel functions of the complex argument, and \( N_{ph} = (\exp(\omega/kT_{p}) - 1)^{-1} \) is the averaged number of phonons and \( T_{p} \) stands for the phonon temperature. Indeed, the thermal equilibrium between the electrons in the electrodes and phonons in the molecule can be broken due to smaller heat capacity of the phonons. \( \tilde{G}_{i\sigma}^{r}(\varepsilon) \) is the dressed retarded Green function [45] for the lesser and greater Green functions, as follows [33]

\[ \tilde{G}_{i\sigma}^{r}(\varepsilon) = \sum_{k=0}^{2} \rho_{k} \left( \frac{1 - N_{i-\sigma}}{E_{i\sigma} - \Pi_{k}} + \frac{N_{i\sigma}}{E_{i\sigma} - U_{ii} - \Pi_{k}} \right) \]

where \( E_{i\sigma} = \varepsilon - \varepsilon_{i\sigma} + 1/2(\tilde{\Gamma}_{i\sigma}^{L} + \tilde{\Gamma}_{i\sigma}^{R}) \), and, the summation is over all possible configurations in which the level \( j \) (\( j \neq i \)) is empty, \( \rho_{0} = 1 + n_{j,\sigma}n_{j,-\sigma} > (N_{j,\sigma} + N_{j,-\sigma}) \), singly, \( \rho_{1} = N_{j,\sigma} + N_{j,-\sigma} \), or doubly, \( \rho_{2} = n_{j,\sigma}n_{j,-\sigma} > (N_{j,\sigma} + N_{j,-\sigma}) \), occupied. \( \rho_{k} \) denotes the probability factor of a configuration expressed by one-particle \( N_{i\sigma} = n_{i,\sigma}d_{i,\sigma} > \rho \) and two-particle \( n_{i,\sigma}n_{i,-\sigma} > \rho \) occupation numbers. \( \Pi_{k} \) denotes the sum of Coulomb repulsions seen by an electron in level \( i \) due to other electrons in configuration \( k \), in which the level \( j(j \neq i) \) is empty \( \Pi_{0} = 0 \), singly, \( \Pi_{1} = U_{12} \), or doubly, \( \Pi_{2} = U_{12} \).

In the linear response theory for the electronic current and heat flux (equation [39]), the electrical conductance is equal to \( G_{e} = \frac{e^{2}}{h} L_{11} \), thermopower is \( S = \frac{1}{e^{2}} L_{12} \), and the thermal conductance is given by \( \kappa_{e} = \frac{1}{e^{2}} (L_{22} - \frac{e^{2}}{h} L_{11}) \). The linear response coefficients are given by [46]

\[ L_{11} = \frac{T_{e}}{h} \sum_{j\sigma} \int d\varepsilon \left( \frac{\Gamma_{j,\sigma}^{L}}{\Gamma_{j,\sigma}^{L} + \Gamma_{j,\sigma}^{R}} \right) ImG_{j\sigma}^{r}(\varepsilon)(-\frac{\partial f(\varepsilon)}{\partial \varepsilon}) T_{e} \]  

(7a)

\[ L_{12} = \frac{T_{e}^{2}}{h} \sum_{j\sigma} \int d\varepsilon \left( \frac{\Gamma_{j,\sigma}^{L}}{\Gamma_{j,\sigma}^{L} + \Gamma_{j,\sigma}^{R}} \right) ImG_{j\sigma}^{r}(\varepsilon)(\frac{\partial f(\varepsilon)}{\partial T_{e}}) \]  

(7b)

\[ L_{22} = \frac{T_{e}^{2}}{h} \sum_{j\sigma} \int d\varepsilon \left( \frac{\Gamma_{j,\sigma}^{L}}{\Gamma_{j,\sigma}^{L} + \Gamma_{j,\sigma}^{R}} \right) ImG_{j\sigma}^{r}(\varepsilon)(\frac{\partial f(\varepsilon)}{\partial T_{e}}) \]  

(7c)

For simulation purposes, we use half band width, \( D \), as energy unit and set \( \omega = D/50 \), and \( U_{ii} = 2U_{12} = D/10 \). We also take the renormalized tunneling
rate, $\tilde{\Gamma}^{i}_{\alpha\sigma}$, as an input parameter and ignore the narrowing the width of the tunneling rate due to the EPI and assume the wave functions of the molecular levels are identical, i.e. $\Gamma^{1}_{\alpha\sigma} = \Gamma^{2}_{\alpha\sigma}$. It has been shown that the EPI does not narrow the width of tunneling rate in some cases [47, 48].

$\Gamma^{i}_{\alpha\sigma} = 0$, $2\omega$, and $\Delta = 2\omega$ is the level spacing.

3 Results and discussions

Figure 1a describes the electrical conductance, $G_e$, as a function of temperature in the absence and presence of the electron-phonon interaction. Results show that $G_e$ is uniformly increased by increase of temperature. However, behavior of it is strongly dependent on the electron and phonon temperatures and EPI. One can divide figure 1a to three parts. In part 1, low temperatures, $kT_e < 0.2\omega$, the electrical conductance resulting from the EP nonequilibrium is more. Figure 1b

![Figure 1: (a) Electrical conductance as a function of electron temperature for $\lambda = 0$ (solid line), $\lambda = 1, T_p = T_e$ (dashed line), and $T_p = 5T_e$ (dash-dotted line). (b)-(d) show DOS in the parts1-3, respectively. $-\frac{\partial f(\epsilon)}{\partial \epsilon}$ is plotted in gray. $\Gamma_{\alpha\sigma} = 0.2\omega$, and $\Delta = 2\omega$ is the level spacing.](image-url)
can help us understand the reason. In low temperatures the DOS of the molecule exhibits a vibrational absorption sideband (dash-dotted line) located near the chemical potential of the leads. Such peak is not observed in the elastic transport (solid line) or in the presence of the thermal equilibrium between electrons and phonons (dashed line). Note that there are no phonons in the molecule when phonons and electrons are in the thermal equilibrium because of \( kT_p << \omega \). In region 2, mediated temperatures, \( 0.2 < kT_e < \omega \), the electrical conductance of the elastic transport is more. However, EP nonequilibrium can enhance \( G_e \) in comparison with the EP equilibrium. It is worth noting that \( G_e \) resulted from the EPI is independent of the temperature difference between electrons and phonons for \( kT_e = \omega \). In region 3, high temperatures, \( kT_e > \omega \), \( G_e \) approaches saturated values. The DOS of the molecule and \( -f'(\varepsilon) \) are plotted in figures 1a-d for parts 1-3, respectively. \( f'(\varepsilon) \) is a Lorentzian function whose center is located in \( \mu \) and its width depends on the electron temperature. Therefore, \( f'(\varepsilon) \) becomes wider with increase of the temperature so that more part of the DOS involves in the electron transport.

Figure 2: Thermal conductance as a function of gate voltage. Inset shows the DOS when \( V_g = -1/2(\Delta + \tilde{U}_1 + 2\tilde{U}_{12}) \). \( T_e = 0.3\omega \).
The electrical conductance, $\kappa_e$, is plotted in figure 2 as a function of the gate voltage. In $\lambda = 0$, the electrical conductance has seven peaks. Four peaks are located in resonance energies i.e. $V_g = \varepsilon_1^0$, $V_g = -(\Delta + \tilde{U}_{12})$, $V_g = -\varepsilon_2^0$, and $V_g = -\varepsilon_0^1$, $V_g = -(\Delta + \tilde{U}_{12} + 2\tilde{U}_{12})$, in which the electrical conductance is maximum because electrons can easily tunnel to the molecule. Other peaks are located in electron-hole symmetry points, i.e. $V_g = -1/2(\Delta + \tilde{U}_{12})$, $V_g = -1/2(\Delta + \tilde{U}_1 + 2\tilde{U}_{12})$, and $V_g = -1/2(\Delta + \tilde{U}_1 + \tilde{U}_2 + 3\tilde{U}_{12})$. In these points, thermopower is zero. In the electron-hole symmetry points, electrons and holes participate in the charge and energy transport with the same weight. Although they carry the charge in the opposite directions, they carry the energy in the same direction resulting in the appearance of the peak in the thermal conductance spectrum. In addition, it is observed that the height of the peaks is strongly dependent on the electron population of the molecule, so that the peaks are lower in the voltages $V_g = \varepsilon_1^0$, and $V_g = -(\Delta + \tilde{U}_2 + 2\tilde{U}_{12})$ which the molecule is, respectively, approximately empty or fully occupied. The peaks are higher when the molecule is partially occupied. The dependence of the DOS on the one- and two-electron populations gives rise to such behavior. In the presence of the EPI, the height of the peaks is significantly reduced. Furthermore, peaks located in the electron-hole symmetry points are not well observed. Inset shows the DOS in $V_g = -1/2(\Delta + \tilde{U}_{12})$. It is clearly observed the DOS is completely symmetric around the chemical potential of the leads in the elastic transport, while the EPI disturbs the symmetry leading to the disappearing the peaks of the thermal conductance in the electron-hole symmetry points. However, interaction of the EP nonequilibrium can slightly increase $\kappa_e$ due to the existence of the phonon absorption side peaks.

Figure 3 describes the behavior of the thermopower and figure of merit as a function of temperature in the absence and presence of the EPI. It is observed the thermopower is increasingly enhanced in the low temperatures, whereas it is reduced in the high temperatures. Because thermopower has the main contribution in the figure of merit, $ZT$ follows the same behavior. Furthermore, results show that the thermopower is independent of the EPI if $kT_e = \omega$. In low temperatures, holes participate in the generation of the current because $\varepsilon_1$ is below the resonance and electrons from the colder lead (right lead) can tunnel to the warmer one (left lead). Note that $S$ in the unit of $k/e$ is negative because of negative electron charge. With increase of temperature resulting in the excitation of the electrons toward above the chemical potential, electrons from the warmer lead can tunnel to the colder one using the level $\varepsilon_2$. It is so interesting that the sign of the thermopower changes faster in the presence of the EPI. It comes from the fact that the electrons and holes can more easily tunnel from one lead to the other by the phonon absorption processes. In addition, the magnitude of $ZT$ is significantly reduced in the presence of the EPI. However, EP nonequilibrium can enhance $ZT$ when $0.6\omega < kT_e < \omega$ because of the increase of the thermopower (figure 3a). $ZT$ approaches the lower values in the high temperatures due to the inter-level and intra-level Coulomb repulsions (proximity effect). Such behavior was analyzed for a triple quantum dot system.
Figure 3: (a) Thermopower and (b) figure of merit as a function of electron temperature. Parameters are the same as fig.1.

by Kuo and co-workers [17].

The dependence of the figure of merit on the phonon temperature and EP coupling strength is analyzed in figure 4. In \( \lambda = 0 \), \( ZT \) is independent of the phonon temperature so that its magnitude is constant and maximum. With increase of \( \lambda \) the magnitude of \( ZT \) is significantly reduced by increase of \( T_p \). However, in weak \( \lambda \), \( \lambda < 0.4\omega \), \( ZT \) is nearly constant but in the strong \( \lambda \), \( ZT \) is suppressed because of the reduction of the thermopower and increase of the thermal conductance.

The Lorentz ration, \( L/L_0 \), where \( L_0 = \pi^2 k^2/3e^2 \) is plotted in figure 5 as a function of the molecule energy levels and in figure 6 as a function of temperature. The Coulomb interactions give rise to the violation of the Wiedemann-Franz law. It is observed that the Lorentz ratio oscillates as a function of the energy level. When the molecule is completely full or empty, the Lorentz ratio is one for elastic transport because the transport in this regime is dominant by higher order tunneling, while it is bigger than unity for the EP nonequilibrium due to the phonon assisted tunneling. The Lorentz ratio is significantly
increased in the Coulomb blockade regime. On the other hand, the dependence of the DOS on the one- and two-electron populations leads to the asymmetry of the Lorentz ratio. The EP nonequilibrium increases the Lorentz ratio near the chemical potential of the leads. The behavior of the Lorentz ratio as a function of temperature is different in the absence and presence of the EPI. In the presence of the EP nonequilibrium, the Lorentz ratio is lesser than one because the electrical conductance is increased due to the phonon absorption-assisted tunneling, while the Lorentz ratio is increased in the elastic transport. The reason of the difference was investigated in figure 1. In high temperatures, the Lorentz ratio decreases significantly because the electrical conductance is increased. Such behavior was previously reported for the single-level quantum dots [15].

4 Summary

We analyze the thermoelectric properties of a two-level molecule by means of equation of motion technique within the Green function formalism. The influence of the Coulomb interactions, electron-phonon coupling, and temperature on the figure of merit is examined. The electron temperature of the bulky electrodes can be different from the phonon temperature because of the smaller heat capacity of the phonons so that the electron-phonon nonequilibrium thermody-
Figure 5: Lorentz ratio as a function of gate voltage. Parameters are the same as fig. 2.

namics may govern the system. The temperature difference results in the novel and interesting phenomena. It is observed that the electron-phonon interaction results in the reduction of the number of peaks in the thermal conductance due to the disturbance of the symmetry of the DOS near the chemical potential of the leads. Furthermore, the Coulomb repulsions and electron-phonon interaction result in the violation of the Wiedemann-Franz law.

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Figure 6: Dependence of Lorentz ratio on the electron temperature.

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