Luttinger liquid and polaronic effects in electron transport through a molecular transistor

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Electron transport through a single-level quantum weakly dot coupled to Luttinger liquid leads is considered in the master equation approach. It is shown that for a weak or moderately strong interaction the differential conductance demonstrates resonant-like behavior as a function of bias and gate voltages. The inelastic channels associated with vibron-assisted electron tunnelling can even dominate electron transport for a certain region of interaction strength. In the limit of strong interaction resonant behavior disappears and the differential conductance scales as a power low on temperature (linear regime) or on bias voltage (nonlinear regime).

1. Introduction

Last years electron transport in molecular transistors became a hot topic of experimental and theoretical investigations in nanoelectronics (see e.g. [1,2]). From experimental point of view it is a real challenge to place a single molecule in a gap between electric leads and to repeatedly measure electric current as a function of bias and gate voltages. Being in a gap the molecule may form chemical bonds with one of metallic electrodes and then a considerable charge transfer from the electrode to the molecule takes place. In this case one can consider the trapped molecule as a part of metallic electrode and the corresponding device does not function as a single electron transistor (SET). Much more interesting situation is the case when the trapped molecule is more or less isolated from the leads and preserves its electronic structure. In a stable state at zero gate voltage the molecule is electrically neutral and the chemical potential of the leads lies inside the gap between HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) states. This structure demonstrates Coulomb blockade phenomenon [3,4] and Coulomb blockade oscillations of conductance as a function of gate voltage (see review papers in [5] and references therein). In other words a molecule trapped in a potential well between the leads behaves as a

quantum dot and the corresponding device exhibits the properties of SET. The new features in a charge transport through molecular transistors as compared to the well-studied semiconducting SET appear due to «movable» character of the molecule trapped in potential well (the middle electrode of the molecular transistor). Two qualitatively new effects were predicted for molecular transistors: (i) vibron-assisted electron tunnelling (see e.g. [6,7]) and, (ii) electron shuttling [8] (see also Rev. 9).

Vibron (phonon)-assisted electron tunnelling is induced by the interaction of charge density on the with dot local phonon modes (vibrons) which describe low-energy excitations of the molecule in a potential well. This interaction leads to satellite peaks (side bands) and unusual temperature dependence of peak conductance in resonant electron tunnelling [10]. For strong electron–vibron interaction the exponential narrowing of level width and as a result strong suppression of electron transport (polaronic blockade) was predicted [10,11]. The effect of electron shuttling appears at finite bias voltages when additionally to electron–vibron interaction one takes into account coordinate dependence of electron tunnelling amplitude [8,9].

Recent years carbon nanotubes are considered as the most promising candidates for basic element of future

nanoelectronics. Both C_{60}-based and carbon nano-tube-based molecular transistors were already realized in experiment [12,13]. The low-energy features of $I–V$ characteristics measured in experiment with C_{60}-based molecular transistor [12] can be theoretically explained by the effects of vibron-assisted tunnelling [7].

It is well known that in single-wall carbon nanotubes (SWNT) electron–electron interaction is strong and the electron transport in SWNT quantum wires is described by Luttinger liquid theory. Resonant electron tunnelling through a quantum dot weakly coupled to Luttinger liquid leads for the first time was studied in Ref. 14 were a new temperature scaling of maximum conductance was predicted: $G(T) \propto T^{1/g-2}$ with interaction dependent exponent (g is the Luttinger liquid correlation parameter).

In this paper we generalize the results of Refs. 10 and 14 to the case when a quantum dot with vibrational degrees of freedom is coupled to Luttinger liquid quantum wires. The experimental realization of our model system could be, for instance, C_{60}-based molecular transistors with SWNT quantum wires.

In our model electron–electron and electron–phonon interactions can be of arbitrary strength while electron tunnelling amplitudes are assumed to be small (that is the vibrating quantum dot is weakly coupled to quantum wires). We will use master equation approach to evaluate the average current and noise power. For noninteracting electrons this approximation is valid for temperatures $T >> \Gamma_0$, where Γ_0 is the bare level width. For interacting electrons the validity of this approach (perturbation theory on Γ_0) for high-T regime of electron transport was proved for $g < 1/2$ (strong interaction) [15] and when $1 - g << 1$ (weak interaction) [16].

We found that at low temperatures: $\Gamma_0 << T << \hbar\omega_0$ ($\hbar\omega_0$ is the characteristic energy of vibrons) the peak conductance scales with temperature accordingly to Furusaki prediction [14]: $G(T) \propto (\Gamma_\lambda / T)(T / \Lambda)^{1/g-1}$ ($\Lambda \simeq \varepsilon_F$ is the Luttinger liquid cutoff energy). The influence of electron–phonon interaction in low-T region results in renormalization of bare level width: $\Gamma_\lambda = \Gamma_0 \exp(-\lambda^2)$, where λ is the dimensionless constant of electron–phonon interaction. In the intermediate temperature region: $\hbar\omega_0 \le T \le \lambda^2 \hbar\omega_0$, ($\lambda >> 1$), Furusaki scaling is changed to $G(T) \propto (T)^{1/g-3/2}$ and at high temperatures when all inelastic channels for electron tunnelling are open we again recovered Furusaki scaling with nonrenormalized level width (Γ_0).

For nonlinear regime of electron tunnelling we showed that zero-bias peak in differential conductance, presenting elastic tunnelling, is suppressed by Coulomb correlations in the leads. This is manifestation of the Kane–Fisher effect [14,15]. When interaction is moderately strong ($1/2 \le g < 1$) the dependence of differential conductance on bias voltage is non-monotonous due to

the presence of satellite peaks. For $g > 1/2$ the zero-bias peak can be even more suppressed than the satellite peaks, which dominate in this case. This is the manifestation of the interplay between the Luttinger liquid effects in the leads and the electron–phonon coupling in the dot. For strong interaction $g < 1/2$ satellites are also suppressed and the differential conductance at low temperatures ($T << \hbar\omega_0$) scales as $dI/dV \propto V^{1/g-2}$. This scaling coincides with the Furusaki prediction, where temperature is replaced by the driving voltage (eV) which becomes the relevant energy scale for $eV >> T, \hbar\omega_0, \Gamma$. It means that the influence of vibrons on the resonant electron tunnelling through a vibrating quantum dot can be observed only for weak or medium strong interaction ($1/2 < g < 1$) in the leads.

2. The Model

The Hamiltonian of our system (vibrating quantum dot weakly coupled to Luttinger liquid leads, see Fig. 1) consists of three parts

$$\mathcal{H} = \mathcal{H}_{LL} + \mathcal{H}_{QD} + \mathcal{H}_T. \qquad (1)$$

Here $\mathcal{H}_{LL} = \sum_{j=L,R} \mathcal{H}_l^{(j)}$ describes quantum wires adiabatically connected to electron reservoirs. Quantum wires (left-L and right-R) are supposed equal and modelled by Luttinger liquid Hamiltonians with equal Luttinger liquid parameters $1/g_{L(R)}$: $1/g_L = 1/g_R = 1/g$ (see e.g. [14])

$$\mathcal{H}_l^{L(R)} = \mathcal{H}_l = \hbar v_c \int_0^\infty a_k^+ a_k k \, dk. \qquad (2)$$

Here $a_k^+ (a_k)$ are the creation (annihilation) operators of bosons which describe the charge density fluctuations propagating in the leads with velocity $v_c \sim v_F$. These operators satisfy canonical bosonic commutation relations $[a_k, a_{k'}^+] = \delta(k - k')$. In what follows we consider for simplicity the case of spinless electrons.

The Hamiltonian of vibrating single level quantum dot takes the form (see e.g. [10])

$$\mathcal{H}_{QD} = \varepsilon_0 f^+ f + \varepsilon_i (b^+ + b) f^+ f + \hbar\omega_0 b^+ b, \qquad (3)$$

where ε_0 is the energy of electron level on the dot, $\hbar\omega_0$ is the energy of vibrons, ε_i is the electron–vibron interaction energy, $f^+ (f)$ and $b^+ (b)$ are fermionic (f) and bosonic (b) creation (annihilation) operators with canonical commutation relations $\{f, f^+\} = 1$, $[b, b^+] = 1$.

The tunnelling Hamiltonian is given by standard expression

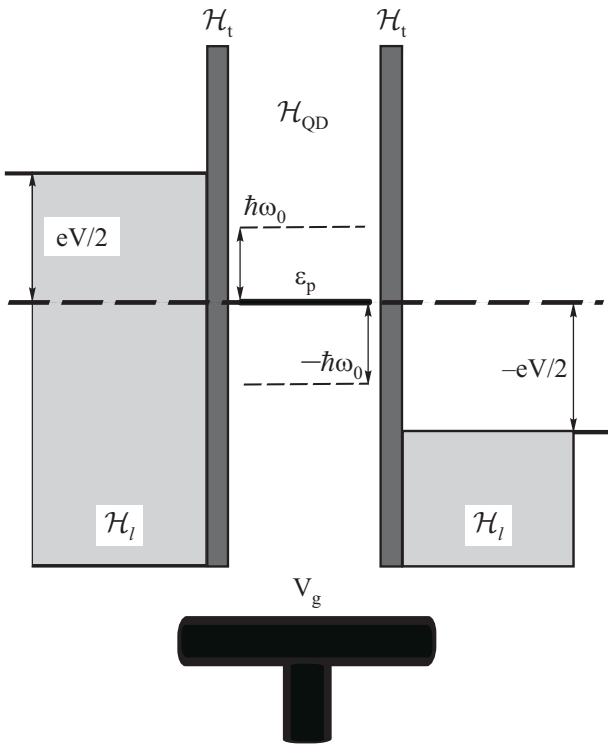$$\mathcal{H}_T = \sum_{j=L,R} \{t_j f^+ \Psi(j) + \text{h.c.}\}, \qquad (4)$$

Fig. 1. The schematic picture of the two-terminal electron transport through a vibrating quantum weakly dot coupled (via narrow dielectric regions H_t) to the Luttinger liquid leads ($\mathcal{H}_l^{L(R)} = \mathcal{H}_l$) with the chemical potentials $\varepsilon_F \pm eV/2$ (V is the driving voltage). All the energies are counted from the Fermi energy, which chosen to be zero. Electrons tunnel from one lead to another by hopping on and off the level dot with the energy ε_P (elastic channel) and due to electron–vibron coupling they can emit or absorb vibrons (vibron–assisted tunnelling). Inelastic channels are represented as side-levels with energies $\varepsilon_{P\pm} = \varepsilon_P \pm \hbar\omega_0$. The position of the levels dot with respect to the Fermi energy can be uniformly shifted by applying voltage V_g to the «gate» electrode.

where t_j is the electron tunnelling amplitude and $\Psi(j)$, $j = L, R$ is the annihilation operator of electron at the end point of $L(R)$-electrode. This operator could be written in a «bosonised» form (according to [14])

$$\Psi(L(R)) = \sqrt{\frac{2}{\pi\alpha}} \exp\left[\int_0^\infty dk \frac{e^{-\alpha k/2}}{\sqrt{2K_\rho k}}(a_k - a_k^+)\right], \quad (5)$$

here α is a short-distance cutoff of the order of the reciprocal of the Fermi wave number k_F and $K_\rho = (2/g-1)^{-1}$ is the interaction parameter in the «fermionic» form of the Luttinger liquid Hamiltonian (2), it defines the Luttinger liquid parameter g which is varied between 0 and 1: the case $g = 1$ describes the «noninteracting» (Fermi-liquid) leads, than in the case $g \to 0$ the interaction in the leads goes to infinity.

Hamiltonian (3) is «diagonalized» to $\mathcal{H}_d = \varepsilon_P f^+ f + \hbar\omega_0 b^+ b$ by the unitary transformation (see e.g. [17]) $U = \exp(i\lambda p n_f)$, where $p = i(b^+ - b)/\sqrt{2}$, $n_f = f^+ f$ and the dimensionless parameter $\lambda = -\sqrt{2}\varepsilon_i/\hbar\omega_0$ characterizes electron–vibron coupling. The unitary transformation results in: (i) the shift of fermionic level (polaronic shift) $\varepsilon_P = \varepsilon_0 - \varepsilon_i^2/\hbar\omega_0$ and (ii) the replacement of tunnelling amplitude in (3) $t_j \to t_j \exp(-i\lambda \cdot p)$. The model Eqs. (1)–(5) can not be solved exactly and one needs to exploit certain approximations to go further.

We will use «master equation» approximation (see e.g. [5]) to evaluate the average current and noise power in our model. It is in this approximation that average current separately for the model with interacting leads [14] and for vibrating quantum dot with noninteracting leads [18] was calculated earlier. Master (rate) equation approach exploits such quantities as the probability for electron to occupy level dot and the transition rates. It neglects quantum interference in electron tunnelling and therefore describes only the regime of sequential electron tunnelling which is valid when the width of electron level $\Gamma_0 \ll \min(T, eV)$. In other words, in our case «master equation» approach is equivalent to the lowest order of perturbation theory in Γ_0.

For interacting electrons the validity of master equation approach for high-T regime of resonant electron tunnelling can be justified for strong repulsive interaction $g < 1/2$ [14]. It is correct also for weak interaction $1-g \ll 1$ as one can check by comparing the results of Refs. 14 and 16, where resonant tunnelling through a double-barrier Luttinger liquid was considered for weak electron–electron interaction. Notice, that the results [18] of exact solution known for $g = 1/2$, where a mapping to free-fermion theory can be used [5], do not agree with the high-T scaling of $G(T)$ [14] extrapolated to this special point $g = 1/2$. The free-fermion scaling $G(T) \propto T^{-1}$ found for $g = 1/2$ (master equation approach predicts T-independent value [14]) could be a special feature of this exactly solvable case. We will assume that beyond the close vicinity to $g = 1/2$ the master equation approach for high-T behavior of conductance is a reasonable approximation.

3. Transition rates and the average current

In master equation approach the average current through a single level quantum expressed dot in terms of transition rates takes the form

$$I = e\frac{\Gamma_{01}^R \Gamma_{10}^L - \Gamma_{01}^L \Gamma_{10}^R}{\Gamma_\Sigma}, \quad (6)$$

where $\Gamma_{01}^{R(L)}$ is the rate of electron tunnelling from the to dot right (left) electrode, $\Gamma_{10}^{R(L)}$ describes the reverse process and $\Gamma_\Sigma = \Gamma_{01} + \Gamma_{10}$, $\Gamma_{if} = \Gamma_{if}^L + \Gamma_{if}^R$ ($i, f = 0,1$). To

evaluate these rates in our approach we will use Fermi «Golden Rule» (quantum mechanical perturbation theory) for tunnelling Hamiltonian obtained from Eq. (4) after the unitary transformation: $\mathcal{H}_T \Rightarrow \mathcal{H}_t$

$$\mathcal{H}_t = \sum_{j=L,R} \{t_j \Psi^+(j) f \exp(-i\lambda \cdot p) + \text{h.c.}\}. \qquad (7)$$

The standard calculation procedure results in the following expressions for tunnelling rates

$$\Gamma_{10}^{(j)} = \left|\frac{t_j}{\hbar}\right|^2 \int_{-\infty}^{\infty} dt \langle V(t)V^+(0)\rangle_b \langle \Psi_j^+(t)\Psi_j(0)\rangle_f \exp(i(\varepsilon_P - \varepsilon_F + eV_j)t/\hbar), \qquad (8)$$

$$\Gamma_{01}^{(j)} = \left|\frac{t_j}{\hbar}\right|^2 \int_{-\infty}^{\infty} dt \langle V^+(t)V(0)\rangle_b \langle \Psi_j(t)\Psi_j^+(0)\rangle_f \exp(-i(\varepsilon_P - \varepsilon_F + eV_j)t/\hbar), \qquad (9)$$

where $V_L - V_R = V$ is the bias voltage and $j = L, R$. Notice that in the perturbation calculation on the bare level width $\Gamma_0 \propto |t_{L,R}|^2$, we neglect the level width in the Green function of the level dot. Besides, in this approximation averages over bosonic and fermionic operators in formulas for tunnelling rates are factorized and, thus, the averages $\langle \ldots \rangle_b$ over bosonic variables

$$V = \exp(-i\lambda \cdot p), \quad p = \frac{i}{\sqrt{2}}[b^+ - b] \qquad (10)$$

can be calculated with the quadratic Hamiltonian $\mathcal{H}_b = \hbar\omega_0 b^+ b$. In what follows we will assume that vibrons are characterized by equilibrium distribution function: $n_b(T) = [\exp(\hbar\omega_0/T) - 1]^{-1}$. Averages $\langle \ldots \rangle_f$ over fermionic operators in Eqs. (8), (9) are calculated with the Luttinger liquid Hamiltonian (2). The corresponding correlation functions in Eqs. (8), (9) are well known in the literature (see e.g. [10,14])

$$\langle V(t)V^+(0)\rangle_b = \exp(-\lambda^2(1+2n_B)) \times$$

$$\times \left\{\sum_{l=-\infty}^{\infty} I_l[2\lambda^2\sqrt{n_B(1+n_B)}]\exp[-il\omega_0(t + i\hbar/2T)]\right\}, \quad (11)$$

$$\langle \Psi_j^+(t)\Psi_j(0)\rangle_f \simeq \frac{\Lambda}{\hbar v_F}\left\{\frac{i\Lambda}{\pi T}\sinh\left[\frac{\pi T t}{\hbar}\right]\right\}^{-1/g}. \qquad (12)$$

Here $I_l(z)$ is a modified Bessel function, $\Lambda \sim \varepsilon_F$ is a ultraviolet cutoff energy, g is the Luttinger liquid correlation parameter.

By putting correlation functions (11),(12) in Eqs. (8), (9) and evaluating time integrals we get the following equations for tunnelling rates $\Gamma_+^{(j)} = \Gamma_{10}^{(j)}$ and $\Gamma_-^{(j)} = \Gamma_{01}^{(j)}$, $(j = L, R)$

$$\Gamma_\pm^{(j)} = \frac{\Gamma_j}{2\pi\hbar}\left(\frac{2\pi T}{\Lambda}\right)^{1/g-1}\frac{\exp[-\lambda^2\coth(\hbar\omega_0/2T) \pm \Delta_j/2T]}{\Gamma(1/g)} \times$$

$$\times \left\{\sum_{l=-\infty}^{\infty} I_l\left[\frac{\lambda^2}{\sinh(\hbar\omega_0/2T)}\right]\left|\Gamma\left(\frac{1}{2g} + i\frac{(\pm\Delta_j - \hbar\omega_0 l)}{2\pi T}\right)\right|^2\right\}, \qquad (13)$$

where $\Gamma_{L(R)}$ is the partial level width (see, for example, [14]) $\Gamma_j = (2\pi c_j t_j^2/\alpha\Lambda)\langle f^+ f\rangle = \text{const}$ $(j = L, R)$, $\Gamma_L + \Gamma_R = \Gamma_0$, $\Delta_j = \varepsilon_F - \varepsilon_P + eV_j$; here $\Gamma(z)$ is Gamma function.

At first we consider different limiting cases when it is possible to obtain simple analytical expressions for the average current (6). Notice, that electric current depends on the gate voltage V_g through the corresponding dependence of level energy $\varepsilon_P(V_g)$. It is convenient for the further analysis to choose the value of gate voltage at which the current at low bias is maximum as: $\varepsilon_P(V_g) = \varepsilon_F$. In what follows we also put $V_L = -V_R = V/2$.

For noninteracting leads ($g = 1$) and noninteracting quantum dot ($\lambda = 1$) it is easy to derive from Eqs. (6), (13) the well-known formula for the maximum (resonant) current at temperatures $T \gg \Gamma_{L(R)}$

$$I(V) \simeq \frac{e\Gamma}{\hbar}\tanh\left(\frac{eV}{4T}\right), \qquad (14)$$

where $\Gamma = \Gamma_L\Gamma_R/(\Gamma_L + \Gamma_R)$ is the effective level width. It is evident that at high voltages: $eV \gg T$ the current through a single level dot does not depend on the bias voltage and its value is totally determined by the effective level width Γ.

For a vibrating quantum dot ($\lambda \neq 0$) weakly coupled to noninteracting leads ($g = 1$) our approach reproduces the results of Ref. 10. In the temperature region we are interesting in ($T \gg \Gamma_{L(R)}$) the general formulae derived in [10] can be rewritten in a more clear and compact form. In particular, by using for $g = 1$ in Eq. (11) the well-known representation for Gamma function (see e.g. [19])

$$\left|\Gamma(\frac{1}{2} + iz)\right|^2 = \frac{\pi}{\cosh(\pi z)}, \qquad (15)$$

it is easy to obtain the following expression for the maximum (peak) conductance

$$G_\lambda(T) = G(T) F_\lambda\left(\frac{\hbar\omega_0}{T}\right), \qquad (16)$$

where

$$G(T) \simeq \frac{\pi}{2} G_0 \frac{\Gamma}{T}, \quad G_0 = \frac{e^2}{h} \qquad (17)$$

is the standard resonance conductance of a single-level quantum at dot $T \gg \Gamma_{L(R)}$. The dimensionless function $F_\lambda(x)$ takes the form

$$F_\lambda(x) = \exp[-\lambda^2(1 + n_B(x))] \times$$

$$\times \left\{ I_0(z(x)) + 2\sum_{l=1}^{\infty} \frac{I_l(z(x))}{\cosh^2(lx/2)} \right\}, \qquad (18)$$

h e r e $z(x) \equiv 2\lambda^2\sqrt{n_B(x)[1 + n_B(x)]}$ a n d $n_B(x) = (\exp(x) - 1)^{-1}$. At low temperature region $\Gamma \ll T \ll \hbar\omega_0$, when there are no thermally activated vibrons in the dot ($n_B \ll 1$) only the first term in the brackets contribute to the sum and: $F_\lambda(T \ll \hbar\omega_0) \simeq \exp(-\lambda^2)$. We see, that zero-point fluctuations of the position dot result in renormalization of the level width $\Gamma_\lambda = \Gamma \exp(-\lambda^2)$. For strong electron–vibron coupling this phenomenon (polaronic narrowing of level width) leads to polaronic (Franck–Condon) blockade of electron transport through vibrating quantum dot [11]. The temperature behavior of peak conductance (16) was considered in Ref. 20.

Now we will study the general case when interacting quantum dot ($\lambda \neq 0$) is connected to interacting leads ($g < 1$). Analytical expressions for conductance in this case can be obtained in the limits of low ($\Gamma_{L(R)} \ll T \ll \hbar\omega_0$) and high ($T \gg \hbar\omega_0$) temperatures.

At low temperatures the main contribution to the sum over «l» in Eq. (13) comes from elastic transition $l = 0$. All inelastic channels ($l \neq 0$) are exponentially suppressed for $eV, T \ll \hbar\omega_0$. At $T \ll g\hbar\omega_0$ the peak conductance takes the form

$$G(T) \simeq \frac{\sqrt{\pi}}{2} G_0 \frac{\Gamma_\lambda}{T} \left[\frac{\Gamma(1/2g)}{\Gamma(1/2g + 1/2)} \right] \left(\frac{\pi T}{\Lambda}\right)^{1/g-1}. \qquad (19)$$

We see that at low temperatures conductance scales with temperature according to Furusaki's prediction [14]: $G(T) \sim T^{1/g-2}$. The influence of electron–vibron coupling results in multiplicative renormalization of bare level width $\Gamma_\lambda = \Gamma \exp(-\lambda^2)$.

At high temperatures: $T \gg \hbar\omega_0$ one can use the well known asymptotic expansion for Bessel function $I_l(z) \simeq \exp(z)/\sqrt{2\pi z}$, which can be used in summation Eqs. (18), (13) until $l^2 \leq z$. Besides, in this temperature region the summation in Eq. (13), can be replaced by integration and the corresponding integral can be taken exactly

$$\int_{-\infty}^{\infty} |\Gamma(a + iz)|^2 \, dz = \pi 2^{1-2a} \Gamma(2a). \qquad (20)$$

This allows us to derive the following expression for the temperature dependence of peak conductance in the intermediate temperature region $\hbar\omega_0 \ll T \leq \lambda^2\hbar\omega_0, (\lambda \geq 1)$

$$G(T) \simeq \frac{\pi}{2} G_0 \left[\frac{\Gamma \exp(-\lambda^2\hbar\omega_0/4T)}{\lambda\sqrt{\hbar\omega_0 T}} \right] \left(\frac{\pi T}{\Lambda}\right)^{1/g-1}. \qquad (21)$$

Notice that in the considered temperature region the polaronic blockade is already partially lifted $\Gamma_\lambda(T) = \Gamma \exp(-\lambda^2\hbar\omega_0/4T) \sim \Gamma$ at $T \sim \lambda^2\hbar\omega_0$ and conductance scales with temperature as $G(T) \sim T^{1/g-3/2}$. At last, at temperatures $T \gg \lambda^2\hbar\omega_0$ when all inelastic channels for electron transport are open, the polaronic blockade is totally lifted [20] and we reproduce again Furusaki scaling. It is clear from our asymptotic formulae (19),(21) that both in low- and in high- temperature regions the contributions of electron–electron and electron–vibron interactions to the conductance are factorized. In general case these contributions are not factorized, as one can see from Eqs. (8), (9) and from Eq. (13) for tunnelling rates, and we can expect interplay of Kane–Fisher effect and the effect of phonon(vibron)-assisted tunnelling.

To see this interplay we consider nonlinear (differential) conductance $G(V) = dI/dV$. It is well known that Kane–Fisher effect is pronounced for the energies close to the Fermi energy. For differential conductance it means that the zero-bias (elastic) resonance peak is suppressed with the increase of electron–electron interaction, while satellite peaks are less affected by the interaction. When electron–electron interaction is weak or moderately strong ($1/2 \leq g < 1$) the dependence of differential conductance on the bias voltage (for $\lambda \simeq 1$) is not a monotonous function due to the presence of satellite peaks (see Fig. 2,a,b). The resonant behavior disappears for strong interaction $g < 1/2$ (Fig. 2,b), when at low temperatures $T \ll \hbar\omega_0$ differential conductance scales with bias voltage as $G(V) \propto V^{1/g-2}$ in accordance with the Luttinger liquid prediction for nonlinear electron transport through a single-level quantum dot. For instance, if we put $1/g = n, (n = 2,3,\dots)$ and tune the level energy to the resonance point $\varepsilon_0 = \lambda^2\hbar\omega_0$ — («resonant» location of the level in the presence of «polaronic» shift), we obtain for the differential conductance $G(V)$ the following expression for $eV/\hbar\omega_0 \gg (1/g-2)$

$$G(V) \simeq 4\pi G_0 \frac{\Gamma_\lambda}{\Lambda} \left[\frac{1}{(n-1)!} \right] \left(\frac{eV}{2\Lambda}\right)^{n-2}, \qquad (22)$$
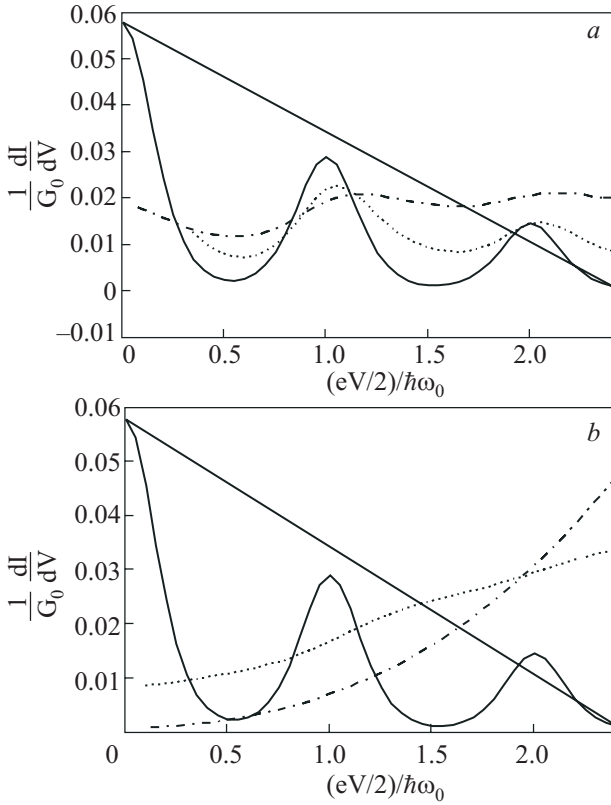
Fig. 2. Differential conductance (in the units of G_0) as a function of driving voltage (in the units of $\hbar\omega_0$). Here we put $\Gamma/kT = 0.01$; $\hbar\omega_0/kT = 10$; $\lambda^2 = 1$; and tune the level energy to the resonant position $\varepsilon_0 = \lambda^2 \hbar\omega_0$ ($\varepsilon_P = 0$). Solid lines correspond to the case of noninteracting leads $g = 1$ (*a*) and (*b*); dot line ($g = 0.8$), dash-line dot ($g = 0.6$) (*a*), dot line ($g = 0.45$), dash-dot ($g = 0.25$) (*b*). Zero-bias (elastic) resonance peak is gradually suppressed with the increase of electron–electron correlations (decrease of Luttinger liquid parameter g) while the satellite peaks survive until $g > 1/2$ (*a*). For $g < 1/2$ the resonance-like behavior of differential conductance disappears and conductance scales as a power-law of the bias voltage (*b*).

where $\Gamma_\lambda = \Gamma \exp(-\lambda^2)$. One can readily see that expression (22) reproduces Furusaki temperature scaling Eq. (19) when eV is replaced by T.

Analogous interplay of Kane–Fisher and polaronic effects one can see in Fig. 3,*a,b*, where differential conductance is plotted as a function of level energy ε_0 (or, equivalently, as a function of gate voltage). For noninteracting leads ($g = 1$) the resonance conductance peaks correspond to the level positions at $\varepsilon_{P\pm} = \varepsilon_F \pm eV/2$ (in our plot we put: $eV = 5\hbar\omega_0$). This elastic resonance peak is suppressed by electron–electron interaction in the leads ($g < 1$). The dependence $G(V_g)$ for weak and moderately strong interaction still reveals resonance structure with 4 satellites in our case, Fig. 3,*a*. The inelastic resonance peaks disappear at $g < 1/2$ and maximum of differential conductance corresponds at $g \ll 1$ to the level position at
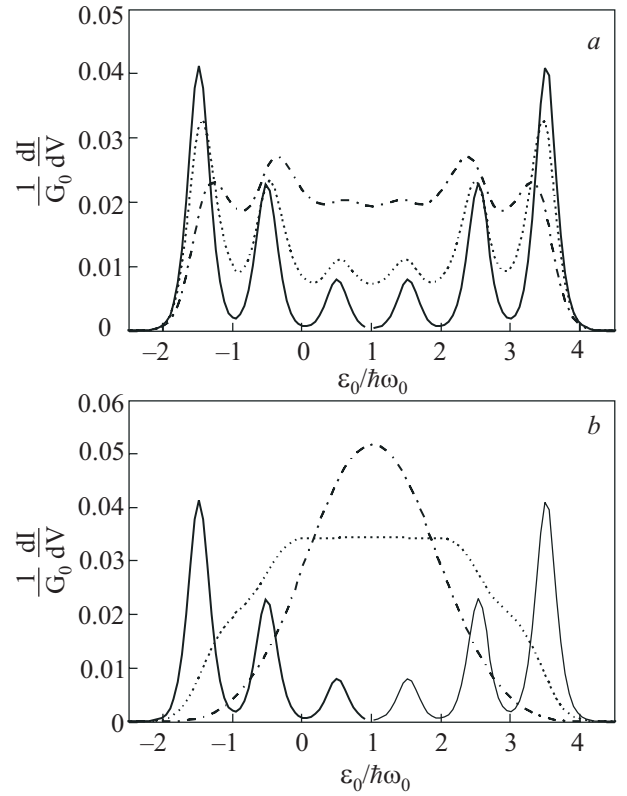

Fig. 3. Differential conductance (in the units of G_0) as a function of level energy ε_0, counted from the Fermi energy. The bias voltage $eV/\hbar\omega_0 = 5$ is sufficiently high to excite vibrons and to support electron transport through inelastic channels. All parameters are the same as for Fig. 2,*a* and *b*, correspondingly.

$\varepsilon_P(V_g) = \varepsilon_F$, that is exactly in the middle between chemical potentials of left and right electrodes (Fig. 3,*b*).

It is important to stress here once more that for moderately strong electron–electron interaction in the leads the inelastic tunnelling can dominate in electron transport. One can see from Figs. 2,3 that there is region of coupling constants when the first satellite peak is higher than the «main» (zero-bias) resonant peak, which corresponds to elastic ($l = 0$) tunnelling channel. It is the most significant prediction, we have made in this paper.

4. The noise power

The knowledge of tunnelling rates Eqs. (8), (9) allows us to evaluate not only the average current Eq. (6) but the noise power as well. We will follow the method developed in Refs. 21 and 22 where quantum noise was calculated for resonant electron transport through a quantum weakly dot coupled to noninteracting electrodes.

The noise power is defined (see e.g. [23]) as

$$S(\omega) = 2 \int_{-\infty}^{\infty} dt \, \exp(i\omega t) \langle \Delta I(t) \Delta I(0) \rangle, \qquad (23)$$

where $\Delta I(t) = I(t) - I$ (I is the average current). The noise defined in Eq. (23), in the case of sequential tunnelling through a quantum dot, can be expressed in terms of tunnelling rates. For a single level quantum this dot formula for low frequency noise $S = S(\omega = 0)$ takes the form

$$S = 2eI - \frac{4I^2}{\Gamma_\Sigma} + 4e^2 \frac{\Gamma_{01}^L \Gamma_{10}^R}{\Gamma_\Sigma}, \qquad (24)$$

here the average current I is determined by Eq. (6). The noise power Eq. (24) depends on temperature and bias voltage $S(T,V)$ and contains both thermal (Jonson–Nyquist) noise $S_{JN}(T) \equiv S(T, V = 0) = 4TG(T)$ (G is the conductance) and the nonequilibrium (shot) noise $S_{\rm sh}(T,V)$. Since the thermal noise is totally determined by temperature dependence of conductance, we will study in what follows only shot noise and Fano factor $F = S_{\rm sh}/2eI$. In particular, Fano factor in our case can be represented as follows

$$F = \left\{ 1 - \frac{2I}{e\Gamma_\Sigma} + \frac{2e}{I}\left(\frac{\Gamma_{01}^L \Gamma_{10}^R}{\Gamma_\Sigma} - \frac{TG}{e^2}\right)\right\}. \qquad (25)$$

For noninteracting leads ($g = 1$) and noninteracting quantum dot ($\lambda = 0$) one readily gets from Eqs. (13), (24) a simple expression for the «full» noise (S) of a single electron transistor (SET). On resonance $\varepsilon_P(V_g) = \varepsilon_F$ and at temperatures $T \gg \Gamma$ one finds

$$S = \left\{ \frac{2e^2\Gamma}{\hbar} \tanh\left(\frac{eV}{4T}\right)\left[1 - \frac{2\Gamma}{\Gamma_\Sigma}\tanh\left(\frac{eV}{4T}\right)\right] + \right.$$
$$\left. + \frac{e^2\Gamma}{\hbar}\left[\frac{\exp(-eV/4T)}{\cosh^2(eV/4T)}\right]\right\}. \qquad (26)$$

From Eq. (26) in the limit $V \to 0$ we obtain $S = S_{JN}(T)$, where $S_{JN}(T) = e^2\Gamma/\hbar = 4TG$ is the thermal noise. In the opposite case $eV \gg T$ we rederive the well-known formulae for the shot-noise and the Fano factor of a single level quantum dot [21–23]

$$S_{\rm sh} = \frac{2e^2\Gamma}{\hbar}\left(1 - \frac{2\Gamma}{\Gamma_\Sigma}\right), \quad F = 1 - \frac{2\Gamma}{\Gamma_\Sigma}. \qquad (27)$$

These formulae (26), (27) can be also re-derived from the general expression for the full noise of noninteracting electrons (see e.g., Eq. (61) in Ref. 23)

$$S(V,T) = \frac{e^2}{\hbar} \int d\varepsilon \, \{ T_t(\varepsilon)[f_L(1 - f_L) + f_R(1 - f_R)] + T_t(\varepsilon)[1 - T_t(\varepsilon)](f_L - f_R)^2 \}, \qquad (28)$$

where $T_t(\varepsilon)$ is the transmission coefficient and $f_j = \{\exp[(\varepsilon - \mu_j)/T] + 1\}^{-1}$ is the equilibrium distribution function of electrons in the leads (μ_j is the chemical potential; $j = L, R$). In the case of single level quantum dot $T_t(\varepsilon)$ takes the form Breit–Wigner tunnelling probability

$$T_t(\varepsilon) = \frac{\Gamma_L \Gamma_R}{(\varepsilon - \varepsilon_P)^2 + (\Gamma_L + \Gamma_R)^2/4}. \qquad (29)$$

For a weak tunnelling when $\Gamma_{L(R)}$ are the smallest energy scales in the problem the Lorentzian shape of the Breit–Wigner resonance shrinks to δ-function

$$T_t(\varepsilon)|_{\Gamma_{L,R} \to 0} \simeq 2\pi\Gamma\delta(\varepsilon - \varepsilon_P). \qquad (30)$$

With the help of Eqs. (28),(30) for the resonance condition $\varepsilon_P(V_g) = \varepsilon_F$ we easily re-derive Eq. (26). (Notice, that in sequential tunnelling approach the tunnelling transitions through the left and right barriers are assumed to be weak and uncorrelated. Therefore we can safely neglect T_t^2-term in Eq. (28).) It is evident from Eqs. (25), (27) that for noninteracting electrons the Fano factor is sub-Poissonian ($F \leq 1$) and F approaches 1 for strongly asymmetric junction $\Gamma_{L(R)} \gg \Gamma_{R(L)}$ and for $eV \gg T$.

The master equation approach we have used in our analysis holds when electron tunnelling amplitudes are small. For noninteracting electrons this assumption is satisfied when electron energies are far from the resonant energy level, i.e. $T_t(\varepsilon) \ll 1$. The differential shot noise in this case as a function of bias voltage or gate voltage behaves similarly to the differential conductance. Notice however that due to different dependence on temperature the shot noise unlike the thermal one even in sequential tunnelling regime ($T \gg \Gamma$) can not be expressed in terms of conductance.

By comparing Fig. 4,*a* and Fig. 3,*b*, one can see that the above similarity is preserved for interacting electrons ($g \neq 1$, $\lambda \neq 0$) as well. The corresponding Fano factor which is the «shot noise/current» ratio and thus is less sensitive to the details of tunnelling process, for strong electron–electron interaction exhibits a simple behavior (see Fig. 4,*b*). It dips ($F \simeq 1/2$) at symmetric (with respect to chemical potentials of the leads) position of the level dot. Outside this region $F \to 1$ (Poissonian noise). The width of the dip decreases with the increase of interaction, Fig. 4,*b*.
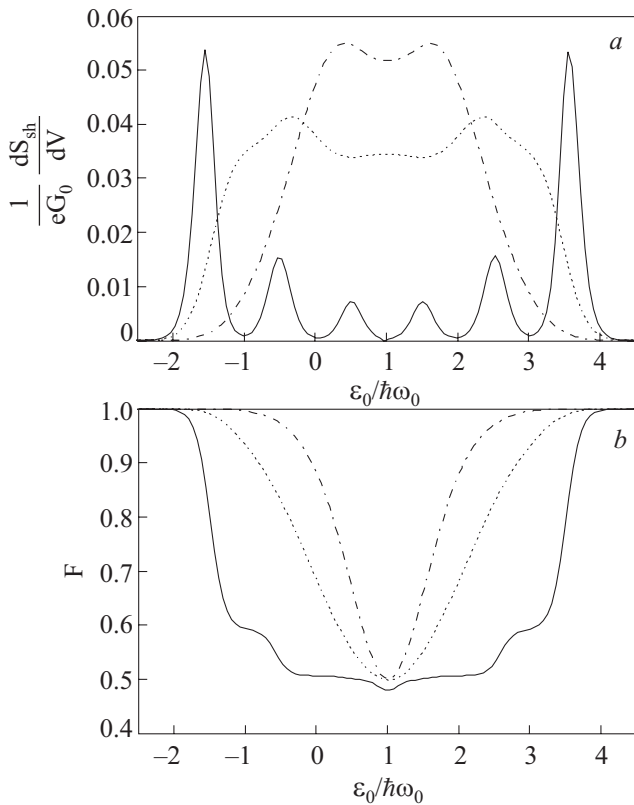
Fig. 4. Differential shot noise power (in the units of eG_0) (*a*) and Fano factor as functions of the level energy ε_0 in the non-linear transport regime $eV / \hbar\omega_0 = 5$ (*b*). Other parameters are the same as on Fig. 2,*b*.

5. Summary

We considered the influence of interaction on transport properties of molecular transistor which was modelled as a vibrating single-level quantum dot weakly coupled to the Luttinger liquid leads. We found interesting interplay between polaronic and Luttinger liquid effects in our system. In particular it was shown that for weak or moderately strong interaction ($1 / 2 < g \leq 1$) the differential conductance demonstrates resonance-like behavior and for moderately strong interaction inelastic channels can even dominate in electron transport through a vibrating quantum dot. For strong interaction ($g \ll 1$) the resonant character of vibron-assisted tunnelling disappears and the differential conductance scales as a power law on temperature (linear regime $T \gg eV$) or on bias voltage (nonlinear regime $eV \gg T$).

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