Theoretical Reproduction of the Lineshapes of Nonlinear Conductance Observed in a Quantum Point Contact

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The nonlinear conductance observed in a quantum point contact is theoretically reproduced for the entire range of applied bias. The single-impurity Anderson model with two reservoirs at different chemical potentials is studied for a sequential change of the gate voltage. The imbalance in the left and right Kondo coupling strength is introduced by the displacement of the Kondo impurity by the electric field produced in the construction of quantum point contact. We reveal the origin of the side peaks and study the behavior of the height and width of the zero-bias anomaly.

Understanding the nonlinear conductance in a system with nanocontact is indispensable in the study of nanoelectronics or nanomagnetism. The Kondo effect is often involved in studying its transport. A typical example of nanocontact is quantum point contact (QPC) or quantum wire [3,4] in which an interesting sequential change of the $dI/dV$, where $I$ and $V$ denote the current and the bias, respectively, lineshape is observed with an increase in the gate voltage $V_G$. However, theoretical understanding for the observed nonlinear conductance is insufficient and unsatisfactory. The purpose of this study is to present the theoretical $dI/dV$ lineshapes that show a similar sequential change of the $dI/dV$ with $V_G$ to the one reported in Ref. [3]. Our theoretical lineshapes remarkably fits the experimental data for the entire range of the applied bias used in the experiments. From this analysis, one may understand the physics of electron transport in a mesoscopic system in which a zero-bias anomaly (ZBA) and side peaks appear in the lineshape of the nonlinear conductance.

In order to explain the observed nonlinear conductance in a QPC, the transport mechanism in a two-reservoir system with a mediating Kondo impurity must be investigated when the system is under steady-state nonequilibrium (SSN). The issues of this study are two-fold: two-reservoir and SSN. The former duplicates all basis vectors describing the back and forth movements of the electron. For this reason, additional resonant tunneling levels, which are the origin of the side peaks, occur. The latter shifts the Fermi level of the reservoir and allows only unidirectional resonant tunneling if the system is in the ground state. This unidirectional resonant tunneling makes the state of SSN different from that of equilibrium.

We obtain the formula for $dI/dV$ by differentiating the current formula provided in Refs. [3] and [4] with respect to the bias. We fix the chemical potential of the Kondo impurity at the Fermi level of one of the metallic reservoirs. Then, the differential conductance at zero temperature is given by

$$\frac{dI}{dV} = \frac{e^2}{\hbar} \sum_{\sigma} \rho_{\sigma\sigma}(eV),$$  \hspace{1cm} (1)

where $e$, $\sigma$, and $\hbar$ denote electronic charge, spin, and the Planck constant divided by 2$\pi$, respectively. Here, $\rho_{\sigma\sigma}(eV)$ is the local density of states of the Kondo impurity at bias $V$. The factor $\Gamma^\text{tot}$ is given by the combination of featureless coupling functions, i.e., $\Gamma^\text{tot} = \Gamma^L \Gamma^R / (\Gamma^L + \Gamma^R)$, where the superscripts $L$ and $R$ stand for left and right reservoirs of a QPC, respectively. We omit the term containing $\partial \rho_{\sigma\sigma}(\omega)/\partial V$ because its contribution to $dI/dV$ is negligible. We show its negli- gence in a different study.

The spectral function of an up-spin electron, for example, at the Kondo impurity is given by $\rho_\uparrow(\omega) = (1/\pi) \text{Re}[(M_\uparrow)^{-1}_{33}]$, where

$$M_\uparrow = \begin{pmatrix}
-\omega' & \gamma_{LL} & \gamma_{LR} & \gamma_{JR} \\
\gamma_{LL} & -i\omega' & \gamma_{JL} & \gamma_{JL}
\end{pmatrix}.$$

(2)

Here, $\omega' \equiv \omega - \epsilon_j - U\langle n_{i\downarrow} \rangle$, where $\epsilon_j$, $U$, and $\langle n_{i\downarrow} \rangle$ denote the energy level of the Kondo impurity, Coulomb interaction, and the average number of down-spin electrons occupying the level $\epsilon_j$, respectively. All the matrix elements, except the eight $U$-elements, have additional self-energy terms, $\beta_{mn}[\Sigma^L_\omega + \Sigma^R_\omega] = 2\beta_{mn}\Delta$, for a flat wide band, where $\Delta \equiv (\Gamma^L + \Gamma^R)/4$ and $\Gamma^R \propto |V_0|^2$, where $V_0$ denotes the hybridization strength between the Kondo impurity and the right reservoir. The coefficient $\beta_{mn}$ is given in [8]. We use $\Delta$ to indicate the unit of energy.

The matrix elements represented by $\gamma$ are given by

$$\gamma_{LL} = \sum_k i(V_{k\uparrow}c_{k\uparrow}^+ + V_{k\downarrow}c_{k\downarrow}^+)(c_{\uparrow}\langle u^L_{i\downarrow} j^L_{i\downarrow} \rangle) \times \left\{ \left( \langle \delta j^L_{i\downarrow} \rangle^2 \right)^{1/2} \right\}^{-1/2},$$

$$\gamma_{JR} = \sum_k i(V_{k\uparrow}c_{k\uparrow}^+ + V_{k\downarrow}c_{k\downarrow}^+)(c_{\uparrow}\langle u^L_{i\downarrow} j^L_{i\downarrow} \rangle)$$

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\[ \times \left[ \frac{\langle (\delta j_{iL}^+)^2 \rangle}{\langle (\delta j_{iL}^+)^4 \rangle} \right]^{1/2}, \]

and

\[ \gamma_{LR} = \langle iU (V_{ki}^L c_{ki}^L + V_{ki}^R c_{ki}^R) c_{ki}^\dagger j_{iL}^−, j_{iL}^+ \rangle \]

\[ \times \left[ \frac{\langle (\delta j_{iL}^−)^2 \rangle}{\langle (\delta j_{iL}^−)^4 \rangle} \right]^{1/2}, \]

where the operator \( c_{ki}(i) \) denotes the fermion annihilation at the state-\( k(i) \) in the lead (impurity), \( j_{iL} = i \sum_k (V_{ki}^L c_{ki}^L c_{ki}^R - V_{ki}^L c_{ki}^L c_{ki}^R), \)

\[ j_{iL}^− = \sum_k (V_{ki}^L c_{ki}^L c_{ki}^R + V_{ki}^B c_{ki}^L c_{ki}^R), \]

and \( \delta \) means the deviation from the average. The element \( U_{L}^L \), on the other hand, is given by

\[ U_{L}^L = \frac{iU \langle n_{iL}, j_{iL}^+ \rangle}{2} (1 - \gamma^2) + \langle n_{iL} \rangle \langle j_{iL}^+ \rangle. \]

One may roughly understand the roles of matrix elements as follows: \( \gamma_{LL} / (\gamma_{RR}) \) represents the degree of Kondo coupling; \( \gamma_{LR} \) and \( \gamma_{JR} \) represent connecting mechanism; The real part of \( U \)-elements determines the position of Coulomb peak, whereas the imaginary part gives rise to the asymmetry in the \( df/dV \) lineshape. A symmetric lineshape is obtained when \( \langle n_{iL} \rangle = 1/2 \).

The spectral function \( \rho_{ii}(\omega) \) given by the reduced matrix of Eq. (2) has five peaks in general. The positions of five peaks can be obtained from the zeros of the determinant of \( \mathbf{M}_r \) in the atomic limit: a Kondo peak at \( \omega = 0 \), two Coulomb peaks at \( \omega \approx \pm U/2 \), and two additional resonant tunneling level peaks at \( \omega\prime = \pm ([\gamma_{LL}^2 + \gamma_{RR}^2]/2 + (\gamma_{LR} - \gamma_{JR})^2 + O(U^-2)]^{1/2} \) for a large \( U \). One can also find the spectral weight of each peak. It is interesting to note that the additional tunneling level can have a meaningful amount of spectral weight only when a bias is applied \( (\gamma_{JR} \neq 0) \). Therefore, we call the peak at the additional tunneling level the steady-state resonant tunneling level (SSRTL) peak.

We have discussed the effect of bias, which allows only unidirectional resonant tunneling at the ground state, above. In Fig. 1, we present the graphical illustrations of \( \gamma_{LR} \) and \( \gamma_{JR} \) on the basis of the corresponding operator expressions, which are third order processes of hybridization. Both exchange (black or red (2)) and singlet hopping (blue or red (2)) processes in equilibrium are depicted in Fig. 1. Applied bias makes the second part of Fig. 1 negligible when we calculate the expectation value. Thus, the condition \( \gamma_{LR} > \gamma_{JR} \) is obtained. Note that only singlet hopping process can establish current. Therefore, the unidirectional resonant tunneling (without black (2) on the left part of Fig. 1) dominates the Kondo process under bias. In this study, we do not calculate the values of \( \gamma \). We will use them as free parameters within the condition \( \gamma_{LR} > \gamma_{JR} \).

In order to perform the calculation for the spectral function, we must know what happens in the constriction of a QPC when \( V_G \) changes. Calculations by spin density functional theory \([10, 11]\) show that a magnetic impurity is formed spontaneously at the center or a displaced position in the QPC constriction at a low \( V_G \). When a bias is applied, an electric field will be created in the constriction and the magnetic impurity will be displaced to the direction opposite to the electric field, as shown in Fig. 2 (a). As a result, one has \( \gamma_{LL} > \gamma_{RR} \).

As \( V_G \) increases, the magnetic impurity will move back to the center of the constriction because the number of electrons in the lead increases, as shown in Fig. 2 (b) \( (\gamma_{LL} > \gamma_{RR}) \). When the magnetic impurity reaches near the center of the constriction, we assume that \( \gamma_{LL} = \gamma_{RR} \) is established, as shown in Fig. 2 (c). Upon reaching the center, the magnetic impurity stays there even at a high \( V_G \). However, both \( \gamma_{LL} \) and \( \gamma_{RR} \) increase continuously as \( V_G \) increases further.

According to the scenario discussed above, we determine the specific manner in which the matrix elements \( (U_{L}^L \) and \( \gamma \) and \( \Gamma^{tot} \) change with \( V_G \). One can see that the real part \( \text{Re}[U_{L}^L] \) is composed of the correlation in numerator and the fluctuation in denominator, i.e., \( \text{Re}[U_{L}^L] = C_{U}^L / F_{L}^U \). Since fluctuation is proportional to the number of particles \( N_c \), where \( N_c \) is the number of conduction electrons in a QPC, and \( N_c \propto V_G \) \([12]\), we obtain \( F_{L}^U \propto V_G^{-1/2} \). We propose a specific expression that shows the dependence of \( F_{L}^U \) on \( V_G \): \( F_{L}^U = p \sqrt{V_G - q} \). The constants \( p \) and \( q \) are so determined that \( F_{L}^U = 1 \) for \( V_G = 1 \) and \( F_{L}^U = 6 \) for \( V_G = 17 \), as shown in the first two columns of Table I. The values of \( V_G \) indicate the steps in which \( V_G \) is varied.

In the region where \( \gamma_{LL} > \gamma_{RR} \) (Figs. 2 (a) and 2 (b)), one must consider \( L - R \) unbalance in the strength of Kondo coupling. Only \( C_{U}^L \) that includes \( j_{iL}^+L \) would reflect the \( L - R \) unbalance. We consider linear changes in \( V_G \) for \( C_{U}^L \) up to \( V_G = 9 \). For \( V_G > 9 \), however, we choose \( C_{U}^L = 9 \) as a border separating the \( L - R \) balanced and unbalanced region. We also consider linear relationships for \( \gamma_{LL}(RR) \) and \( \Gamma^{tot} \). We set \( \gamma_{LR} = \gamma_{JR} \) for the unbalanced region, i.e., \( V_G \leq 9 \). However, in the balanced region, \( V_G > 9 \), we consider nonvanishing exchange process in the second part of Fig. 1 and allow \( \gamma_{LR} \) to increase further.

We first fix the values of matrix elements of \( M_r \) for \( V_G = 1 \) as shown in the lowermost row of Table I that afford the lineshape similar to the one obtained experi-
mentally for the lowest $V_G$. The sequential change of the $dI/dV$ lineshape with $V_G$ is obtained by using the values in Table I that are determined by the $V_G$-dependence discussed above. We list the values only for odd numbers of $V_G$ in Table I. Figure 3 (a) shows the characteristics of the sequential change of the nonlinear conductance in a QPC, such as the change of ZBA and the behavior of the side peak with an increase in $V_G$. One can observe two distinct groups of lineshapes, denoted by different colors. As $V_G$ increases, the SSRTL peaks first move inwards, and then move outwards. The behavior of SSRTL changes at $V_G = 9$, at which point the two SSRTL peaks are closest in bias. The values listed in Table I depend on top-gate voltage and sample characteristics. Different sample or top-gate voltage affords different table and the corresponding set of $dI/dV$ lineshapes.

A remarkable comparison with experiment is shown in Fig. 3 (b). We choose the experimental $dI/dV$ curve that is the one with the closest-spaced side peaks of Fig 1 (b) of Ref. [4] for comparison. Our theoretical lineshape is obtained by setting $\gamma_{LL} = \gamma_{RR} = 0.5$, $\gamma_J = \gamma_{LR} = 0.65$, $\text{Re}[U_{j_{\pm}R}^L] = 1.17$, $\text{Im}[U_{j_{\pm}R}^L] = 0.05$, and $\Gamma_{\text{tot}} = 0.62$. Since the experimental curve is slightly asymmetric and the peak is a little bit offset from $V = 0$, we introduce a small nonvanishing $\text{Im}[U_{j_{\pm}R}^L]$. We discuss about asymmetry of the lineshape more below. Perfect fitting is obtained, as shown in Fig. 3 (b).

The ZBA peaks shown in Fig. 3 (a) provide us with another interesting comparison with the experiment. In Fig. 4, we present the height and width of ZBA vs. $G_{\text{max}}$. (b) Full width at half maximum (FWHM) of ZBA vs. $G_{\text{max}}$. The dots are obtained from Fig. 3 (a) and the crosses are the data of Ref. [4] for $V_{\text{top}} = +4$ V. The units of $\Delta h_{\text{ZBA}}$ and $G$ are $2e^2/h$. Inset: Conductance vs. gate voltage.

![FIG. 2: Location of a magnetic impurity (black dot) under bias. The strength of Kondo coupling is represented by the line thickness. (a) Low $V_G$: $\gamma_{LL} > \gamma_{RR}$. Green dots denote electrons in the leads. (b) $V_G$ before balance: $\gamma_{LL} < \gamma_{RR}$. (c) $V_G$ after balance: $\gamma_{LL} = \gamma_{RR}$.]

![FIG. 3: (a) Sequential change in the $dI/dV$ lineshape when $V_G$ changes from 1 to 17. The curve in red ($V_G = 9$) is the border that corresponds to the 0.7 conductance anomaly. (b) Comparison of theoretical data (red line) with the experimental data (crosses) of the closest-spaced side peaks in Fig. 1 (b) of Ref. [4]. Weak asymmetry is given by setting $\text{Im}[U_{j_{\pm}R}^L] = 0.05$. We set $\beta_{11} = 0.252$, $\beta_{22} = \beta_{21} = 0.246$, $\beta_{22} = 0.256$, and other $\beta_{mn} = 0.25$.]

![FIG. 4: Characteristics of ZBA. (a) ZBA height ($\Delta h_{ZBA}$) vs. $G_{\text{max}}$. (b) Full width at half maximum (FWHM) of ZBA vs. $G_{\text{max}}$. The dots are obtained from Fig. 3 (a) and the crosses are the data of Ref. [4] for $V_{\text{top}} = +4$ V. The units of $\Delta h_{\text{ZBA}}$ and $G$ are $2e^2/h$. Inset: Conductance vs. gate voltage.]

| $V_G$ | $F_{U^+}^{L,R}$ | $C_{U^+}^L$ | $C_{U^+}^R$ | $\gamma_{LL}$ | $\gamma_{RR}$ | $\gamma_{LR}$ | $\Gamma$ |
|------|----------------|-------------|-------------|--------------|--------------|--------------|--------|
| 11   | 6              | 1           | 1           | 0.6          | 0.6          | 0.70         | 1      |
| 15   | 2.63           | 1           | 1           | 0.54         | 0.54         | 0.65         | 8.5/9  |
| 13   | 1.92           | 1           | 1           | 0.48         | 0.48         | 0.60         | 8.0/9  |
| 11   | 1.59           | 1           | 1           | 0.42         | 0.42         | 0.55         | 7.5/9  |
| 9    | 1.39           | 1           | 1           | 0.36         | 0.36         | 0.50         | 7.0/9  |
| 7    | 1.25           | 1.4         | 0.8         | 0.42         | 0.30         | 0.50         | 6.5/9  |
| 5    | 1.15           | 1.8         | 0.6         | 0.48         | 0.24         | 0.50         | 6.0/9  |
| 3    | 1.08           | 2.2         | 0.4         | 0.54         | 0.18         | 0.50         | 5.5/9  |
| 1    | 1              | 2.6         | 0.2         | 0.6          | 0.12         | 0.50         | 5.0/9  |
tions \(\langle \delta j^{\pm L,R}_i \rangle^2 \rangle^{1/2}\). These two effects are conflicting in determining the ZBA peak because the former causes inward movement of the SSRTL peaks with taking spectral weight from the ZBA. These conflicting roles of \(V_G\) lead to a local maximum of \(\Delta h_{ZBA}\) in the region \(V_G < 9\) in Fig. 4 (a). However, in the regime \(V_G > 9\) in which the \(L - R\) symmetry is retained, only one role of \(V_G\), enhancing the Kondo peak, remains. Interestingly, however, the unitary limit of conductance prevents the height of ZBA in the region \(V_G > 9\). Abrupt increase in the width of ZBA from \(V_G = 9\), as shown in Fig. 4 (b), is also resulted from this unitary limit. We also plot the maxima of Fig. 3 (a) vs. \(V_G\) in the inset Fig. 4 (b). A slight curve bending is shown near \(0.7\) anomaly (Inset of Fig. 4 (b)) at which the curve characteristics of ZBA height and width are apparently different (Figs. 4 (a), (b)). We also identified that the strengths of the \(L - R\) Kondo coupling are just balanced at the point of 0.7 anomaly (Table I and Fig. 1 (c)). The theoretical skill used in this study can be extended to other mesoscopic systems with a mediating Kondo impurity between two reservoirs under bias.

In conclusion, we obtained the \(dI/dV\) lineshapes observed in a QPC in terms of the Anderson model with two reservoirs. We identified the side peaks of the \(dI/dV\) as the SSRTL peaks. We showed that the sequential change of the \(dI/dV\) lineshape with \(V_G\) is separated into two parts (Figs. 3 (a)) and the border corresponds to the point of 0.7 anomaly (Inset of Fig. 4 (b)) at which the curve characteristics of ZBA height and width are apparently different (Figs. 4 (a), (b)). We also identified that the strengths of the \(L - R\) Kondo coupling are just balanced at the point of 0.7 anomaly (Table I and Fig. 1 (c)). The theoretical skill used in this study can be extended to other mesoscopic systems with a mediating Kondo impurity between two reservoirs under bias.

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