Dynamic conductivity of a quantum well under Coulomb blockade conditions

S. N. Molotkov and S. S. Nazin
Institute of Solid State Physics, Russian Academy of Sciences, 142432, Chernogolovka, Moscow Oblast

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The frequency dependence of the differential conductivity of a quantum well with a bias voltage has a structural feature at a frequency corresponding to the energy of the Coulomb repulsion of two electrons confined in the well.

There are several distinctive features in the conductance between massive electrodes connected by a "bottleneck," i.e., a quantum well or a narrow metal bridge. The most prominent effect is a quantization of the conductance, i.e., the appearance of steps on the current-voltage characteristic.[1]

Two factors lead to these steps. First, there is the ordinary quantum size effect in the levels in the bottleneck.[2] Second, there are the effects which stem from the single-electron charging of the junction (the Coulomb blockade).[3] In both of these limiting cases (intermediate cases are also possible[4]), the reason for the quantization of the current is the discrete nature of the electron spectrum, which itself is a consequence of either the single-particle quantum size effect or an electron–electron interaction. The distinctive features of the electron spectrum should evidently be manifested in the frequency dependence of the conductivity. In the present letter we use the example of a quantum well under Coulomb blockade conditions to show that the dynamic conductivity has some sharp structural features (nearly δ-functions) at frequencies corresponding to the spacing of electron levels, due to Coulomb repulsion in the bottleneck. An unusual aspect of this situation is that the levels appear because of an electron–electron interaction. The very presence of these levels (and thus the structural feature in the conductivity) depends on the static external voltage; there is a threshold value of this voltage below which these effects do not occur. The system behaves as a nonlinear filter controlled by an external voltage.

Let us derive the dynamic conductivity $\sigma(\Omega)$ of a quantum well with two barriers (Fig. 1) under Coulomb blockade conditions. Effects of a Coulomb blockade in such a structure have recently been observed.[5] We will treat the repulsion of two electrons in the well on the basis of a Hubbard Hamiltonian.[6] This approach will be sufficient to demonstrate the appearance of a structural feature in $\sigma(\Omega)$ as the result of an electron-electron interaction. This Hamiltonian is

$$\hat{H}=\sum_{\alpha=L,R}\epsilon_{k\alpha}c_{k\alpha}^{+}c_{k\alpha}+\sum_{\sigma}\epsilon_{0}c_{\sigma}^{+}c_{\sigma}+Un_{\downarrow}n_{\uparrow}+\sum_{\alpha=L,R}(T_{k\alpha}c_{k\alpha}^{+}c_{\sigma}+\text{H.a.}). \quad (1)$$

The subscript α specifies the states in the left-hand (L) and right-hand (R) electrodes; $\epsilon_{k\alpha}$ is the electron spectrum in the banks; ϵ_0 is the energy of a single-particle level in the quantum well; U is the Hubbard repulsion energy of the electrons in the well; and

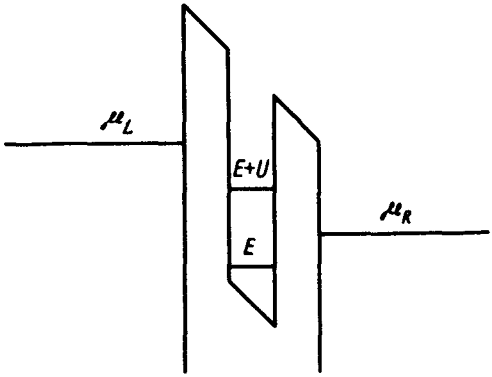

FIG. 1.

$T_{k\alpha}$ are the matrix elements for tunneling into the banks. The static voltage v_0 is dealt with in the usual way, by means of shifts of the chemical potential in the banks: $\mu_L - \mu_R = -ev_0$. If an alternating voltage $u(t)$ is applied against the background of v_0, we should add a term to Hamiltonian (1):

$$\delta\hat{H}(t) = -e\eta u(t) \sum_{\sigma} c_{\sigma}^{+} c_{\sigma} - eu(t) \sum_{k} c_{kR}^{+} c_{kR}. \tag{2}$$

The parameter η reflects the asymmetry of the well. The introduction of η essentially means that we are taking account of the circumstance that the alternating voltage perturbs the level ϵ_0 in the well [the structural feature in $\sigma(\Omega)$ stems from the second term in (2), which is independent of η].

The response of this system to a small signal $u(t)$ (the differential conductivity) against the background of the static finite voltage is calculated in the standard way. By definition, the variable tunneling current is

$$I(t) = -\frac{1}{2} ie \langle [\hat{I}_L(t) + \hat{I}_R(t)] \hat{S}(t) \rangle,$$

$$\hat{I}_{\alpha}(t) = \sum_{\substack{\alpha = L,R \\ \sigma}} (T_{k\alpha} c_{k\alpha}^{+}(t) c_{\sigma}(t) - \text{H.a.}), \tag{3}$$

$$\hat{S}(t) = \hat{T}_c \exp\left[i \int dt' \delta\hat{H}(t') \right];$$

the symbol $\hat{T}_c$ represent chronological ordering on the double time loop.[7] The angle brackets mean an expectation value over the state, with allowance for the interaction U and the tunneling $T_{k\alpha}$. An expansion of the evolution operator $\hat{S}$ up to terms linear in $u(t)$ yields

$$I(t)=\frac{1}{2}e^2\int dt'\left\langle \hat{T}_c\left\{[\hat{I}_L(t)+\hat{I}_R(t)]\left[\eta\sum_\sigma c_\sigma^+(t')c_\sigma(t')\right.\right.\right.$$

$$\left.\left.\left.+\sum_k c_{kR}^+(t')c_{kR}(t')\right]\right\}\right\rangle u(t'). \tag{4}$$

Since the causality condition must be satisfied for this response, we need to single out the retarded component of the correlation function in (4) from the Keldysh matrix. As in Ref. 8, we write the response in the form

$$I(t)=\frac{e^2}{4\pi}\int dt'\Pi^R(t-t')u(t'), \tag{5}$$

where $\Pi^R(t-t')$ is the retarded component of the polarization operator in (4), which is related to the differential conductivity by

$$\sigma(\Omega)=\frac{e^2}{4\pi}\Pi^R(\Omega). \tag{6}$$

Calculations of $\Pi^R(\Omega)$ incorporating (3) reduce to a breakup of paired expectation values of the type $< \hat{T}_c[c_{k\alpha}^+(t)c_\sigma(t)c_\sigma^+(t')c_\sigma(t')] >$. The extraction of the retarded components leads to expressions for the real and imaginary parts of $\sigma(\Omega)$:

$$\begin{aligned}\text{Re }[\sigma(\Omega)]=&-\frac{e^2}{2}\int d\omega\left\{\frac{\gamma_R(\gamma_L-\gamma_R)}{\Omega}f_R^{(-)}\text{Im}[G^R(\omega+\Omega)]\text{Im}[G^A(\omega)]\right.\\&+\eta[\gamma_Lf_L^{(+)}-\gamma_Rf_R^{(+)}]\text{Im}[G^A(\omega+\Omega)G^A(\omega)]\\&-\frac{1}{\gamma}\eta(\gamma_L-\gamma_R)[(\gamma_Lf_L(\omega+\Omega)+\gamma_Rf_R(\omega+\Omega))\text{Im}[G^A\\&\times(\omega+\Omega)]\text{Re }[G^A(\omega)]+(\gamma_Lf_L(\omega)+\gamma_Rf_R(\omega))\text{Re}[G^A\\&\left.\times(\omega+\Omega)]\text{Im}[G^A(\omega)]]+\frac{\gamma_R}{\Omega}f_R^{(-)}\text{Im}[G^R(\omega+\Omega)-G^A(\omega)]\right\},\end{aligned} \tag{7}$$

$$\begin{aligned}\text{Im}[\sigma(\Omega)]=&-\frac{e^2}{2}\int d\omega\left\{\eta\frac{\gamma_R\gamma_L}{\gamma}[f_R^{(-)}-f_L^{(-)}]\text{Re }[G^A(\omega+\Omega)G^A(\omega)]\right.\\&-\frac{\gamma_R(\gamma_L-\gamma_R)}{\Omega}f_R^{(-)}\text{Im}[G^R(\omega+\Omega)G^A(\omega)]+\frac{\gamma_R}{\Omega}f_R^{(-)}\text{Re}[G^R\\&\times(\omega+\Omega)-G^A(\omega)]-\frac{1}{\gamma}\eta(\gamma_L-\gamma_R)[(\gamma_Lf_L^{(-)}+\gamma_Rf_R^{(-)})\text{Im}[G^A\\&\left.\times(\omega+\Omega)]\text{Im}[G^A(\omega)]\right\},\end{aligned}$$

where $f_{L,R}^{(\pm)} = f_{L,R}(\omega+\Omega) \pm f_{L,R}(\omega+\Omega)$, $f_{L,R}(\omega)$ are the distribution functions in the electrodes, and the constants $\gamma_{L,R}$ describe the tunneling coupling with banks. These constants are given by

$$\gamma_{L,R}=\pi\sum_k |T_{k\alpha}|^2\delta(\omega-\epsilon_{kL,R}),\quad \gamma=\gamma_L+\gamma_R. \tag{8}$$

They can be assumed independent of the energy. Here $G(\omega)$ is the Green's function which describes the state of the electrons in the well; their Coulomb repulsion and tunneling into the banks are taken into account. For an isolated center, $G(\omega)$ can be derived exactly.[6] The tunneling into the banks can be dealt with by perturbation theory (as in Refs. 9 and 10, for example). In the derivation of (7) we discarded terms of the type

$$\int d\omega \sum_k |T_{k\alpha}|^2 g^A_{k\alpha}(\omega) g^A_{k\alpha}(\omega+\Omega),$$

which vanish in the case $T_{k\alpha}=$ const [$g^A_{k\alpha}(\omega)$ is the free Green's function for one of the banks]. The appearance of a structural feature in Re $[\sigma(\omega)]$ depends on the average number of electrons at a center, $\langle n\rangle = n_\downarrow + n_\uparrow$, i.e., on the static applied voltage. By definition we have

$$\langle n\rangle=\sum_\sigma \int d\omega\ G^+_\sigma(\omega)/2\pi, \tag{9}$$

where G^+ is the Keldysh Green's function of the electrons in the well. This Green's function can be written in the form[9,10]

$$G^+_\sigma(\omega)=\gamma^{-1}[\gamma_L f_L(\omega)+\gamma_R f_R(\omega)]\rho_\sigma(\omega),$$
$$\rho_\sigma(\omega)=\frac{1}{\pi}\,\mathrm{Im}[G^A_\sigma(\omega)]. \tag{10}$$

The density of states $\rho(\omega)$ also depends on the occupation number $\langle n\rangle$:

$$\rho_\sigma(\omega)=\frac{\gamma\ [\omega-\epsilon_0-U(1-\langle n_{-\sigma}\rangle)]}{(\omega-\epsilon_0)^2(\omega-\epsilon_0-U)^2+[\omega-\epsilon_0-U(1-\langle n_{-\sigma}\rangle)]^2\gamma^2}. \tag{11}$$

It has two sharp peaks at energies $\simeq\epsilon_0$ and $\simeq\epsilon_0+U$. In the limit $\gamma\to 0$ the function $\rho_\sigma(\omega)$ is given by the known expression[6]

$$\rho_\sigma(\omega)=(1-\langle n_{-\sigma}\rangle)\delta(\omega-\epsilon_0)+\langle n_{-\sigma}\rangle\delta(\omega-\epsilon_0-U). \tag{12}$$

We wish to repeat that the height of the peaks depends on $\langle n\rangle$. The average number of electrons at a center is determined by the distribution functions in the banks (by the positions of μ_L and μ_R). It can be controlled by means of the static voltage v_0. Of importance for our purposes is the point that the number of electrons in the well—in contrast with the number at an isolated center—may be a noninteger (at an isolated center we would have $\langle n\rangle=0,1,2$). It follows from (9)–(12) that if v_0 is such that the condition $\mu_L>\epsilon_0+U$ holds, while we have $\mu_R<\epsilon_0+U$ [we are assuming for definiteness a temperature $T=0$ and $f_{L,R}(\omega)=\theta(\mu_{L,R}-\omega)$, then the second term, $\gamma_R f_R(\omega)$ in (10) does not contribute to $\langle n\rangle$ [since the second peak in $\rho(\omega)$, at $\omega=\epsilon_0+U$, does not contribute to the integration over ω]. The occupation number in this case is $\langle n\rangle=\gamma_L/(\gamma_L+\gamma_R)$, and there are simultaneously two peaks in the spectral density

$\rho(\omega)$ (since the conditions $\langle n_{-\sigma}\rangle \neq 0$ and $1-\langle n_{-\sigma}\rangle \neq 0$ hold simultaneously). The same property leads to a step on the static current-voltage characteristic.

The first term in the integral in expression (7) for $\mathrm{Re}[\sigma(\Omega)]$ contains a structural feature at $\Omega \simeq U$ along the frequency scale:

$$\mathrm{Re}\ [\sigma(\Omega)] \simeq \frac{1}{2} e^2 \frac{\gamma_R(\gamma_L-\gamma_R)}{\Omega\pi} \sum_\sigma \int_{\mu_R-\Omega}^{\mu_R} d\omega \rho_\sigma(\omega+\Omega)\rho_\sigma(\omega). \tag{13}$$

Expression (13) simplifies for small values of γ:

$$\mathrm{Re}\ [\sigma(\Omega)] \simeq \frac{1}{2} \frac{e^2}{\pi U} \gamma_R(\gamma_L-\gamma_R) \sum_\sigma \langle n_{-\sigma}\rangle (1-\langle n_{-\sigma}\rangle) \delta(\Omega-U). \tag{14}$$

The structural feature arises under the conditions $\mu_L > \epsilon_0 + U$ and $\mu_R < \epsilon_0 + U$, $\mu_R - \Omega < \epsilon_0$. It is a consequence of a decrease in the distance between the poles in $G^A(\omega+\Omega)$ and $G^R(\omega)$ [see (7)] corresponding to states with energies ϵ_0 and $\epsilon_0 + U$ as $\Omega \to U$. It follows from (14) that this singularity occurs only to the extent that there is an asymmetry of the barriers of the quantum well.

A contribution to $\mathrm{Im}[\sigma(\Omega)]$ with a singularity arises from the last term in the integral in (7). This contribution is

$$\mathrm{Im}[\sigma(\Omega)] \simeq \eta \frac{e^2}{2} \frac{(\gamma_L-\gamma_R)}{\pi\gamma} \sum_\sigma \left(\int_{\mu_R}^{\mu_L} + \int_{\mu_R-\Omega}^{\mu_L-\Omega} \right) \rho_\sigma(\omega+\Omega)\rho_\sigma(\omega) d\omega \tag{15}$$

with $\mu_R > \mu_L - \Omega$ [in the case $\mu_R < \mu_L - \Omega$, the limits in (15) should be replaced by $\mu_L - \Omega$, μ_L and $\mu_R - \Omega$, μ_R (the upper and lower limits, respectively)]. Again in this case, the singularity is present to the extent that the well is asymmetric.

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