Effect of the Coulomb repulsion on the $ac$ transport through a quantum dot

T. Ivanov$^{(a)}$, V. Valetchinov$^{(b)}$, and L. T. Wille$^{(c)}$

$^{(a)}$ Department of Physics, University of Sofia, 5 J. Boucher Blvd, 1126 Sofia, Bulgaria
$^{(b)}$ Department of Physics, Northeastern University, Boston, MA 02115, USA
$^{(c)}$ Department of Physics, Florida Atlantic University, Boca Raton, FL 33431-0991

We calculate in a linear response the admittance of a quantum dot out of equilibrium. The interaction between two electrons with opposite spins simultaneously residing on the resonant level is modeled by an Anderson Hamiltonian. The electron correlations lead to the appearance of a new feature in the frequency dependence of the conductance. For certain parameter values there are two crossover frequencies between a capacitive and an inductive behavior of the imaginary part of the admittance. The experimental implications of the obtained results are briefly discussed.

Ms. No PACS numbers: 73.20Dx, 73.40Gk

The double-barrier resonant tunneling systems (DRBTS) are in the focus of intensive experimental and theoretical investigations. While the main characteristics of the steady-state transport properties of such systems have been well understood in terms of several basic approaches – the kinetic equation approach, by a Landauer-Büttiker-type formula, and via the Wigner-function – some of the features in the time-dependent behavior of the DRBTS still remain unclear. In particular, the long lasting question of the fact whether the tunneling transport through the structure is via an establishing a coherent wave function, or can be viewed as a sequence of quantum tunneling events. The answer to this question is of major importance to the practical applicability of these devices as a high frequency resonators.

In a recent paper Fu and Dudley have utilized a model of non-interacting electrons transmitted through the structure under the influence of a small $ac$ bias superimposed upon the driving $dc$ voltage, having shown that for some values of the system’s parameters the frequency-driven behavior can be simulated by an equivalent electrical circuit with an additional inductive element – feature, which was earlier encountered in the modelling the frequency dependence of the DRBTS. In this context, however, it is important to correctly account for the Coulomb interaction effects due to the repulsion between two electrons simultaneously residing on the resonant level – phenomenon, which was shown to give rise of a numerous effects in the $dc$ transport. In a previous paper we have calculated the linear response admittance of a quantum dot with interacting electrons in the case of a zero $dc$ voltage, thus isolating the effects due to the Coulomb on-site repulsion in an equilibrium state of the system. We have obtained a feature in both the real and the imaginary part of the admittance at $\omega \approx 1\text{GHz}$ for the currently accessible experimental parameters.

In this work we apply a non-equilibrium technique to this problem to deal with the case of a non-zero applied $dc$ voltage. We study the effects of the Coulomb interaction on the relatively low-frequency behavior of the conductance through the dot. It is worth mentioning at this point that the formalism developed here is equally applicable either to the case of symmetrical ($T_L = T_R$) or asymmetrical ($T_L \neq T_R$) coupling of the well to the leads, and can be easily extended to take into account additional effects due to environmental fluctuations (i.e. electron-phonon coupling). The conductance is calculated as a function of the $dc$ voltage and the frequency $\Omega$ of the applied $ac$ bias for $\Omega$ of the order of several $\gamma$, where $\gamma$ is the elastic width of the resonant level.

We found that the Coulomb repulsion has a profound effect on both the frequency-driven conductance and the energy losses over a relatively broad range of parameters. In particular, a new feature in the $ac$ response is found in the case of finite Coulomb repulsion energy $E_c$, which we contribute to the fundamental way in which the well-electrons energy spectrum changes in the presence of electron-electron interactions - and this is in marked contrast to the non-interacting ($E_c \to 0$) limit. The imaginary part of the admittance behaves in a way consistent with the Kramers-Kronig dispersion relations, thus giving rise to an additional feature for a finite $E_c$. We further discuss in some details the experimental implications of the theoretical findings reported here, giving the conditions necessary for observing the predicted effects, and discussing some recent experimental results as well.

The Hamiltonian of the quantum well, coupled to the leads, can be written as

$$H = \sum_{k\sigma} \epsilon_k^L a_{k\sigma}^\dagger a_{k\sigma} + \sum_{p\sigma} \epsilon_p^R b_{p\sigma}^\dagger b_{p\sigma} + \epsilon_e \sum_{\sigma} c_{\sigma}^\dagger c_{\sigma} + E_c n_{\uparrow} n_{\downarrow} + \sum_{k\sigma} (T_{Lk} c_{\sigma}^\dagger a_{k\sigma} + h.c.) + \sum_{p\sigma} (T_{Rp} b_{p\sigma}^\dagger c_{\sigma} + h.c.) \tag{1}$$

It is expressed in terms of the creation (annihilation) operators in the emitter $a_{k\sigma}$, collector $b_{p\sigma}$, and the well ($c_{\sigma}$) with
The well electron Green’s function is obtained in the form (for more details see [15]).

\[ G_r(\omega) = \frac{\omega - \epsilon_{c\sigma} - \Sigma_0 - \Sigma_1}{\omega - \epsilon_c - \Sigma_0 - \Sigma_1 - \epsilon_c - \Sigma_0 - \Sigma_2} \]  

(3)

The explicit expressions for the self-energy parts \( \Sigma_0, \Sigma_1, \Sigma_2 \) in Eqn. (3) can be found in Ref. 15. We use the following notation: \( \epsilon_{c\sigma} = \epsilon_c + E_{c\sigma}(1 - < n_{-\sigma} >) \) where \( < n_{-\sigma} > \) is the average number of well electrons with spin \( \sigma \).

This Green’s function describes two energy levels for the quantum well electrons - a lower level with energy \( \epsilon_c \) and an upper level with energy \( \epsilon_c + \epsilon_u \).

We should stress that the derivation of the Green’s function presented here is valid for temperatures higher than the characteristic temperature for this problem – the Kondo temperature \( T_K \). Lacroix [22] has shown that for temperatures \( T < T_K \) this truncation procedure omits terms which are divergent at the Fermi level. These terms give rise to the Kondo effect.

The distribution Green’s function is calculated assuming that all transient processes after the switching on the \( dc \) bias have decayed. In this case one can consider the distribution Green’s function to be independent on the time \( T \). The result for \( G_c(\omega) \) is found in the following closed form:

\[ G_c(\omega) = -F(\omega) (G_r(\omega) - G_a(\omega)) \]  

(4)

where

\[ F(\omega) = \frac{\sum_k |T_{Lk}|^2 A_c(k, \omega) + \sum_p |T_{Rp}|^2 B_c(p, \omega)}{\sum_k |T_{Lk}|^2 (A_r(k, \omega) - A_a(k, \omega)) + \sum_p |T_{Rp}|^2 (B_r(p, \omega) - B_a(p, \omega))} \]  

(5)

is the new non-equilibrium (but steady-state) distribution of electrons in the quantum well. In this expression \( A_r(a) \) and \( B_r(r) \) are the retarded (advanced) and the distribution Green’s functions in the left (right) lead, respectively.

Next we calculate the current through the quantum well in the presence of a time-dependent electric field. The total current is given by \( I = (I_L + I_R)/2 \) where \( I_L(R) \) is the current through the left(right) barrier, respectively.

\[ I_{\text{ext}}(t) = -\alpha e u(t) \sum_\sigma \epsilon_\sigma^c c_\sigma - e u(t) \sum_\sigma b_\sigma^L b_\sigma^r + h.c., \]  

(2)

where the field operators are taken at the time \( t \). The external field is \( u(t) = u_0 e^{i\omega t} \) and its amplitude is assumed to be very small in order not to disturb the electron distribution in the well. In writing this form of the \( H_{\text{ext}} \) we have set \( \mu_R = 0 \).
\[ I(t) = -\frac{ie}{2} \left( \sum_{k\sigma} \left[ T_{Lk}c_{\sigma}^*(t)a_{k\sigma}(t) - T_{Lk}^*a_{k\sigma}^*(t)c_{\sigma}(t) \right] + \sum_{p\sigma} \left[ T_{Rp}b_{\sigma}^*(t)c_{\sigma}(t) - T_{Rp}^*c_{\sigma}^*(t)b_{\sigma}(t) \right] \right). \] (6)

To obtain this expression we have used the Shockley - Ramo theorem [23].

In order to calculate the current \( i(t) \) due to the external \( ac \) voltage \( u(t) \), we use the linear response formalism. In this way we obtain the admittance of the quantum dot \( Y(\omega) = i(\omega)/u(\omega) \) where \( u(\omega) = u_0(\delta(\omega - \Omega) + \delta(\omega + \Omega)) \) is the Fourier transform of the external \( ac \) bias. The explicit expression for the admittance is obtained in the form:

\[ Y(\Omega) = \int d\omega \{ -2i(\alpha + D_r(\omega, \Omega))(\gamma_L(\omega)f_L(\omega) - \gamma_R(\omega)f_R(\omega))G_r(\omega + \Omega)G_r(\omega) \]
\[ + 2i(\alpha + D_a(\omega, \Omega))(\gamma_L(\omega + \Omega)f_L(\omega + \Omega) - \gamma_R(\omega + \Omega)f_R(\omega + \Omega))G_a(\omega + \Omega)G_a(\omega) \]
\[ - [(\alpha + D_a(\omega + \Omega))F(\omega + \Omega)(G_r(\omega + \Omega) - G_a(\omega + \Omega))G_a(\omega) \]
\[ + (\alpha + D_r(\omega + \Omega))F(\omega)G_r(\omega + \Omega)(G_r(\omega) - G_a(\omega))] \]
\[ \times (A_r(\omega + \Omega) - A_a(\omega) - B_r(\omega + \Omega) + B_a(\omega)) \} \] (7)

\[ \times (A_r(\omega + \Omega) - A_a(\omega) - B_r(\omega + \Omega) + B_a(\omega)) \} \] (7)

In writing Eqn. (8) we have used the following notations:

\[ A_r(\omega) = \sum_k |T_{Lk}|^2 A_r(k, \omega), \] (9)

\[ B_r(\omega) = \sum_p |T_{Rp}|^2 B_r(p, \omega), \] (10)

\[ D_r(\omega, \Omega) = \sum_p |T_{Rp}|^2 B_r(p, \omega + \Omega)B_r(p, \omega). \] (11)

The tunneling matrices \( T_{Lk} \) and \( T_{Rp} \) are related to the level widths for the leads’ electrons via the usual equations

\[ \gamma_L(\omega) = \pi \sum_k |T_{Lk}|^2 \delta(\omega - \epsilon_{L}^k), \gamma_R(\omega) = \pi \sum_p |T_{Rp}|^2 \delta(\omega - \epsilon_{R}^p). \] In the following \( \gamma_L(\omega), \gamma_R(\omega) \) are taken to be independent of \( \omega \).

Now we present our numerical results for the \( ac \) conductance \( \sigma(\Omega) = ReY(\Omega) \) and the energy losses \( ImY(\Omega) \) through the quantum well. We calculate them for \( T > T_K \) assuming that \( E_c \gg T, \gamma = \gamma_L + \gamma_R \) and \( T \gg \gamma \). First we solve self-consistently the equation for the average number of quantum well electrons \( \langle n_\sigma \rangle = \langle n_{-\sigma} \rangle = n = -\int d\omega/2\pi ImG_<(\omega) \) (we consider a non-magnetic solution). We take a broad flat density of states for the leads’ electrons. In Fig. 1 we show the dynamical conductance \( \sigma(\Omega, V) \) calculated for a bare level energy \( \epsilon_{(0)}^c = 0.2E_c \) and for a symmetrical coupling of the leads to the well - \( \gamma_L = \gamma_R \).

For \( \Omega \to 0 \) (dc limit) \( \sigma(V) \) has two maxima. This structure reflects the energy spectrum of the well electrons - there are two channels for the electrons to tunnel through the well. When the number of well electrons is smaller than one \( (n < 0.5) \) the tunneling is predominantly through the lower (resonant) level. For \( n > 0.5 \) the lower level is filled with electrons and they are transferred through the upper level.

In this paper we show that the effect of the electron correlations (the Coulomb repulsion \( E_c \)) can also be observed in the \( \Omega \) dependence of the conductance. For relatively low frequency \( (\Omega \sim 2 - 3\gamma) \) the conductance decreases with \( \Omega \) (similarly to the case of non-interacting electrons) since the electrons cannot follow the applied \( ac \) field. The electrons build-up in the well and fill the upper level (there is more than one electron in the well). This opens an additional tunneling channel through the upper level. Consequently for higher frequencies the tunneling current increases (the feature at \( \sim 8 - 10\gamma \) for relatively low \( dc \) voltage). For larger frequencies the conductance again falls off with \( \Omega \), it becomes negative and tends to zero with negative values. This behaviour is in marked contrast to the non-interacting case. In the latter the conductance is positive (for a resonant level above the right chemical potential) and never changes sign.

When the \( dc \) voltage increases the feature in the \( \Omega \) dependence of \( \sigma \) we have just discussed is almost smeared out. The conductance is a monotonically decreasing function of \( \Omega \) but the non-zero response to the \( ac \) field spreads to substantially higher frequencies compared to the non-interacting case.
For dc voltages in the region of the second peak (at $\Omega \to 0$) when the renormalized level is brought well above $\mu_R$ the conductance is a non-monotonic function of $\Omega$. It slightly increases for $\Omega < 5\gamma$ and then decreases with non-zero values of $\sigma(\Omega)$ up to $\Omega \sim 15\gamma$.

In Fig. 2 we show the imaginary part of the admittance $Im Y(\Omega)$ calculated for two typical cases: a) $\epsilon_c^{(0)} = -0.112E_c$ and b) $\epsilon_c^{(0)} = -0.01E_c$. The applied dc voltage was taken to be $eV = 0.2E_c$ and $\gamma = 0.04E_c$. When the upper level is above the right chemical potential the admittance shows a capacitive behavior - $Im Y(\Omega) > 0$(Fig. 2, curve a)). Note that the sign of the imaginary part of the admittance is opposite to the sign in Ref. [14].

Particularly interesting is the result presented in Fig. 2, curve b). In this case $|\epsilon_c - \mu_R| < \gamma/2$. It shows that there are two frequencies at which a crossover from a capacitive to an inductive behavior (and vice versa) is obtained. At low frequencies the admittance is inductive, then it changes sign and this is the crossover to a capacitive admittance. Fu and Dudley [14] studied the same case in the non-interacting picture of the resonant tunneling. They obtained an inductive behavior - $Im Y(\Omega) < 0$ and no crossover to a capacitive one. Moreover, in the interacting case there is one more crossover frequency at which the admittance changes back from a capacitive to an inductive. When $V = 0$ this frequency is $\Omega \sim \epsilon_c^{(0)} + E_c - \mu_R$. With increasing $V$ the first crossover frequency diminishes and the second increases so that at sufficiently high voltage the behaviour of the admittance will be inductive. The appearance of the second crossover frequency is in agreement with the conclusion of Brandes, Weinmann, and Kramer [16] - at high frequencies the behavior of the admittance is not strongly affected by the electron interactions except the feature at $\Omega \sim E_c$ discussed in [14].

When $|\epsilon_c - \mu_R| > \gamma/2$ (as in Fig. 2, curve a) Fu and Dudley obtained a crossover to an inductive admittance at $\Omega \sim |\epsilon_c - \mu_R|$. With $E_c \neq 0$ this is possible only if $\epsilon_c$ is well below $\mu_R$ and the upper level is above $\mu_R$ [24]. For a quantum dot with both the resonant and the upper level well below the right chemical potential for low $V$ the admittance is inductive. A crossover to a capacitive behavior can be obtained for sufficiently high $V$ at $\Omega \sim \epsilon_c + E_c - \mu_R$ (then the upper level will be moved above $\mu_R$) [24].

All these results clearly indicate that as in the non-interacting case [14] the frequency behavior of DBRTS cannot generally be simulated by any LRC equivalent-circuit model.

To address the experimental detection of the the effects under consideration here, let us recall the range of the three main parameters involved in the model - $E_c \gg T \gg \gamma$. The on-site repulsion energy can be estimated from $E_c \sim e^2/\epsilon L$, where $L$ is the size of the confined region, and $\epsilon$ is the dielectric constant for the GaAs. Thus for a quantum dot with average size of 100 Å, one gets $E_c \sim 1 - 10meV$. It is less evident how to estimate the elastic broadening constant $\gamma$, but we can use the estimation given in Ref. [22] for $\gamma \sim 10 - 20\mu eV$ for a structure of about the same size. Therefore, the type of effects discussed in this study to be detected experimentally, one needs temperatures of few degrees $K$ and a external frequency range up to hundreds $GHz$ - requirements accessible at the present time. Let us only mention at this place that because of the temperature ranges used ($T = 77K$, and room temperature, accordingly) the results of two recent ac experiments (see Refs. [10][11]) did not show the frequency dependence discussed here. This is because the measurements were performed in the regime where the thermal fluctuations prevail over the “Coulomb blockade” effect [21].

We should point out that the expression for the current Eqn. [6] does not include the displacement currents through the parasitic capacitances. They can be accounted for by considering some electrostatic model of the dot. Our aim was to extract the effects of the electron correlations comparing our results with the available works on non-interacting electron tunneling where the displacement currents were not included. One can expect that the parasitic currents would modify the relatively high frequency behavior of the admittance [27].

In conclusion, we have calculated the linear-response admittance of a quantum dot with interacting electrons. We show that the effect of the electron correlations can be observed in the frequency dependence of the conductance where a new feature appears when the electrons tunnel through the upper level. For a certain parameter values there are two frequencies at which the imaginary part of the admittance changes sign i.e. a crossover between a capacitive and an inductive behavior. We discuss the experimental conditions for observation of these effects.

ACKNOWLEDGMENTS

The authors acknowledge the fruitful discussions with Drs. A. Groshev, S. Hershfield, V. Popov, I. Z. Kostadinov, J. Sokoloff. V.V. is thankful to Dr. N. S. Wingreen for making papers available before publication. T.I. was sponsored by a Contract F-225/1992 with the Ministry of Science and Education of Bulgaria.
FIG. 1. Conductance $\sigma$ as a function of the applied $dc$ bias across the structure and the external frequency $\Omega$ calculated for a quantum dot with $\epsilon_c^{(0)} = 0.2E_c$.

FIG. 2. The imaginary part of the dynamical admittance $ImY$ as a function of the frequency $\Omega$ of the external ac signal for two positions of the bare energy level: a) $\epsilon_c^{(0)} = -0.112E_c$ (the solid line), and b) $\epsilon_c^{(0)} = -0.01E_c$ (the dashed line). The applied $dc$ voltage is $eV = 0.2E_c$, and $\gamma = 0.04E_c$. 