The influence of tunneling matrix elements modification due to on-site Coulomb interaction on local tunneling conductivity

V. N. Mantsevich† and N. S. Maslova‡
Moscow State University, Department of Physics, 119991 Moscow, Russia
(Dated: February 1, 2011)

Interplay between changes of energy levels and tunneling amplitudes caused by localized electrons on-site Coulomb interaction depending on non-equilibrium electron filling numbers is analyzed. Specific features of local tunneling conductivity spectra for different positions of localized states energy relative to the Fermi level have been investigated by means of self-consistent mean field approximation in the presence of non-equilibrium effects. The conditions when modifications of tunneling transfer amplitude due to changes of electron filling numbers in the presence of on-site Coulomb interaction should be taken into account in tunneling conductivity spectra have been revealed.

PACS numbers: 71.55.-i
Keywords: D. Coulomb interaction; D. Non-equilibrium filling numbers; D. Impurity; D. Tunneling conductivity spatial distribution

I. INTRODUCTION

Recently great attention is paid to both experimental and theoretical investigations of kinetic processes in nanostructures, in connection with possibility of ultra small size electronic devices fabrication. Comparison between experimental results and theoretical models provide information about tunneling mechanisms in nanoscale junctions due to the presence of localized states [1]. Localized states formed by impurities at surface and interfaces of semiconductors lead to strong modification of local electronic structure and influence the behavior of tunneling characteristics due to on-site Coulomb interaction of the sample and tip conduction electrons with charged localized states [2–4]. Most of the experiments are carried out with the help of scanning tunneling microscopy/spectroscopy technique [2, 5, 6] and theoretical calculations usually deals with Green’s functions formalism [1, 5, 6] or ab-initio calculations [10].

It was predicted theoretically and proved experimentally that on-site Coulomb repulsion of localized electrons leads to the changing of energy values considerably even for deep impurity levels [1, 8]. It was found that taking into account Coulomb interaction of conduction electrons with non-equilibrium localized charges result in non-trivial behavior of tunneling characteristics in the case of STM metallic tip positioned above the impurity atom [5, 11, 12] and also leads to formation of peculiarities in local tunneling conductivity analyzed apart from the impurity [8, 11]. But in all the previous calculation tunneling transfer rates considered as a constant values and influence of the impurity’s non-equilibrium electron filling numbers on tunneling transfer amplitudes due to Coulomb correlations was neglected [6, 8, 12]. However, this effect is a problem of great interest because influence rate depends on the impurity type and solving of this problem gives an opportunity to initialize impurity type with the help of STM technique. Another question of great interest is what effect dominates in tunneling contact: influence of Coulomb interaction on-site or on hopping matrix elements. Correct investigation of this problem shows the way for not only qualitative but also for quantitative theoretical analysis of experimentally measured local tunneling conductivity, but it is necessary to choose the correct starting approximation for each type of impurity atom depending on the localized state energy level position relative to the Fermi level. Previous works demonstrate that for localized states with energy deep below the Fermi level Hubbard-I model [13] suits well and for localized states with energy in the vicinity of Fermi level mean field mixed valence approximation [14] can be applied.

So in this work we present detailed investigation of local tunneling conductivity in vicinity of an impurity paying special attention to the tunneling transfer amplitude dependence from non-equilibrium electron filling numbers due to Coulomb correlations. On-site Coulomb interaction will be also taken into account in our model. Development of theoretical description suggested in [8] and based only on on-site Coulomb interaction should clarify the role of tunneling transfer amplitudes modification due to the influence of impurity’s non-equilibrium electron filling numbers in formation of peculiar features observed experimentally in local tunneling conductivity. We performed calculations for two extreme cases when tunneling takes place through the impurity state with deep energy level and shallow energy level. We applied modified mean field self-consistent approach for the impurity state with shallow energy level and in the case of impurity with deep energy level modified Hubbard-I model was used. We also compared our results with the
calculations based on non-modified models based only on on-site Coulomb interaction. Both approaches were ana-
yzed with the use of the Keldysh formalism [15].

II. THE SUGGESTED MODEL AND MAIN RESULTS

We shall analyze tunneling between the semiconductor
surface and metallic STM tip in the presence of Coulomb
interaction for impurities with deep and shallow energy
levels in comparison with Fermi level. Special attention
will be payed to the impurity atom non-equilibrium
electron filling numbers influence on the values of tun-
neling transfer amplitudes. The standard model system
semiconductor-impurity atom-metallic tip with constant
tunneling transfer amplitudes. The standard model system

\[
H = H_0 + H_{imp} + H_{tun}
\]

Indices \(k\) and \(p\) label the states in the left (semi-
conductor) and right (tip) lead, respectively. The index \(d\)
indicates that impurity electron operator is involved. \(U\)
is the on-site Coulomb repulsion of localized electrons,
\(n_{da} = c_{da}^+ c_{da}\) destroys impurity electron with spin
\(\sigma\). \(H_0\) describes conduction electrons of continuous spec-
trum states in the leads of tunneling contact. \(H_{tun}\)
describes tunneling transitions between the tunneling con-
tact leads through the impurity state. \(H_{imp}\) corresponds
to the electrons in the localized state formed by the im-

We shall start from the case of impurity state with en-
ery level situated deep below the Fermi level. In the
presence of Coulomb interaction tunneling through deep
impurity energy level can be described with the help of
Hubbard-I model [13] (Hamiltonian of this model has the
form \(H_{imp}\)). Taking into account Coulomb interaction
in this model leads to formation of two well separated
impurity energy levels \(\varepsilon_d\) and \(\varepsilon_d + U\) instead of one initial
level \(\varepsilon_d\). It is reasonable to use approximation in which
the strongest interaction of the considered model - the
on-site Coulomb repulsion \(U\) - is included in \(G_{0R}^{dd}\). So we can write down expression for \(G_{0R}^{dd}\) supposing tunneling transfer amplitudes to be independent from lo-
calized state non-equilibrium filling numbers:

\[
G_{0R}^{dd}(\omega) = \frac{1}{\omega - \varepsilon_d - \Sigma(\omega)}
\]

\[
\Sigma(\omega) = \frac{n_{d-}\omega - \varepsilon_d}{\omega - \varepsilon_d - (1 - n_{d-}) U}
\]

Using system of Dyson equations one can get expres-
sion for impurity retarded Green’s function.

\[
G_{0R}^{dd}(\omega) = \frac{1}{\omega - \varepsilon_d - \Sigma(\omega) - t(\gamma_{kd} + \gamma_{pd})}
\]

Where \(\sum_{p} t_{pd}^2 Im G_{0R}^{pd} = \gamma_{pd}\) and \(\sum_{k} t_{kd}^2 Im G_{0R}^{kd} = \gamma_{kd}\). Expression for local tunneling conductivity in the case of constant transfer amplitudes was found in [17] and has the form:

\[
\frac{dI}{dV}(\omega) = \frac{\gamma_{kd}\gamma_{pd}}{\gamma_{kd} + \gamma_{pd}} Im G_{0R}^{dd}(\omega)
\]

If one wants now to analyze modification of tunneling transfer amplitudes due to the dependence from impu-

rity’s non-equilibrium electron filling numbers, it is nec-
nessary to rewrite part \(H_{tun}\) of the initial Hamiltonian \(H\)
which corresponds to tunneling transitions between the
tunneling contact leads through the impurity state. Due
to Coulomb repulsion energy level position depends on
electron filling numbers. Impurity energy increases with
the increasing of filling numbers and it leads to the de-
creasing of tunneling amplitudes between tunneling con-
tact leads through the impurity energy level. So higher
energy level corresponds to the smaller value of tunneling
transfer amplitude and tunneling amplitude now depends
on electron presence or absence on the energy level.

\[
H_{tun} = \sum_{k,d} t_{kd} c_{k\sigma}^+ c_{d\sigma} + \sum_{p,d} t_{pd} c_{d\sigma}^+ c_{p\sigma} + h.c.
\]

where expressions for \(t_{eff}^{kd}\) and \(t_{eff}^{pd}\) have the form:

\[
t_{eff}^{kd} = (T_1(1 - <n_{d-\sigma}>) + T_2 <n_{d-\sigma}>)
\]

\[
t_{eff}^{pd} = (t_1(1 - <n_{d-\sigma}>) + t_2 <n_{d-\sigma}>)
\]

When impurity energy level is free from electrons tun-
neling transitions from semiconductor continuous spec-
trum states to STM tip through impurity atom are de-
scribed by transfer amplitudes \(T_1\) and \(T_2\). If impurity
energy level is occupied by electron with spin tunneling
transitions between continuous spectrum states through
impurity state can be described by tunneling transfer
amplitudes \(T_2\) and \(t_2\). Due to this assumption initial
Hubbard-I model [13] can be modified and expression
for retarded Green’s function will have the form:
In this case relaxation rates can be written in the following way \( \gamma_{eff}^{<} = \sum_{k} t_{kd}^{eff} ImG_{dd}^{R\sigma} \) and \( \gamma_{eff}^{>} = \sum_{p} t_{pd}^{eff} ImG_{dd}^{\sigma R} \). Expression for local tunneling conductivity will then have the form:

\[
\frac{dI}{dV}(\omega) = \frac{\gamma_{eff}^{<} \gamma_{eff}^{>}}{\gamma_{eff}^{<} + \gamma_{eff}^{>} + i\omega + \Sigma} ImG_{dd}^{R\sigma}
\]  

(8)

Calculating expression for \( ImG_{dd}^{R\sigma}(\omega) \) requires solution of self-consistent system of equations. Two of them are equations for \( ImG_{dd}^{R\sigma}(\omega) \), obtained from expression 7 and three equations determine impurity atom non-equilibrium electron filling numbers:

\[
n_{d\pm\sigma} = \frac{-1}{\pi} \int d\omega n_{d\pm\sigma}(\omega) ImG_{dd}^{R\pm\sigma}(\omega, n_{d\pm\sigma})
\]

\[
n_{d\sigma}(\omega) = n_{d-\sigma}(\omega) = \frac{\gamma_{eff}^{<} n_{0}^{<}(\omega) + \gamma_{eff}^{>} n_{0}^{>}(\omega)}{\gamma_{eff}^{<} + \gamma_{eff}^{>}}
\]

(9)

where \( n_{0}^{<}(\omega) \) and \( n_{0}^{>}(\omega) \) are equilibrium filling numbers in the tunneling contact leads.

FIG. 1: Local tunneling conductivity as a function of applied bias voltage calculated for the impurity atom with deep energy level. Gray line corresponds to the case when tunneling transfer amplitudes depend on impurity filling numbers \( t_{1} = 0.20, t_{2} = 0.29, T_{1} = 0.30, T_{2} = 0.35 \). Black line corresponds to the case when tunneling transfer amplitudes have constant values and only on-site Coulomb interaction is taken into account \( t_{kd} = 0.35, t_{pd} = 0.29 \). For all the figures parameters values \( \varepsilon_{d} = -0.80, U = 3 \) are the same.

FIG. 1 shows tunneling conductivity as a function of applied bias voltage for impurity with energy level deep below Fermi level. It means that relation between energy level value and energy level width due to the tunneling processes is about unit. In this case Coulomb interaction effects accompanied by the assumption that non-equilibrium electron filling numbers modify tunneling transfer amplitudes can be described with the use of modified mean-field mixed valence approximation 18, 19 and consequently Hamiltonian depends on average electron filling numbers. So one has to rewrite the Hamiltonian \( H_{tun} \) in the form 5. More over impurity energy level position depends on Coulomb interaction of the non-equilibrium electron density. A new impurity energy level position is a result of initial energy level position shift on the value \( U < n_{d-\sigma} > \). Non-equilibrium impurity atom filling numbers \( n_{d-\sigma} \) must satisfy self-consistency condition 9 where \( \gamma_{eff}^{<} \) and \( \gamma_{eff}^{>} \) are determined by expressions 6 and \( G_{dd}^{R\sigma}(\omega) \) in the mean field approximation has the following form:

\[
G_{dd}^{R\sigma}(\omega) = \frac{1}{\omega - \varepsilon_{d} - U - n_{d-\sigma} + i(\gamma_{eff}^{<} + \gamma_{eff}^{>})}
\]

(10)

After determining new position of impurity energy
level we can calculate expressions for $Im G_{\epsilon d}^{R\sigma}(\omega)$ from $[10]$ and finally evaluate local tunneling conductivity for shallow impurity taking into account Coulomb interaction effects and tunneling transfer amplitudes modification influenced by the impurity non-equilibrium electron filling numbers with the use of expression $[8]$

![Image of a graph showing local tunneling conductivity as a function of applied bias voltage.]

FIG. 2: Local tunneling conductivity as a function of applied bias voltage calculated for the impurity atom with shallow energy level. Gray line corresponds to the case when tunneling transfer amplitudes depend on impurity filling numbers $t_1 = 0.40$, $t_2 = 0.49$, $T_1 = 0.60$, $T_2 = 0.68$. Black line corresponds to the case when tunneling transfer amplitudes have constant values and only on-site Coulomb interaction is taken into account $t_{kd} = 0.68$, $t_{pd} = 0.49$. For all the figures parameters values $\varepsilon_d = -0.80$, $U = 3$ are the same.

Calculation results are presented on Fig.2. Tunneling conductivity as a function of applied bias voltage demonstrates that taking into account modification of tunneling transfer amplitudes due to the influence of impurity’s non-equilibrium electron filling numbers (Fig.2 gray line) in addition to Coulomb interaction leads to important changes in comparison with the case of constant tunneling rates and on-site Coulomb interaction (Fig.2 black line). Decreasing of resonant peak width and a negligible decreasing of the tunneling conductivity amplitude takes place for modified self-consistent mean field approximation due to the influence of impurity’s non-equilibrium electron filling numbers on tunneling transfer amplitudes and consequently on relaxation rates. Describing tunneling through the impurity state with energy level in the vicinity of Fermi level it is necessary to mention that width of peculiarities in tunneling conductivity is determined by the value of relaxation rates $\gamma_{kd}^{\epsilon_f}$ and $\gamma_{pd}^{\epsilon_f}$. Continuous energy shift of the resonant peak to the higher values of applied bias voltage exists mostly due to on-site Coulomb interaction of localized electrons ($U < n_{d-a} \gg \gamma^{\epsilon_f}$) and can be seen both for taking and not taking into account tunneling matrix elements modification. It is clearly evident that resonant peak shift for modified tunneling amplitudes is smaller than in the case of constant tunneling amplitudes also because of relaxation rates modification.

III. CONCLUSION

In this work we have analyzed the role of tunneling transfer amplitudes modification caused by the shift of energy level with changing of non-equilibrium electron filling numbers in the presence of on-site Coulomb interaction in formation of anomalous features in local tunneling conductivity. The influence of this effect on local tunneling conductivity have been analyzed for different location of localized states energy relative to Fermi level. We have studied two extreme cases when tunneling takes place through the impurity state with energy level position deep below Fermi level and through impurity state with energy level in the vicinity of Fermi level by means of modified Hubbard-I model and modified self-consistent mixed valence mean field approximation correspondingly.

For impurity state with energy level deep below the Fermi level modification of tunneling transfer amplitudes in addition to on-site Coulomb interaction results in significant changing of resonant peaks amplitudes and width in comparison with non-modified Hubbard-I model. Resonant peculiarities demonstrate strong amplitudes decreasing. We also observed considerable increasing of resonant peculiarities width.

Impurity state with energy in the vicinity of Fermi level also demonstrates significant changes in local tunneling conductivity in comparison with the case of constant tunneling rates due to modification of tunneling transfer amplitudes in addition to on-site Coulomb interaction. We observed width changing of resonant peak, slight decreasing of the tunneling conductivity amplitude and smaller resonant peak shift to higher value of applied bias voltage.

Obtained results give us possibility to conclude that on-site Coulomb interaction strongly influence local tunneling conductivity measured in the vicinity of impurity atom and Coulomb interaction influence on hopping matrix elements leads to corrections of peculiarities shape, amplitude and width in modified conductivity.

This work was supported by RFBR grants and by the National Grants for technical regulation and metrology.

[1] P.I. Arseyev, N.S. Maslova et al., *JETP Letters*, 68, 299, (1998)
[2] R. Dombrowski, C. Wittneven, M. Morgenstern et al., *Appl. Phys. A*, 66, S203-S206, (1998)
[3] J. Sullivan, G. Boishin, L. Whitman et al., *Phys. Rev. B*, 68, 235324, (2003)
[4] G. Mahieu, B. Grandidier, D. Deresmes et al., *Phys. Rev. Lett.*, 94, 026407, (2005)
[5] J. Inglesfield, M. Boon, S. Crampin, *Condens. Matter*, 12, L489-L496, (2000)
[6] N.S. Maslova, V.I. Panov, S.I. Oreshkin et al., *JETP Letters*, 67, 130, (1998)
[7] W. Hofstetter, J. König, H. Schoeller, *Phys. Rev. Letters*, 87, 156803, (2001)
[8] V.N. Mantsevich, N.S. Maslova, *Solid State Communications*, 150, 2072, (2010)
[9] V.N. Mantsevich, N.S. Maslova, *JETP Letters*, 91, 150, (2010)
[10] M. Qian, M. Gothelid, B. Johnsson, *Phys. Rev. B*, 66, 155326, (2002)
[11] V. Madhavan, W. Chen, T. Jamneala et al., *Science*, 280, 567, (1998)
[12] P.I. Arseyev, N.S. Maslova et al., *ZheTF*, 121, 225, (2002)
[13] J. Hubbard, *Proc. Roy. Soc.*, 276, 238, (1963)
[14] P.W. Anderson, *Phys. Rev.*, 115, 1439, (1959)
[15] L.V. Keldysh, *Sov. Phys JETP*, 20, 1018, (1964)
[16] V.N. Mantsevich, N.S. Maslova, *JETP Letters*, 89, 609, (2009)
[17] P.I. Arseyev, N.S. Maslova, *ZETF*, 102, 575, (1992)
[18] Y. Meir, N. Wingreen et al., *Phys. Rev. Letters*, 70, 2601, (1993)
[19] N. Sivan, N. Wingreen, *Phys. Rev. B*, 54, 11622, (1996)