The effect of Coulomb correlations on non-equilibrium charge redistribution tuned by tunneling current

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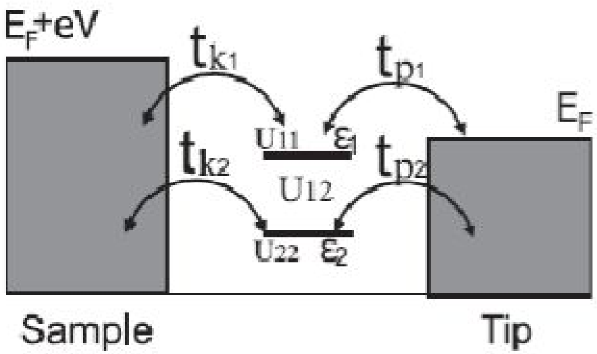
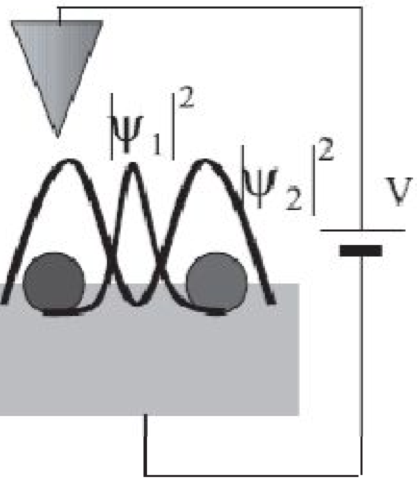
Two-level system

a



b



$$\hat{H} = \sum_{i\sigma} \varepsilon_i n_{i\sigma} + \sum_{k\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_{p\sigma} \varepsilon_p c^+_{p\sigma} c_{p\sigma}$$

$$+ \sum_{ij\sigma\sigma'} U^{\sigma\sigma'}_{ij} n_{i\sigma} n_{j\sigma'} +$$

$$+ \sum_{ki\sigma} t_{ki} (c^+_{k\sigma} c_{i\sigma} + h.c.) + \sum_{pi\sigma} t_{pi} (c^+_{p\sigma} c_{i\sigma} + h.c.)$$

Current

$$I = I_{k\sigma} = \sum_{i\sigma} I_{ki\sigma} = i \sum_{ki\sigma} t_{ki} (< c^+_{k\sigma} c_{i\sigma} > - < c^+_{i\sigma} c_{k\sigma} >)$$

Current calculations

$$i\frac{\partial c^{+}_{k\sigma}c_{i\sigma}}{\partial t}=(\varepsilon_i-\varepsilon_k)\cdot c^{+}_{k\sigma}c_{i\sigma}+U_{ii}n_{i-\sigma}\cdot c^{+}_{k\sigma}c_{i\sigma}+U_{ij}(n_{j\sigma}+n_{j-\sigma})\cdot c^{+}_{k\sigma}c_{i\sigma}$$

$$-t_{ki}\cdot(n_{i\sigma}-\hat{f}_k)+\sum_{k'\neq k}t_{k'i}c^{+}_{k\sigma}c_{k'\sigma}+\sum_{i\neq j}t_{kj}c^{+}_{j\sigma}c_{i\sigma}=0$$

$$\hat{f}_k=c^{+}_{k\sigma}c_{k\sigma}$$

$$n_{1-\sigma}(1-n_{2-\sigma})(1-n_{2\sigma})c^{+}_{k\sigma}c_{1\sigma}=$$

$$\{(t_{k1}\cdot(n_{1\sigma}-\hat{f}_k)+\sum_{k'\neq k}t_{k'1}c^{+}_{k\sigma}c_{k'\sigma}+t_{k2}c^{+}_{2\sigma}c_{1\sigma})\cdot n_{1-\sigma}(1-n_{2-\sigma})(1-n_{2\sigma})\}\cdot\{\varepsilon_1-\varepsilon_k+U_{11}\}^{-1}$$

Simplifications due to $\hat{n}_i^2=1$

$$(1-n_{1-\sigma})(1-n_{2-\sigma})(1-n_{2\sigma})+n_{1-\sigma}(1-n_{2-\sigma})(1-n_{2\sigma})+$$

$$+\sum_{\sigma'}n_{2\sigma'}(1-n_{1-\sigma})(1-n_{2-\sigma'})+\sum_{\sigma'}n_{1-\sigma}n_{2\sigma'}(1-n_{2-\sigma'})+n_{2-\sigma}n_{2\sigma}(1-n_{1-\sigma})+n_{1-\sigma}n_{2-\sigma}n_{2\sigma}=1$$

Current in terms of correlators

$$I_{k1\sigma} = i\, t_{ki} (< c^{+}_{k\sigma} c_{1\sigma} > - < c^{+}_{1\sigma} c_{k\sigma} >)$$

$$\begin{aligned} I_{k1\sigma} = \Gamma_{k1} \{ &\langle n_{1\sigma} \rangle - \langle (1-n_{1-\sigma})(1-n_{2-\sigma})(1-n_{2\sigma}) \rangle f_k(\varepsilon_1) - \langle n_{1-\sigma}(1-n_{2-\sigma})(1-n_{2\sigma}) \rangle \cdot f_k(\varepsilon_1 + U_{11}) - \\ -&\langle n_{2\sigma}(1-n_{2-\sigma})(1-n_{1-\sigma}) \rangle \cdot f_k(\varepsilon_1 + U_{12}) - \langle n_{2-\sigma}(1-n_{2\sigma})(1-n_{1-\sigma}) \rangle \cdot f_k(\varepsilon_1 + U_{12}) - \\ -&\langle n_{1-\sigma} n_{2\sigma}(1-n_{2-\sigma}) \rangle \cdot f_k(\varepsilon_1 + U_{11} + U_{12}) - \langle n_{1-\sigma} n_{2-\sigma}(1-n_{2\sigma}) \rangle \cdot f_k(\varepsilon_1 + U_{11} + U_{12}) - \\ -&\langle n_{2\sigma} n_{2-\sigma}(1-n_{1-\sigma}) \rangle \cdot f_k(\varepsilon_1 + 2U_{12}) - \langle n_{1-\sigma} n_{2-\sigma} n_{2\sigma} \rangle \cdot f_k(\varepsilon_1 + U_{11} + 2U_{12}) \} + \end{aligned}$$

$$+ t_{k1} t_{k2} \nu_{0k} c^{+}_{2\sigma} c_{1\sigma} + \sum_{k' \neq k} \langle t_{k1} t_{k'1} c^{+}_{k\sigma} c_{k'\sigma} \rangle \times [....]$$

Stationarity conditions

$$\frac{\partial}{\partial t} \langle n_{i\sigma} n_{j\sigma'} \rangle = 0 \qquad \frac{\partial}{\partial t} \langle n_{j\sigma} n_{j-\sigma} n_{i-\sigma'} \rangle = 0$$

Triple correlators as functions of pair correlators

Equations for the pair correlators

$$K_{11} \equiv \langle n_{1\sigma} n_{1-\sigma} \rangle \quad K_{22} \equiv \langle n_{2\sigma} n_{2-\sigma} \rangle \quad K_{12} \equiv \langle n_{1\sigma} n_{2\sigma} \rangle$$

$$\begin{pmatrix} A \end{pmatrix} \times \begin{pmatrix} K_{11} \\ K_{12} \\ K_{22} \end{pmatrix} = \begin{pmatrix} F \end{pmatrix}$$

$$F = \begin{pmatrix} n_1^T(\varepsilon_1 + U_{11}) \cdot n_{1\sigma} \\ n_2^T(\varepsilon_2 + U_{22}) \cdot n_{2\sigma} \\ \frac{\Gamma_1}{\Gamma_1 + \Gamma_2} n_1^T(\varepsilon_1 + U_{12}) n_{2\sigma} + \frac{\Gamma_2}{\Gamma_1 + \Gamma_2} n_2^T(\varepsilon_2 + U_{12}) n_{1\sigma} \end{pmatrix}$$

$$a_{12} = 2 \cdot n_1^T(\varepsilon_1 + U_{11}) - n_1^T(\varepsilon_1 + U_{11} + U_{12}) - 2 \cdot \frac{\Gamma_2}{\Gamma_1} \cdot n_2^T(\varepsilon_2 + U_{22} + U_{12}) \cdot \Phi_1$$

$$\Phi_i = \frac{n_i^T(\varepsilon_i + U_{ii}) - n_i^T(\varepsilon_i + U_{ii} + \cdot U_{ij})}{3 + n_i^T(\varepsilon_i + 2 \cdot U_{ij}) - n_i^T(\varepsilon_i + U_{ii} + 2 \cdot U_{ij})} + \frac{n_i^T(\varepsilon_i + U_{ii} + 2 \cdot U_{ij})}{3 + n_i^T(\varepsilon_i + 2 \cdot U_{ij}) - n_i^T(\varepsilon_i + U_{ii} + 2 \cdot U_{ij})}$$

$$n_i^T(\varepsilon) = \frac{\Gamma_{ki} f_k(\varepsilon) + \Gamma_{pi} f_p(\varepsilon)}{\Gamma_{ki} + \Gamma_{pi}}$$

For large U we neglect triple correlators

$$I_{k1\sigma} = \Gamma_k \cdot \{ \langle n_{1\sigma} \rangle - (1 - \langle n_{1\sigma} \rangle - 2\langle n_{2\sigma} \rangle + K_{22} + 2K_{12}) \cdot f_k(\varepsilon_1) -$$
$$- (\langle n_{1\sigma} \rangle - 2K_{12}) \cdot f_k(\varepsilon_1 + U_{11}) - 2 \cdot (\langle n_{2\sigma} \rangle - K_{12} - K_{22}) \cdot f_k(\varepsilon_1 + U_{12}) \}$$

Solutions for the pair correlators look like:

$$K_{12} = \frac{\frac{1}{2} n^T(\varepsilon_1 + U_{12}) \cdot (1 - n^T(\varepsilon_2 + U_{22})) \cdot n_{2\sigma} + \frac{1}{2} n^T(\varepsilon_2 + U_{12}) \cdot (1 - n^T(\varepsilon_1 + U_{11})) \cdot n_{1\sigma}}{1 + n^T(\varepsilon_1 + U_{12}) \cdot (\frac{1}{2} - n^T(\varepsilon_2 + U_{22})) + n^T(\varepsilon_2 + U_{12}) \cdot (\frac{1}{2} - n^T(\varepsilon_1 + U_{11}))}$$

$$U_{ij} \to \infty$$

$$n_{1\sigma} = \frac{n_1^T(\varepsilon_1)(1 - n_2^T(\varepsilon_2))}{(1 + n_1^T(\varepsilon_1))(1 + n_2^T(\varepsilon_2)) - 4n_1^T(\varepsilon_1)n_2^T(\varepsilon_2)}$$

$$n_{2\sigma} = \frac{n_2^T(\varepsilon_2)(1 - n_1^T(\varepsilon_1))}{(1 + n_1^T(\varepsilon_1))(1 + n_2^T(\varepsilon_2)) - 4n_1^T(\varepsilon_1)n_2^T(\varepsilon_2)}$$

1) $n_2^T = 1/2 \quad n_1^T = 0$

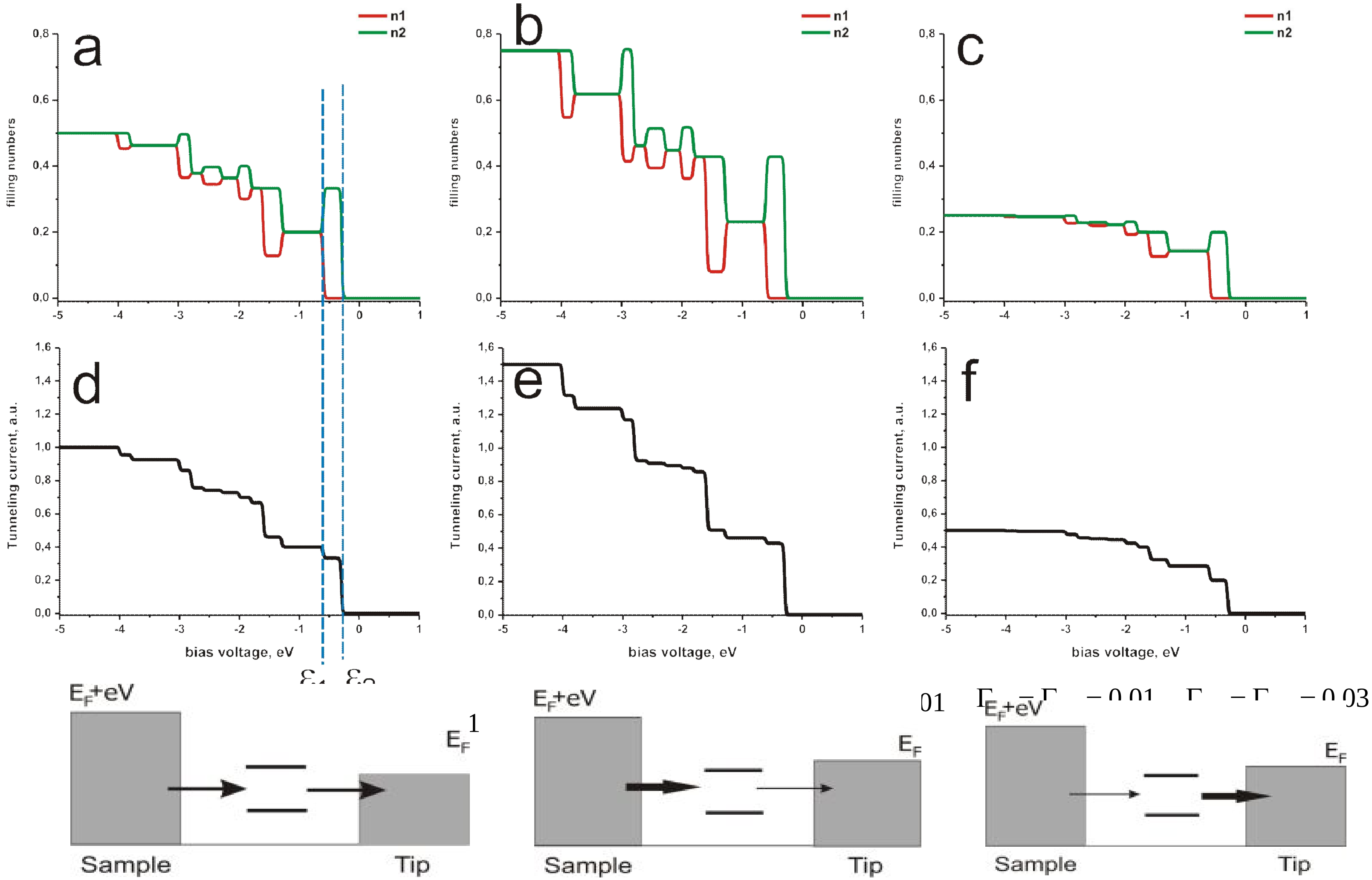
$n_1 = 0 \quad n_2 = 1/3$

2) $n_2^T = 1/2 \quad n_1^T = 1/2$

$n_2 = n_1 = 1/5$

$$I_k = \frac{4\Gamma_k \Gamma_p}{\Gamma_k + \Gamma_p} \frac{(f_p(\varepsilon_1) - f_k(\varepsilon_1))(1 - n_2^T(\varepsilon_2)) + (f_p(\varepsilon_2) - f_k(\varepsilon_2))(1 - n_1^T(\varepsilon_1))}{(1 + n_1^T(\varepsilon_1))(1 + n_2^T(\varepsilon_2)) - 4n_1^T(\varepsilon_1)n_2^T(\varepsilon_2)}$$

Tunneling characteristics and charge distribution

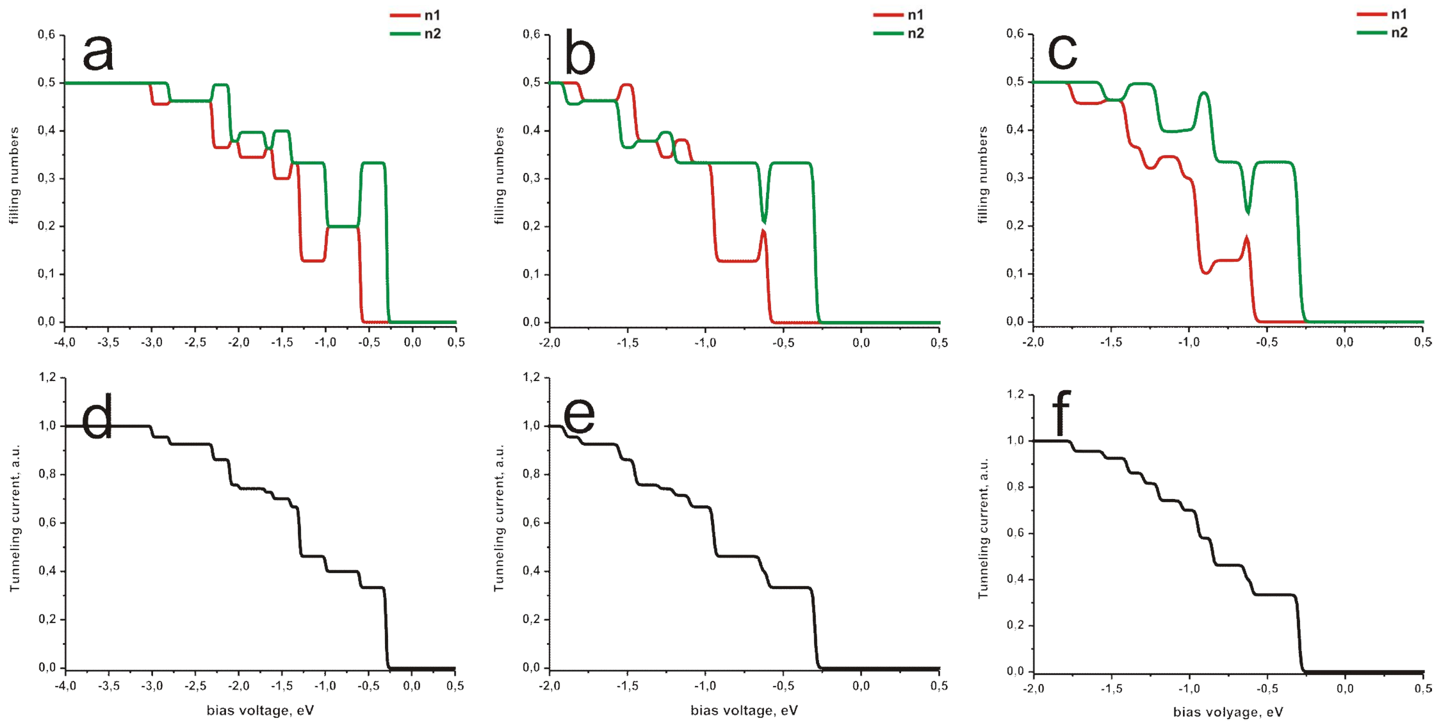


12 steps for V=

$$\varepsilon_1 \qquad \varepsilon_1 + U_{12} \qquad \boldsymbol{\varepsilon_1 + U_{11}}$$

$$\varepsilon_1 + U_{11} + U_{12} \qquad \varepsilon_1 + 2U_{12} \qquad \varepsilon_1 + U_{11} + 2U_{12}$$

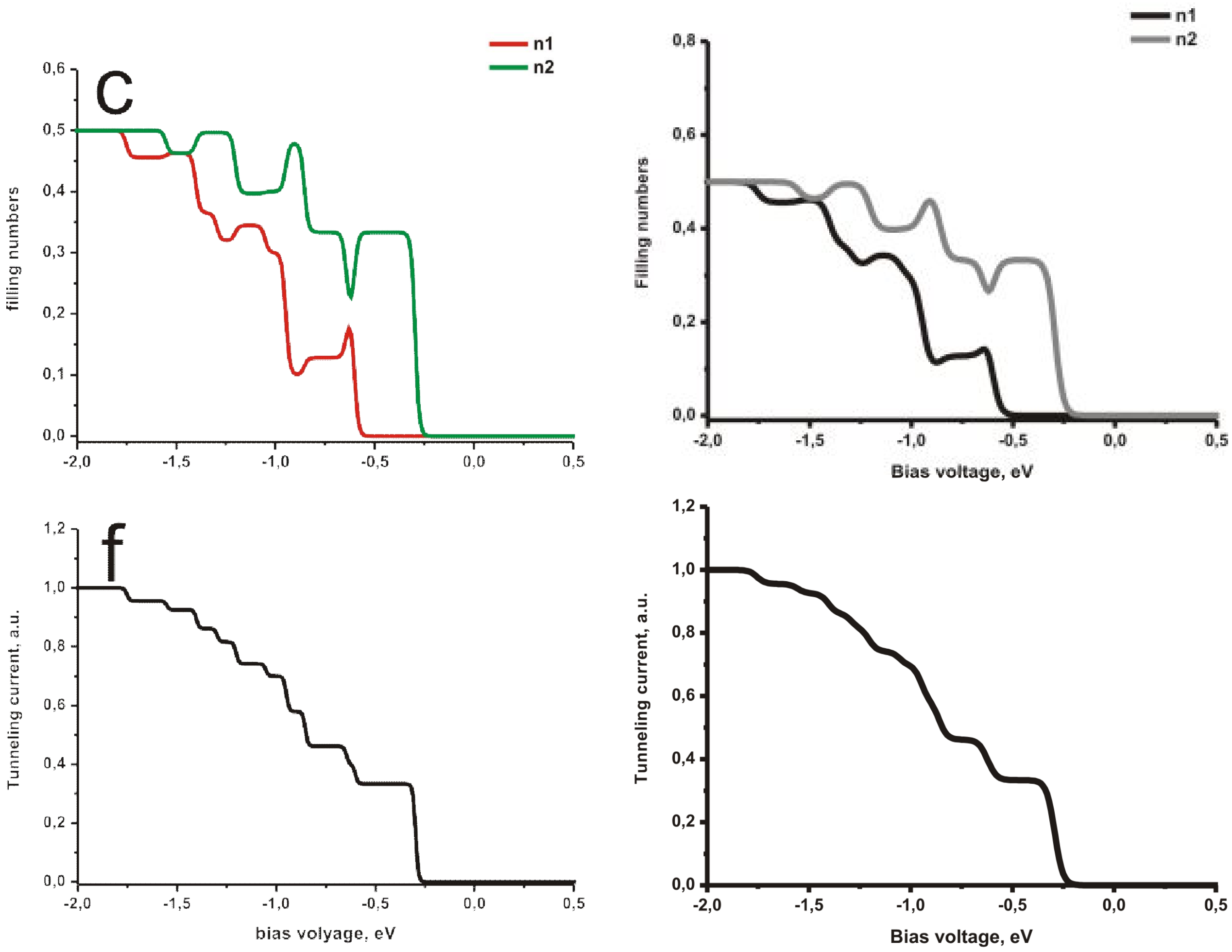
U dependence



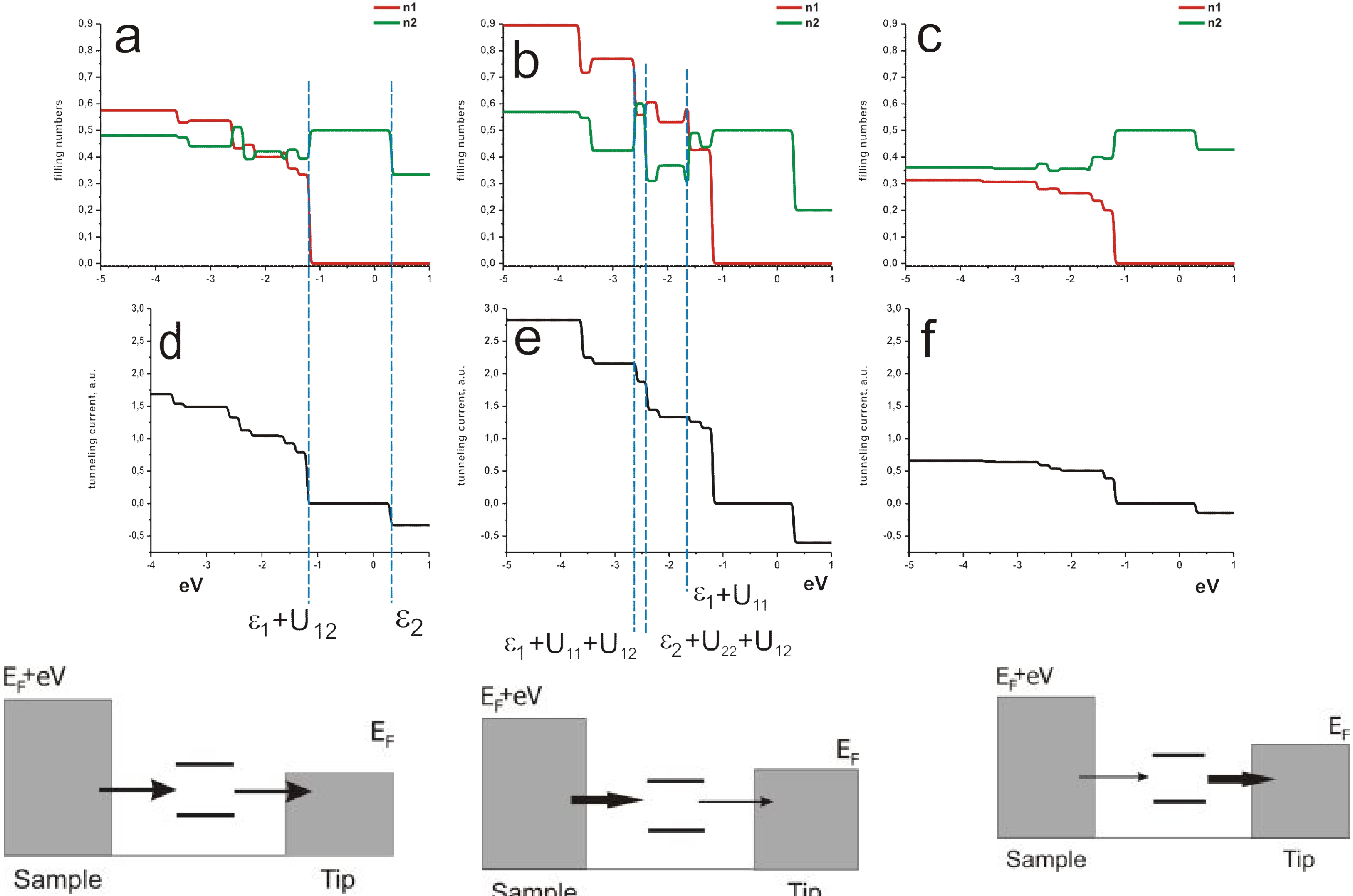
$U_{12} = 1.0 \;\; U_{11} = 1.5 \;\; U_{22} = 1.6 \qquad U_{12} = 0.4 \;\; U_{11} = 0.5 \;\; U_{22} = 0.65 \qquad U_{12} = 0.15 \;\; U_{11} = 0.25 \;\; U_{22} = 0.4$

$$\tau_1 = -0.1 \;\; \tau_2 = -0.3$$

Temperature smoothing

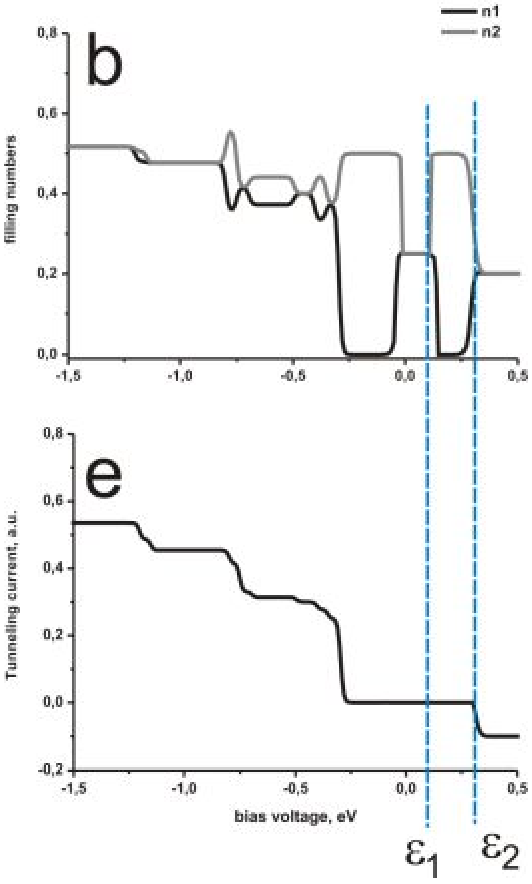


Inverse occupation



$$\tau_1=0.2\ \ \tau_2=-0.3\ \ U_{12}=1.0\ \ U_{11}=1.4\ \ U_{22}=1.7$$

Charge redistribution inside Coulomb blockade step



$$\tau_1 = -0.1 \ \tau_2 = -0.3 \ U_{11} = 0.5 \ U_{22} = 0.65 \ U_{12} = 0.4$$

Negative differential conductivity

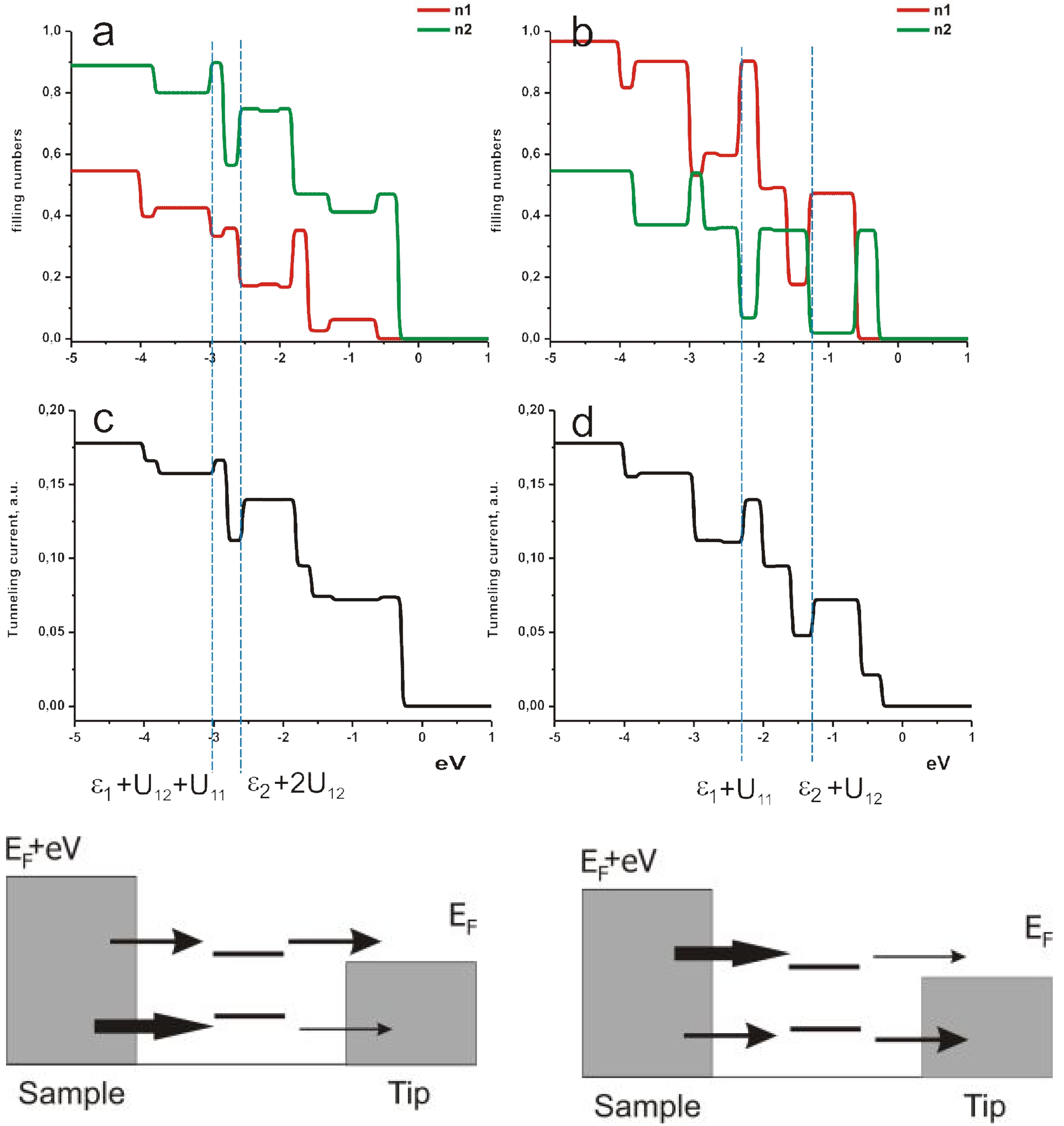
$$\tau_1 = 0.6$$

$$\tau_2 = 0.3$$

$$U_{12} = 1.0$$

$$U_{11} = 1.5$$

$$U_{22} = 1.6$$



Some conclusions

Systems with several states - Coulomb blockade systems with “internal gate” controlled by the tunneling current

Possibility to control charge distribution by tunneling current

Negative differential conductivity