“*Electron transport through degenerate electron level in single-molecular junction in the presence of electron-vibrational coupling and attractive electron-electron correlations*”

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Electron transport through a molecular junction consisted of a single molecule coupled to macroscopic leads is studied in the nonequilibrium regime. The molecule is modeled as a degenerate energy level with an electron-vibrational interaction (EVI) and attractive electron-electron correlation which lifts the degeneracy. The level occupancy and differential conductance are calculated with account of molecule-lead coupling at low temperature and finite voltage.

We assume that the relaxation of the vibrational mode is faster than the tunneling rate so the vibrational mode can relax between each tunneling events according to thermal boson distribution. It is the so called antiadiabatic regime.

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We use the method of the transport spectroscopy which consists of calculating the differential conductance dI/dVsd as a function of the bias voltage, Vsd , and the gate voltage, Vg, that forms the 2D-map which is called the stability diagram. The transport spectroscopy allows a full spectroscopy of the level structure of the molecule.

The cases of doubly degenerate and 4-fold-degenerate orbitals on the molecule were analyzed by calculating stability diagrams for each of the split levels.

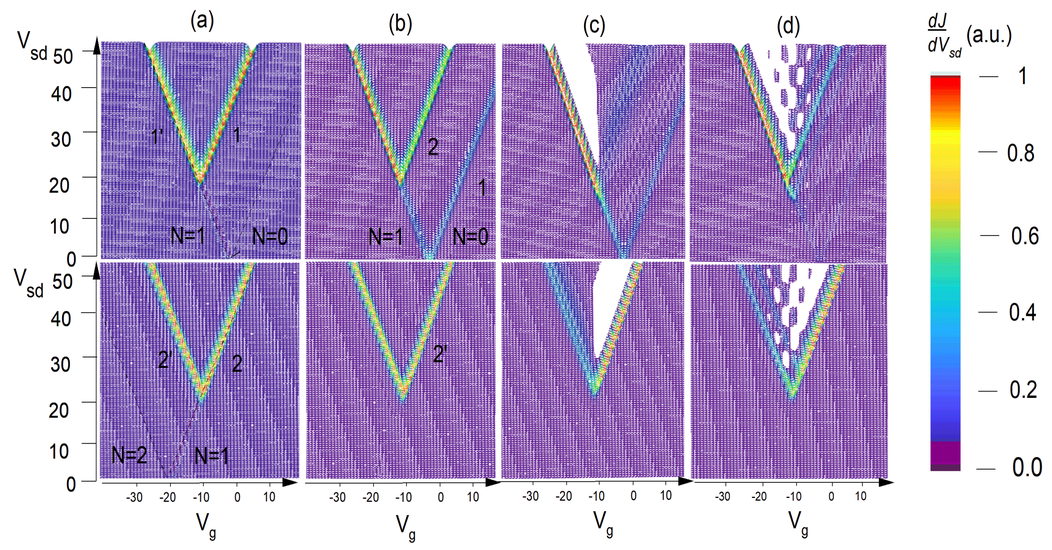

Fig.1. Stability diagrams for the transport of electrons through a doubly degenerate orbital on the molecule that splits by electron-electron interaction.

- The top panel corresponds to tunnelling to two levels (E1 and E2) by the attractive through the level E1 and the bottom level – through the level E2.

Coulomb (a) depicts the case without EVI. The bright lines form the V-shape region that defines the regions of the Coulomb blockade (outside the V-shape) and the steady current (within the V-shape). The edges of the V-shape correspond to the level alignment with the source lead (positive slope) or the drain lead (negative slope).

- When the EVI is included even of a weak strength (coulomb (b)), a new transition appears for the E_1 level beginning with zero bias voltage. This level will be occupied as a result of coupling of electron with vibrons.
- The coulomb (c) shows the case of moderate strength of the EVI. When an electron tunnels from the source lead to the E_1 level (top panel) , the vibrational sidebands are running parallel to the right edge of the V-shape. When electron tunnels from the E_2 level to the drain lead (bottom panel), the vibrational sidebands are running parallel the left edge.
- For the strong EVI (coulomb (d,)) vibrational excitations form a progression of conductance resonances, which become current drops (regions of negative differential conductance (NDC)) as soon as the other orbital contributes to the current.

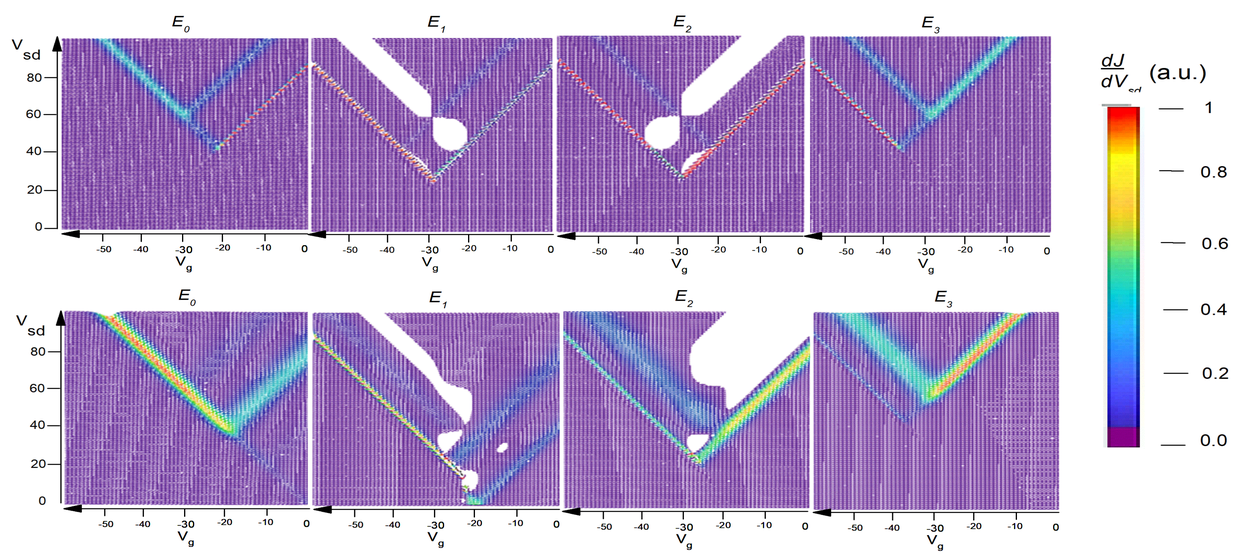

Fig.2. The stability diagrams for the electron transport though the 4-fold degenerate orbital on the molecule that splits into four levels (E_0, E_1, E_2, E_3) by the attractive electron correlations are shown. Top panels correspond to the case without EVI. Bottom panels – to the case with moderate strength of the EVI.

- In the top panel for the level E_1 (**the EVI is absent**), the less intensive line running parallel to the right edge of the V-shape is seen. This line corresponds to the addition of an electron to the orbital where a spin-up electron already present. The incoming electron must have spin-down and it will occupy the excited state. The white line seen in the plot, corresponds to the case, when the spin-up electron tends to occupy the ES-level that already already has a spin-up electron, but it is not permitted by the Pauli principle.
- The V-shape of the E_2-level coincides with that of the level E_1, so the incoming electron has spin-down. The excited state occupies with a spin-up electron. The appearance of the white line has the same reason as for E_1-level.
- Tunneling through levels C and E_3, as seen in the Fig.2, takes place through the excited states: for E_0 – through ES(1), for E_3 – through ES(2). The ES(1) state is aligned to the Fermi level of the S lead, so its width will depend on the thermal spread in contrast to the ES(2) which is situated below the Fermi level.
- If **the EVI is taken into account (**bottom panels in Fig.2), we can see that tunnelling through the levels E_1 and E_2 has common features with the case of doubly degenerate level on the molecule. In the diagram for tunnelling through the E_0 level, we can see that electron flows through several splitting levels because of the thermal distribution. In the case of the E_3 level, the tunnelling occurs through the lowest level and its excited state as in the case without EVI.

The results of the work were published in the journal [1].

- [1] E.A. Ponezha*, Low Temp. Phys*., **2024 ,** V. 50, p. 448.