Forschungszentrum Karlsruhe
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Tunneling transport through molecules and coupled quantum dots

Jasmin Aghassi [1,2], *Axel Thielmann* [1], *Matthias H. Hettler* [1], *Gerd Schön* [1,2]

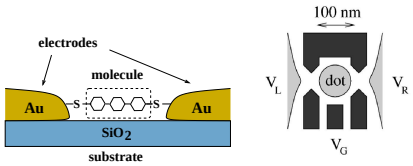
[1] Forschungszentrum Karlsruhe, Institut für Nanotechnologie

[2] Institut für Theoretische Festkörperphysik, Universität Karlsruhe

I. Motivation

- Quantum dots and molecules as potential building blocks for future nanoelectronic devices
- Problem: coupling of molecule to electrodes unknown and not easily controllable in nanoscopic devices.
- Combined measurement of current and shot noise provides additional information about couplings, interaction, etc.

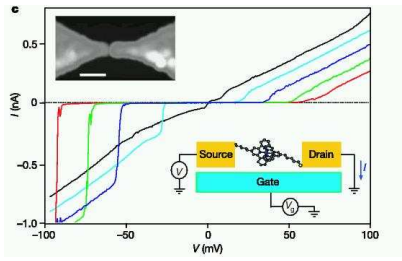
II. Physical Realization



l.h.s.: deposition of molecule between two fixed electrodes (Reed et al., Science **278**, 252 (1997))

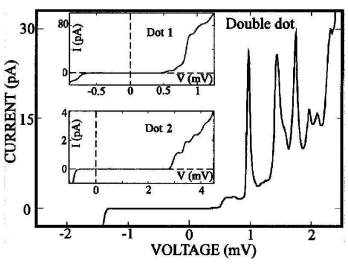
r.h.s.: schematic picture of a lateral quantum dot structure

III. Experiments



J. Park , A.N. Pasupathy, *et.al.*, Nature **417**, 722 (2002)

- electrodes probed via electron beam lithography and electromigration
- molecule is a Co ion bonded to ligands → coupling to the electrodes can be controlled

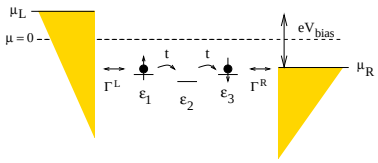


van der Wiel *et al.*, Rev. Mod. Phys. **75**, 1 (2003)

- lateral coupled quantum dots ("artificial molecules")
- single-electron phenomena such as Coulomb blockade observed

IV. Model

Sketch of couplings for three coupled quantum dots



- $\hat{H} = \hat{H}_{\rm L} + \hat{H}_{\rm R} + \hat{H}_{\rm dots} + \hat{H}_{\rm T,L} + \hat{H}_{\rm T,R}$ with:

$$\hat{H}_r = \sum_{k\sigma} \varepsilon_{k\sigma r} a^\dagger_{k\sigma r} a_{k\sigma r},$$

$$\hat{H}_{{\rm T},r} = \sum_{ik\sigma} (t_i^r a^\dagger_{k\sigma r} c_{i\sigma} + h.c.),$$

$$\hat{H}_{\rm dots} = \sum_{i\sigma} \varepsilon_i n_{i\sigma} - t \sum_{<ij>\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.)$$
$$+U \sum_i n_{i\uparrow} n_{i\downarrow} + U_{nn} \sum_{<ij>\sigma\sigma'} n_{i\sigma} n_{j\sigma'}$$

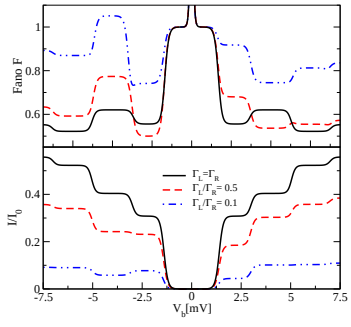
- $\hat{H}_{\rm L}$, $\hat{H}_{\rm R}$: left and right electrode with non-interacting electrons ($r = {\rm L}, {\rm R}$).
- $\hat{H}_{\rm dots}$: molecule or dot term with i (spin-dependent) molecular sites ($n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$).
- $\hat{H}_{\rm T,L}$, $\hat{H}_{\rm T,R}$: tunneling between the dot system and electrodes.
- Energies: level energies (ε_i), intra-dot (U) and inter-dot (U_{nn}) Coulomb repulsion, kinetic (hopping) energy t)
- coupling strength $\Gamma_i^r = 2\Pi |t_i^r|^2 \rho_e$ with t_i^r being the tunneling amplitude and ρ_e is DOS

V. Numerical Results

A. Two coupled quantum dots

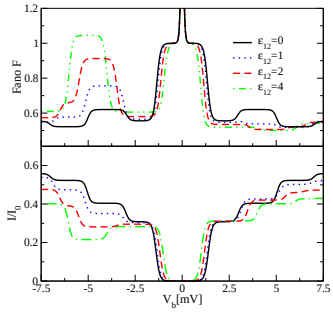
Fano factor $F = \frac{S}{2eI}$ for symmetric bias voltage and $\varepsilon_1 = \varepsilon_2 = -5.5, t = 2, U = 10, U_{nn} = 5$, $k_{\rm B}T = 0.05$ (all units in meV). Step positions determined by energy parameters and plateau heights by couplings $\Gamma_{\rm L}, \Gamma_{\rm R}$. The total coupling scale is set to $\Gamma_R = 0.05 k_B T$.

Asymmetric coupling $\Gamma_{\rm L} \neq \Gamma_{\rm R}$



For strong asymmetries super-Poissonian Noise (F>1) and negative differential conductance (NDC) develop at the same bias (energy) positions

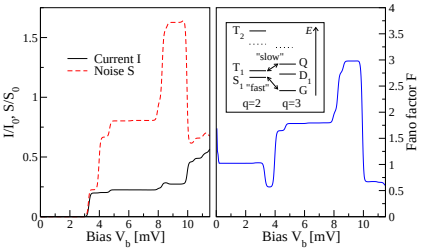
Strong level detuning, in particular $\varepsilon_{12} = \varepsilon_1 - \varepsilon_2 > t$, leads to super-Poissonian noise and NDC



B. Three coupled quantum dots

Strong non-local Coulomb interactions $U_{nn} > t$

Current and Noise for symmetric coupling $\Gamma_{\rm R} = \Gamma_L$ with parameters $\varepsilon_i = -10$, $t = 2$, $U = 10$, $U_{nn} = 5$, $k_{\rm B}T = 0.025$ (units in meV) and more complex many body wavefunctions (Singlets S, Doublets D, Triplets T, Quadruplets Q)

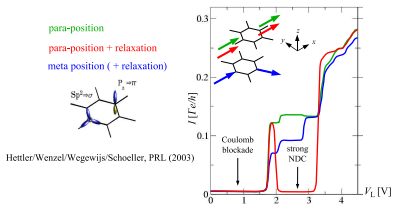


Super-Poissonian noise and Fano factors without simultanous suppression of the current

→ competition of "fast" and "slow" transport channels leads to strongly enhanced noise
→ effect depends on the ratio $\frac{U_{nn}}{t}$ and is entirely due to internal electronic level structure

C. Towards a description of Molecules

Six site model for aromatic molecules like benzene rings including relaxation processes of photons



Transport highly sensitive to different coupling positions (para and meta position)

In the case of paraposition strong NDC is observed → occupation of a blocking state of the molecule

References:

Thielmann *et. al.*, Phys. Rev. Lett. **95**, 146806 (2005), Aghassi *et. al.*, Phys. Rev. B **73**, 195323 (2006), Aghassi *et. al.* cond-mat/0505345 (to be published in Appl. Phys. Lett.)