CB Conductance Peak Spacings: Interplay of Spin and Dot-Lead Coupling

Serguei V. Vorojtsov and Harold U. Baranger

Department of Physics, Duke University, Box 90305, Durham NC 27708-0305, USA

GOAL: Determine How Peak Spacings Change as Dot-Lead Coupling, $|t|^2$ Increases

CONCLUSION: Even/Odd Parity Effect is Smaller For Real Quantum Dots Than For Ones Described by CI Model

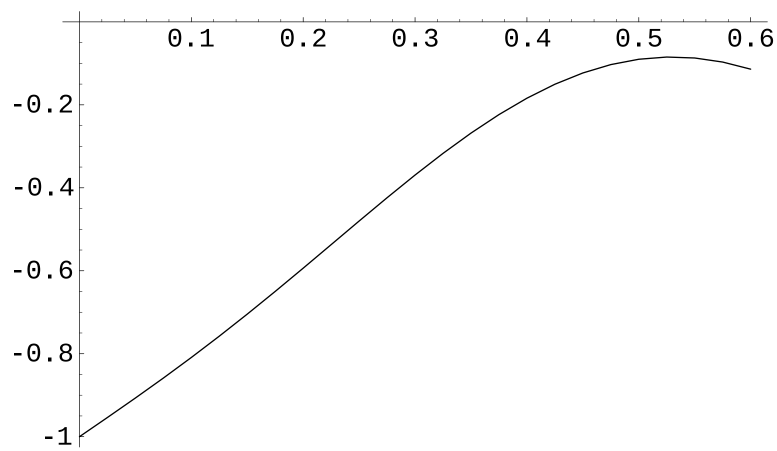
RESULT

$U \equiv$ peak spacing normalized by $2E_c$. Odd spacing change:

$$\left\langle U_{odd}^{(2)} \right\rangle = \frac{g_L + g_R}{8\pi^2} \frac{\Delta}{E_C} \left[C_T(j) \ln \frac{2E_C}{T} + C_\Delta(j) \ln \frac{2E_C}{\Delta} + O(1) \right]$$

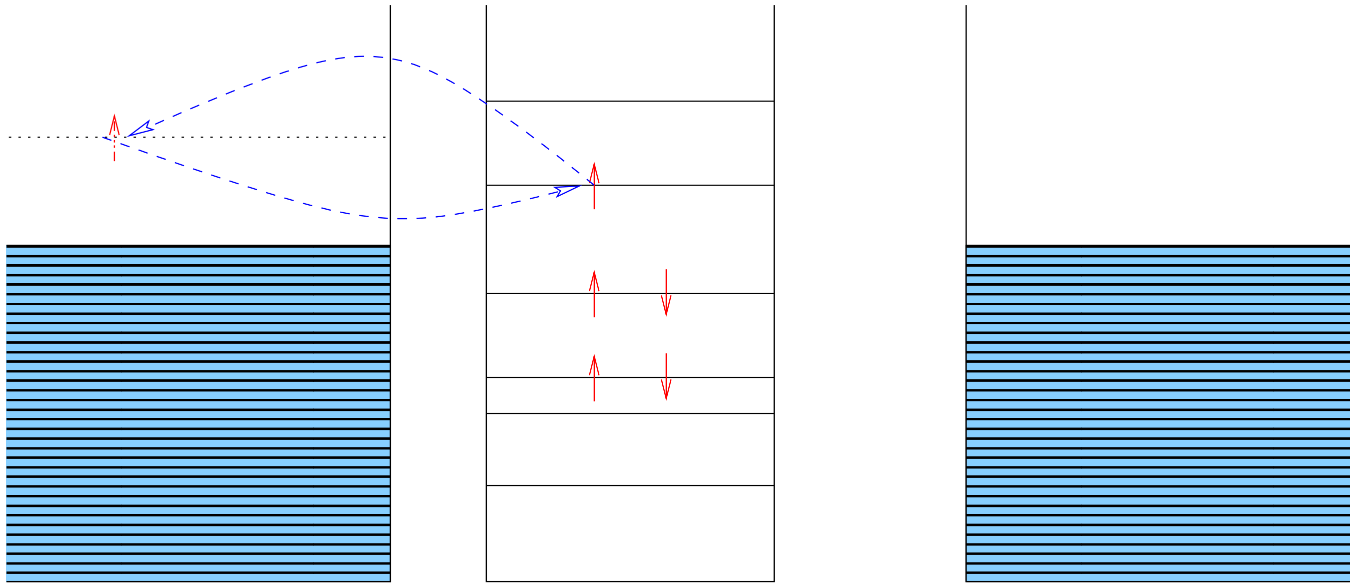
where $j \equiv J_s/\Delta$ – exchange interaction constant normalized by mean single-particle spacing.

Plot of $\left\langle U_{odd}^{(2)} \right\rangle \Big/ \left| \left\langle U_{odd}^{(2)} \right\rangle_{j=0} \right|$ **at** $E_c/\Delta = 20$**,** $\Delta/T = 10$**:**



VIRTUAL EXCITATIONS

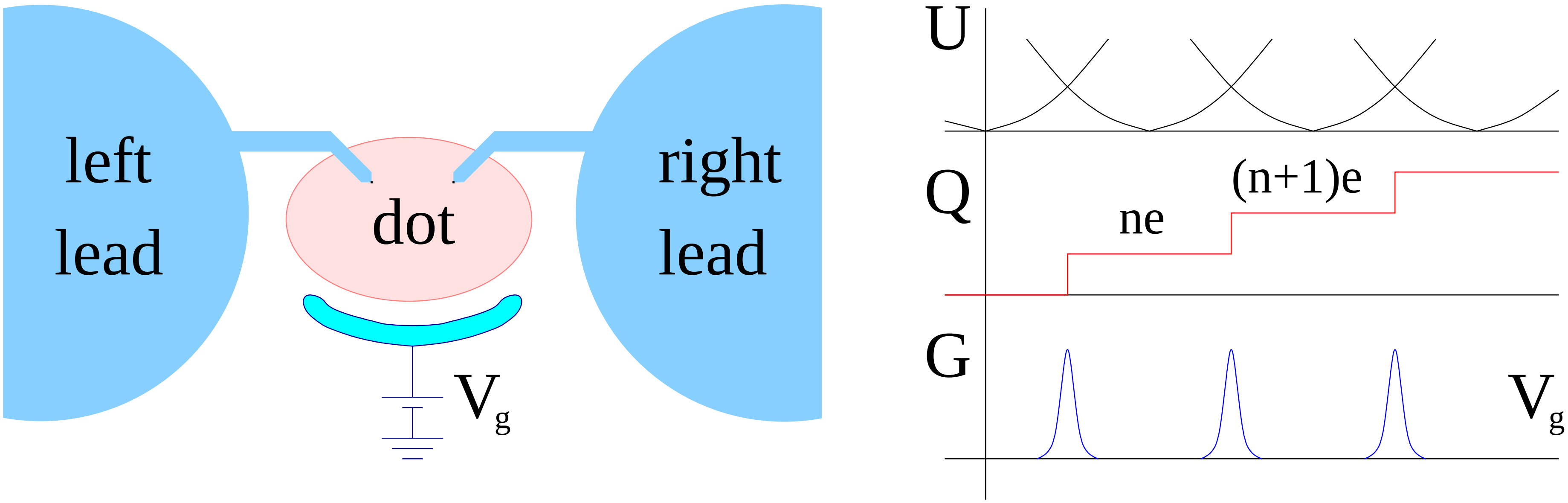
Dot-lead coupling changes states of the system:



- most dramatic: Kondo effect
- here: *virtual excitations* change energy of dot

⇒ study through Coulomb blockade peak spacings

COULOMB BLOCKADE PEAK SPACING



- weakly coupled leads: Q jumps sharply $(G_{L,R} \ll \frac{e^2}{h};\ T \ll \frac{e^2}{C})$
- Q jumps and G has peak when:

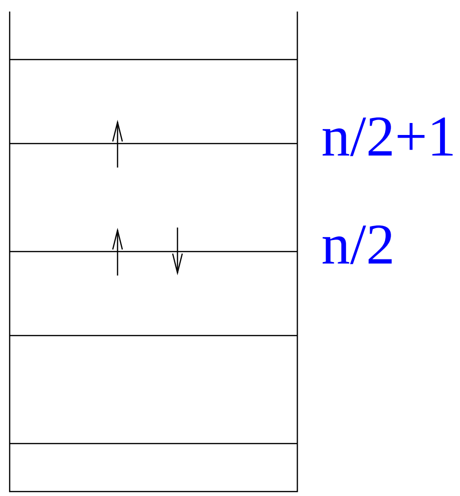
$$E_{gr}(n) - \frac{C_g}{C} enV_g^* = E_{gr}(n+1) - \frac{C_g}{C} e(n+1)V_g^*$$

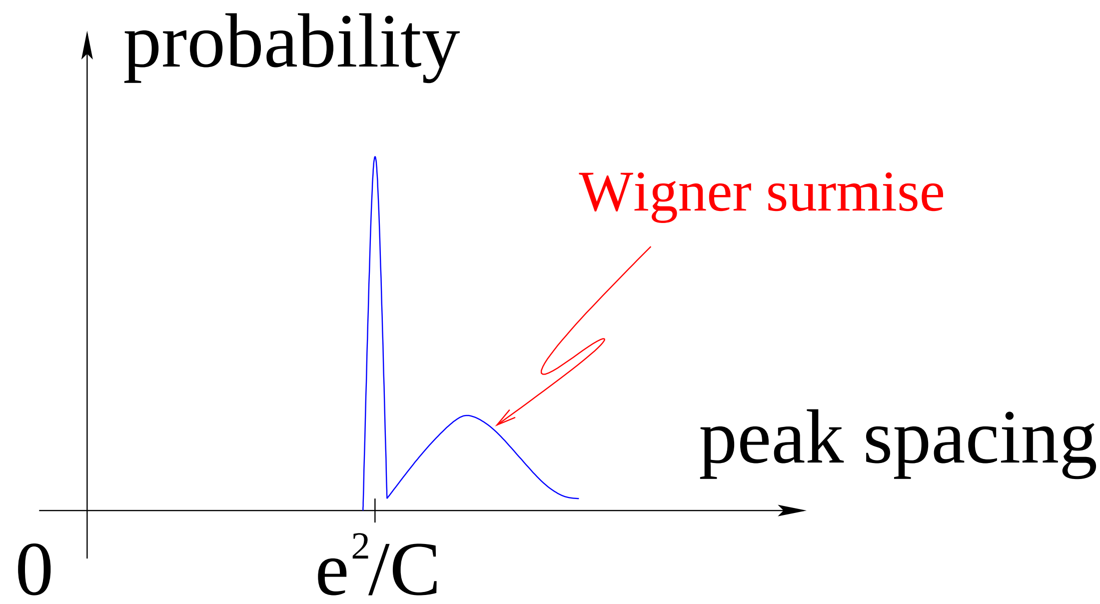
- position $\propto E_{gr}(n+1) - E_{gr}(n)$; spacing $\propto \Delta^2 E_{gr}(n)$

MODEL FOR E_{gr}: CONSTANT INTERACTION

$$\hat{H}_{CI} = \underbrace{\sum_{\alpha\sigma} \epsilon_\alpha \hat{n}_{\alpha\sigma}}_{\text{SINGLE PARTICLE}} + \underbrace{\frac{e^2\hat{n}^2}{2C}}_{\text{CHARGING}} \Rightarrow \Delta^2 E_{gr} = \begin{cases} \frac{e^2}{C}, & n \text{ is odd} \\ \frac{e^2}{C} + \epsilon_{\frac{n}{2}+1} - \epsilon_{\frac{n}{2}}, & n \text{ is even} \end{cases}$$

- chaotic dot $\Rightarrow$ take $\{\epsilon_\alpha\}$ from Random Matrix Theory (RMT)





Large even/odd parity effect!

MODEL FOR E_{gr}: UNIVERSAL HAMILTONIAN

$$\hat{H}_{UH} = \sum_{\alpha\sigma} \epsilon_\alpha \hat{n}_{\alpha\sigma} + E_c \hat{n}^2 \underbrace{-J_s \hat{\mathbf{S}}^2}_{\text{EXCHANGE!}}$$

Derivation: RMT for single particle + RPA for interactions

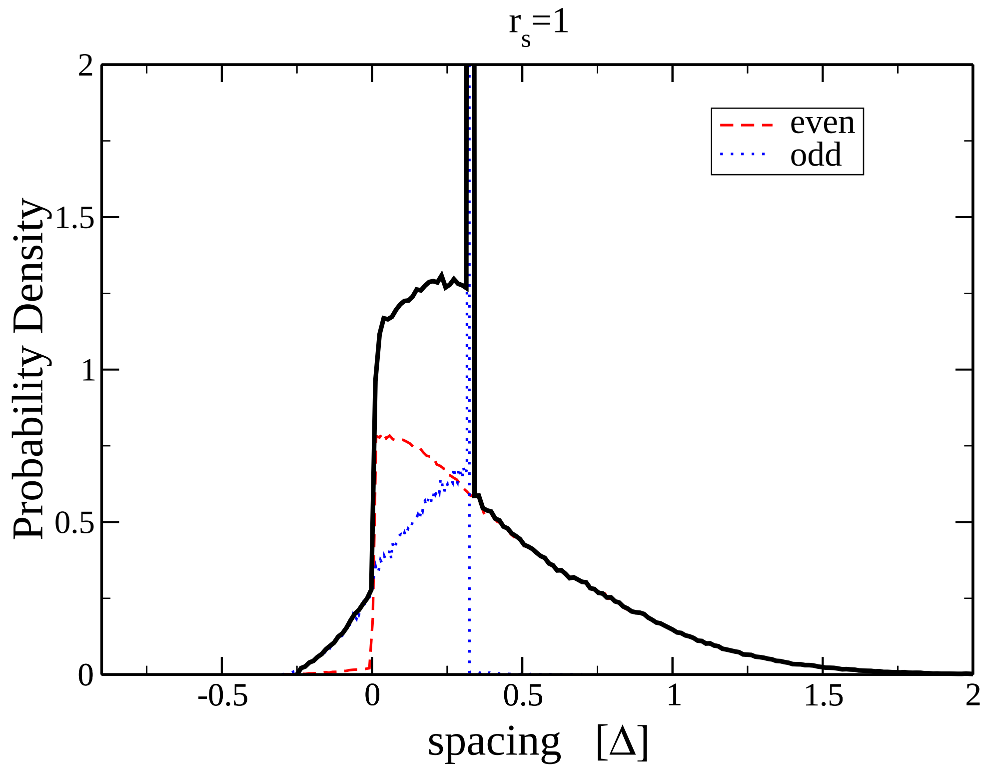
[for review see Aleiner, Brouwer and Glazman, cond-mat/0103008]

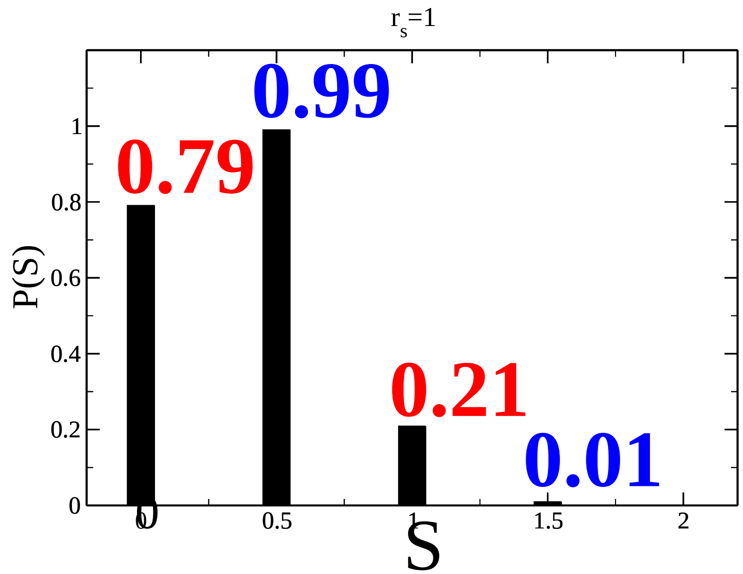
Has 3 energy scales:

- $E_c \equiv e^2/2C$ is largest
- $\Delta \equiv$ mean single-particle spacing $\ll E_c$
- $J_s < \Delta$ (example: $J_s = 0.32\Delta$ for $r_s = 1.5$ in RPA)

Important: $-J_s\hat{\mathbf{S}}^2$ term causes $S > 1/2$ (Hund's rule)

Peak Spacing Distribution Within $\hat{H}_{UH}$





[from Denis Ullmo and Harold U. Baranger, cond-mat/0103098]

Big deviation from CI model: even/odd effect smaller

- $S > 1$ not needed for $r_s \lesssim 1.5$

DOT-LEAD COUPLING EFFECT

Virtual excitations shift ground state:

- condition for peak positions (spacing) acquire corrections

In CI model:

- substantial effect
- peak spacing shift of order $\Delta \times \frac{g_{dot-lead}}{2\pi^2} \ln \frac{2E_c}{T}$
- increases even/odd parity effect

[Alexei Kaminski and Leonid I. Glazman, Phys. Rev. B. **61**, *15927 (2000)]*

But CI model is wrong:

- $S > 1/2$ in valleys are possible
- position of $n^{th}-$peak depends on *spin sequence:* $(S_n \to S_{n+1})$
- n^th-valley peak spacing depends on: $(S_{n-1} \to S_n \to S_{n+1})$

What is the effect within Universal Hamiltonian Model?

OUR MODEL

Hamiltonian: $\hat{H} = \hat{H}_{dot} + \hat{H}_{leads} + \hat{H}_{tun}$

- $\hat{H}_{dot} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + E_c(\hat{n} - N)^2 - J_s \hat{\mathbf{S}}^2$
- $\hat{H}_{leads} = \sum_{p\sigma} \epsilon_p \hat{n}_{p\sigma} + \sum_{q\sigma} \epsilon_q \hat{n}_{q\sigma}$
- $\hat{H}_{tun} = \sum_{kp\sigma} t_{kp}(\hat{c}^{\dagger}_{k\sigma}\hat{c}_{p\sigma} + h.c.) + \sum_{kq\sigma} t_{kq}(\hat{c}^{\dagger}_{k\sigma}\hat{c}_{q\sigma} + h.c.)$

is considered as a pertubation

Model assumptions:

- $T_K < T \ll \Delta \ll E_c, \quad T_K$ is Kondo temperature
- $G_{L,R} \ll e^2/h$
- J_s is small $\Rightarrow S > 1$ not needed
- $\delta\epsilon_{n/2}$ and $\delta\epsilon_{n/2+l}$ are uncorrelated if $l > 1$, $\delta\epsilon_{n/2} \equiv \epsilon_{n/2+1} - \epsilon_{n/2}$

IDEA OF OUR CALCULATION

2 ingredients in average odd peak spacing, $\langle U_{odd} \rangle$:

- *peak spacing* for given spin sequence, $e.g.\ \ U(0 \to 1/2 \to 1)$
- *probability* that spin sequence occurs, $e.g.\ \ P(0 \to 1/2 \to 1)$

$$\langle U_{odd} \rangle = \sum_{spin\ seqs.} P(seq.)\ \ U(seq.)$$

Peak Spacing For Given Spin Sequence:

- dimensionless gate voltage: $N \equiv C_g V_g / e$
- $(n+1)^{st}$ peak occurs at $N^{(0)}_{n+1}$: $E^{(0)}_n(N^{(0)}_{n+1}) = E^{(0)}_{n+1}(N^{(0)}_{n+1})$

where $E^{(0)}_{n+1}(N)$ is eigenvalue of $\hat{H}_0 = \hat{H}_{dot} + \hat{H}_{leads}$

$\Rightarrow N^{(0)}_{n+1}$ depends on S_n and S_{n+1}

- $U^{(0)}_{n+1} = N^{(0)}_{n+2} - N^{(0)}_{n+1}$ *depends on* $(S_n, S_{n+1}, S_{n+2})-$*sequence*

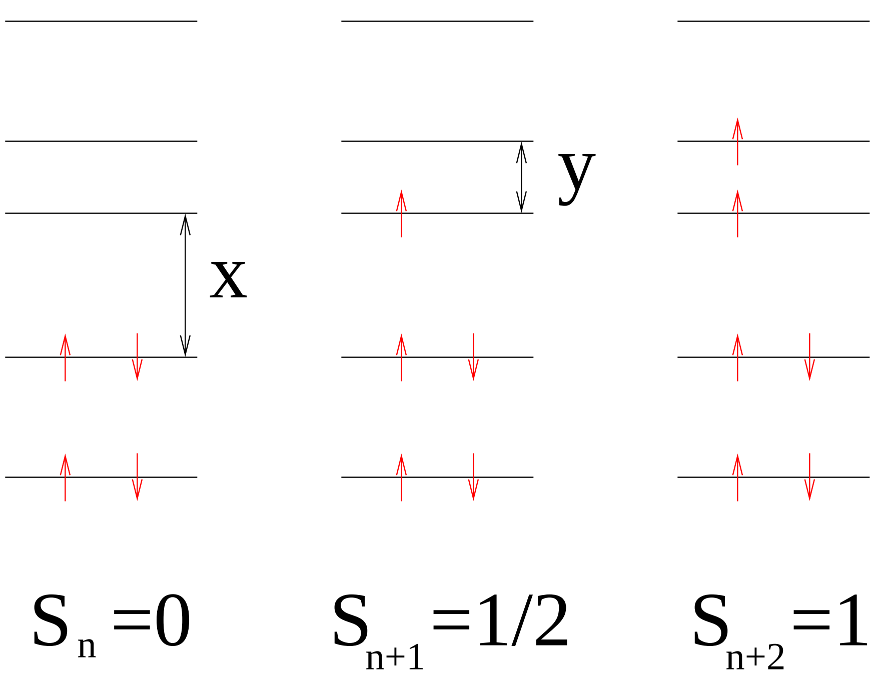
Probability of Spin Sequence In Odd Case:

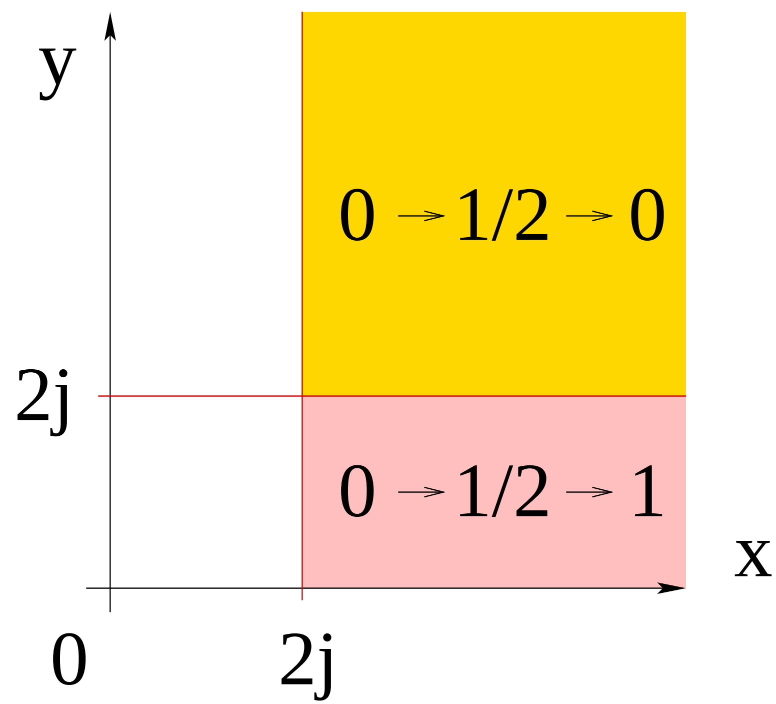
- depends on 2 adjacent level spacings in the dot, *e.g.*

if $x > 2j$ and $y < 2j \Rightarrow (0 \rightarrow 1/2 \rightarrow 1)$ occurs

- RMT gives $P(x, y)$ distribution

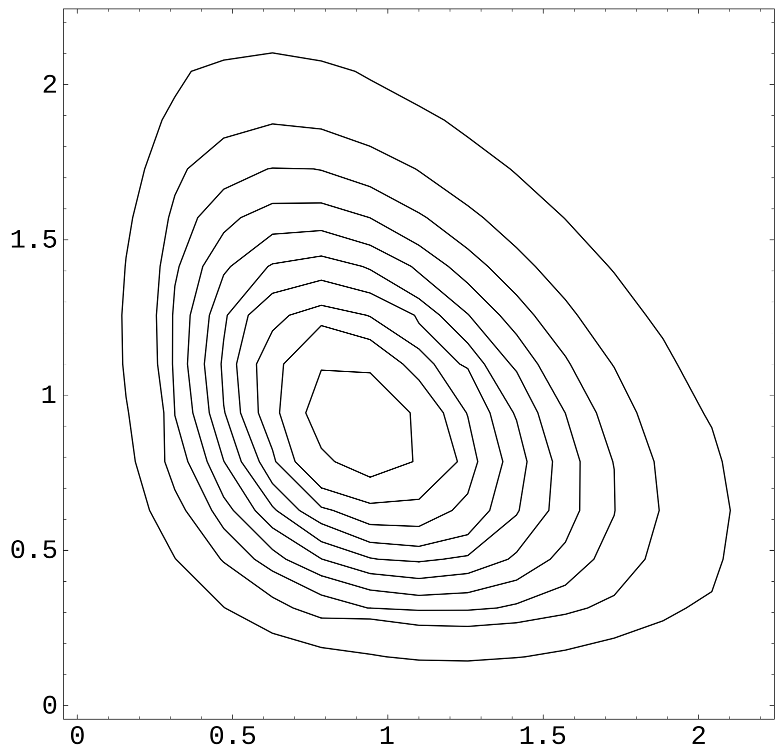
- $$P^{(0)}(seq.) = \underbrace{\int\int}_{\text{SEQ. REGION}} dx\, dy\, P(x,y)$$





$P(x,y)$ is derived using 3×3 random matrix in GUE:

$P(x,y) = Ax^2y^2(x+y)^2e^{-\alpha(x^2+y^2+xy)}$, where $A \approx 7.94$, $\alpha \approx 1.21$



[Damir Herman and Harsh Mathur, unpublished (2001)]

- This formula proved to be a good approximation

[D. Herman, H. Mathur, G. Usaj, T. Ong, H. Baranger, unpublished (2001)]

DOT-LEAD COUPLING

changes both peak spacings and spin sequence probabilities

Change In Peak Spacings

- due to *virtual excitations* energy changes: $E_{n+1} = E^{(0)}_{n+1} + E^{(2)}_{n+1}$
- peak positions get corrected, *e.g.* $N^{(2)}_{n+1}\left(0 \to \frac{1}{2}\right)$

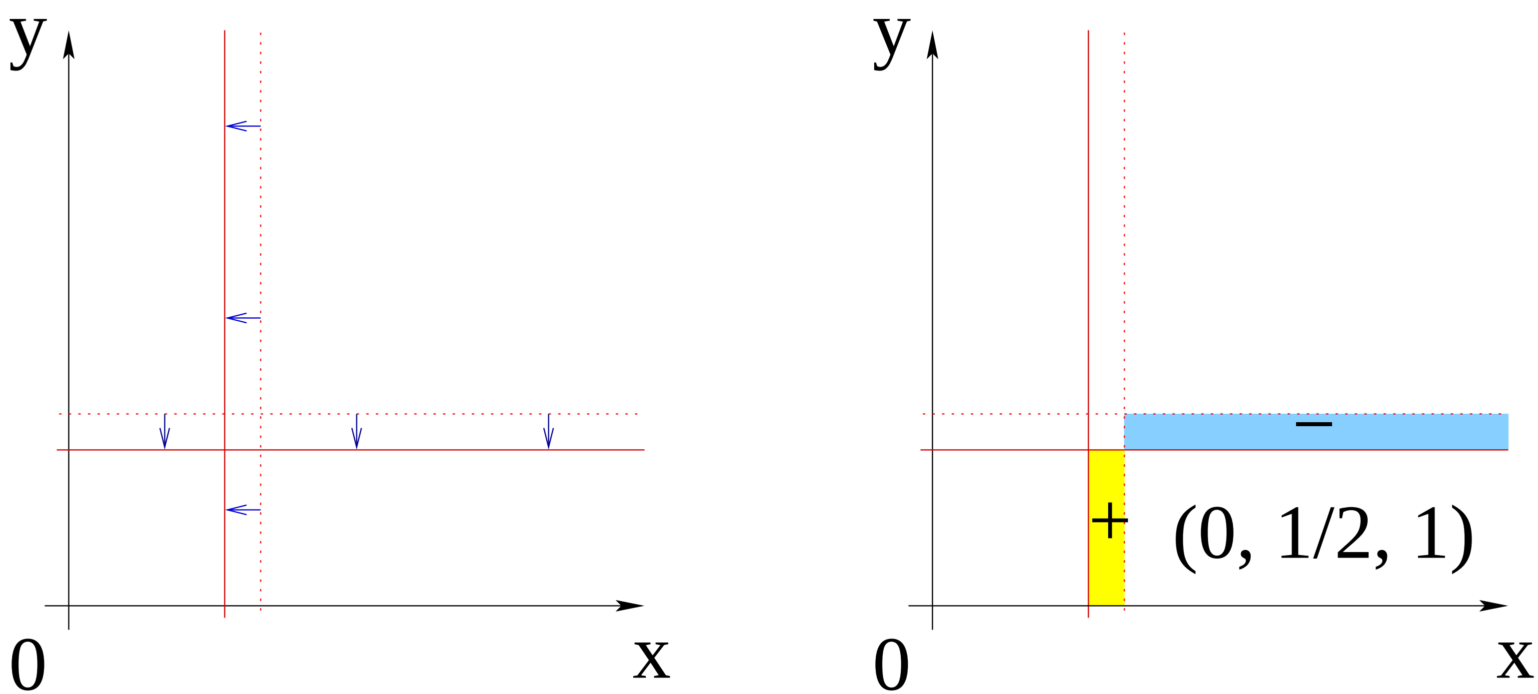
$$= \frac{1}{8\pi^2}\frac{\Delta}{E_c}\sum_{\alpha=L,R} g_\alpha \left[-2\sum_{k\neq\frac{n}{2}+1} sign(\epsilon_{\frac{n}{2}+1}-\epsilon_k)\frac{|\psi_k(\mathbf{r}_\alpha)|^2}{\left\langle|\psi_k(\mathbf{r}_\alpha)|^2\right\rangle}\ln\left(\frac{2E_c}{\left|\epsilon_{\frac{n}{2}+1}-\epsilon_k\right|}+1\right)\right.$$
$$\left. + \frac{\left|\psi_{\frac{n}{2}+1}(\mathbf{r}_\alpha)\right|^2}{\left\langle\left|\psi_{\frac{n}{2}+1}(\mathbf{r}_\alpha)\right|^2\right\rangle}\ln\frac{2E_c}{T} + \frac{3}{2}\sum_{k=\frac{n}{2}-\frac{2E_c}{\Delta}+1}^{\frac{n}{2}}\frac{|\psi_k(\mathbf{r}_\alpha)|^2}{\left\langle|\psi_k(\mathbf{r}_\alpha)|^2\right\rangle}\ln\left(1-\frac{2J}{\epsilon_{\frac{n}{2}+1}-\epsilon_k}\right)\right]$$

- as well as peak spacings: $U_{n+1} = U^{(0)}_{n+1} + U^{(2)}_{n+1}$

Change In Spin Sequence Probabilities

- $E_n^{(0)}(S=0) = E_n^{(0)}(S=1) \Rightarrow \epsilon_{n/2+1} - \epsilon_{n/2} = 2J_s \; (x = 2j)$
- *virtual excitations* change energies by $E_n^{(2)}(S)$

$\Rightarrow$ boundaries shift: $x' = 2j - (2\pi)^{-2}(g_L + g_R) \ln(2J_s/T)$



- spin sequence probabilities acquire corrections, *e.g.*

$$P^{(2)}(0,1/2,1) = \underbrace{\int\int}_{+\ \text{REGION}} dx\, dy\, P(x,y) - \underbrace{\int\int}_{-\ \text{REGION}} dx\, dy\, P(x,y)$$

Comment: Calculating $E^{(2)}$ we sum over all virtual processes. Logarithms in $U^{(2)}$ and $P^{(2)}$ is the result of integration over continuous states in the leads.

Adding Up Two Contributions

averaged odd spacing change:

$$\left\langle U^{(2)}_{odd} \right\rangle = \sum_{spin\ seqs.} \left\{ P^{(0)}(seq.)U^{(2)}(seq.) + P^{(2)}(seq.)U^{(0)}(seq.) \right\}$$

- both contributions are of the same order

averaged even spacing change: $\left\langle U^{(2)}_{even} \right\rangle = -\left\langle U^{(2)}_{odd} \right\rangle$