The Kondo state in quantum point contacts and the local moment in semiconductor quantum dots - two sides of the same phenomenon.

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(February 9, 2022)

This is a three step work: i) we explain why quantum point contacts are similar to ballistic quantum dots; ii) we introduce the virtual Kondo state in both systems; iii-1st) this state explains 0.7 structure in point contacts; iii-2nd) formation of the local moment on this state is described by the nearly symmetric Anderson model, we solve it for finite size system having in mind quantum dots. We found one large level spacing \( \Delta^* \propto (U/\Gamma)^{1/2} \gg \Delta \), where \( U \) is the charging energy of the virtual state, \( \Gamma \) is the spectral width of this state and \( \Delta \) is the mean level spacing of whole system. The theory explains periodicity of abnormal level spacing vs gate potential. The theory is in agreement with many experiments.

I. WHY QUANTUM POINT CONTACTS ARE SIMILAR TO CHAOTIC QUANTUM DOTS.

In this work we develop common view on two types of experiments, first, differential conductivity of quantum point contacts [1–3], and second, fluctuations of level spacing in semiconductor quantum dots [4–8]. The challenge in the former case is to understand the plato of differential conductance \( dI/dV \approx 0.7(2e^2/h) \), which indicates presence of the Kondo state [3]. The Kondo state can appear from a magnetic impurity, as in the case of metallic point contact [10], however the point contact was made by electrodes on top of clean 2d electron gas [1–3].

There are two possibilities: either magnetic moment is formed on the localized Kondo state or the magnetic moment is formed due to the Stoner instability of electron system [12–14]. However, the clean semiconductor quantum dots do not have magnetic impurities and formation of the Kondo state is unrealistic. The Stoner instability occurs under very restrictive condition met only in some experiments [16,17].

The anticipated Kondo state can be found in both systems, quantum point contact and semiconductor quantum dot, as a virtual state bouncing along shortest axis of the system. This state is marked by dashed line in Fig. 1a for contact geometry and in Fig. 1b for real potential of rectangular quantum dot [18,19]. We assume that the system is ballistic, \( l \gg l_p \), where \( l \) is the mean free path and \( l_p \) is the length of the virtual state. This state is very unstable indeed, the electron lifetime on such orbit \( h/\Gamma \) is of the order of the time of flight \( l_p/v_F \), in other words level uncertainty of such state is of the order of level spacing \( \Gamma \sim \pi h^2 k_F/m l_p \),

where \( k_F \) is the Fermi momentum and \( m \) is the effective mass. This state is important for two main reasons i) it has good coupling to all other “chaotic” wave functions spread across whole system; the enhancement factor is approximately \( \log(k_F l_p) \).

In this way conductance of the point contact at zero bias is given by resonant conductance of Kondo state. The level spacing of the quantum dot is almost the same as of a non-interacting system. When the Fermi level reaches “symmetric” limit position, the virtual state can be doubly occupied. The system becomes effectively non-interacting. At this gate potential one observes kink of the level spacing in the

FIG. 1. Local moment (Kondo state) is formed on unstable periodic trajectory between tips of quantum point contact (a) or across quantum dot (b). This orbit traps electrons for some time and have high charging energy.

The sweep of the gate potential in both dots and contacts raise the Fermi level; the singly occupied Kondo state floats on the Fermi level [20]. In this way conductance of the point contact at zero bias is given by resonant conductance of Kondo state. The level spacing of the quantum dot is almost the same as of a non-interacting system. When the Fermi level reaches “symmetric” limit position, the virtual state can be doubly occupied. The system becomes effectively non-interacting. At this gate potential one observes kink of the level spacing in the
II. HAMILTONIAN OF THE VIRTUAL STATE.

Single electron wave functions $\psi_j(\vec{r})$ of a classically chaotic system are inhomogeneous. Consider an unstable periodic orbit $p$ in a system with two degrees of freedom. Such an orbit contributes to the density of states at the energy $\epsilon$ the sum

$$\frac{-T_p}{2\pi\hbar}\Im\sum_{n=1}^{\infty}\frac{1}{\sinh(\Lambda_p m/2)}e^{imS_p(\epsilon+i\theta)/\hbar},$$

(1)

where $T_p = \partial S_p/\partial \epsilon$ is the period of the orbit, $S_p(\epsilon)$ is the action of the orbit, $\Lambda_p > 0$ is the bent symmetry exponent.

Let us assume that $p$ is the only periodic orbit in the system. In this particular case $p$ contributes a sequence of Lorentzians $\sum_n^\Lambda_p \hbar$ to the density of states:

$$\sum_n T_p(\epsilon) \frac{\Lambda_p \hbar}{[S_p(\epsilon) - 2\pi n \hbar]^2 + (\Lambda_p \hbar/2)^2}.$$  

(2)

Each term in the sum can be regarded as the spectral function of the “scar” state

$$A_n(\epsilon) = \frac{1}{\pi} \frac{\Gamma_n}{(\epsilon - \epsilon_n)^2 + \Gamma_n^2},$$

(3)

where $\Gamma_n = \Lambda_p \hbar/(2T_p(\epsilon_n))$.

This spectral function tell us that it is possible to construct a non-stationary solution $\psi_n(\vec{r})$ to the Schroedinger equation in the vicinity of orbit $p$. This solution, let us call it “scar”, would decay to “flat” states with the rate $\Gamma_n/\hbar$. The matrix elements of the decay process $V_{jn}$ are not known, but it is clear that

$$\Gamma_n = \pi \sum_j |V_{jn}|^2 A_n(\epsilon_j),$$

(4)

where $\epsilon_j$ are energies of the exact wave functions. Fortunately we will not need explicit values of $V_{jn}$ in further calculations.

In what follows let us assume that electrons fill the system up to the Fermi energy at zero temperature. Let $n = 1$ is the first “scar” state below the Fermi energy $E_F$. The Hamiltonian for states in the vicinity of the Fermi level is

$$\hat{H} = \sum_{\sigma} \left\{ \epsilon_j a_{j\sigma}^\dagger a_{j\sigma} + V_{jn} a_{j\sigma}^\dagger a_{n\sigma} + \text{h.c.} \right\},$$

(5)

$$D_d = (\epsilon_d + \epsilon_{d-1})/2,$$

(6)

and formulation of the Anderson impurity model is accomplished by adding the correlation energy

$$\hat{H}_{\text{corr}} = U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow},$$

(7)

with

$$U = \int d\vec{r}_1 d\vec{r}_2 |\psi_d(\vec{r}_1)|^2 |\psi_d(\vec{r}_2)|^2 \frac{\epsilon^2}{|\vec{r}_1 - \vec{r}_2|^2}.$$  

(8)

It should be much larger than the charging energy of the dot, $U_j$, given in general by

$$U_j = \int d\vec{r}_1 d\vec{r}_2 |\psi_j(\vec{r}_1)|^2 |\psi_j(\vec{r}_2)|^2 \frac{\epsilon^2}{|\vec{r}_1 - \vec{r}_2|^2}.$$  

(9)

and almost the same for all flat states $\psi_j$.

The contribution of $p$ to the Green function of the non-interacting system has the form $G(r, r') \sim e^{iW(x) y^2/\hbar}$, where $W(x)$ is the coordinate along the orbit $p$, the $y$ axis is perpendicular to the orbit $p$ at the point $x$, and $W(x)$ is connected with the second derivatives of the action. Then, the width of the “scar” state is estimated as $\sim \sqrt{\hbar/W}$. It is clear that $W(x) \sim k|\vec{r}|$, where $k = 2\pi m e\hbar^2/\hbar$ and $m$ is the mass of the particle, see for example the analysis of chaotic billiards.

The integral Eq. (6) for the wave function concentrated in the rectangle of the width $\sim \sqrt{l_p/k}$ and length $l_p$ gives $U \sim \sqrt{k l_p} \log(k l_p - 1)$. For experiment of Sivan et al. $k l_p \sim 100$ and the correlation energy $U$ is large.

To summarize the section both a quantum dot and a point contact can have virtual quasi one-dimensional state at the energy $\epsilon_d$; the charging energy of the state is $U$. This state is well coupled to the finite number of “flat” chaotic states in certain energy interval. So we have all ingredients of the Anderson impurity model. It allows to compute valence of the impurity state and other thermodynamic properties. Our primary interest is the compressibility of the electron system at formation/disappearance of magnetic moment. This regime is described by the almost symmetric limit of the model, see the next section.
III. THE LEVEL SPACING IN PRESENCE OF THE KONDO STATE.

The purpose of this section is to compute the ground state energy $E_N$ of $N$-particle chaotic system in presence of the Kondo interaction with quasi-one-dimensional state. Then we will compute the chemical potential $\mu_N = E_{N+1} - E_N$ and the inverse compressibility (the level spacing) of whole system $\Delta^* = \mu_N - \mu_{N-1}$. This quantity is interesting in vicinity of the symmetric regime, when spin is just disappears and we expect strong fluctuations.

Wiegmann have solved this problem in one dimension. However dimensionality of the system is not important since $j$-states do not interact with themselves. In order to apply the Wiegmann solution we need to postulate the constant energy spacing $2\Delta$ between $j$-states. This approximation is not bad in chaotic systems due to level repulsion.

At the zero magnetic field the ground state is described by the set of rapidities $\{\lambda_\alpha\}_{\alpha=0}^M$, where $M+1$ is number of down spins. The rapidities satisfy

$$J_\alpha + \frac{1}{\pi} \sum_{\beta=0}^M \arctan(\lambda_\alpha - \lambda_\beta) = -\frac{1}{\Delta} [x(\lambda_\alpha) + O(\Delta)] \quad (10)$$

$$x(\lambda) = \epsilon_d + U/2 - (U\Gamma)^{1/2}(\lambda + (\lambda^2 + 1/4)^{1/2})^{1/2} \quad (11)$$

$\Gamma = |V|^2$ is also constant. We keep here terms in the lowest order in $\Delta$. The integer numbers $\{J_\alpha\}_{\alpha=0}^M$ completely describe the state of the system with $N = 2(M+1)$ particles. The energy of the system is just

$$E = 2 \sum_{\alpha=0}^M x(\lambda_\alpha) \quad (12)$$

The ground state corresponds to subsequent values of $J_\alpha$, fixed by the condition

$$J_\alpha < J_M, \quad \lambda_\alpha < \lambda_M, \quad x(\lambda_\alpha) > x(\lambda_M) = D \quad (13)$$

where $D$ is the bottom of the energy band, see Fig. 3.

The ground state is a bit more complicated for odd number of particles, $N = 2M + 1$. In this case $\alpha = 0 \ldots M - 1$, and we introduce new rapidity $\tilde{\lambda}$:

$$J_\alpha + \frac{1}{\pi} \sum_{\beta=0}^{M-1} \arctan(\lambda_\alpha - \lambda_\beta) + \frac{1}{\pi} \arctan(2\lambda_\alpha - 2\tilde{\lambda}) = -\frac{1}{\Delta} x(\lambda_\alpha) \quad (14)$$

$$\tilde{x}(\tilde{\lambda}) = \epsilon_d + U/2 - (2U\Gamma\tilde{\lambda})^{1/2} = D \quad (15)$$

$$E = \tilde{x}(\tilde{\lambda}) + 2 \sum_{\alpha=0}^{M-1} x(\lambda_\alpha) \quad (16)$$

In order to compute the chemical potential we need both solutions Eq. (12) and Eq. (16), because one additional electron changes number of particles from odd to even or
vise versa. Fortunately, the difference between the odd-electron solution and the even-electron solution is small, something happens at the bottom of the band, and not near the Fermi surface. For this very reason we will define the chemical potential as half of energy one needs to add two particles to a system with even number of particles:

$$
\mu_N \equiv \frac{E_{N+2} - E_N}{2}, \quad \Delta_\sigma = \frac{\mu_N - \mu_{N-2}}{2}.
$$

Here $\Delta_\sigma$ is the level spacing of interacting system.

When the level spacing of non-interacting system is small $\Delta \to 0$, one can solve Eq. (10) by making use of the continuous approximation. It is justified by the condition

$$
|\lambda_{\alpha+1} - \lambda_\alpha| \ll 1 \quad \forall \alpha.
$$

So we replace sum Eq. (10) by integral

$$
J_\alpha + \frac{1}{\Delta} \int_{\lambda_0}^{\lambda_M} \arctan(\lambda_\alpha - \lambda') \sigma(\lambda') d\lambda' = -\frac{1}{\Delta} x(\lambda_\alpha),
$$

where $\sigma(\lambda) \sim \frac{\Delta/\pi}{\lambda_{\alpha+1} - \lambda_\alpha}$. Taking derivative with respect to $\lambda_\alpha$ we arrive at the integral equation

$$
\sigma_\lambda + \frac{1}{\pi} \int_{\lambda_0}^{\lambda_M} \frac{\sigma_\lambda(x') d\lambda'}{1 + (\lambda - \lambda')^2} = -\frac{1}{\pi \Delta} \frac{d}{d\lambda} x(\lambda_\alpha),
$$

which can be formally solved in whole range $\lambda \in [-\infty, \lambda_M]$. For large $\lambda_M$ we can write equation with $\alpha = M$ as $J_M + M/2 \approx -D/\Delta$, then all $J_\alpha$s become fixed $J_\alpha = -D/\Delta - 3M/2 + \alpha$. Introducing Eq. (21) from $-\infty$ to $\lambda_\alpha$ (again $\lambda_M$ is large) we get equation for $\lambda_\alpha$:

$$
\pi \int_{-\infty}^{\lambda_\alpha} \tilde{\sigma}_\lambda d\lambda = \epsilon_d + U/2 - D - 2M\Delta + \alpha \Delta.
$$

where we made use of $x(-\infty) = \epsilon_d + U/2$.

The general (Wienner-Hopf) solution of Eq. (21) is available in the Wiegmann paper. The particular case $\lambda_0 = -\infty$ and $\lambda_M = \infty$ can be solved by Fourier transform method and the result is

$$
\sigma_\lambda = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{1}{\cosh(\pi \lambda - \pi k^2/(2UT))} \, (22)
$$

it changes a little when $\lambda_0, \lambda_M$ are finite but large. For large negative $\lambda$ the solution behaves exponentially

$$
\sigma_\lambda \approx \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{\pi \lambda - \pi k^2/(2UT)} = \sqrt{2UT} e^{\pi \lambda} \, (23)
$$

Then we can compute the lowest rapidity $\lambda_0$ from Eq. (22)

$$
\lambda_0 = \frac{1}{\pi} \log \epsilon_d + U/2 - D - 2M\Delta \sqrt{2UT} \, (24)
$$

and indeed it goes to $-\infty$ in the symmetric limit of the Anderson model

$$
\epsilon_d + U/2 - D - 2M\Delta \to 0, \text{ (it is enough to have } |\epsilon_d + U/2 - D - 2M\Delta| \ll \sqrt{2UT}).
$$

The general solution of Eq. (22) works for any $\lambda_0$ if $\lambda < \lambda_0$. Then we combine Eq. (24) with Eq. (20) and obtain compressibility

$$
\frac{dN}{d\mu} = \frac{1}{\Delta} \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{\tilde{\mu} - \pi^2/4\tilde{\mu}^3}{\cosh((\pi^2/4 - \tilde{\mu}^2)/2\tilde{\mu}^2 - k^2/2)} \, (25)
$$

where $\tilde{\mu} = (\mu - \epsilon_d - U/2)/\sqrt{2UT/\pi}$. The compressibility is zero at symmetric limit, see Fig. 3.

In the vicinity of symmetric limit one has simple expressions for chemical potential and level spacing

$$
\mu_N = x(\lambda_0) = \epsilon_d + U/2 - \sqrt{\frac{\pi UT/8}{\log(\sqrt{2UT}/A_N)}}, \quad \Delta = \frac{\Delta_{\sigma}}{A_N} \sqrt{\frac{\pi UT/32}{\log^4(\sqrt{2UT}/A_N)}},
$$

$$
A_N = \epsilon_d + U/2 - D - (N - 2)\Delta \, (26)
$$

The level spacing $\Delta_\sigma$ diverges for any fixed $\Delta$ in the vicinity of the symmetric limit. This result indicates that system is unstable near $\mu = \epsilon_d + U/2$, and experimentally one observes kinks of level spacing.

The kink of the level spacing means that the system becomes non-interacting, the chemical potential get its $U = 0$ value

$$
\mu_N|_{U=0} = N\Delta + D \, , (28)
$$

and the observed kink is
\[ \Delta_\ast = \mu_N|_{U=0} - \mu_{N-2}, \]
\[ = \sqrt{\frac{\pi UT}{8}} \log(\sqrt{2UT}/A_{N-2}) - A_N. \]  

(29)

The maximal possible kink of the level spacing is

\[ \Delta_{\text{max}} = \sqrt{\frac{\pi UT}{4}} \log(UT/2\Delta) \gg \Delta. \]  

(30)

It goes to zero in thermodynamic limit \( \Delta \to 0 \), but remains large. We will derive Eqs. (30, eq:model.res2) in the rest of the section.

The problem is that the condition Eq. (3) is broken for the lowest \( \lambda_0 \) near the symmetric limit. Since for \( \lambda_0 \to -\infty \) the density of the rapidities goes to zero exponentially, so \( |\lambda_1 - \lambda_0| \propto e^{\pi |\lambda_0|} \Delta/\sqrt{UT} \) can be very large for any fixed \( \Delta \). The main idea of the present paper is to introduce one rapidity \( \lambda_0 \) separated from all the rest \( \lambda_1 \ldots \lambda_M \). We should assume \( |\lambda_0 - \lambda_1| \gg 1 \) in Eq. (19) with \( \alpha = 0 \):

\[ J_0 - \frac{M}{2} - \frac{1}{\Delta} \int_{\lambda_1}^{\lambda_M} \sigma_\lambda d\lambda \frac{\lambda_0 - \lambda}{\lambda_0 - \lambda} = -\frac{1}{\Delta} \epsilon_d + U/2 - \sqrt{\frac{UT}{8|\lambda_0|}}. \]  

(31)

where we expanded \( \arctan() \). The integral equation for region of "dense" rapidities becomes

\[ \sigma_\lambda + \frac{\Delta/\pi}{1 + (\lambda - \lambda_0)^2} \frac{1}{\pi} \int_{\lambda_1}^{\lambda_M} \frac{\sigma_\lambda d\lambda'}{1 + (\lambda' - \lambda)^2} = -\frac{1}{\pi} \frac{dx}{d\lambda}. \]  

(32)

In the lowest order in \( 1/\lambda_0 \) we neglect the integral in Eq. (31) and obtain \( x(\lambda_0)/\Delta = M/2 - J_0 = 2M + D \) that is equivalent to Eq. (24). Lowest rapidities are

\[ \lambda_0 \approx -\frac{UT}{8A_N^2}, \quad \lambda_1 = \frac{1}{\pi} \log \left( A_{N-2}/\sqrt{2UT} \right), \]  

(33)

where \( \lambda_1 \) goes to \(-\infty \) much slowly than \( \lambda_0 \). Within the approximation made here \( \lambda_1 \) of system of \( N + 2 \) particles coincides with \( \lambda_0 \) of system of \( N \) particles. Then the obtained pseudogap Eq. (30) is just \( x(\lambda_0) - x(\lambda_1) \).

In conclusion of the section we have found the anomalously large spacing between energy levels of electron gas interacting with impurity. This is a finite size effect, which requires special treatment. The pseudogap appears at the Fermi energy when the model approaches complete particle-hole symmetry, \( \mu \approx \epsilon_d + U/2 \).

**IV. EXPERIMENTAL DATA AND CONCLUSIONS.**

Let us consider experiment, where one fills the system by particles. The Fermi level goes up \( \mu(N) \sim N\Delta + D \), where \( N \) is the number of particles inside the system, and \( D \) is the band offset. At the value \( N = N_d \) given by equation

\[ \mu(N_d) = \epsilon_d + U/2 \]  

(34)

we arrive at the symmetric Anderson model. Just below this value of \( N \) the Fermi energy makes a large jump given by Eq. (29). Later we will measure the \( \Delta_* \) in terms of mean level spacing

\[ \delta_* = \Delta_*/\Delta \approx \sqrt{(\pi/4)x/\log x}, \quad x = UT/2\Delta^2 \gg 1. \]  

(35)

The Fermi energy will jump again near \( N = N_{d+1} \). The distance between jumps is \( N_{d+1} - N_d \approx (\epsilon_{d+1} - \epsilon_d)/\Delta \) is inverse proportional to the length of the orbit \( l_p \):

\[ \delta N = N_{d+1} - N_d \approx \frac{2L}{l_p} \sqrt{2\pi N_{d+1}}. \]  

(36)

This formula was derived for \( \Delta = \pi h^2/(mA) \), where \( L \) is size of the quantum dot, \( A \approx L^2 \) is its area and \( \delta N \ll N_{d+1} \).

The experimental data from few references is summarized in Table 1. The first block contains data taken from cited papers, then we provide estimation of \( k_F, \Delta, \Gamma, U, \delta N, \) and \( \delta_* \). Last computed values are \( \epsilon_{d+1} - \epsilon_d \) taken from charts of \( E_{N+1} - E_N \) vs \( N \) reported in cited papers.

Typically \( l_p \sim 2L \) and we will use \( \delta N = \sqrt{2\pi N_{d+1}} \). The Coulomb energy of the virtual state is \( U \approx E_C \log k_F l_p \) where \( E_C \) is the charging energy of the dot, and \( k_F \) is wave number on Fermi surface. The coupling \( \Gamma \) is of the order of level spacing of virtual state, at least it larger than level spacing of host system: \( \Delta \lesssim \Gamma \lesssim \delta_{d+1} - \delta_d \). For this reason Table 1 contains two values for \( \Gamma \) - minimal and maximal estimates. Last computed value is \( \delta_* \), which eventually have minimal and maximal estimates obtained from Eq. (25). We see that our theory works well for clean samples [44], and it is not applicable for disordered quantum dots [44]. The virtual state is absent in perfectly rectangular quantum dot [44] (without shape deformations) as well.

The conductance of a quantum point contact (QPC) with the Kondo state inside has been computed recently[43] and the model explained all the experimental data. Existence of the Kondo state in a QPC is very plausible, and therefore we expect to see Kondo state inside quantum dots too. The present theory should not be confused with Kondo effect due to charging of entire dot. However the intersting feature of both types of experiments (Kondo state on "scar" and Kondo state inside entire dot) is that the gate voltage allows to scan all regimes of Anderson model [44].

To summarize, inhomogenities of chaotic wave functions can be gathered together into an additional state of small size. In this way one arrives at Anderson’s impurity model with finite number of free electron states. At certain value of the chemical potential the model has
complete particle-hole symmetry. The chemical potential does not approach this value gradually, but rather irregularly. The energy scale of this effect is a new combination of the parameters of Anderson’s model and the mean level spacing. This scenario is a possible explanation of the irregularities observed experimentally in quantum dots.

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Table I. Measured data / Intermediate calculations/ Observed values of $\delta N$ and $\delta_*$ energies are given in meV, length are given in $\mu$m and wavenumbers in $\mu$m$^{-1}$.

| Ref. | $N$ | $A$ | $L$ | $E_C$ | $k$ | $\Delta$ | $U$ | $\Gamma$ | $\delta N$ | $\delta_*$ |
|------|-----|-----|-----|------|-----|---------|-----|--------|----------|----------|
| 4    | 100 | 0.15| 0.5 | 0.6  | 65  | 0.02    | 2.0 | 0.02 - 0.5 | 25       | 3 - 10    |
| 5    | 100 | 0.13| 1.2 | 1.0  | 83  | 0.05    | 8.0 | 0.04 - 2.0 | 25       | 4 - 16    |
| 6    | 100 | 0.17| 0.9 | 0.59 | 3   | 0.04    | 4.6 | 1.0 - 1.0 | 15       | 5 -       |
| 7    | 3   | 10   | 2   | 6    | 3 - 10 | 4 - 16 | 3 - 7 | 3 - 13  | 2 -       |
| 8    | 10  | 2   | 5   | 6    | 10   | 6 - 8   | 2   | 6       |          |

† – circumference ‡ – the sample # 1