KONDO EFFECT IN THE TRANSPORT THROUGH A QUANTUM DOT: EXTENDED NONCROSSING APPROXIMATION APPROACH*

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We calculate the conductance through a single quantum dot coupled to metallic leads, modeled by the spin 1/2 Anderson model. We adopt the finite-U extension of the noncrossing approximation method. Our results are in good agreement with exact numerical renormalization group results both in the high temperature and in the Kondo (low temperature) regime. Thanks to this approach, we were able to fit fairly well recently reported measurements [1]. in a quantum dot device. We show that, contrarily to what previously suggested, the conductance of this particular device can be understood within the spin 1/2 Anderson model, in which the effects of the multilevel structure of the dot are neglected.

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The recent observation [2,3] of the Kondo effect [4] in quantum dot (QD) devices has opened the possibility to control the Kondo effect experimentally, and a new exciting field of research [5]. It was shown that — below a Kondo temperature $T_{\rm K}$ of the order of 100 mK — the linear response conductance of a QD device, G, approaches $2e^2/h$ (unitary limit) if the number n of electrons confined in the QD is odd, and it becomes very small if n is even [3]. This even/odd effect seems to be a general feature of most [6] QD devices. In the present paper we focus our attention on those devices for which Kondo anomalies appear *only* for odd n [1–3], and in particular on the experimental data reported very recently in Ref. [1].

In order to describe a QD coupled to its leads, we adopt the spin 1/2 Anderson model [7]

$$H = \sum_{(\boldsymbol{k},\sigma)\in \mathrm{S,D}} \varepsilon_{\boldsymbol{k}}\, c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \varepsilon_0 \sum_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{(\boldsymbol{k},\sigma)\in \mathrm{S,D}} \left(V_{\boldsymbol{k}\sigma}\, c^{\dagger}_{\boldsymbol{k}\sigma} d_{\sigma} + \mathrm{h.c.} \right). \quad (1)$$

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Here $c^{\dagger}_{\boldsymbol{k}\sigma}$ ($c_{\boldsymbol{k}\sigma}$) creates (destroys) a conduction electron with momentum $\boldsymbol{k}$, energy $\varepsilon_{\boldsymbol{k}}$ and spin σ in one of the two leads, which we label with S (source) and D (drain); $d^{\dagger}_{\sigma}$ (d_{σ}) creates (destroys) an electron with spin σ on the QD; $V_{\boldsymbol{k}\sigma}$ is the hybridization between QD and conduction states (which we suppose to be $\boldsymbol{k}$ independent, $|V_{\boldsymbol{k}\sigma}| = V_{\mathrm{S(D)}}$ for $\boldsymbol{k} \in$ S or D), ε_0 is the energy of a single electron localized on the QD and U is the Coulomb interaction among electrons on the same orbital level. In the present model the energy ε_0 is not fixed, but on the contrary it is tuned by a gate voltage, V_g, coupled to the QD through a capacitor. As a first approximation we assume a linear relation, $\varepsilon_0 = \alpha V_g + \mathrm{const}$. The gate voltage (and thus ε_0) controls the number of electrons confined in the QD at low temperature. In the linear response regime ($V_{\mathrm{SD}} \ll V_g$, where V_{SD} is the source-drain bias) the conductance, G, may be written in a Landauer-like form [8]

$$G(T, V_g) = \frac{2e^2}{h} \int_{-\infty}^{+\infty} \pi \Gamma \left(-\frac{1}{\pi} \mathrm{Im}\{G^{\mathrm{R}}(\varepsilon + i\eta)\} \right) \left(-\frac{\partial f}{\partial \varepsilon} \right) \mathrm{d}\varepsilon. \qquad (2)$$

Here we have assumed for simplicity that the couplings to the leads are symmetric. The actual QD-leads coupling strength is thus $\Gamma = \pi N(\varepsilon_{\mathrm{F}}) V^2$, where $V = (V_{\mathrm{S}}^2 + V_{\mathrm{D}}^2)^{1/2}$, and $N(\varepsilon_{\mathrm{F}})$ is the density of states per spin at the Fermi level [7]. In addition, f is the Fermi distribution function and $G^{\mathrm{R}}(\varepsilon + i\eta)$ is the retarded local Green function, *i.e.* the Fourier transform of the time-dependent function $G^{\mathrm{R}}(t) = -\mathrm{i}\,\theta(t)\langle|\{d(t), d^{\dagger}(0)\}|\rangle$. In order to calculate the local density of states (DOS), that is $\rho = -\mathrm{Im}\{G^{\mathrm{R}}(\varepsilon + i\eta)\}/\pi$, we adopt the noncrossing approximation method in its finite-U extension (UNCA) [9]. This method allows us to explore the empty orbital, ($n \sim 0$, $-\varepsilon_0 < -\Gamma$), the Kondo ($n \sim 1$, $\Gamma < -\varepsilon_0 < U - \Gamma$) and the doubly occupied ($n \sim 2$, $-\varepsilon_0 > U + \Gamma$) regimes. Further details on the method used to calculate $G^{\mathrm{R}}(\varepsilon + \mathrm{i}\eta)$ can be found in Refs [9,10].

The main purpose of the present work is to understand the experimental data of Ref. [1]. The results of our (new) calculations are shown in Fig. 1(a) and (b) for two different choices of parameters. The parameters of Fig. 1(a) are our best fit of the experimental data. We notice that the conductance as a function of ε_0/U is directly related to experimental data because of the linear relation between ε_0 and V_g. The results in Fig. 1(a) and (b) are in good agreement with previously reported exact numerical renormalization group (NRG) calculations (see Fig. 2 of Ref. [11]). The figure shows that, at high temperature ($T \gg T_{\mathrm{K}}$, see *e.g.* $T = 900$ mK), there are two Coulomb blockade peaks at energies $\varepsilon_0/U \sim 0$ and $\varepsilon_0/U \sim -1$, as observed experimentally by different groups [1–3]. Each peak corresponds to the addition of one electron to those confined in the QD. When the temperature is lowered, the peaks approach each other, and the conductance gradually increases for

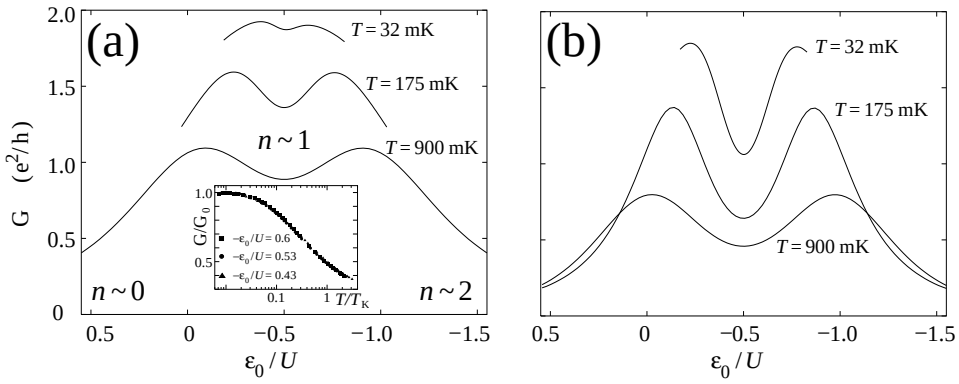

Fig. 1. Linear-response conductance as a function of ε_0/U and for different temperatures [12]. (a) Parameters: $\Gamma = 0.262$ meV and $U = 0.8$ meV. Inset: G/G_0 as a function of T/T_K and for different choices of ε_0/U. Here G_0 is the value of G at the lowest temperature that can be reached with the UNCA; T_K is such that $G(T_\mathrm{K}) \equiv G_0/2$. (b) Parameters: $\Gamma = 0.120$ meV and $U = 0.7$ meV.

$n \sim 1$, while it decreases for $n = 0$ and $n = 2$. At very low temperature ($T \ll T_\mathrm{K}$, see *e.g.* Fig. 1(a), $T = 32$ mK) the Coulomb blockade peaks merge into a plateau at $G \sim 2e^2/h$, which is located in the parameter region for which $n \sim 1$.

In the Kondo regime, the conductance is expected to be a universal function of T/T_K. In the inset of Fig. 1(a) we show the calculated universal curve G/G_0 for three different choices of ε_0/U in the Kondo regime (that is ε_0/U between -0.4 and -0.6). The ratio G/G_0 is proportional to $\ln(T/T_\mathrm{K})$ for $T \sim T_\mathrm{K}$. At very low temperature ($T \ll T_\mathrm{K}$) $G/G_0 \propto (T/T_\mathrm{K})^2$, as expected in the Fermi-liquid regime [4] and as found experimentally [1,3].

The conductance of the spin 1/2 Anderson model was calculated with the NRG technique in Ref. [1], and directly compared with the reported experimental data. Although very good agreement was reached at low temperature, it was shown that at high temperature the theoretical conductance strongly underestimates the experimental value. For the same choice of parameters of the Anderson model, we find the same discrepancy (see Fig. 1(b) and Fig. 2 of Ref. [1]). It was then suggested in Ref. [1] that multilevel effects could be responsible of this discrepancy. Here we explored another possibility. We suggest that the experimental data *can* be fitted within the spin 1/2 Anderson model, provided that an appropriate choice of parameters is made. We found the best agreement for $\Gamma = 0.262$ meV (about two times larger than the one used in Fig. 1(b)) and $U = 0.8$ meV. The results obtained with these optimal parameters are shown in Fig. 1(a), and they are in excellent agreement with experiments both at high and low temperature.

In conclusion, we have calculated the conductance of a system made of a QD coupled to two leads, described by the spin 1/2 Anderson model. We adopted the UNCA, and we found good agreement with exact NRG results [11] and experiments [2,3]. We have shown that recent experiments [1], contrarily to what previously proposed, *can* be understood in the framework of the spin 1/2 Anderson model, in which the effects of the multi-level structure of the dot is neglected. Although the spin 1/2 Anderson model can be solved exactly by using the NRG, we believe that the UNCA is more suitable than NRG for extensions to realistic systems, and it could become an important tool to interpret experiments in which the realistic electronic structure of the QDs plays a crucial role (*e.g.* the Kondo effect in quantum dots for integer spin [6]).

REFERENCES

[1] S. De Franceschi, W.G. van der Wiel, T. Fujisawa, J.M. Elzerman, W. Izumida, S. Tarucha, L.P. Kouwenhoven, *Proceedings of the Moriond Conference*, ed. T. Martin, G. Montambaux, J. Tran Thanh Van, EDPS Sciences, Les Arc 2001, pp. 361.

[2] D. Goldhaber-Gordon, H. Shtrikman, D. Mahalu, D. Abusch-Magder, U. Meirav, M.A. Kastner, *Nature* **391**, 156 (1998); S.M. Cronenwett, T.H. Oosterkamp, L.P. Kouwenhoven, *Science* **281**, 540 (1998).

[3] W.G. van der Wiel, S. De Franceschi, T. Fujisawa, J.M. Elzerman, S. Tarucha, L.P. Kouwenhoven, *Science* **289**, 2105 (2000).

[4] A.C. Hewson, *The Kondo Problem to Heavy Fermions*, Cambridge University Press, Cambridge (UK) 1993.

[5] L.P. Kouwenhoven, L.I. Glazman, *Phys. World* **14**, 33 (2001).

[6] In some QDs, Kondo-like anomalies have been observed also for even n [J. Schmid, J. Weis, K. Eberl, K. von Klitzing, *Phys. Rev. Lett.* **84**, 5824 (2000); S. Sasaki, S. De Franceschi, J.M. Elzerman, W.G. van der Wiel, M. Eto, S. Tarucha, L.P. Kouwenhoven, *Nature* **405**, 764 (2000)]. These anomalies have been related to the formation of integer spin states with $S \geq 1$.

[7] L.I. Glazman, M.É. Raĭkh, *Pis'ma Zh. Eksp. Teor. Fiz.* **47**, 378 (1988) [*JETP Lett.* **47**, 452 (1988)].

[8] Y. Meir, N.S. Wingreen, *Phys. Rev. Lett.* **68**, 2512 (1992).

[9] T. Pruschke, N. Grewe, *Z. Phys.* **B74**, 439 (1989).

[10] D. Gerace, E. Pavarini, L.C. Andreani, *Phys. Rev.* **B65**, 155331 (2002).

[11] W. Izumida, O. Sakai, S. Suzuki, *J. Phys. Soc. Jpn.* **70**, 1045 (2001).

[12] At low temperature, in the empty orbital and in the doubly occupied regimes, a spurious peak appears in the UNCA local DOS close to the Fermi level. This is a known shortcoming of the UNCA [9]. Thus results at temperatures $T = 175$ mK (Fig. 1(a)) and $T = 32$ mK (Fig. 1(a) and (b)) are shown only in the regions in which the UNCA is reliable.