Comment on "Conductance scaling in Kondo-correlated quantum dots: Role of level asymmetry and charging energy"

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In a recent work [Merker, Kirchner, Muñoz, and Costi, Phys. Rev. B **87**, 165132 (2013)], the authors compared the results of numerical renormalization group (NRG) and a perturbative approach for the dependence on temperature T and magnetic field B of the conductance through a quantum dot described by the impurity Anderson model, for small T and B. We show that the equation used to extract the dependence on B from NRG results is incorrect out of the particle-hole symmetric case. As a consequence, in the Kondo regime, the correct NRG results have a weaker dependence on B and the disagreement between both approaches increases.

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Recent experimental studies for the conductance through one quantum dot for low applied bias voltage V and temperature T [1,2], stimulated further theoretical work on the subject [3–10]. Using a Fermi liquid approach—based on perturbation theory in U (PTU)—and Ward identities, Oguri had determined exactly the scaling up to second order in T and V for the symmetric impurity Anderson model (SIAM) in which the energy level $E_d = U/2$ [11,12]. Further work considered the effect of higher order contributions using different approximations, such as PTU [3], $1/N$ expansion [5], noncrossing approximation [6], or decoupling of equations of motion [7]. The effect of asymmetric coupling to the left and right leads $\Gamma_L \neq \Gamma_R$, and asymmetric drop in the bias voltage has been calculated up to second order in T and V using Fermi liquid approaches, for the SIAM [3,4,8]. The more general expression was given first by Sela and Malecki [4] and reproduced by us using renormalized PTU [8]. These results are exact up to terms of total second order in V and T.

Some of these results were extended for $E_d \neq U/2$ using two different approaches [8,9]. A controversy between the authors of both works exists [13–15]. We claim that the lesser and greater self-energies and Green functions in Ref. [9] are incorrect. In turn, Muñoz *et al.* [14] claim that a Ward identity is not satisfied in Ref. [8]. However, direct evaluation shows that the Ward identity is in fact fulfilled [8(b),15].

While the conductance can be expressed in terms of the retarded Green function only (which is by construction correct in the SIAM), if the lesser and greater quantities are not correct conservation of the current is not guaranteed when particle-hole symmetry is broken. Therefore, the results out of the SIAM of Muñoz, Bolech, and Kirchner [9] might be incorrect. However when both approaches can be compared, for the linear term in V, they give the same result [13]. In any case, for more general multilevel models, for example when interference phenomena are important [16–18], lesser quantities cannot be eliminated from the conductance, and their correct evaluation becomes crucial.

Taking into account the above objections, the recent study of Merker *et al.* [10] is certainly of interest. The authors compare the approach of Muñoz *et al.* [9] for the temperature and magnetic field B dependence of the conductance G, with accurate numerical-renormalization-group (NRG) calculations at equilibrium ($V = 0$). For the dependence on B, the authors combine NRG results for the total occupation of the localized level $n_d = n_{d\uparrow} + n_{d\downarrow}$ with the Friedel sum rule for finite B [19,20]:

$$\rho_\sigma(0,B) = \frac{\sin^2(\pi n_{d\sigma})}{\pi\Delta}, \tag{1}$$

which relates the spectral density of the localized level for a given spin $\rho_\sigma(\omega,B)$ at the Fermi level $\omega = 0$ with the corresponding occupancy. Since the conductance for each spin $G_\sigma(B)$ at $T = 0$ is proportional to $\rho_\sigma(0,B)$, expanding $n_{d\sigma}$ up to second order in B and replacing in Eq. (1) one obtains the corresponding expansion in the total conductance $G = G_\uparrow + G_\downarrow$. Specifically

$$n_{d\sigma}(B) = \frac{n_d}{2} + \frac{\chi B}{g\mu_B}\sigma + \frac{\partial^2 n_d}{\partial B^2}\frac{B^2}{4} + O(B^3), \tag{2}$$

where χ is the magnetic susceptibility, $\sigma = 1\,(-1)$ for spin up (down), and the quantities in the second member except B are evaluated at $B = 0$.

The last term is missed in Ref. [10]. While this term vanishes for the SIAM, because $n_d = 1$ there as a consequence of electron-hole symmetry, it becomes increasingly important out of the SIAM, for which the perturbative approach of Ref. [9] was developed. In this work we examine the effects of this term. An important consequence is that the results presented in Ref. [10] (Fig. 8, for example) as coming from NRG are misleading, because one expects that they are highly accurate, but since they were obtained indirectly neglecting the last term in Eq. (2), they should be corrected. We also show that inclusion of this term increases the disagreement with the perturbative approach of Ref. [9] out of the SIAM in the Kondo regime.

Replacing Eq. (2) in Eq. (1) one obtains up to order B^2,

$$\frac{G_\sigma(B)}{G_\sigma(0)} = \frac{\rho_\sigma(0,B)}{\rho_\sigma(0,0)} = 1 + c\frac{2\pi\chi B}{g\mu_B}\sigma + (c^2-1)\left(\frac{\pi\chi B}{g\mu_B}\right)^2 + c\frac{\pi}{2}\frac{\partial^2 n_d}{\partial B^2}B^2, \tag{3}$$

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$$c = \cot\left(\frac{\pi n_d}{2}\right). \tag{4}$$

Adding both spins, and defining c_B and T_0 by [10]

$$\frac{G(B)}{G(0)} = 1 - c_B\left(\frac{g\mu_B B}{T_0}\right)^2, \tag{5}$$

$$\chi = \frac{(g\mu_B)^2}{4T_0}, \tag{6}$$

one obtains

$$c_B = \frac{\pi^2}{16}(1-c^2) - c\frac{\pi}{2}\left(\frac{T_0}{g\mu_B}\right)^2\frac{\partial^2 n_d}{\partial B^2}. \tag{7}$$

For $n_d < 1$, $c > 0$. In addition, $\partial^2 n_d/\partial B^2$ is also positive, as shown by exact Bethe ansatz results [21]. This means that the last term of Eq. (7), missed in Ref. [10] has the effect of decreasing the results for c_B reported as NRG ones in that work (Figs. 6 and 8). This in turn means that in the Kondo regime ($-E_d \gg \Delta$ and $E_d + U \gg \Delta$) the disagreement between NRG and the the perturbative approach of Ref. [9] increases (Fig. 8 of Ref. [10]). Only well inside the intermediate valence and weak coupling regime $-0.75 < E_d/\Delta < 0$, $U/\Delta < 1.5$, the comparison might be good.

To estimate the effect of the correction, we have calculated c_B for $U \to \infty$ in the slave-boson mean-field approximation (SBMFA). This approach fulfills Fermi liquid properties [like Eq. (1)] and is expected to be semiquantitatively valid at low energies. In particular for large N and low temperatures it compares very well with exact results [22]. In the SBMFA, the solution of the Anderson model at $T = 0$ reduces to the self-consistent solution of the following two equations for the Lagrange multiplier λ and the width of the quasiparticle spectral density $\tilde{\Delta}$ [20]:

$$\begin{aligned} \frac{\lambda}{\Delta} &= -\frac{1}{2\pi}\sum_\sigma \ln\left(\frac{\epsilon_\sigma^2 + \tilde{\Delta}^2}{W^2}\right), \\ \frac{\tilde{\Delta}}{\Delta} &= 1 - \sum_\sigma n_{d\sigma}, \end{aligned} \tag{8}$$

where

$$\begin{aligned} \epsilon_\sigma &= E_d + \lambda - \sigma g\mu_B B/2, \\ n_{d\sigma} &= \frac{1}{\pi}\arctan\left(\frac{\tilde{\Delta}}{\epsilon_\sigma}\right), \end{aligned} \tag{9}$$

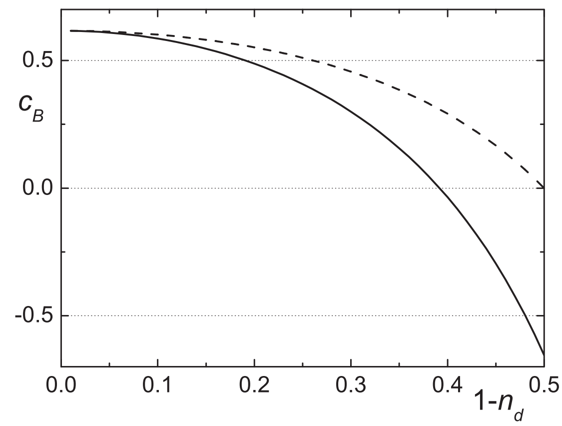

FIG. 1. Full line: coefficient of the magnetic field dependence of the conductance [see Eq. (5)]. Dashed line: the same, including only the first term in Eq. (7).

and $-W$ is the bottom of the conduction band assumed constant.

After solving the problem for $B = 0$, the derivatives with respect to B are obtained solving a system of linear equations, obtained differentiating Eqs. (8) and (9). The resulting c_B is represented in Fig. 1 as a function of the occupation and compared with the result of the first term of Eq. (7), which corresponds to that used in Ref. [10]. We have chosen $W = 50\Delta$. With this choice $n_d = 0.99$ for $E_d = -5.42\Delta$ and $n_d = 0.5$ for $E_d = -2.21\Delta$. As expected, both results coincide for $n_d \to 1$ and the first term of Eq. (7) changes sign for $n_d = 0.5$. Instead, the correct result changes sign for $n_d \simeq 0.61$, corresponding to $E_d \simeq -2.7\Delta$, and decreases strongly to negative values as $1 - n_d$ (or E_d) is further increased, moving to the intermediate valence region.

In the Kondo regime, the perturbative approach of Ref. [9] gives values of c_B which lie above those given by the first term of Eq. (7) (which would correspond to the dashed line of Fig. 1 for large U) [10]. This fact and the disagreement with the temperature dependence of G suggest that the approach of Muñoz, Bolech, and Kirchner [9], at least in its present form, fails to correctly extend the results for the SIAM for general values of E_d in the Kondo regime.

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