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

L. Merker,[1] S. Kirchner,[2,3] E. Muñoz,[4] and T. A. Costi[1]
[1]*Peter Grünberg Institut and Institute for Advanced Simulation, Research Centre Jülich, 52425 Jülich, Germany*
[2]*Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany*
[3]*Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany*
[4]*Facultad de Física, Pontificia Universidad Católica de Chile, Casilla 306, Santiago 22, Chile*

(Received 8 April 2014; revised manuscript received 22 July 2014; published 13 August 2014)

The Comment of A. A. Aligia claims that the superperturbation theory (SPT) approach [E. Muñoz, C. J. Bolech, and S. Kirchner, Phys. Rev. Lett. **110**, 016601 (2013)] formulated using dual fermions [A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. B **77**, 033101 (2008)] and used by us to compare with numerical renormalization group (NRG) results for the conductance [L. Merker, S. Kirchner, E. Muñoz, and T. A. Costi, Phys. Rev. B **87**, 165132 (2013)], fails to correctly extend the results of the symmetric Anderson impurity model (SIAM) for general values of the local level E_d in the Kondo regime. We answer this criticism. We also compare new NRG results for c_B, with c_B calculated directly from the low-field conductance, with new higher-order SPT calculations for this quantity, finding excellent agreement for all E_d and for $U/\pi\Delta$ extending into the strong coupling regime.

DOI: 10.1103/PhysRevB.90.077102 PACS number(s): 75.20.Hr, 71.27.+a, 72.15.Qm, 73.63.Kv

Motivated by recent experiments on conductance scaling in correlated quantum dots exhibiting the Kondo effect [1–3], we recently presented a detailed study of the low-temperature and low-field scaling properties of the linear conductance of a quantum dot described by the single level Anderson impurity model [4]. Scaling in physical properties is a hallmark of the Kondo effect [5]. Within a Kondo model description of a quantum dot the conductance $G(T,B)$ is a universal function of T/T_0 and B/T_0 over all temperatures T and magnetic fields B, with microscopic parameters (such as the Kondo exchange J) only entering through the dynamically generated low-energy scale T_0, defined via the $T=0$ static susceptibility $\chi = (g\mu_{\rm B})^2/4k_{\rm B}T_0$, where Boltzmann ($k_{\rm B}$) and Bohr magneton ($\mu_{\rm B}$) factors shall, henceforth, be set to unity. In particular, at low T and low B the conductance $G(T,B) = G(0,0)[1 - c_T(T/T_0)^2 - c_B(B/T_0)^2]$ is universal in the sense that the coefficients $c_T = \pi^4/16 = 6.0880...$ and $c_B = \pi^2/16 = 0.6168...$ are independent of microscopic details. Actual quantum dot devices, however, have a finite charging energy, and they are more realistically described by an Anderson impurity model. In Ref. [4] we investigated the effect of the charging energy and level position in the Anderson model on the values of c_T and c_B by using the numerical renormalization group (NRG) approach [6–8]. Furthermore, we compared the values of these coefficients with those obtained within the recently developed superperturbation theory (SPT) [9] within the dual fermion formalism [10–12].

Both the SPT approach of Muñoz *et al.* [9] and the renormalized perturbation theory approach of Aligia in Ref. [13] apply to equilibrium and nonequilibrium transport through an Anderson impurity, whereas the NRG is applicable only for linear transport. A controversy between the authors of the works in Refs. [9,13] exists with Aligia claiming [14] that "lesser and greater selfenergies and Green functions in Ref. [9] (of the preceding comment) are incorrect. ...the results ...of Muñoz, Bolech and Kirchner might be incorrect. However, when both approaches can be compared ...they give the same result," a claim first made in Refs. [13,15], and refuted in Refs. [16,17]. Interested readers can follow explicitly the latter by using the detailed Supplemental Material of Ref. [9]. Muñoz *et al.* [16] showed that the source of this controversy lies in a Ward identity that is not satisfied in Refs. [13,15], as can be explicitly checked from Refs. [16,17].

In the preceding Comment [14], Aligia makes two claims on our Ref. [4], to which we respond below. Specifically, these claims are that,

(1) "the results presented in Ref. [10] (of the preceding comment) 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."; and

(2) the SPT of Ref. [9] "fails to correctly extend the results for the SIAM for general values of E_d in the Kondo regime."

We will address these claims in turn.

The expression that we used for calculating $c_B = \frac{\pi^2}{16}[1 - \cot^2(\pi n_d/2)]$ in Ref. [4] from a numerical renormalization group calculation of the local level occupancy n_d made use of a Fermi liquid argument where we took only the linear in B corrections to the local level occupancy n_d, resulting in an approximate expression for c_B. Aligia points out that there is an additional contribution to c_B that results from a B^2 correction to n_d. Taking this into account results in a modification of our expression for c_B given by Eq. (7) of Ref. [14],

$$c_B = \frac{\pi^2}{16}\left[1 - \cot^2(\pi n_d/2)\right] - \frac{\pi}{2}\cot(\pi n_d/2) T_0^2 \frac{\partial^2 n_d}{\partial B^2}. \quad (1)$$

The last term in Eq. (1) is, in general, finite and vanishes only for the symmetric Anderson impurity model. In order to address this point in more detail, we compare the results of Fig. 8 of Ref. [4] with full NRG calculations in which c_B is calculated directly from the conductance and thus includes the second derivative of the local occupation with respect to the applied field in Eq. (1). The results are shown in Fig. 1. The old and new NRG results differ significantly only for local level positions far from the Kondo regime and become identical in the symmetric Kondo regime. Note that the inclusion of the

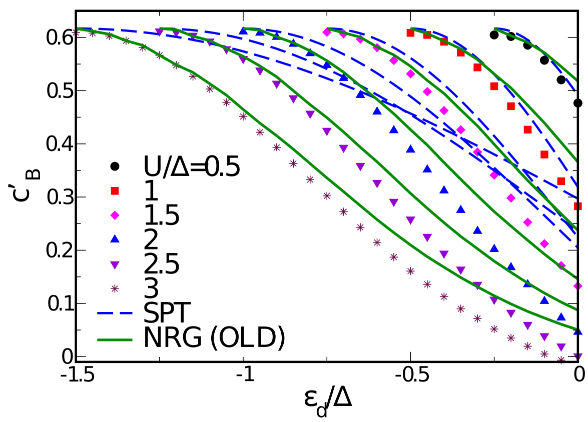

FIG. 1. (Color online) SPT (dashed lines) and NRG (solid lines) results for c_B as defined in Fig. 8 of Ref. [4]. Symbols represent the NRG results for c_B including the second derivative of the occupation with respect to the field. For small U/Δ this term improves the comparison with the SPT.

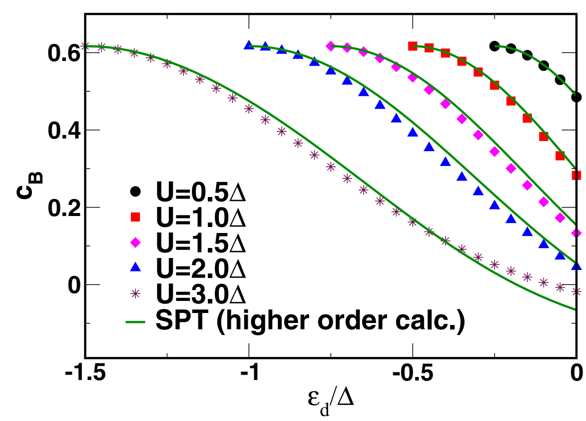

FIG. 2. (Color online) Transport coefficient c_B versus ϵ_d/Δ for various values of U/Δ. The symbols are based on NRG calculations (same as in Fig. 1). The straight lines are the results from the SPT summing up the full Dyson equation (and not just the terms contributing to quadratic order as in Ref. [4]). Note that the NRG results here include all contributions to c_B. Note also the good agreement between these higher-order SPT results with NRG results for all ε_d for $U/\Delta = 3$. This U/Δ value corresponds to a renormalized Coulomb interaction $\tilde{u} \approx 0.761$ close to the strong coupling Kondo limit $\tilde{u} = 1$.

second term in the NRG improves the comparison between SPT and NRG at least for the $U/\Delta < 1.5$ data. This is expected since the SPT includes all terms contributing to c_B (up to the order considered in $\tilde{\varepsilon}_d$ and the renormalized interaction). For small U/Δ, the resulting $\tilde{\varepsilon}_d$ is small and considering terms up to only order $O(\tilde{\varepsilon}_d^2)$ in the SPT works well for all $-U/2 < \epsilon_d < 0$.

The SPT is perturbative in the deviation from particle-hole symmetry around the strong coupling (or Kondo) fixed point. This can be seen, e.g., in Figs. 3 and 4 of Ref. [4], where agreement is found for all values of U/Δ but also from the agreement between SPT and NRG for $-U/2 \approx \tilde{\varepsilon}_d$ in Figs. 7 and 8 of Ref. [4]. As we already discussed on p. 6 of our paper, "Although we show comparisons also in the region $\tilde{\varepsilon}_d \gg 1$, by construction the SPT calculation is perturbative in $\tilde{\varepsilon}_d$ and agreement can only be expected in the limit $\tilde{\varepsilon}_d \ll 1$, which we find." [4]. The claim of Aligia in the concluding sentence that "SPT fails to correctly extend the results for the SIAM for general values of E_d in the Kondo regime" is unfounded and misleading. Our precise claim about SPT away from particle-hole symmetry is that cited above. Moreover, we also anticipated on p. 6 of our paper that "agreement between NRG and SPT... can be increased by going to higher order, however, this lies beyond the scope of this paper." This extension of the SPT to higher orders is accomplished by analytically summing all ladder diagrams entering the renormalized dual fermion expansion, thus summing arbitrary terms in $\tilde{\varepsilon}_d$. We have recently carried through this calculation [18]. It is important to note that this calculation can be performed both for equilibrium and nonthermal steady state properties and is current conserving by construction. Figure 2 compares the higher-order extension of the SPT with the full NRG results for the quantity c_B. As expected, the inclusion of higher orders in $\tilde{\varepsilon}_d$ systematically improves the agreement for all $U/\pi\Delta$ up to the strong coupling Kondo regime $U/\pi\Delta \approx 1$ and for $-U/2 \leqslant \tilde{\varepsilon}_d \leqslant 0$. [The results for the case $U/\Delta = 3$ in Fig. 2 correspond to a renormalized Coulomb interaction $\tilde{u} \approx 0.761$ (see Ref. [4]) close to the strong coupling Kondo value of 1.]

In summary, we presented new NRG results for c_B, calculated directly from the low-field conductance, which includes the second term in Eq. (1). This term is finite, but small, in the Kondo regime and vanishes at the symmetric point. SPT calculations include this correction term to each order and we presented new higher-order SPT calculations demonstrating the good agreement with NRG calculations for all E_d and for values of $U/\pi\Delta$ extending up to the strong coupling Kondo regime.

[1] M. Grobis, I. G. Rau, R. M. Potok, H. Shtrikman, and D. Goldhaber-Gordon, Phys. Rev. Lett. **100**, 246601 (2008).
[2] A. V. Kretinin, H. Shtrikman, D. Goldhaber-Gordon, M. Hanl, A. Weichselbaum, J. von Delft, T. Costi, and D. Mahalu, Phys. Rev. B **84**, 245316 (2011).
[3] G. D. Scott, D. Natelson, S. Kirchner, and E. Muñoz, Phys. Rev. B **87**, 241104 (2013).
[4] L. Merker, S. Kirchner, E. Muñoz, and T. A. Costi, Phys. Rev. B **87**, 165132 (2013).
[5] A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, 1993).
[6] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[7] H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B **21**, 1003 (1980).
[8] R. Bulla, T. A. Costi, and T. Pruschke, Rev. Mod. Phys. **80**, 395 (2008).
[9] E. Muñoz, C. J. Bolech, and S. Kirchner, Phys. Rev. Lett. **110**, 016601 (2013).

[10] A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. B **77**, 033101 (2008).
[11] H. Hafermann, C. Jung, S. Brener, M. I. Katsnelson, A. N. Rubtsov, and A. I. Lichtenstein, Europhys. Lett. **85**, 27007 (2009).
[12] C. Jung, A. Lieder, S. Brener, H. Hafermann, B. Baxevanis, A. Chudnovskiy, A. Rubtsov, M. Katsnelson, and A. Lichtenstein, Ann. Phys. **524**, 49 (2012).
[13] A. A. Aligia, J. Phys.: Condens. Matter **24**, 015306 (2012).
[14] A. A. Aligia, Phys. Rev. B **90**, 077101 (2014).
[15] A. A. Aligia, Phys. Rev. Lett. **111**, 089701 (2013).
[16] E. Muñoz, C. J. Bolech, and S. Kirchner, Phys. Rev. Lett. **111**, 089702 (2013).
[17] E. Muñoz, C. J. Bolech, and S. Kirchner, arXiv:1308.0638.
[18] E. Muñoz *et al.* (unpublished).