Here I present briefly some facts about nonequilibrium renormalized perturbation theory (RPT), correcting recent misleading statements in Ref. 1 and discuss some results of this work using rSPT at equilibrium.

In RPT, the bare renormalized local spectral density from which renormalized retarded \( \tilde{\Sigma}^r(\omega) \) and lesser \( \tilde{\Sigma}^< (\omega) \) self energies are calculated is given by [2, 3]

\[
\tilde{\rho}_0(\omega) = \frac{\Delta/\pi}{(\omega - \tilde{\epsilon}_d)^2 + \Delta^2},
\]

(1)

where \( \tilde{\epsilon}_d \) is the renormalized d level, which using Friedel sum rule (FSR) for zero temperature \( T \) and voltage \( V \) can be related to the local occupancy \( n_d \) [2, 3]:

\[
\tilde{\epsilon}_d = \Delta \cot(\pi n_d/2),
\]

(2)

where here zero applied magnetic field \( B \) is assumed.

In Ref. 1, Muñoz et al. review some results of equilibrium rSPT. In the appendix they discuss a Ward identity (WI) in general. In particular, they argue that in Ref. [3], \( \tilde{\rho}_0(\omega) \) contains a voltage dependence that invalidates the WI. This statement is unfounded. In fact Eq. (11) in Ref. [3] was derived using FSR [3], which is only valid for \( T = V = 0 \). Therefore to assume that \( n_d \) is calculated self-consistently [see Eq. (52) of Ref. 1] in Ref. [3] to modify \( \tilde{\rho}_0 \) is preposterous. Moreover in Ref. [3], it is stated that “The parameters of the original model are renormalized and their values can be calculated exactly from Bethe ansatz results [44–48], or accurately using NRG [49–53]” (both techniques are only valid at \( V = 0 \) and “an accurate knowledge of thermodynamic quantities from the Bethe ansatz or NRG permits a precise determination of \( z = \rho(0)/\tilde{\rho}_0(0), \) and the renormalized interaction through the Wilson ratio \( R = 1 + \hat{U} \tilde{\rho}_0(0) \).” The constant \( \tilde{\rho}_0(0) \) enters the explicit expression of \( \tilde{\Sigma}^< (\omega) \) given by Eq. (20) of Ref. [3] (E20R3). E20R3 was shown to satisfy the WI in Ref. [1]. The results were generalized to finite temperature in Ref. [2], where also the nonequilibrium heat current of a nanodevice was discussed using renormalized parameters \( \Delta, \tilde{\epsilon}_d \) and \( \hat{U} \) obtained from NRG following the method of Hewson et al. [6] as described in Ref. [7], where also \( \Delta, \tilde{\epsilon}_d \) and \( \hat{U} \) for several values of the original parameters were tabulated. In all these works of course \( \tilde{\epsilon}_d \) is constant independent of voltage and temperature.

Previous results of some of the authors [8] claimed that \( \tilde{\Sigma}^< (\omega) = 2f(\omega)\text{Im} (\tilde{\Sigma}^r (\omega)) \), where \( f(\omega) \) is an average of the Fermi function at the two leads. This expression is incorrect and leads to spurious jumps in \( \tilde{\Sigma}^< (\omega) \) at \( T = 0 \) [4]. In Ref. [1] this result is corrected. In fact Eq. (41) for \( \tilde{\Sigma}^< (\omega) \) of Ref. [1] is identical to Eq. (16) of Ref. [3] and when evaluated to order \( V^2 \) at \( T = 0 \) leads to the correct result, E20R3. For finite small \( T, \tilde{\Sigma}^< (\omega) \) and \( \text{Im} (\tilde{\Sigma}^r (\omega)) \) are evaluated in Ref. [5].

The repeated attempts of Muñoz and Kirchner to undermine Ref. [3] have been inconsistent over the time.

First, in Ref. [8] they stated “A problem with this approach is that it fails to recover \( p - h \) symmetry at \( \tilde{u} = 1 \) and gives a linear in \( T \) term in the spectral density away from half filling \( n = 1 \), in contradiction to certain Ward identities.” However, Eq. (30) of Ref. [8] precisely shows that previous rigorous results for \( n_d = 1 [10] \) are recovered, including the particle-hole \( (p - h) \) symmetric case. Concerning the \( T \) dependence, Ref. [3] is dedicated to \( T = 0 \). In the small section 3.5 a brief comment is given on the effect of the Hartree term on the dressed unrenormalized spectral density \( \rho(\omega) \) (which does not enter the WI’s) in self-consistent ordinary (not renormalized) perturbation schemes [3] (b), but this has not been used and in any case, terms linear in \( T \) are absent for \( V = 0 \). The extension to finite \( T \) is done in Ref. [5].

Second, in Ref. [11] they “proved” that \( \tilde{\Sigma}^< (\omega) \) for \( T = 0 \) given by E20R3 does not satisfy the WI based on a (wrong) expansion of \( \tilde{\Sigma}^< (\omega) \) around \( \omega = V = 0 \) (no mention of the dependence of \( \tilde{\epsilon}_d \) on \( V \) alleged in Ref. [11] was made at this stage). They state the violation of the WI in Refs. [6, 8] “is most clearly seen by noticing the linear-in-\( \omega \) and linear-in-V terms in E20R3.” This point is clarified in Ref. [4] and Ref. 29 of Ref. [3]. The derivatives involved in the WI were calculated explicitly for \( T = 0 \) (Ref. [4]) and arbitrary \( T \) (Ref. [4]), showing that the WI’s are fulfilled.

Third, as explained above, in Ref. [1] they now take the same expression [Eq. (16) of Ref. [3]] that leads to E20R3, but invent that \( \tilde{\rho}_0(\omega) \) contains a dependence on \( V \).

As shown above, the nonequilibrium RPT scheme, which in the most complete form is given in Ref. [1], is correct and satisfies the WI’s. However, it has important limitations. One of them is that it is restricted to \( eV \ll k_BT_K \). For this reason, alternative approaches are usually preferred, like the non-crossing approximation (see e.g. Refs. [12, 10], which reproduces well the scaling relations with temperature \( T \) and \( V \) in the Kondo regime [10].
Ref. [1] presents also equilibrium results using rSPT for the first term in the expansion of the conductance as a function of $(T/T_0^*)^2$ ($c_T'$) and also a function of $(g\mu_B B/k_B T_0^*)^2$ ($c_B'$), where the Kondo scale is defined as $T_0^* = (g\mu_B B)^2/(4\chi(0))$, being $\chi(0)$ the magnetic susceptibility for the symmetric Anderson model $\varepsilon_d = -U/2$, for which $n_d = 1$. I use the notation of a previous paper of the authors on the subject [Eqs. (20) and (21) of Ref. [17]; see also Ref. [2] for some corrections to this work]. One realizes that including a sum of ladder diagrams the results presented improve considerably when compared to NRG results. However, as I argue below, the results are still somewhat disappointing.

One point to be noted is that out of the symmetric point $\varepsilon_d = -U/2$, it would be more natural to use the energy scale $T_0 = (g\mu_B B)^2/(4\chi)$ for the actual value of $\varepsilon_d$ to define the expansion coefficients. This leads to $c_T'$ and $c_B'$ as defined in Ref. [17]. The symmetric point, and therefore $T_0^*$ might not be experimentally accessible. This is the case of some molecular system in which $U$ is very large [13]. Moreover, since $\chi$ decreases ($T_0$ increases) fast when moving to the intermediate valence region $\varepsilon_d \sim 0$, the $c'$ are considerably smaller (by a factor $(T_0^*/T_0^*)^2$) than the $c$. As a consequence, while the $c$ have an increasing downward curvature as $\varepsilon_d$ increases from $-U/2$ to 0 [11], the $c'$ have an inflexion point [1] and become in general much smaller for $\varepsilon_d < 0$. Since at the other end of the plotted values, $\varepsilon_d = -U/2$ the coefficients are fixed by Fermi liquid properties, the end points of $c'$ are rather fixed and it is hard to see deviations from any two curves of $c'$, while they are more evident if $c$ is represented. In Ref. [3] the authors plot with the names $c_T$ and $c_B$ what they had called $c_T'$ and $c_B'$ in Ref. [17].

In Fig. 1 I show the results for $c_B'$ represented in Fig. 1 of Ref. [7] rescaled by the factor $(T_0^*/T_0^*)^2$ to represent $c_B'$. The results of a very simple interpolative perturbative approach (IPA) [18] seem excellent and better than the rSPT results shown in Fig. 2 of Ref. [1] particularly for $\varepsilon_d < -0.5\Delta$. However, in Fig. 1 of Ref. [7] one can see that the IPA results are systematically lower than the more precise obtained using DMRG or combining NRG and RPT. The origin of this difference is twofold, errors in evaluating $T_0^*$ within IPA and the factor $(T_0^*/T_0^*)^{-2}$. The difference between IPA and DMRG results for $c_B$ increases as $\varepsilon_d$ moves away of the symmetric point and reaches $12\%$ of the maximum value of $c_B$ for $\varepsilon_d = 0$. This difference is reduced to $2.6\%$ when $c_B'$ is plotted.

While the IPA might be considered acceptable for $U = 3\Delta$ and improves considerably as $U$ is lowered [1], the main problem is that the IPA [7] (and it seems to be also the case rSPT [1]) rapidly deteriorates as $U$ increases. In the Kondo limit $-\varepsilon_d, \varepsilon_d + U \gg \Delta$, one knows that the spectral density displays two charge-transfer peaks for $\omega \sim \varepsilon_d$ and $\omega \sim \varepsilon_d + U$ of total width $4\Delta$ and a Kondo peak at the Fermi level of width of the order of $2\Delta$ [14]. For $U = 3\Delta$ (the largest value of $U$ considered in Ref. [1]), these peaks cannot be separated. More accurate methods seem necessary to treat the Kondo case [2].

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{Coefficient $c_B'$ of $G/G_0 = 1 - c_B'(g\mu_B B/k_B T_0^*)^2$ vs $\varepsilon_d$ for $U = 3\Delta$ obtained by different methods.}
\end{figure}

[1] E. Muñoz, F. Zamani, L. Merker, T. A. Costi, and S. Kirchner, Journal of Physics: Conf. Series \textbf{807}, 092001 (2017).
[2] A. C. Hewson, Phys. Rev. Lett. \textbf{70}, 4007 (1993).
[3] A. A. Aligia, J. Phys. Condens. Matter \textbf{24}, 015306 (2012); Corrigendum \textbf{29}, 069501 (2017).
[4] A. A. Aligia, [arXiv:1310.8324]
[5] A. A. Aligia, Phys. Rev. B \textbf{89}, 125405 (2014).
[6] A. C. Hewson, A. Oguri, and D. Meyer, Eur. Phys. J. B \textbf{40}, 177 (2004).
[7] I. J. Hamad, C. Gazza, J. A. Andrade, A. A. Aligia, P. S. Cornaglia, and P. Roura-Bas, Phys. Rev. B \textbf{92}, 195113 (2015).
[8] E. Muñoz, C. J. Bolech, and S. Kirchner, Phys. Rev. Lett. \textbf{110}, 016601 (2013).
[9] A. A. Aligia, Phys. Rev. Lett. \textbf{111}, 089701 (2013).
[10] E. Sela and J. Malecki, Phys. Rev. B \textbf{80}, 233103 (2009).
[11] E. Muñoz, C. J. Bolech, and S. Kirchner, Phys. Rev. Lett. \textbf{111}, 089702 (2013).
[12] N. S. Wingreen and Y. Meir, Phys. Rev. B \textbf{49}, 11040 (1994).
[13] S. Florens, A. Freyn, N. Roch, W. Wernsdorfer, F. Balestro, P. Roura-Bas and A. A. Aligia, J. Phys. Condens. Matter \textbf{23}, 243202 (2011); references therein.
[14] A. A. Aligia, P. Roura-Bas, and S. Florens, Phys. Rev. B \textbf{92}, 035404 (2015); references therein.
[15] L. Tosi, P. Roura-Bas, and A. A. Aligia, Phys. Rev. B \textbf{88}, 235427 (2013); P. Roura-Bas, L. Tosi, and A. A. Aligia, Phys. Rev. B \textbf{93}, 115139 (2016).
[16] P. Roura-Bas, Phys. Rev. B \textbf{81}, 155327 (2010).
[17] L. Merker, S. Kirchner, E. Muñoz, and T. A. Costi, Phys. Rev. B \textbf{87}, 165132 (2013).
[18] H. Kajueter and G. Kotliar, Phys. Rev. Lett. \textbf{77}, 131(1996).