Comment on "Fano Resonance for Anderson Impurity Systems"

In a recent Letter, Luo *et al.* [1] analyze the Fano line shapes obtained from scanning tunneling spectroscopy of transition metal impurities on a simple metal surface, in particular, of the Ti/Au(111) and Ti/Ag(100) systems [2]. As the key point of their analysis, they claim that there is not only a Fano interference effect between the impurity d orbital and the conduction electron continuum, as derived in Ref. [3], but that the Kondo resonance in the d-electron spectral density has by itself a *second* Fano line shape, leading to the experimentally observed spectra. In the present note we point out that this analysis is conceptually incorrect. Therefore, the quantitative agreement of the fitted theoretical spectra with the experimental results is meaningless. The nomenclature and the equation numbers below refer to Ref. [1], unless stated otherwise.

Luo *et al.* adopt an effective Fermi liquid (FL) picture, where the impurity spectrum is comprised of three well-defined quasiparticle states, the single-particle levels at energies ε_d and $\varepsilon_d + U$, respectively, and the Kondo resonance near the Fermi energy ε_F. The latter arises from resonant spin-flip scattering of the impurity electrons from the conduction electrons, induced by the interplay of hybridization V and on-site Coulomb interaction U. Luo *et al.* describe this phenomenologically by means of a Dyson equation (4) which defines the potential scattering T matrix $T_d(\omega)$ of the impurity electrons. We point out that a microscopic derivation of Eq. (4) does not exist, since interaction effects (U, V) are to some degree already incorporated in Luo *et al.*'s "bare" impurity Green's function $G_d^0(\omega)$, Eq. (5), and therefore Wick's theorem is not valid here. Nevertheless, such an effective treatment may be valid in the Kondo FL regime, where the high- and low-energy scales are separated. However, the implications drawn from it in [1] are erroneous in three major points.

(1) FL theory [4] as well as numerous exact numerical renormalization group (NRG) calculations (see, e.g., Ref. [5]) demonstrate that in the Kondo as well as in the mixed valence regime the full impurity Green's function $G_d(\omega)$ has a simple peak structure near ε_F. It has, in general, a slight asymmetry caused by potential scattering, but by no means the peak-dip shape of a Fano resonance. Therefore, $G_d(\omega)$ is approximately given near ε_F by

$$G_{d\sigma}(\omega) \approx \frac{\Gamma_K/\Delta}{\omega - \varepsilon_K + i\Gamma_K}, \qquad |\omega| \lesssim T_K, \qquad T = 0. \quad (1)$$

$T_d(\omega)$ is then uniquely determined by Eq. (4); i.e., it has a complicated energy dependence which can be extracted from Eq. (1) of this Comment in combination with Eqs. (4), (5). In contrast, Luo *et al.* assume *ad hoc*, c.f. Eq. (7), that $T_d(\omega)$ has the energy dependence of Eq. (1) of this Comment, in clear contradiction to the correct statements given above. To illustrate this fact, we point out that Eq. (8) reduces to the known Kondo resonance form only in the particle-hole symmetric case ($U = 2|\varepsilon_d|$), or in the limit $\Delta/|\varepsilon_d| \ll 1$, $U \gg 2|\varepsilon_d|$, where $q_d(\omega)$ diverges at the position of the Kondo resonance, but fails to do so for all other cases in the Kondo regime. Consequently, the subsequent fitting of the experimental spectra is invalid.

(2) Luo *et al.* describe the Ti/Au(111) and Ti/Ag(100) systems [2] as being in the mixed valence regime, ($\Delta/\varepsilon_d \approx 1$), where their Fano-like factor $q_d(\omega) = -\mathrm{Re}G_d^0(\omega)/\mathrm{Im}G_d^0(\omega)$ is finite near ε_F. However, in this regime, there is no separation between low-energy spin-flip scattering and high-energy Coulomb and hybridization processes, which is the basis for Luo *et al.*'s analysis. Instead, in the mixed valence regime, the ε_d peak of the impurity spectrum and the Kondo resonance are known (e.g., from exact NRG calculations [4,5]), to merge to a single peak near ε_F of width $\sim\Delta$, and there is no distinction between Δ and Γ_K, again in contrast to Eq. (8). We note in passing that the quantitative agreement of Luo *et al.*'s results with NRG calculations shown in their Fig. 3 pertain only to quantities which are determined by high-energy physics and are, thus, not relevant for the present points of criticism.

(3) The fitting of Luo *et al.*'s expressions to the Ti/Au(111) and Ti/Ag(100) systems yields a width of the "mixed valence" resonance peak of $\Delta = 54.5$ meV and $\Delta = 29.2$ meV, respectively. This is inconsistent with the expectation that for transition metal impurities on metal surfaces the width Δ of the single-particle resonance is at least 1 order of magnitude larger. The narrow widths of the experimental spectral peaks suggests, that these are, in fact, Kondo peaks. We have theoretical evidence, that the complex line shape observed in Ti/Au(111) and Ti/Ag(100) [2] is due to the multiple Kondo resonances arising from the crystal-field split local orbitals of the transition metal impurity. This will be discussed elsewhere.

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