Fano Resonance for Anderson Impurity Systems

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We present a general theory for the Fano resonance in Anderson impurity systems. It is shown that the broadening of the impurity level leads to an additional and important contribution to the Fano resonance around the Fermi surface, especially in the mixed valence regime. This contribution results from the interference between the Kondo resonance and the broadened impurity level. Being applied to the scanning tunneling microscopic experiments, we find that our theory gives a consistent and quantitative account for the Fano resonance line shapes for both Co and Ti impurities on Au or Ag surfaces. The Ti systems are found to be in the mixed valence regime.

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The Fano resonance [1] is a ubiquitous phenomenon observed in different fields including atomic and condensed matter physics. This resonance results from the interference between a continuum and an embedded discrete level and is characterized by an asymmetry factor q for the line shape [1]. Recently, the interest in the Fano resonance has been renewed in the study of the Kondo effect by the scanning tunneling microscope (STM) measurements. Experimentally, the tunneling spectra of $3d$ transition metal atoms on noble metal surfaces manifest themselves as Fano resonances near the Fermi level ε_F [2–6]. In the Kondo regime, for example, in the systems of Co atoms on Au [2], Cu [4,5], or Ag [6] surfaces, this resonance is believed to result from the interference between the Kondo resonance and the conduction electrons [7–11]. However, in other impurity systems, such as Ti atoms on Au [12] or Ag [13] surfaces, the line shape appears much more complicated and cannot be explained without invoking a broadened impurity level near the Fermi surface [12,13]. In this case, the interference between the Kondo resonance and the conduction electrons is dramatically modified by the broadened impurity level, and a microscopic picture for the Fano resonance has not been established.

In this Letter, we study the effect of the Fano resonance on the density of states of conducting electrons in the Anderson impurity systems by explicitly taking account of the broadening effect of impurity levels. It is shown that the line shape of Fano resonance at the Fermi level is determined by two interference processes. One is the interference between the Kondo resonance and the broadened impurity level that serves effectively as an open (quasicontinuum) channel; the other is the interference between the Kondo resonance and the conduction band. While the contribution from the former interference channel is very small in the Kondo regime where the impurity levels lie well below or above the Fermi energy, it becomes important in the mixed valence regime, where the impurity levels are located within the linewidth from the Fermi energy. In previous studies, attention has been paid to the Fano resonance observed in the Kondo regime [2–6], but the recent measurement data for Ti/Au [12] and Ti/Ag [13] appear not to fall into this category. We will show that, by incorporating the broadening effects, we can also give quantitative account for the line shapes of the Fano resonance in these cases.

For an Anderson impurity system, as schematically shown in Fig. 1, the hybridization of the impurity with the conduction electrons leads to the broadening of the impurity levels. At low temperatures, the conduction electrons screen the impurity spin, and a Kondo resonance emerges near ε_F [14]. The impurity density of states is a superposition of the density of states of the broadened levels and that of the Kondo resonance. In the Kondo limit, the broadening effect can be neglected, and the Fano resonance is predominantly due to the interference between a Lorentzian-shaped Kondo resonance and the conduction band. However, in the mixed valence regime,

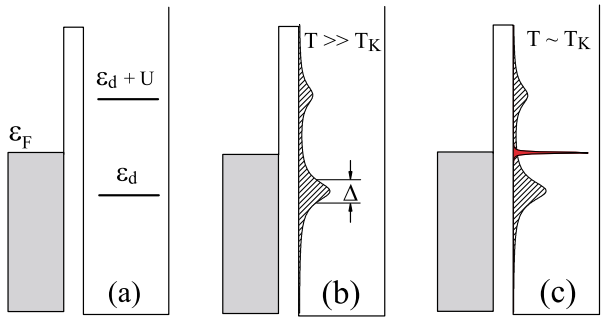

FIG. 1 (color online). Energy spectra for an Anderson impurity system. (a) The conduction band with two impurity levels ε_d and $\varepsilon_d + U$ without hybridization. (b) With hybridization, the two impurity levels are broadened with width Δ. (c) In the Kondo regime below the Kondo temperature T_K, a sharp Kondo resonance is developed at the Fermi level.

the density of states at ε_F due to the broadening becomes significant. This broadened impurity level opens effectively an alternative quasicontinuum channel and leads to an additional contribution to the Fano resonance by interfering with the Kondo resonance.

To demonstrate the above picture, let us consider the Anderson impurity model defined by [15]

$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_\sigma \varepsilon_d d^\dagger_\sigma d_\sigma + U d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow + V \sum_{k,\sigma} (c^\dagger_{k\sigma} d_\sigma + \text{H.c.}), \quad (1)$$

where $c^\dagger_{k\sigma}$ and $d^\dagger_\sigma$ are the creation operators for the conduction and impurity electrons, respectively. V is the hybridization integral, and the impurity level broadening is given by $\Delta = \pi\rho_0|V|^2$, where ρ_0 is the density of states of conduction electrons at ε_F.

The physical quantity measured by the STM is essentially the local density of states of conduction electrons around the impurity site ($r = 0$). Because of the impurity scattering, the correction to the retarded Green's function for the conduction electrons reads

$$\delta G_c(r, \omega) = |V|^2 G^0_c(r, \omega) G_d(\omega) G^0_c(-r, \omega), \quad (2)$$

where $G^0_c(r, \omega)$ and $G_d(\omega)$ are the retarded Green's functions for the conduction electrons and impurity, respectively. This leads to a correction to the local density of states for conduction electrons:

$$\delta\rho_c(r, \omega) = -\frac{1}{\pi} \text{Im}\, \delta G_c(r, \omega) = -\Delta\rho_0[(q_c^2 - 1)\,\text{Im}\, G_d(\omega) - 2q_c\,\text{Re}\, G_d(\omega)], \quad (3)$$

where $q_c = -\text{Re}\, G^0_c(r, \omega)/\text{Im}\, G^0_c(r, \omega)$.

In the Kondo limit, $G_d(\omega)$ consists of approximately three well-separated Lorentzian poles [7]. Two of them are located at ε_d and $\varepsilon_d + U$, and the third one is the Kondo resonance at the Fermi level. In this case, Eq. (3) can be recast into the standard form for the Fano resonance with an asymmetry factor q_c [7]. The Fano resonance can then be interpreted as a result of the interference between the Kondo resonance and the conduction band.

When $|\varepsilon_d - \varepsilon_F|$ is of order Δ or smaller, the Lorentzian pole approximation for the Kondo resonance is no longer valid since the broadening provides a new channel for the interference and should be reflected in $G_d(\omega)$. Using the Dyson equation, it can be shown that the impurity Green's function $G_d(\omega)$ is given by

$$G_d(\omega) = G^0_d(\omega) + G^0_d(\omega) T_d(\omega) G^0_d(\omega), \quad (4)$$

where $T_d(\omega)$ denotes an effective scattering potential by the Kondo resonance. $G^0_d(\omega)$ includes the contribution from the hybridization:

$$G^0_d(\omega) = \frac{1 - n/2}{\omega - \varepsilon_d + i\Delta} + \frac{n/2}{\omega - \varepsilon_d - U + i\Delta}, \quad (5)$$

where $n = \langle n_{d\uparrow} + n_{d\downarrow} \rangle$ is the average occupation number on the impurity site. From the imaginary part of G_d, the density of states of the impurity is found to be

$$\rho_d(\omega) = \rho_{d,0}(\omega) - \pi\rho^2_{d,0}(\omega)[(q_d^2 - 1)\,\text{Im}\, T_d(\omega) - 2q_d\,\text{Re}\, T_d(\omega)], \quad (6)$$

where $q_d = -\text{Re}\, G^0_d(\omega)/\text{Im}\, G^0_d(\omega)$ and $\rho_{d,0}(\omega) = -\text{Im}\, G^0_d(\omega)/\pi$.

The scattering matrix T_d is a complicated function of ω. However, around the Kondo energy, T_d is mainly determined by the Kondo resonance pole and is approximately given by

$$T_d(\omega) \approx \frac{\Gamma_K}{\pi\rho_{d,0}(\varepsilon_K)} \frac{1}{\omega - \varepsilon_K + i\Gamma_K} + t_{\text{incoh}}, \quad (7)$$

where ε_K is the energy of the Kondo resonance and Γ_K is its width. t_{incoh} denotes the incoherent contribution. Substituting (7) into (6) and ignoring the t_{incoh} term, we obtain

$$\rho_d(\omega) \approx \rho_{d,0}(\varepsilon_K) \frac{(\tilde{\varepsilon} + q_d)^2}{\tilde{\varepsilon}^2 + 1}, \quad (8)$$

where $\tilde{\varepsilon} = (\omega - \varepsilon_K)/\Gamma_K$. Equation (8) is a generalization of the standard formula for the Fano resonance [1]. The difference is that the asymmetry factor q_d is now ω dependent. It is natural to interpret this formula as a result of the interference between the Kondo resonance (serving as the discrete channel) and the broadened impurity levels (serving effectively as the open channel), although both channels belong to the same physical object.

Equation (8) captures the main feature of the density of states of d electrons in the Kondo limit, i.e., $|\varepsilon_d - \varepsilon_K| \gg \Delta$. Around the Fermi level $|q_d| \to \infty$ and ρ_d takes a simple Lorentzian form:

$$\rho_d(\omega) \approx \frac{\Gamma_K}{\pi\Delta} \frac{\Gamma_K}{(\omega - \varepsilon_K)^2 + \Gamma_K^2}. \quad (9)$$

In this case the broadening effect is weak. This is actually the starting point of Ujsaghy *et al.* for the Fano resonance analysis [7]. On the other hand, if $|\varepsilon_d - \varepsilon_K| \sim \Delta$, $\rho_d(\omega)$ is no longer a Lorentzian around ε_K; neither can it be written as a sum of a Lorentzian function similar to Eq. (9) and $\rho_{d,0}$. This shows that the Fano resonance of conduction electrons described by Eq. (3) is of a more complex form, and cannot be expressed as a simple sum of two Fano resonances, as assumed in Refs. [7,8].

The above analysis indicates that two asymmetry factors, q_c and q_d, are needed in order to characterize the Fano resonance of conduction electrons in the Anderson impurity model. The introduction of this additional

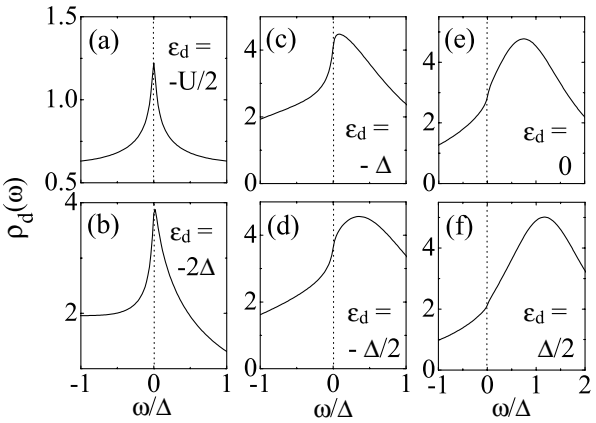

FIG. 2. $\rho_d(\omega)$ for different ε_d with $U = 4\pi\Delta$.

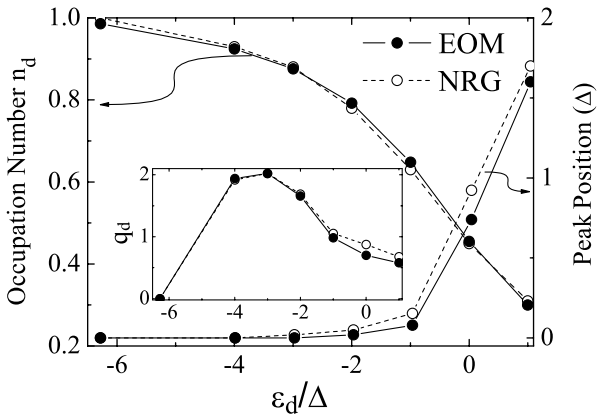

FIG. 3. Comparison of the results obtained with EOM and NRG approaches for the impurity electron occupation number, the peak position, and q_d at the Fermi level (inset). The NRG results are extracted from Table I and Figs. 5 and 8 in Ref. [18].

asymmetry factor q_d is vital for the description of the Fano resonance in the mixed valence regime.

To elucidate more explicitly the broadening effect, we have evaluated the impurity density of states using the equation of motion (EOM) approach [16,17]. Figure 2 shows $\rho_d(\omega)$ for several limiting cases. In the Kondo regime, the Kondo peak located at ε_F is known to be symmetric for the particle-hole symmetric case [Fig. 2(a)] and asymmetric otherwise [Fig. 2(b)]. However, in the mixed valence or empty orbital regime [Figs. 2(c)–2(f), the sharp Kondo resonance peak is washed out and is replaced by a kink at ε_F when ε_d is above ε_F. These are consistent with the numerical renormalization group (NRG) results [18]. By further comparison with the NRG results, we found that the height of the peak in ρ_d obtained with the EOM is underestimated. However, the results for the peak position of ρ_d, the impurity electron occupancy, and the key parameters for characterizing the Fano resonance q_d are all in good agreement with the NRG calculations (Fig. 3). In the mixed valence regime, $\rho_d(\omega)$ cannot be written as a Lorentzian, similar to Eq. (9), even after subtracting the contribution from the broadened impurity levels.

Now let us apply our theory to the STM experiments for Co or Ti atoms on noble metal surfaces. The tunneling conductance measured by STM is proportional to the local density of states of conduction electrons $\rho_0 + \delta\rho_c(\omega)$.

For Co atoms on the Au (111) surface [2], the model parameters determined by density functional theory [7] are $\varepsilon_d - \varepsilon_F = -0.84$ eV, $U = 2.84$ eV, $\Delta = 0.2$ eV and $n = 0.8$. This impurity system is in the Kondo regime [7]. However, as $|\varepsilon_d - \varepsilon_F|$ is bigger than Δ only by a factor of 4, the broadening effect can still have a small but finite contribution. From the above parameters, the Fano factor for the d electrons is found to be $q_d(\varepsilon_F) \approx 2.6$. Taking all the above parameters as input, we have analyzed the experimental data published in Ref. [2] using Eqs. (3)–(5) and (7). As shown in Fig. 4, our result agrees well with the experimental data. The fitting parameters used are $q_c = 1.4$, $\varepsilon_K = 4.0$ meV, and $\Gamma_K = 5.6$ meV. Our result also agrees with the theoretical calculation by Ujsaghy *et al.* [7]. However, the Fano factor q_c we obtained is bigger than theirs, $q_c = 0.66$, which indicates that the broadened impurity level has a sizable contribution to the Fano resonance, even if the system is in the Kondo regime. Furthermore, the other parameters we obtained are also slightly different from theirs. In addition, it should be pointed out that, although Eq. (3) in Ref. [7] captures the main feature of the Fano resonance in the Kondo limit, the spectral weight of the ε_d level, deduced from the parameters given in Ref. [7], is $Z_d \sim 11$ which is larger than the upper limit of Z_d physically allowed.

For Ti/Au(111) [12] and Ti/Ag(100) [13], the tunneling spectra cannot be simply fitted by the standard Fano formula. The authors of Refs. [12,13] proposed to use two Fano resonances to fit the tunneling conductance. In particular, they assumed that there is a narrow Fano resonance, taking as the Kondo resonance, at ε_F, and a broader Fano resonance slightly above ε_F, originated from a bare Ti d resonance. From the fitting, they found that the normalized energy of Ti d level $\bar{\varepsilon}_d \sim 36$ meV and

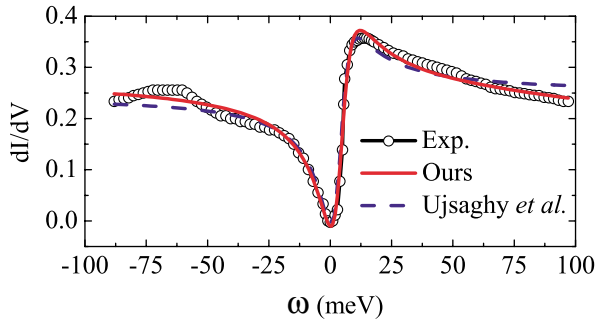

FIG. 4 (color online). Comparison between our theoretical result and the STM measurement data for Co/Au [2]. The result of Ref. [7] is also shown for comparison (dashed line).

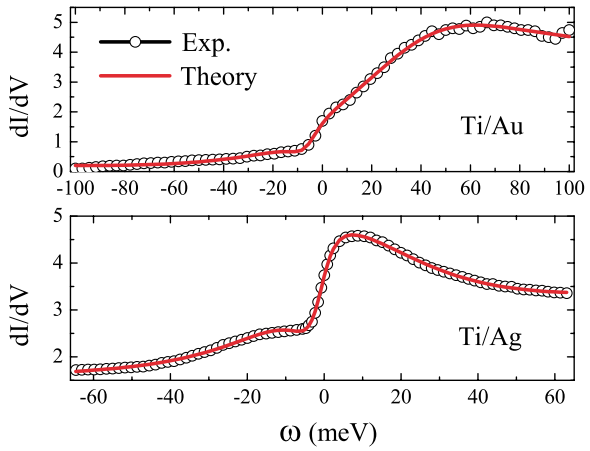

FIG. 5 (color online). Comparison between theoretical fitting curves and the STM measurement data for Ti/Au(111) [12] and Ti/Ag(100) [13].

the broadening parameter $\Delta = 127$ meV for Ti/Au(111), and $\bar{\varepsilon}_d \sim 10$ meV and $\Delta = 78$ meV for Ti/Ag(100). Their results indicate clearly that the broadening effect is rather strong in these systems. However, as mentioned earlier, when the broadening of the d level is larger than the separation between ε_d and ε_F, it is not appropriate, even approximately, to separate the bare d resonance with the Kondo resonance.

We have also analyzed the tunneling spectra for Ti/Au(111) and Ti/Ag(100) using our formula. Figure 5 compares our theoretical results with the experimental data. Our theoretical curves agree quantitatively with the experimental results [12,13]. From the fitting (set $\varepsilon_F = 0$), we find that $n = 0.35$, $\varepsilon_d = 34.7$ meV, $\Delta = 54.5$ meV, $U = 81$ meV, $\varepsilon_K = -5.8$ meV, $\Gamma_K = 7.4$ meV, $q_c = 1.6$, and $q_d = -0.7$ for Ti/Au(111), and $n = 0.6$, $\varepsilon_d = 0.97$ meV, $\Delta = 29.2$ meV, $U = 120.9$ meV, $\varepsilon_K = -1.5$ meV, $\Gamma_K = 5.4$ meV, $q_c = 0.9$, and $q_d = -0.13$ for Ti/Ag(100). In agreement with [12,13], we find that ε_d lies very close to the Fermi level. Furthermore, for both cases $|q_d| < q_c$, therefore, the Fano resonance is strongly modified by the broadening of the impurity levels. Our result shows that Ti/Au and Ti/Ag are all in the mixed valence regime. This can, in principle, be verified by density functional band structure calculations [19].

In summary, we have established a unified microscopic picture for the Fano resonance in both Kondo and mixed valence regimes in the Anderson impurity systems. It is shown that the broadened impurity levels can effectively interfere with the Kondo resonance to affect significantly the density of states measured by the STM, especially in the mixed valence regime. Our theory gives a quantitative account for the STM spectra of Co/Au as well as Ti/Au or Ti/Ag systems. Our work is also of great interest for the interpretation of experimental data in more complex impurity systems explored in recent years, such as quantum dots [20,21].

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