The 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 tunnelling microscopic experiments, we find that our theory gives a consistent and quantitative account for the Fano resonance lineshapes for both Co and Ti impurities on Au or Ag surfaces. The Ti systems are found to be in the mixed valence regime.

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 a discrete level embedded and is characterized by an asymmetry factor $q$ for the lineshape [1]. Recently, the interest in the Fano resonance has been renewed in the study of the Kondo effect by the scanning tunnelling microscope (STM) measurements. Experimentally, the tunnelling spectra of 3d transition metal atoms on noble metal surfaces manifest themselves as Fano resonances near the Fermi level $\varepsilon_F$ [2, 3, 4, 5]. 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, 8]. However, in other impurity systems, such as Ti atoms on Au [7] or Ag [8] surfaces, the lineshape appears much more complicated and cannot be explained without invoking a broadened impurity level near the Fermi surface $\varepsilon_F$. 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 lineshape 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 (quasi-continuum) 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 because 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, 3, 4, 5, 6], but the recent measurement data for Ti/Au [7] and Ti/Ag [8] appear not to fall into this category. We will show that by incorporating the broadening effects, we can also give quantitative account for the lineshapes 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 $\varepsilon_F$. 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, the density of states at $\varepsilon_F$ due to the broadening becomes significant. This broadened impurity level opens effectively an alternative quasi-continuum 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

\begin{figure}[h]
\centering
\includegraphics[scale=0.5]{fig1.png}
\caption{Energy spectra for an Anderson impurity system: (a) The conduction band with two impurity levels $\varepsilon_d$ and $\varepsilon_d + U$ without hybridization; (b) With hybridization, the two impurity levels are broadened with width $\Delta$; (c) In the Kondo regime below the Kondo temperature $T_K$, a sharp Kondo resonance is developed at the Fermi level.}
\end{figure}
Anderson impurity model defined by [14]

\[
H = \sum_{k,\sigma} \varepsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \sum_\sigma \varepsilon_d d_{\sigma}^\dagger d_{\sigma} + U d_{\uparrow} d_{\downarrow} + V \sum_{k,\sigma} (c_{k\sigma}^\dagger d_{\sigma} + h.c.),
\]

where \(c_{k\sigma}^\dagger\) and \(d_{\sigma}^\dagger\) 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 \(\rho_0\) is the density of states of conduction electrons at \(\varepsilon_F\).

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

\[
\delta G_c(r, \omega) = |V|^2 G^0_c(r, \omega) G_d(\omega) G^0_c(−r, \omega),
\]

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:

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

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

In the Kondo limit, \(G_d(\omega)\) consists of approximately three well-separated Lorentzian poles [1]. Two of them are located at \(\varepsilon_d\) 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 \(q_d\) [2]. 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 \(\Delta\) 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

\[
G_d(\omega) = G^0_d(\omega) + G^0_d(\omega) T_d(\omega) G^0_d(\omega),
\]

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

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

where \(n = \langle n_d \rangle + \langle n_d \rangle\) 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

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

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 \(\omega\). However, around the Kondo energy, \(T_d\) is mainly determined by the Kondo resonance pole and is approximated by

\[
T_d(\omega) \approx \frac{\Gamma_K}{\pi \rho_d,0(\varepsilon_K) \omega - \varepsilon_K + i\Gamma_K} + t_{\text{incoh}},
\]

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

\[
\rho_d(\omega) \approx \rho_{d,0}(\varepsilon_K) \left( \frac{\bar{\varepsilon} + q_d}{\bar{\varepsilon} + 1} \right)^2,
\]

where \(\bar{\varepsilon} = (\omega - \varepsilon_K)/\Gamma_K\). Eq. (5) is a generalization of the standard formula for the Fano resonance [1]. The difference is that the asymmetry factor \(q_d\) is now \(\omega\)-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 \(\rho_d\) takes a simple Lorentzian form

\[
\rho_d(\omega) \approx \frac{\Gamma_K}{\pi \Delta} \left( \frac{\varepsilon_K}{\omega - \varepsilon_K} \right)^2 + \frac{\Gamma_K}{\pi \Delta}.
\]

In this case the broadening effect is weak. This is actually the starting point of Ujjah et al. for the Fano resonance analysis [9]. On the other hand, if \(|\varepsilon_d - \varepsilon_K| \sim \Delta\), \(\rho_d(\omega)\) is no longer a Lorentzian around \(\varepsilon_K\), neither can it be written as a sum of a Lorentzian function like 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 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 [17, 18]. Fig. 2 shows \(\rho_d(\omega)\) for several limiting cases. In the Kondo regime, the Kondo peak located at \(\varepsilon_F\) is known to be symmetric for the particle-hole symmetric case (Fig. 2a) and asymmetric otherwise (Fig. 2b). However, in the mixed valence or empty orbital regime (Fig. 2c-f), the sharp Kondo resonance peak is washed out and is replaced by a kink at \(\varepsilon_F\) when \(\varepsilon_d\) is above \(\varepsilon_F\). These are consistent with the numerical renormalization group.
(NRG) results [16]. By further comparison with the NRG results, we found that the height of the peak in \( \rho_d(\omega) \) obtained with the EOM is underestimated. However, the results for the peak position of \( \rho_d \), 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, like Eq. (9), even after subtracting the contribution from the broadened impurity levels.

\[
\rho_d(\omega) = \frac{N}{2 \pi} \left| \frac{\gamma}{\omega - \epsilon + i \Gamma} \right|^2 \\
\text{for } \omega \gg \Gamma, \eta, \epsilon
\]

\( F = \frac{N}{2 \pi} \left| \frac{\gamma}{\omega - \epsilon + i \Gamma} \right|^2 \\
\text{for } \omega < \Gamma, \eta, \epsilon
\]

\( q_e = 1.4, \epsilon_K = 4.0 \text{ meV} \) and \( \Gamma_K = 5.6 \text{ meV} \). Our result also agrees with the theoretical calculation by Ujsaghy et al. [17]. However, the Fano factor \( q_c \) we obtained is bigger than theirs \( q_c \approx 0.66 \), which indicates that the broadened impurity level has a sizeable 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. [17] captures the main feature of the Fano resonance in the Kondo limit, the spectral weight of the \( \epsilon_d \) level, deduced from the parameters given in Ref. [17], is \( Z_d \approx 1 \) which is larger than the upper limit of \( Z_d \) physically allowed.

For Ti/Au(111) [7] and Ti/Ag(100) [8], the tunnelling spectra cannot be simply fitted by the standard Fano formula. The authors of Refs. [7, 8] proposed to use two Fano resonances to fit the tunnelling conductance. In particular, they assumed that there is a narrow Fano resonance, taking as the Kondo resonance, at \( \epsilon_F \), and a broader Fano resonance slightly above \( \epsilon_F \), originated from a bare Ti \( d \)-resonance. From the fitting, they found that the normalized energy of Ti \( d \)-level \( \epsilon_d \sim 36 \text{ meV} \) and the broadening parameter \( \Delta = 127 \text{ meV} \) for Ti/Au(111), and \( \epsilon_d \sim 10 \text{ meV} \) and \( \Delta = 78 \text{ meV} \) 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 \( \epsilon_d \) and \( \epsilon_F \), it is not appropriate, even approximately, to separate the bare \( d \)-resonance with the Kondo resonance.

We have also analyzed the tunnelling spectra for

\[
\rho_d(\omega) = \frac{N}{2 \pi} \left| \frac{\gamma}{\omega - \epsilon + i \Gamma} \right|^2 \\
\text{for } \omega \gg \Gamma, \eta, \epsilon
\]

\( \text{for } \omega < \Gamma, \eta, \epsilon
\]

\( F = \frac{N}{2 \pi} \left| \frac{\gamma}{\omega - \epsilon + i \Gamma} \right|^2 \\
\text{for } \omega < \Gamma, \eta, \epsilon
\]
FIG. 5: Comparison between theoretical fitting curves and the STM measurement data for Ti/Au(111) and Ti/Ag(100) using our formula. Fig. compares our theoretical results with the experimental data. Our theoretical curves agree quantitatively with the experimental results. From the fitting set with the experimental results [7, 8], we find that \( \varepsilon_d \) lies very closely 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].

We are grateful to M. F. Crommie for kindly providing us with the experimental data. We also acknowledge fruitful discussions with B. G. Liu, Y. L. Liu and G. M. Zhang and useful correspondence with T. A. Costi, A. Zawadowski, and O. Ujsaghy. This work is supported in part by the Special Funds for Major State Basic Research Projects of China and by the National Natural Science Foundation of China.

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