Workshop on correlations, criticality, and coherence in quantum systems

Kondo and Fano resonances in correlated impurity systems

Hong-Gang Luo(罗洪刚)
Lanzhou University & CSRC, Beijing, China

Evora, Oct. 6-10, 2014

Outline:

1. Brief background
   What are Kondo and Fano resonances?

2. Experimental observations of Kondo resonance

3. Theoretical picture(Kondo and mixed valence regimes)

4. Kondo resonance of adatom on the graphene surface

5. Summary

Outline:

1. Brief background
   What are Kondo and Fano resonances?

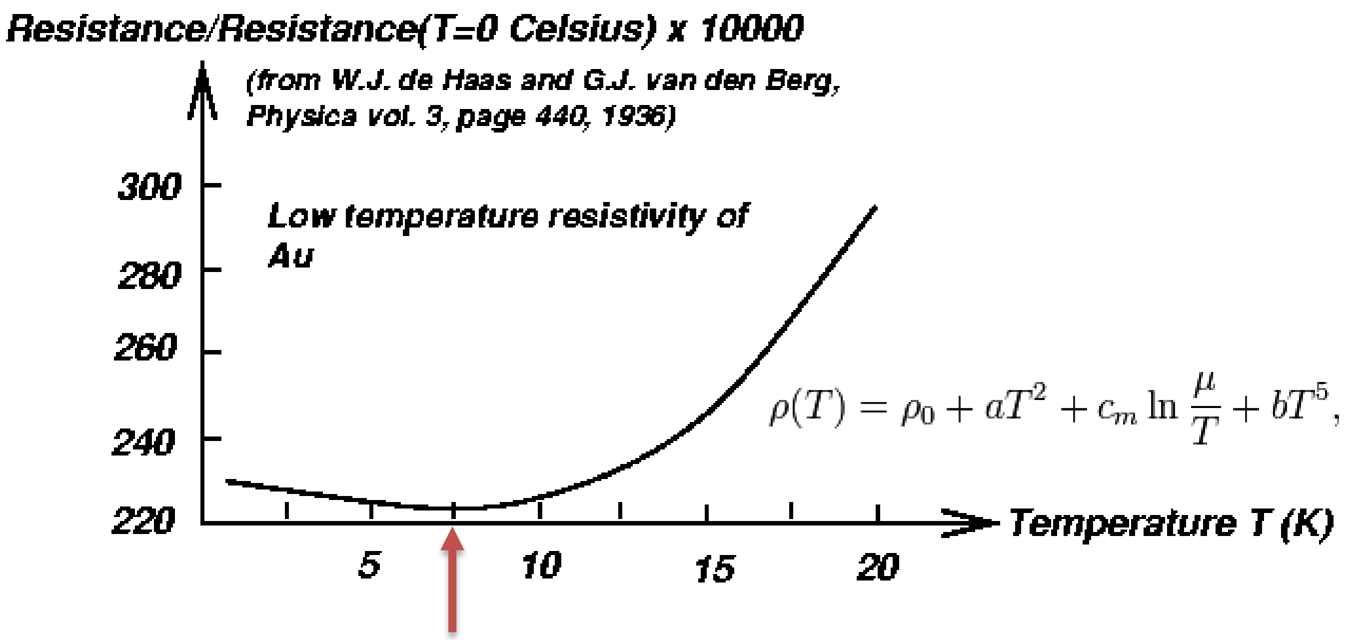
2. Experimental observations of Kondo resonance

3. Theoretical picture(Kondo and mixed valence regimes)

4. Kondo resonance of adatom on the graphene surface

5. Summary

In 1930's resistance minimum was found

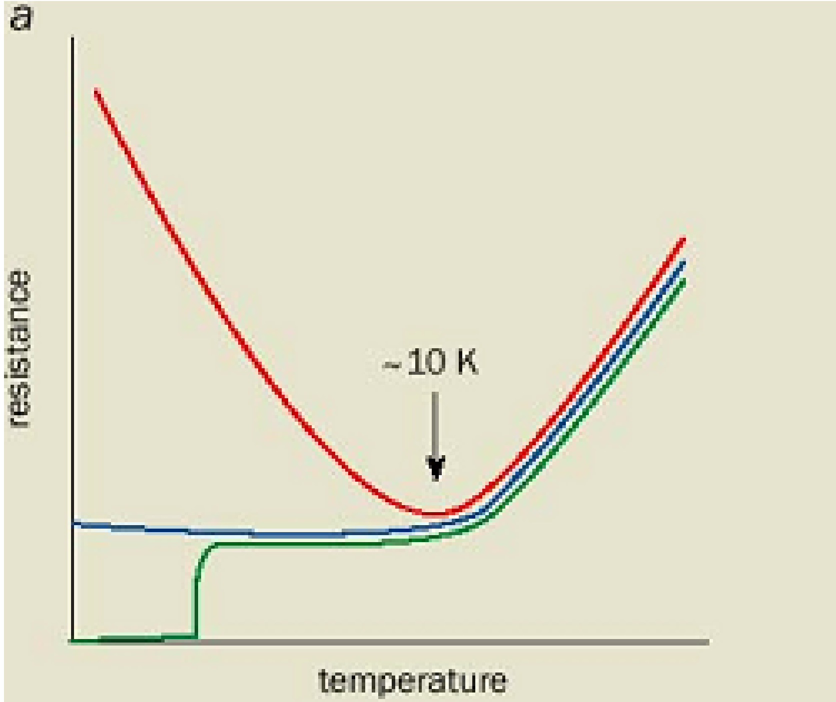


$$\rho(T) = \rho_0 + aT^2 + c_m \ln \frac{\mu}{T} + bT^5,$$

Resistance Minimum

http://en.wikipedia.org/wiki/Kondo_effect

Kondo Effect in Alloys

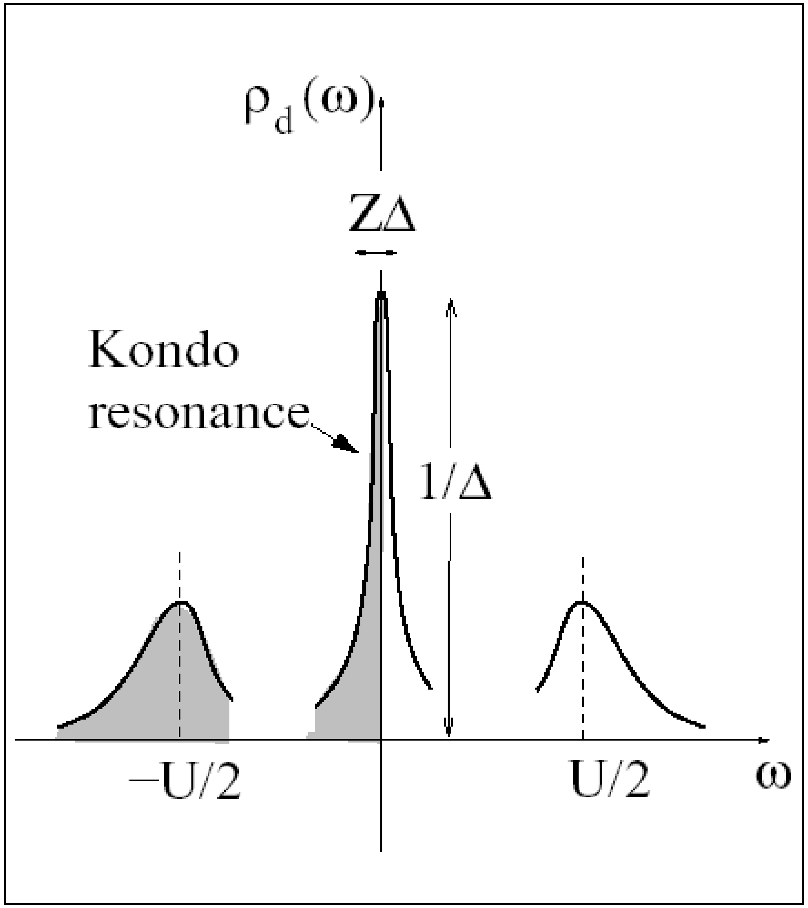


- Effect discovered in the 30's
- Leading by magnetic impurity known in 50's
- 1964 Kondo's explanation of resistance minimum

$$H_I = J\vec{\sigma}(0) \cdot \vec{S} \qquad \frac{1}{\tau} \propto [J\rho + 2(J\rho)^2 \ln \frac{D}{T}]^2$$

J. Kondo, 1964

Density of states from the Anderson model



Around the Fermi level, there is a narrow peak of height of 1/Δ but vanishingly small weight Z<<1.

This is Kondo resonance.

But for the alloy systems, one can not directly observed this resonance peak from, for example, the transport measurements.

Question: what shape of this peak?

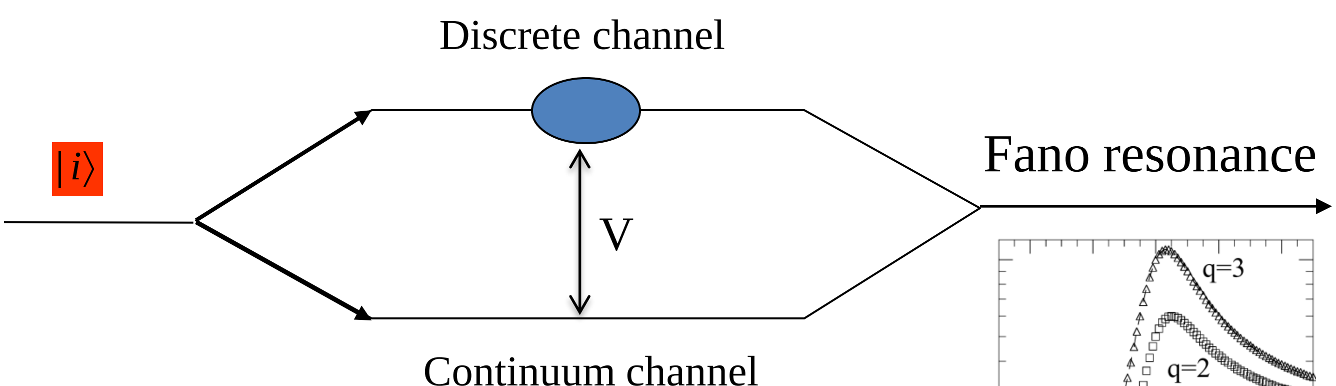
Why?

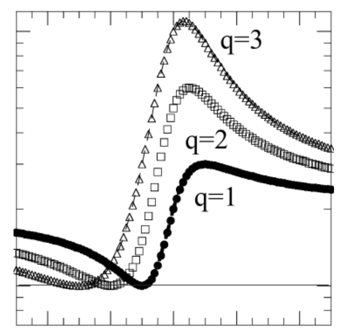
Friedel sum rule: $\rho_d(0) = \frac{1}{\Delta}\sin\frac{\pi\langle n_d\rangle}{2}$

Fano resonance (U. Fano, 1961)

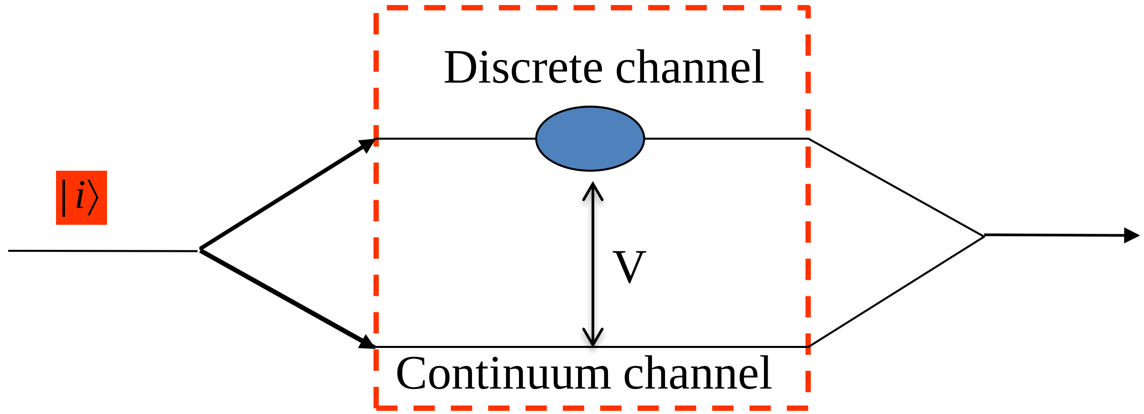
A quantum interference phenomenon between a discrete level and a continuum

U. Fano





The absorption spectrum



$$H = \varepsilon_d d^+ d + \sum_k \varepsilon_k c_k^+ c_k + V \sum_k (c_k^+ d + h.c.)$$

$$|\varphi_d\rangle = d^+ |0\rangle$$

$$|\phi_k\rangle = c_k^+ |0\rangle$$

Schrödinger equation (U. Fano, 1961):

$$\begin{cases} H|\Psi_E\rangle = E|\Psi_E\rangle \\ |\Psi_E\rangle = a|\varphi_d\rangle + \sum_k b_k |\phi_k\rangle \end{cases} \Longrightarrow \begin{cases} a = \frac{\sin\Delta}{\pi V} \\ b_k = \frac{\sin\Delta}{\pi}\frac{1}{E-\varepsilon_k} - \delta(E-\varepsilon_k)\cos\Delta \end{cases}$$

The transition probability (U. Fano, 1961)

$$\boxed{\langle \Psi_E \mid T \mid i \rangle = \tfrac{1}{\pi V} \langle \Phi \mid T \mid i \rangle \sin\Delta - \langle \phi \mid T \mid i \rangle \cos\Delta}$$

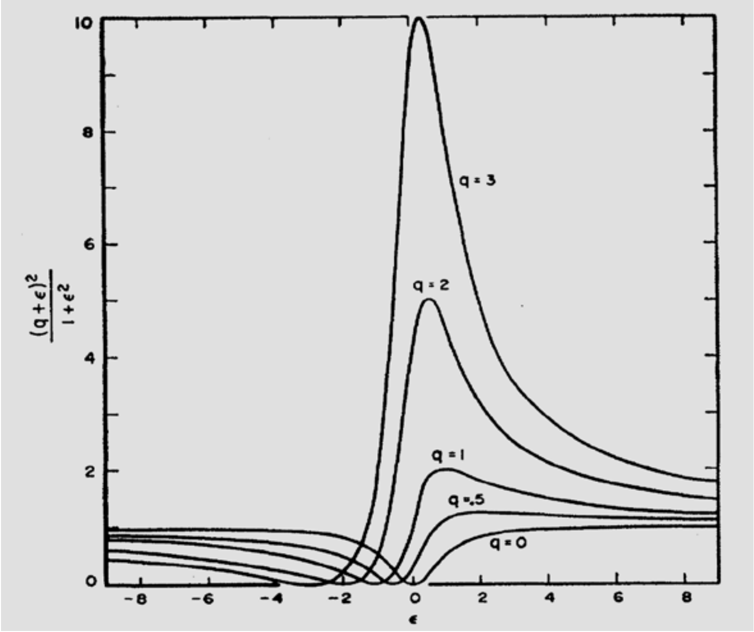
"Modified" discrete channel   Continuum channel

$$\Phi = \varphi_d + P\sum_k \tfrac{V\phi_k}{E-\varepsilon_k}$$

$$\phi = \sum_k \delta(E-\varepsilon_k) \mid \phi_k \rangle$$

The absorption spectrum

$$\frac{|\langle \Psi_E | T | i \rangle|^2}{|\langle \phi | T | i \rangle|^2} = \frac{(q+\varepsilon)^2}{1+\varepsilon^2}$$



$\varepsilon = -\cot\Delta$ Reduced energy

$q = \frac{\langle \Phi | T | i \rangle}{\pi V \langle \phi | T | i \rangle}$ Fano asymmetry parameter

A very highly cited paper: 5427

Fundamentally, Fano resonance is a quantum interference phenomenon, which can be realized in various systems!

Effects of Configuration Interaction on Intensities and Phase Shifts

Phys. Rev. **124**, 1866 – Published 15 December 1961

U. Fano

ABSTRACT
AUTHORS
REFERENCES

ABSTRACT

The interference of a discrete autoionized state with a continuum gives rise to characteristically asymmetric peaks in excitation spectra. The earlier qualitative interpretation of this phenomenon is extended and revised. A theoretical formula is fitted to the shape of the resonance of He observed in the inelastic scattering of electrons. The fitting determines the parameters of the resonance as follows: ev, ev, . The theory is extended to the interaction of one discrete level with two or more continua and of a set of discrete levels with one continuum. The theory can also give the position and intensity shifts produced in a Rydberg series of discrete levels by interaction with a level of another configuration. The connection with the nuclear theory of resonance scattering is indicated.

DOI: http://dx.doi.org/10.1103/PhysRev.124.1866

Received 14 July 1961 Published in the issue dated December 1961

To be expressed message below

Kondo meets Fano

Outline:

1. Brief background
   What are Kondo and Fano resonances?

2. Experimental observations of Kondo resonance

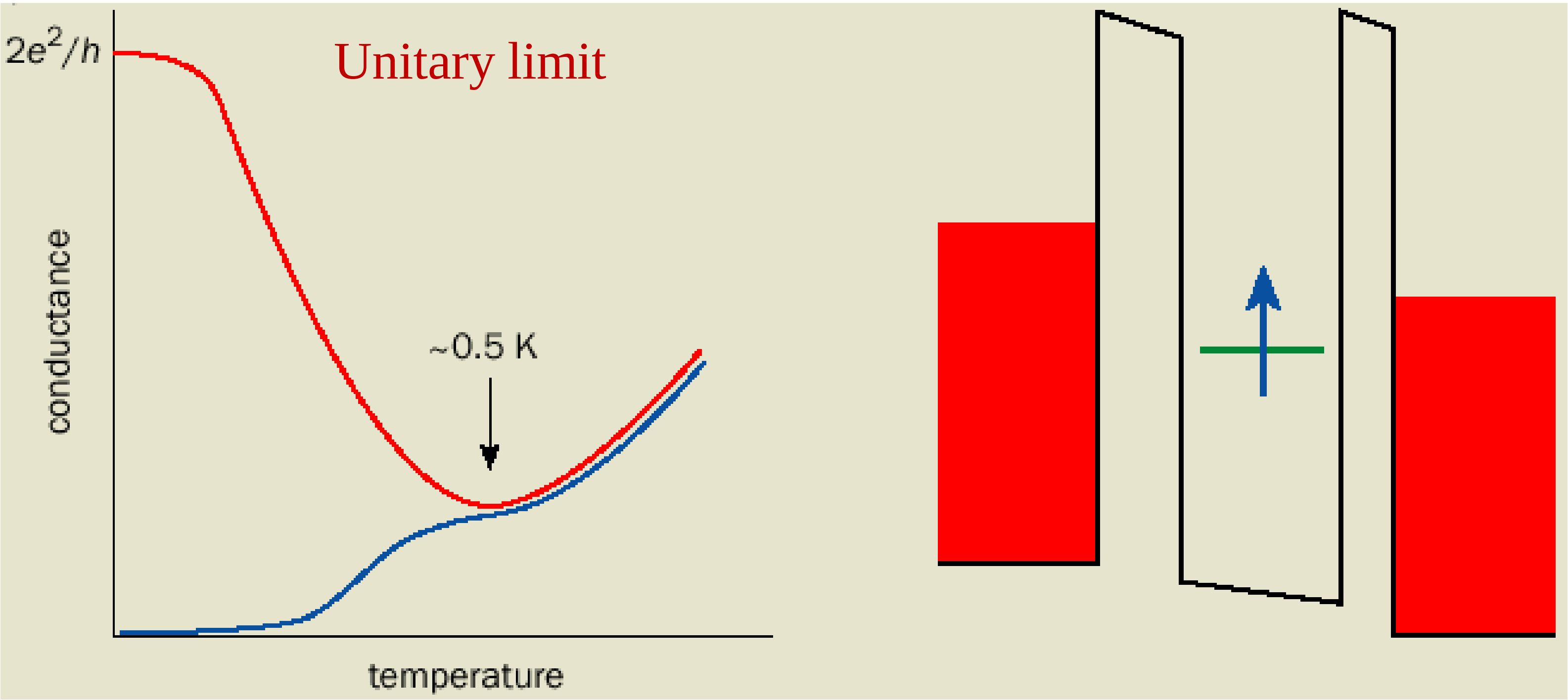
3. Theoretical picture(Kondo and mixed valence regimes)

4. Kondo resonance of adatom on the graphene surface

5. Summary

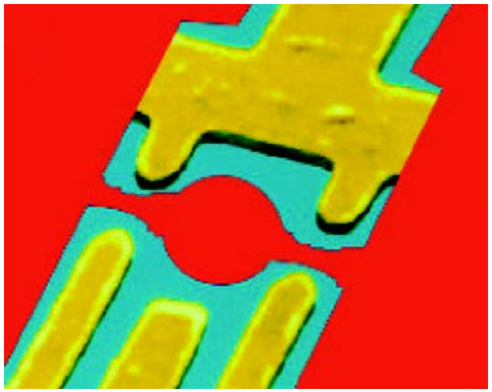
Revival of Kondo physics in quantum dots

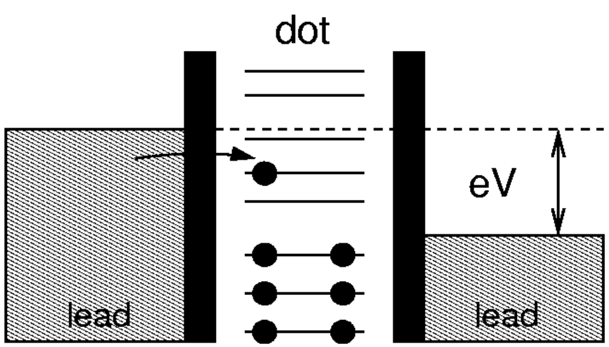
L. Kouwenhoven and L. Glazman, 2001



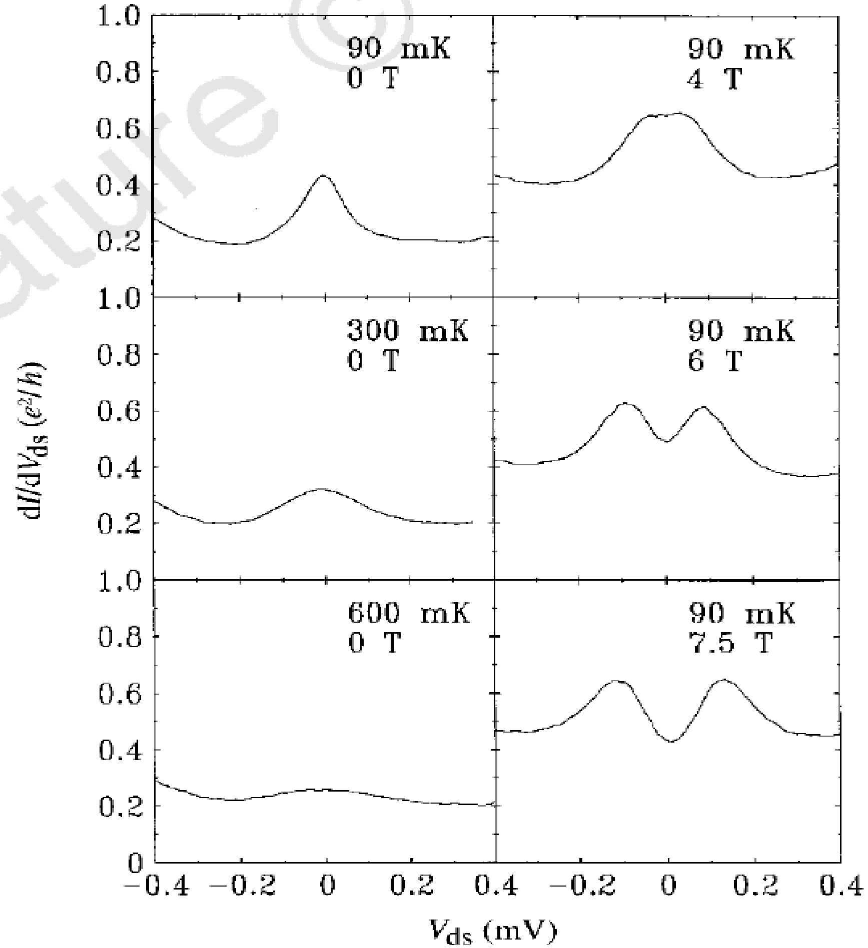
Theory:
T. K. Ng & P. A. Lee;   L. I. Glazman & M. E. Raikh, (1988)

The first experimental observation of the Kondo resonance in semiconductor quantum dots



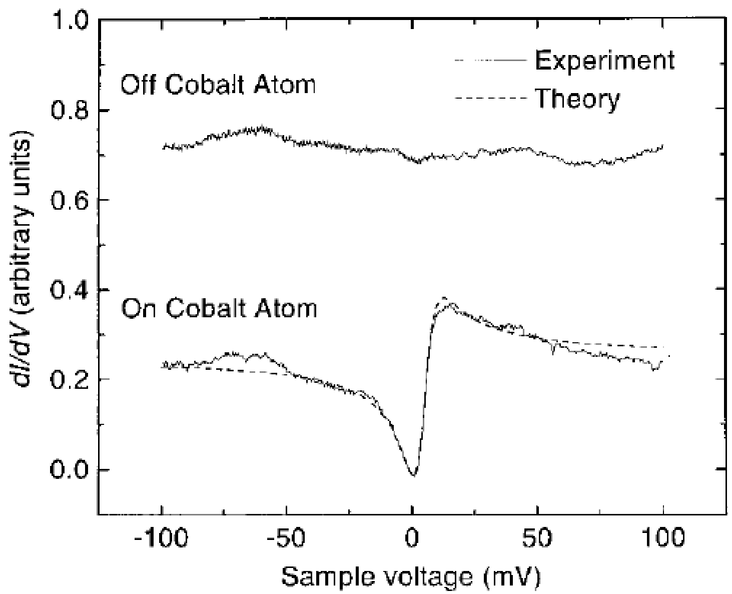


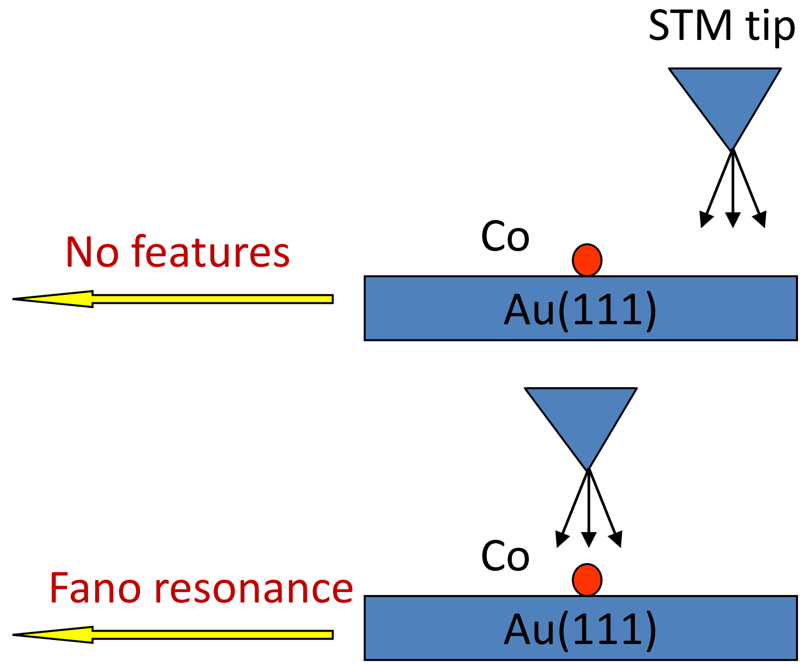
Kondo resonance

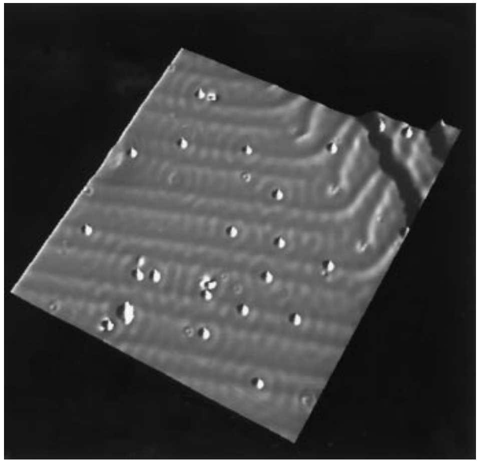


D. Goldhaber-Gordon, *et. al*. Nature **391**, 156 (1998)

The first STM + single magnetic atom system



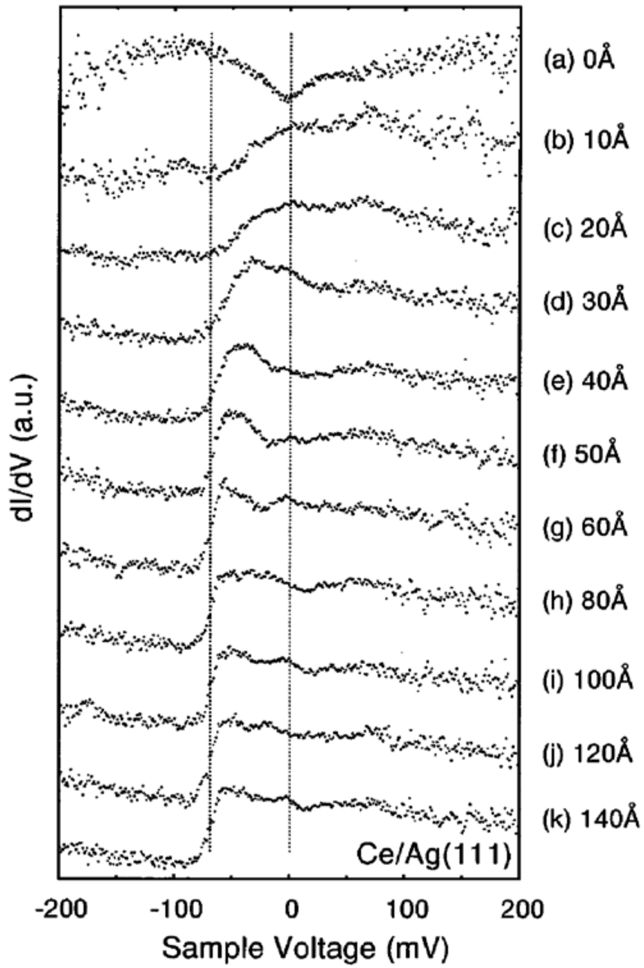


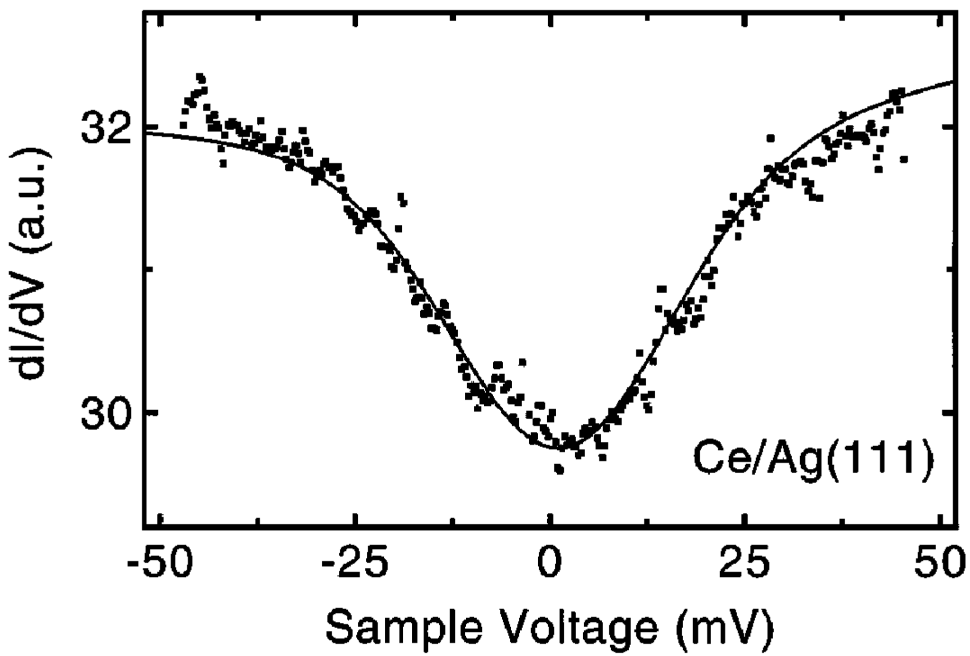


$$R(\varepsilon) = R_0(\varepsilon)\frac{(q + \varepsilon')^2}{1 + \varepsilon'^2},\ \varepsilon' = \frac{\varepsilon - \varepsilon_0}{\Gamma/2}$$

V. Madhavan, W. Chen, T. Jamneala, M. F. Crommie, N. S. Wingreen, Science **280**, 567 (1998)

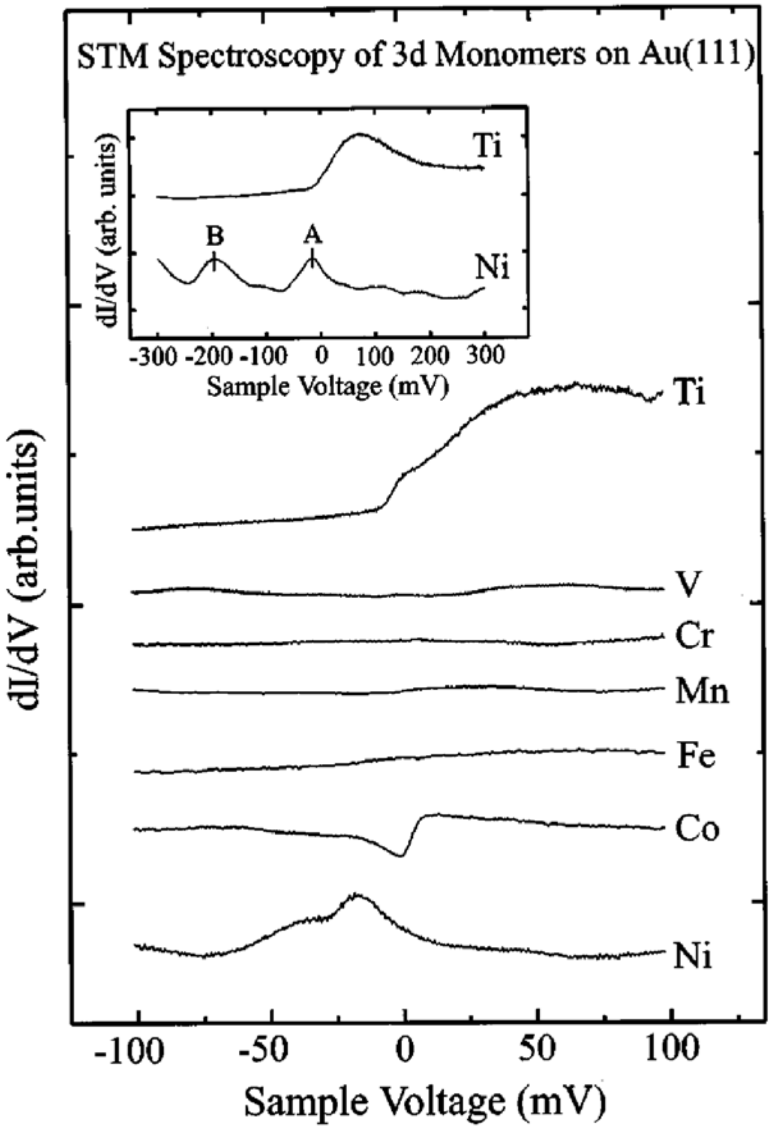
Ce/Ag(111)





J. Li et al., Phys. Rev. Lett. **80**, 2893 (1998)

More experiments



Different transition atoms
→different features

→ e.g., for Ti, there is a shoulder around the Fermi level on the broaden background.

Why ?

T. Jamneala et al. Phys. Rev. B 61, 9990 (2000)

Existing theory and simple Fano-fits

Simple extension of the original Fano resonance theory to the correlated systems:

The discrete channel:

The Kondo resonance (KR)

$$\varepsilon' = \frac{\varepsilon - \varepsilon_K}{\Gamma_K / 2}$$

ε_K: position of the KR

Γ_K: width of the KR

The continuum channel:

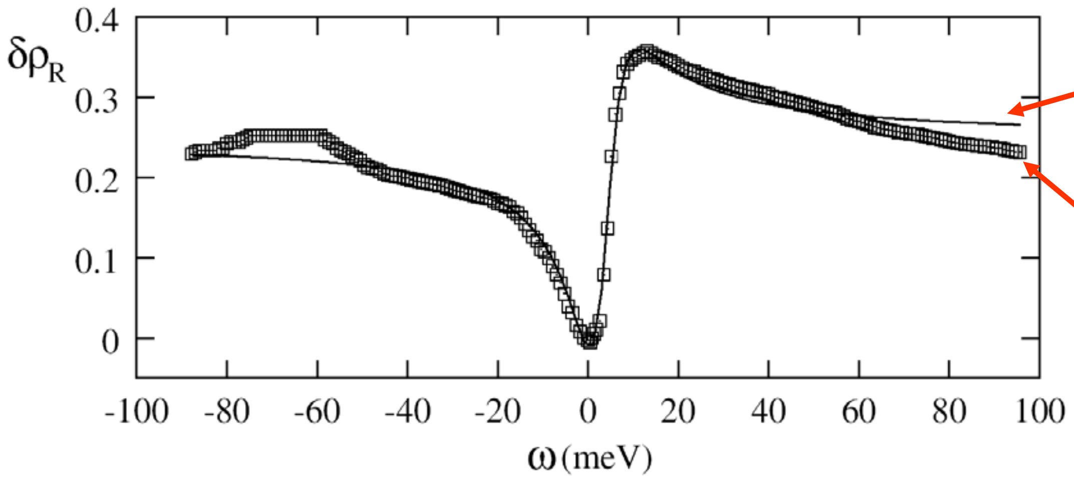
The conduction electrons

Simple Fano-fit formula:

$$R(\varepsilon) = R(\varepsilon_0)\frac{(q+\varepsilon')^2}{1+\varepsilon'^2}$$

q: Fano asymmetry parameter

By the simple Fano-fits, most of experimental data can be fitted. For example:



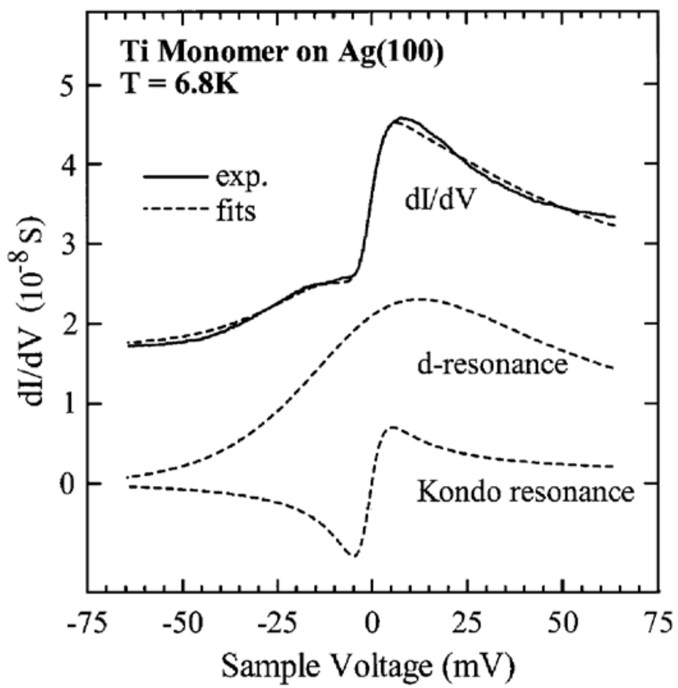
Simple Fano-fit

Exp. Data Co/Au(111)

O. Ujsaghy *et al*., PRL **85**, 2557 (2000)

Fit parameters:
$q = 0.66$
$\varepsilon_K \sim 3.6\text{meV}$
$T_K \sim 5.0\text{meV}$

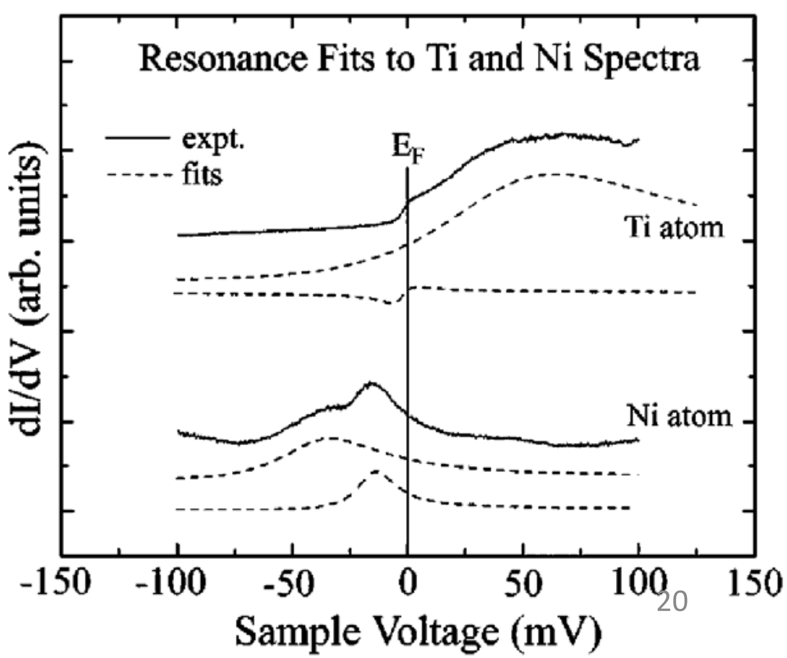
Single magnetic atom on the metal surface



Need two simple Fano-fits

K. Nagaoka et al., PRL 88, 077205 (2002)

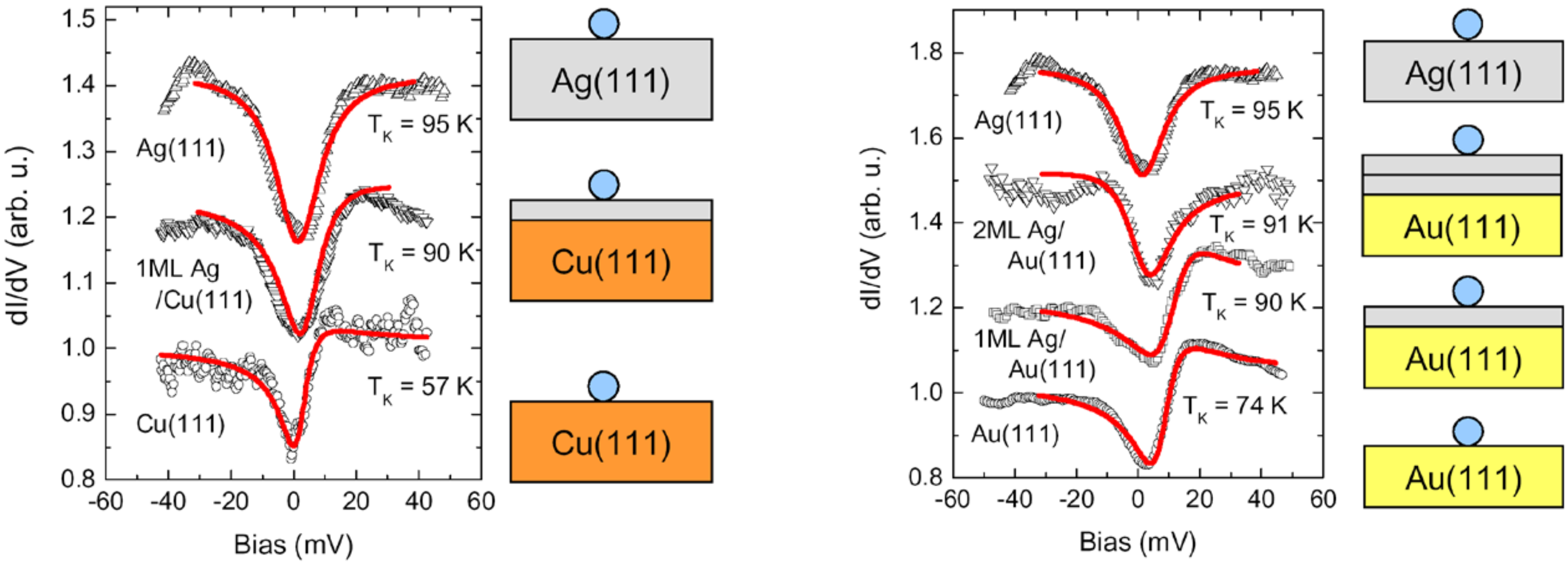
The same for Ti/Au(111)



T. Jamneala, PRB 61, 9990 (2000)

Kondo effect of Co adatoms on Ag monolayers on noble metal surfaces

M.A. Schneider, P. Wahl, L. Diekhöner, L. Vitali, G. Wittich, and K. Kern
Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany



substrate	T_K	q	E_0	m^*	$E_{L_{2'}}$	E_{L_1}	ϕ
Cu(111)	54±2 K[10,12]	0.2	-0.44 eV[19]	$0.38m_0$[19]	-0.9 eV[23]	4.25 eV[23]	4.94 eV[23]
Au(111)	76±8 K [*,7]	0.7	-0.51 eV[20]	$0.27m_0$[20]	-1.0 eV[23]	3.6 eV[23]	5.55 eV[23]
Ag(111)	92±6 K[13]	0.0	-0.065 eV[19]	$0.40m_0$[19]	-0.4 eV[23]	3.9 eV[23]	4.56 eV[23]
1ML Ag/Au(111)	88±10 K [*]	0.8	-0.27 eV[24]	$0.3\ m_0$[24]	-1.0 eV	3.6 eV	"
2ML Ag/Au(111)	95±10 K [*]	-0.1	-0.2 eV[24]	$0.4\ m_0$[24]	"	"	"
1ML Ag/Cu(111)	92±10 K [*]	0.15	-0.23 eV[22]		-0.9 eV	4.25 eV	"

I agree, that the Fano-Fit does not always work very well.
(M.A. Schneider, private communication)

Cond-mat/0409390

A puzzle: in some systems mentioned above, where is the continuum channel?

No "*visible*" continuum channel has been identified in some systems such as the single electron transistor (Gores *et al.*, 2000) and the SWNT (Babic and Schonenberger, 2004).

Our observation:

- All existing discussions neglected the broadening impurity level.
- Obviously, the broadening impurity level has a contribution to the density of states near the Fermi level.

Outline:

1. Brief background
   What are Kondo and Fano resonances?

2. Experimental observations of Kondo resonance

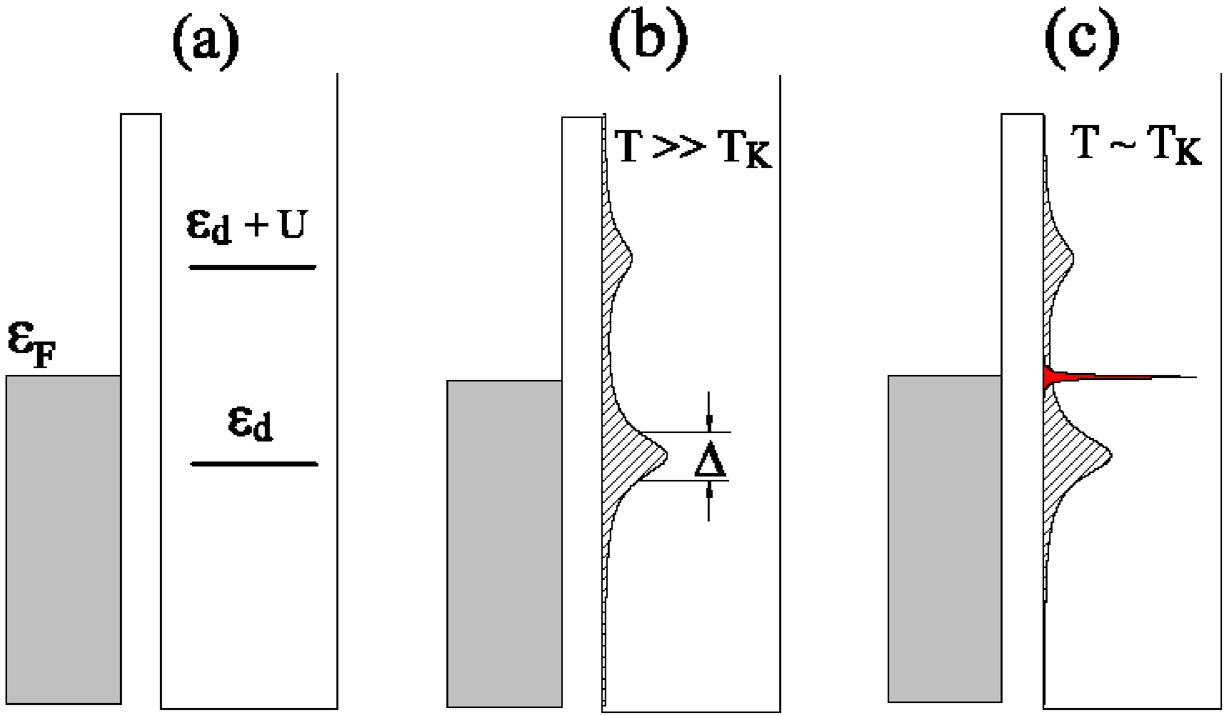
3. Theoretical picture(Kondo and mixed valence regimes)

4. Kondo resonance of adatom on the graphene surface

5. Summary

Anderson impurity system

$$H = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^+ c_{k\sigma} + \sum_{\sigma} \varepsilon_d d_\sigma^+ d_\sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma} (V_{kd} c_{k\sigma}^+ d_\sigma + h.c.)$$

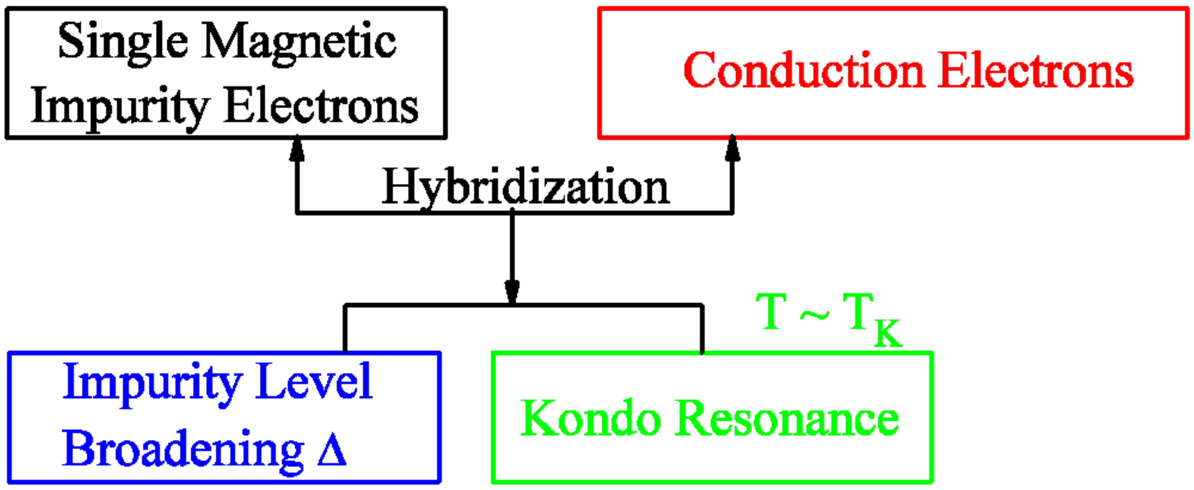


Three regimes: Kondo regime ($\varepsilon_d << -\Delta$)
mixed valence regime ($|\varepsilon_d| \leq \Delta$)
empty orbital regime ($\varepsilon_d > \Delta$)

$$\Delta = \pi \rho_0 |V|^2$$

Physical picture and some formula

Three interference channels: red, green, and blue



H.G. Luo, T. Xiang, X.Q. Wang, Z.B. Su, and L. Yu,
PRL 92, 256602 (2004), see also cond-mat/ 0311533

The Physical quantity measured by STM: $\rho_c(r,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G_c(r,\omega)$

$$\boxed{\delta G_c(r,\omega) = |V|^2\, G_c^0(r,\omega) G_d(\omega) G_c^0(-r,\omega)}$$

Conduction electron Green's function   Impurity electron Green's function

Define: $\boxed{q_c = -\frac{\mathrm{Re}\,G_c(r,\omega)}{\mathrm{Im}\,G_c(r,\omega)}}$

$$\Rightarrow \quad \delta\rho_c(r,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,\delta G_c(r,\omega)$$

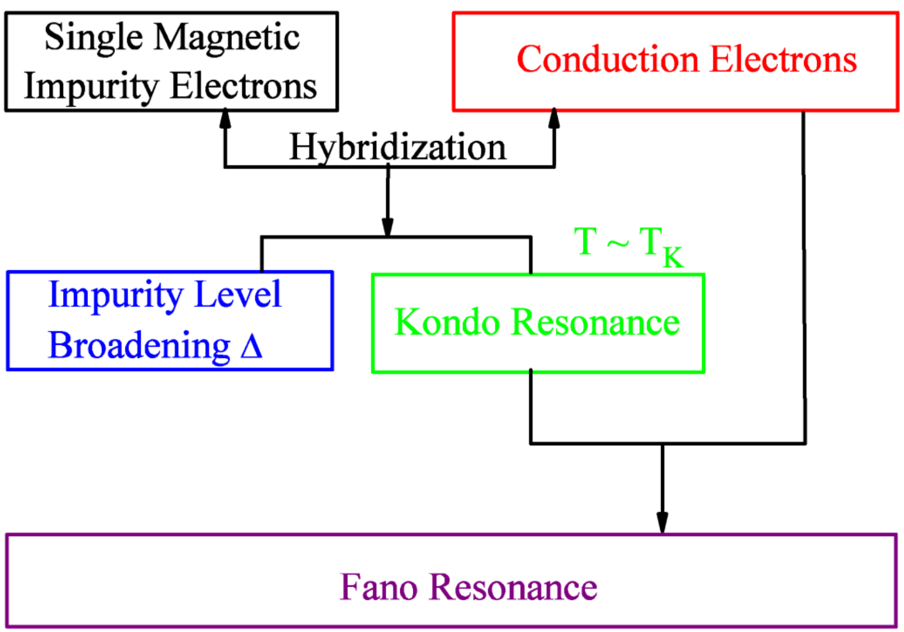
$$\boxed{= -\Delta\rho_0[(q_c^2 - 1)\,\mathrm{Im}\,G_d(\omega) - 2q_c\,\mathrm{Re}\,G_d(\omega)]}$$

Near the Fermi level, if $G_d(\omega)$ is approximated by the Kondo resonance,

$$G_d(\omega) \sim \frac{1}{\omega - \varepsilon_K + i\Gamma_K}$$

$$\Rightarrow \delta\rho_c \sim \frac{\Delta\rho_c}{\Gamma_K}\left(\frac{(\varepsilon+q_c)^2}{\varepsilon^2+1} - 1\right)$$

$$\propto \frac{(\varepsilon+q_c)^2}{\varepsilon^2+1}, \varepsilon = \frac{\omega-\varepsilon_K}{\Gamma_K}$$



Fano resonance by Zawadowski's group

PRL **85**, 2557 (2000)

$$G_d(\omega) \sim \frac{1}{\omega - \varepsilon_K + i\Gamma_K}$$

In the Kondo regime: OK!

In the mixed valence regime: not enough.

The impurity level broadening must be considered.

Scattering matrix representation for *d*-electrons

$$G_{d\sigma}(\omega) = \frac{1}{[G^0_{d\sigma}(\omega)]^{-1} - \Sigma_\sigma(\omega)}$$

$$\Downarrow$$

$$G_{d\sigma}(\omega) = G^0_{d\sigma}(\omega) + G^0_{d\sigma}(\omega)T_\sigma(\omega)G^0_{d\sigma}(\omega)$$

$$T_\sigma(\omega) = \frac{\Sigma_\sigma(\omega)}{1-\Sigma_\sigma(\omega)G^0_{d\sigma}(\omega)}$$

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

If $G^0{}_d(\omega) = X_d(\omega) + i\,Y_d(\omega)$, then

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

$$q_d(\omega) = -\frac{X_d(\omega)}{Y_d(\omega)}$$

asymmetry parameter

If T is a resonance peak

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

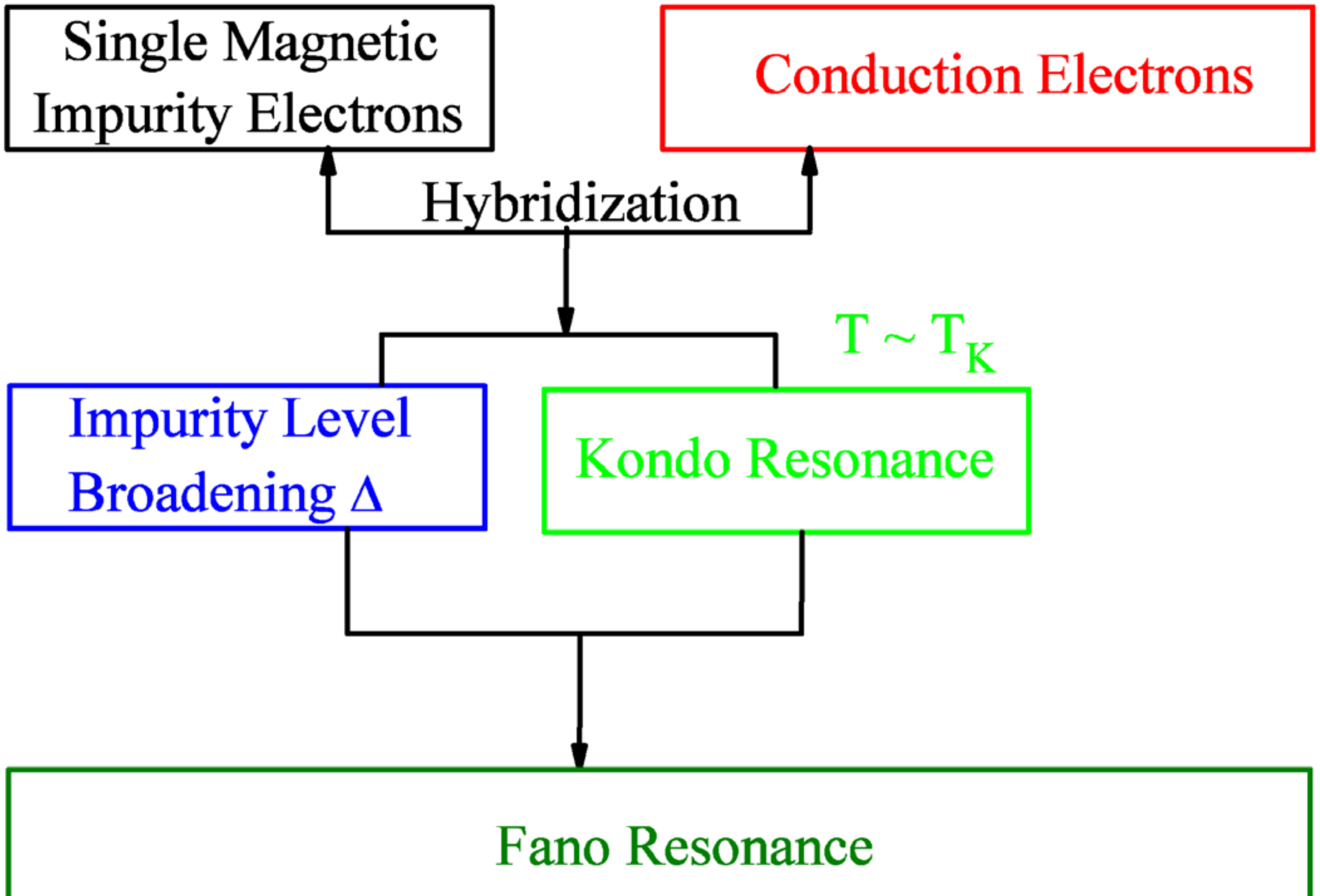
$$\rho_d(\omega) \approx \rho_{d,0}(\varepsilon_K)\frac{(\tilde{\varepsilon} + q_d)^2}{\tilde{\varepsilon}^2 + 1}$$

Fano resonance

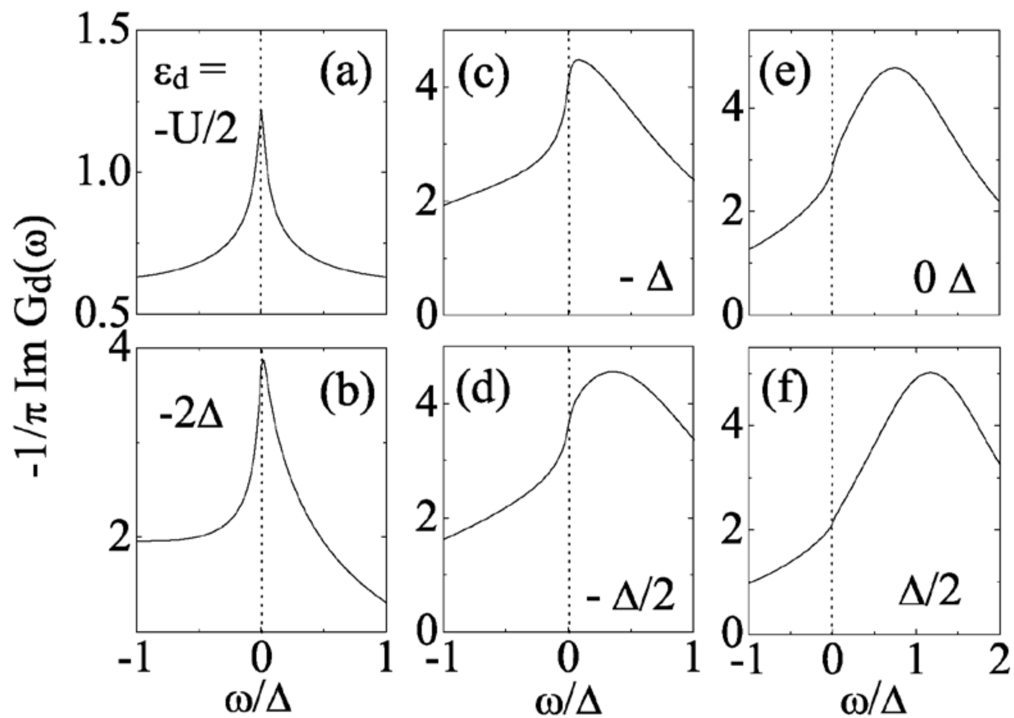
$$\tilde{\varepsilon} = (\omega - \varepsilon_K)/\Gamma_K$$

Note: This expression is only ok in the Kondo regime

The interference between the Kondo resonance and the broadened impurity level



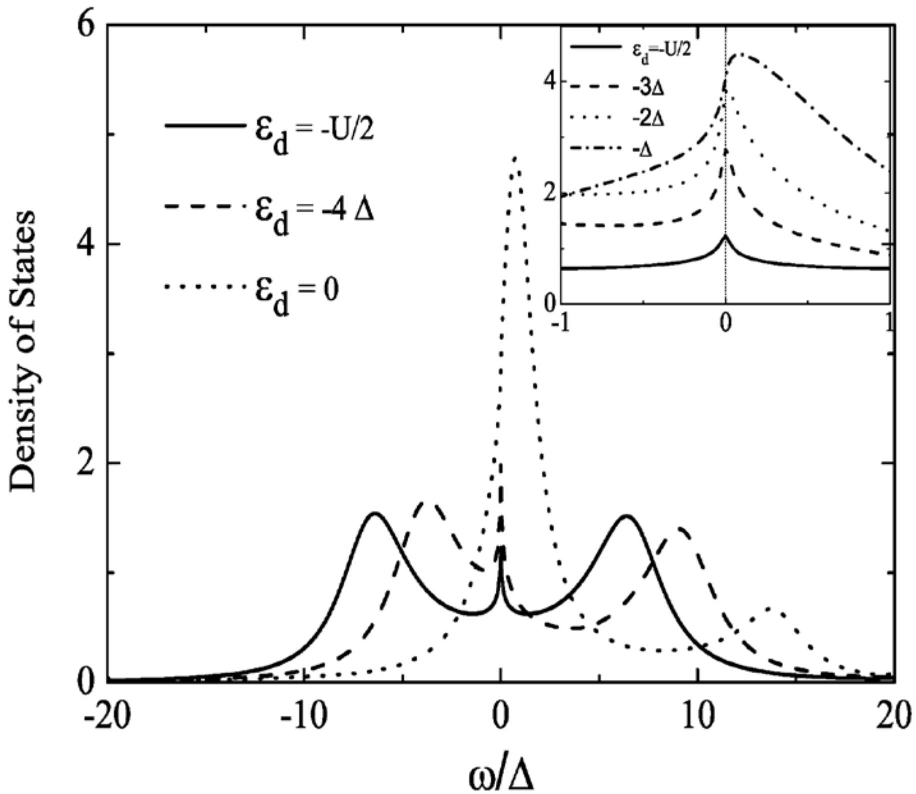
Interference between the broadened impurity level and the Kondo resonance → Kondo peak shows Fano-like lineshape

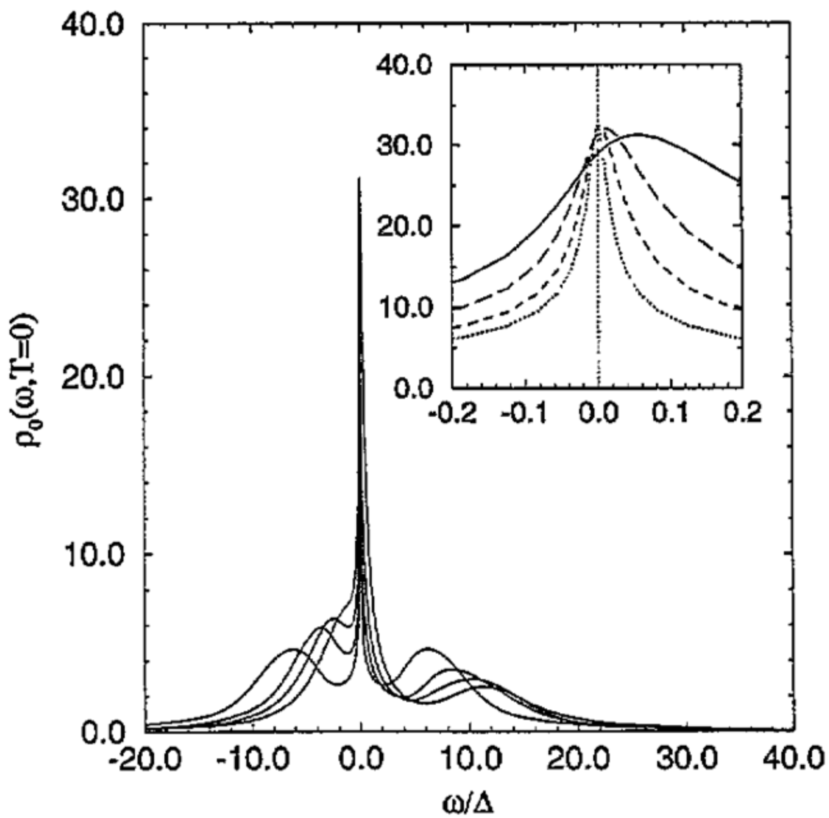


Kondo resonance shows Fano-like lineshape

From the equation of motion (EOM) method

Comparison of Equation of Motion Results with Numerical RG

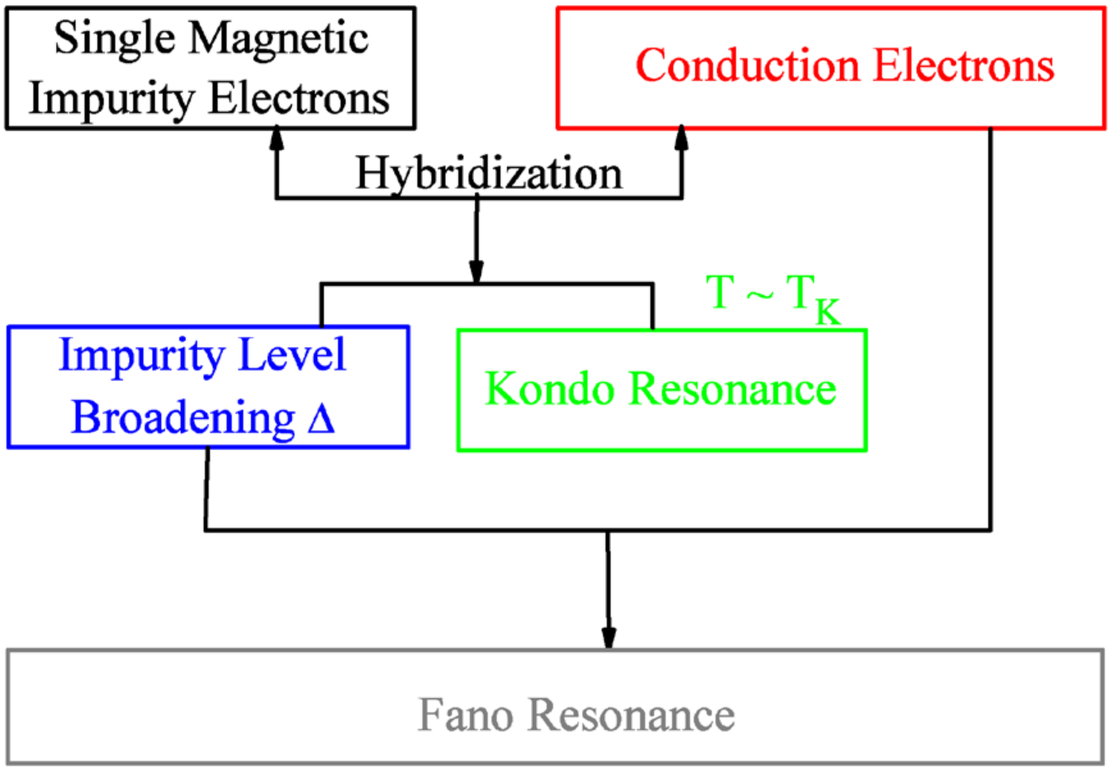




EOM results

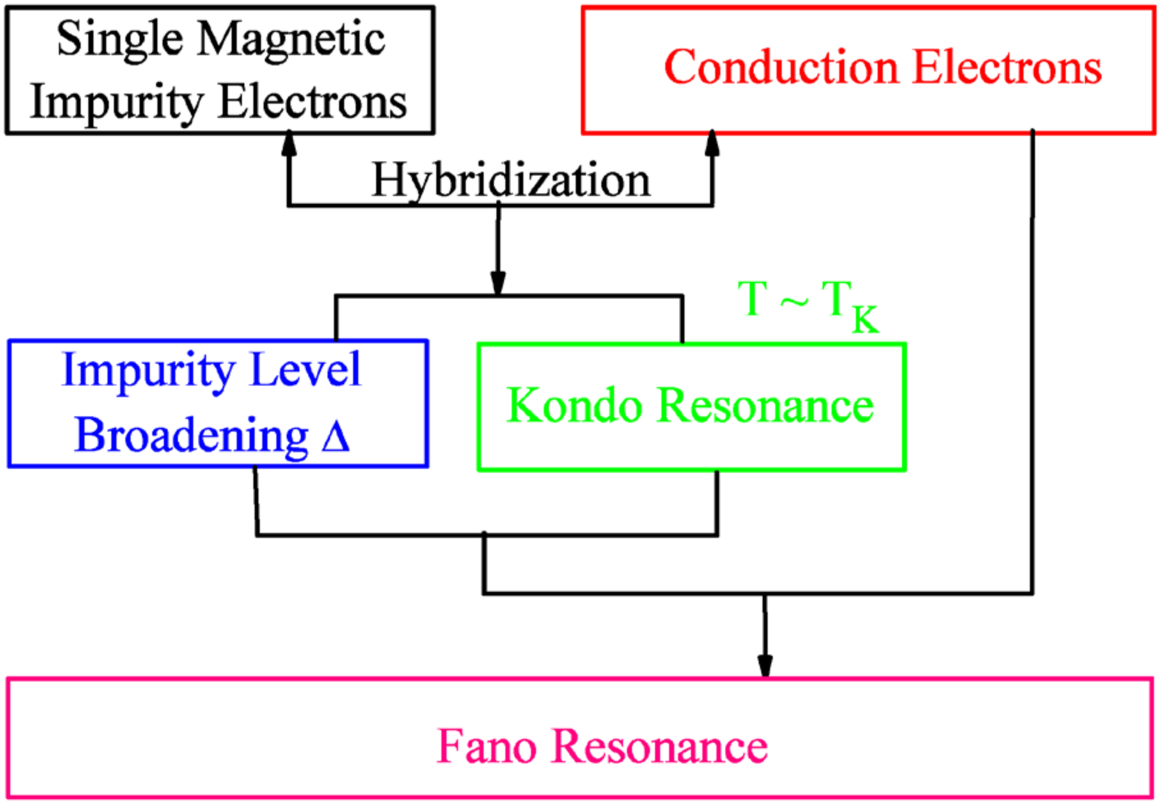
NRG (Costi et al, 1994)

Interference between the broadened impurity level and the conduction electrons



The Fano resonance proposed originally by Fano for non-interacting systems

In general, three channels should be considered.



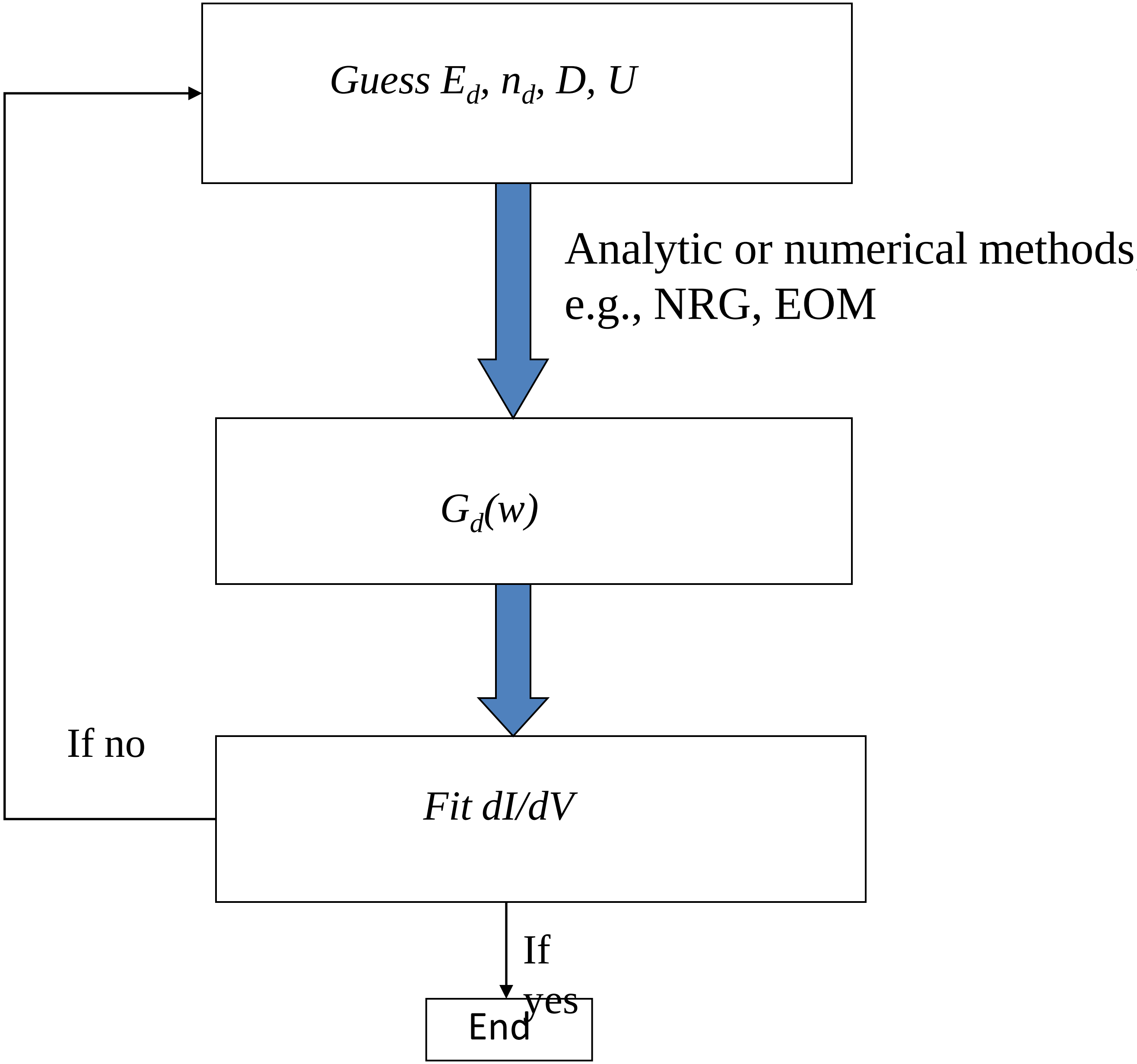
Comparison with the experimental data:

$$\frac{dI}{dV} \propto$$

$$\rho_c = c1 - c2\left\{(q_c^2 - 1)\,\mathrm{Im}[G_d(\omega)] - 2q_c\,\mathrm{Re}[G_d(\omega)]\right\}$$

Two ways to get $G_d(\omega)$

a) Self-consistent calculation



b) Direct fit by using T-matrix:

$$G_d(\omega) = G_d^0(\omega) + G_d^0(\omega) T_d(\omega) G_d^0(\omega)$$

$$G_d^0(\omega) = \frac{1-n/2}{\omega - \varepsilon_d + i\Delta} + \frac{1-n/2}{\omega - \varepsilon_d - U + i\Delta}, \; q_d = -\frac{\mathrm{Re}[G_d^0(\omega)]}{\mathrm{Im}[G_d^0(\omega)]}$$

$$T_d(\omega) = \frac{T_K}{\pi \rho_{d,0}} \left(\frac{1}{\omega - \varepsilon_K + i T_K} + t_{incoh.} \right)$$

Luo et al., PRL 92, 256602 (2004)

Note: The form of T_d(w) is only suit for the Kondo regime.
In the mixed valence regime, it overestimates the asymmetry of the Kondo resonance

Kolf et al., PRL 96, 019701 (2006)

Correctly, $T_d(\omega)$ should be replaced by

$$T_d(\omega) \approx \frac{a e^{i\delta}}{\omega - \varepsilon_K + i\Gamma_K} + t_{\mathrm{incoh}}$$

In the Kondo limit, $\delta \sim 0$, $a \sim \Gamma_K/\pi \rho_{d,0}$

Luo et al, PRL 96, 019702 (2006)

Key fit parameters:

$\varepsilon_d, \Delta, U, n$ — Impurity related parameters, may be calculated by first principle or fitted directly; determining q_d

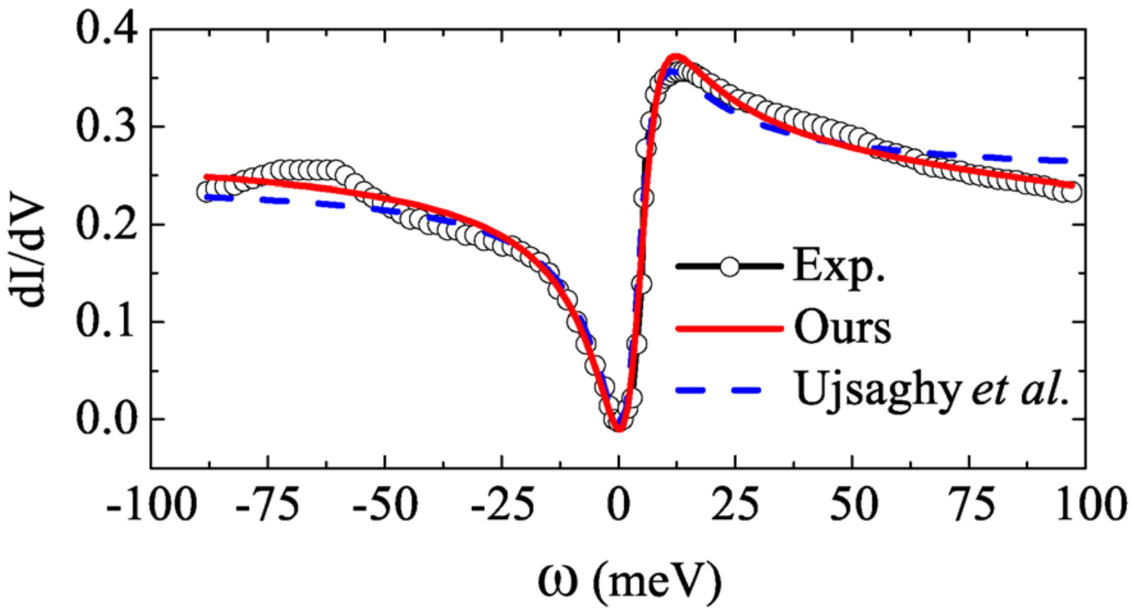
ε_K, T_K — Kondo resonance parameters

q_c — Conduction electron asymmetry parameter

a) Co/Au(111), Kondo regime

$\varepsilon_d - \varepsilon_F = -0.84\,eV$, $U = 2.84\,eV$, $\Delta = 0.2\,eV$ and $n = 0.8$. This impurity system is in the Kondo regime[9].

DFT calculation



q_d=2.6

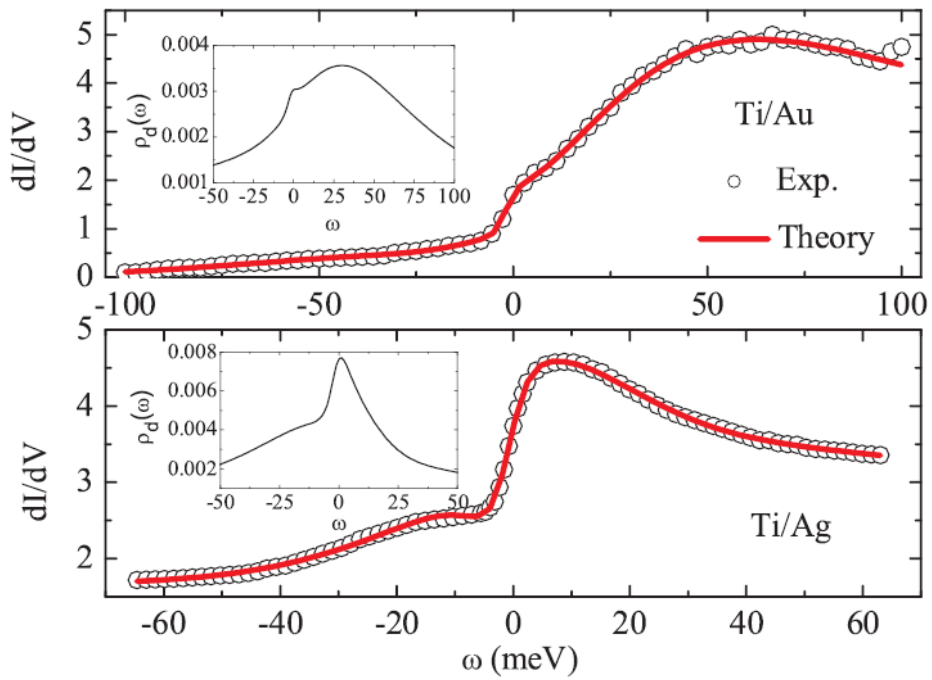
Small contribution by the broadening impurity level

$q_c = 1.4$, $\varepsilon_K = 4.0\,meV$ and $\Gamma_K = 5.6\,meV$

Comparable to the previous parameters obtained by Ujsaghy et al.:

$q_c = 0.66$, ε_K=3.6 *meV*, Γ_K=5.0 *meV*

b) Ti on the surfaces of Au and Ag, mixed valence regime



In both cases, $|q_d|<|q_c|$

Larger contribution by the broadening impurity level than the conduction electrons

systems, assuming $U \to \infty$ for simplicity. The fitting parameters are $(n, \varepsilon_d, \Delta, \varepsilon_K, \Gamma_K, a, \delta, q_c) = (0.38, 2.3, 65.0, -1.9, 4.0, 28.2, 2.7, 2.0)$ for Ti/Au and $(0.53, 13.4, 38.8, -1.4, 5.2, 144.9, 3.0, 1.8)$ for Ti/Ag ($\varepsilon_F = 0$ and the unit of energy is meV). Figure 1 shows that the experimental

Outline:

1. Brief background
   What are Kondo and Fano resonances?

2. Experimental observations of Kondo resonance

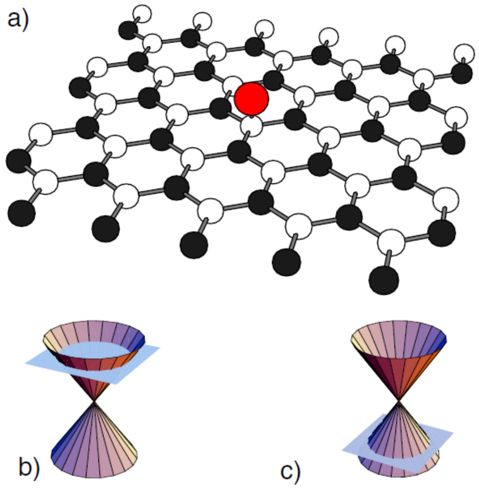
3. Theoretical picture(Kondo and mixed valence regimes)

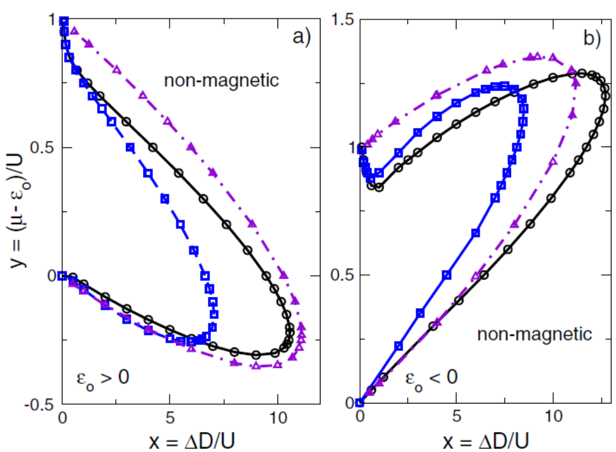
4. Kondo resonance of adatom on the graphene surface

5. Summary

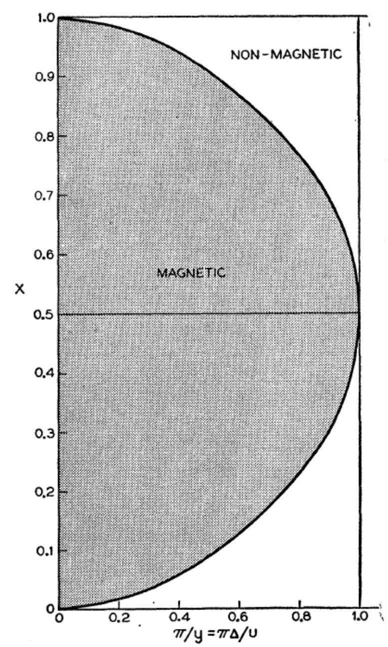
Kondo effect on the graphene substrate (Li et al., 2013)

Localized Magnetic States in Graphene



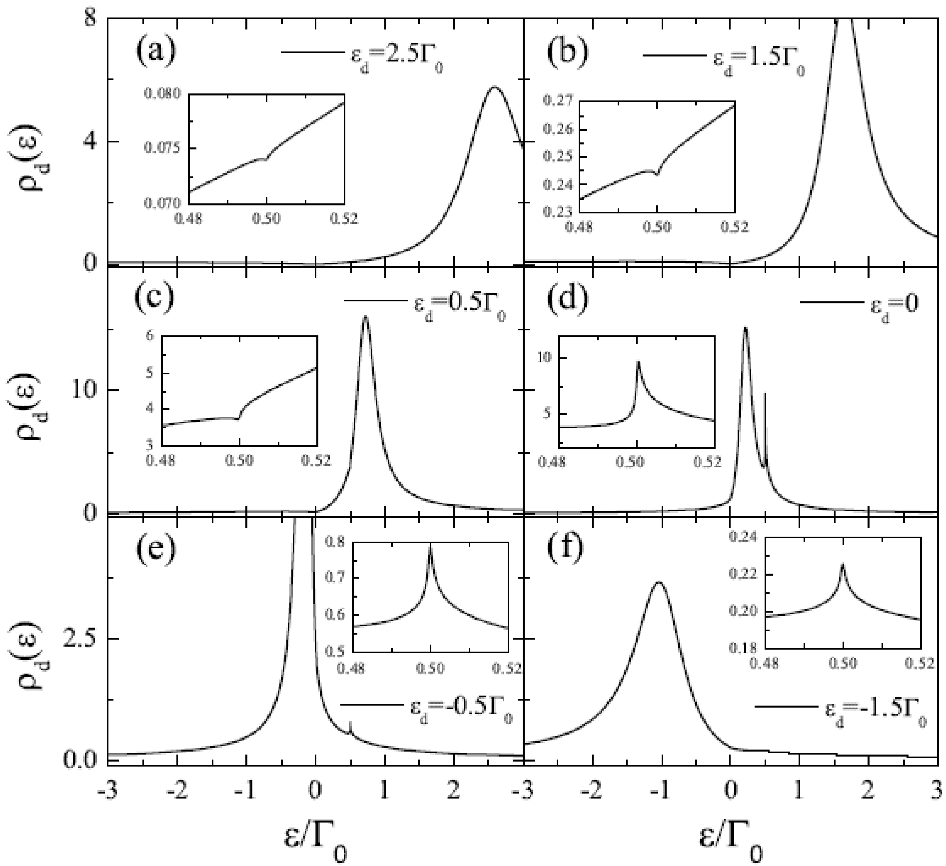


Bruno Uchoa, Valeri N. Kotov, N. M. R. Peres, and A. H. Castro Neto, PRL 101, 026805 (2008)



P. W. Anderson, 1961

Density of states of adatom



Why anti-resonance in mixing valence or even empty orbital regimes?

$$G_\sigma(\varepsilon) \approx \frac{1-\langle n_{\bar{\sigma}}\rangle}{\varepsilon-\varepsilon_{\mathrm{d}}+\mathrm{i}\Gamma_{\mathrm{g}}(\varepsilon)-B_{\bar{\sigma}}(\varepsilon)}$$

$$G(\varepsilon) \approx G^0(\varepsilon)+G^0(\varepsilon)\,T(\varepsilon)\,G^0(\varepsilon).$$

$$T(\varepsilon) \approx \frac{\Gamma_{\mathrm{K}}}{\pi\rho_0(\varepsilon)}\frac{1}{\varepsilon-\varepsilon_{\mathrm{K}}+\mathrm{i}\Gamma_{\mathrm{K}}}$$

$$\rho(\varepsilon) \approx \rho_0(\varepsilon_{\mathrm{K}})\frac{(\tilde{\varepsilon}+q_{\mathrm{d}})^2}{\tilde{\varepsilon}^2+1}$$ Fano resonance

The essential reason for this is that the impurity level is broadened extensively due to the linear density of states around the Dirac points, which provides a finite background.

L. Li, Y.-Y. Ni, Y. Zhong, T.-F. Fang, and H.-G. Luo, NJP **15**, 053018 (2013) (**IOP Select**); arXiv:1204.2696 (2012)

Summary

1) Kondo meets Fano, important in mixed valence regime

2) Adatom on the surface of graphene has an intriguing feature in mixed valence, even in the empty orbital regime.

Thank you for your attention !