δ interference of two Friedel resonances

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(Received 29 March 2010; revised manuscript received 12 July 2010; published 13 August 2010)

When a single resonator is coupled to a continuous spectrum one obtains a resonance of finite half width. Such a resonance is known in many fields of physics. The Friedel resonance is an example where a *d* impurity is dissolved in a simple metal. If two resonators are coupled to the continuous spectrum the resonances interfere. For identical coupling and similar frequencies one obtains two effective resonances. The coupling of one of them to the continuum can be tuned to zero yielding a δ-like resonance.

DOI: 10.1103/PhysRevB.82.073102 PACS number(s): 71.23.An, 71.28.+d, 72.10.Fk

A Friedel resonance describes generally a transition-metal impurity dissolved in a host metal. It was investigated by Friedel more than half a century ago[1] and plays a very important role in solid-state physics. In most cases one has not one but many impurities in a host metal, each being a resonance for the conduction electrons. It is generally assumed without much further consideration that one can just multiply the resonance density of states (DOS) of a single impurity with the number of impurities.

Recently the author investigated the density of state of a magnetic impurity in the Friedel artificially inserted resonance (FAIR).[2] Here as in numerical renormalization group (NRG) theory one replaces the conduction band by a relatively small number of Wilson states. The remaining continuum does not couple to the impurity and is neglected (although it has a finite coupling to the discrete Wilson states)

As a result the excitations spectrum is discrete. This is, of course, a consequence of the finite state approximation because the real spectrum is continuous. In NRG one broadens the discrete spectrum artificially with a Gauss curve or a logarithmic Gauss curve.[3–6] In some papers one has tried to overcome the imperfection of this method by sweeping the energies of the Wilson states over a finite-energy range.[7]

A more appropriate procedure would be to calculate the coupling of the discrete excited states to the neglected continuous states. That represents a rather complex multi-Friedel resonance problem where all the excited states represent resonance states with different energies. To obtain a feeling of what happens if one has several Friedel resonances (each coupling to the continuum) I investigated some example on my PC. I found a rather amazing result. Two Friedel resonances with the same coupling matrix elements to the conduction band show a strong interference. If the two resonance energies are also identical then this yields two resonance where one is a delta function.

The physics behind this phenomenon is rather straight forward. Just nobody appears to have noticed this before. I believe that this phenomenon could be experimentally very valuable because in certain geometries it should be rather simple to prepare such identical resonances. Sharp resonances provide important markers in physics. For example, in solid-state physics the sharp Kondo resonance has been used in a number of beautiful experiments to observe the propagation of electrons in real space,[8] to see the Fermi surface of the host[9] and to measure magnetic-energy shifts.[10] In this Brief Reports I propose to build a sharp resonance out of two broad ones. The ability to fine-tune the strength and width of the resonance will be very useful in similar experiments.

Let us consider a Friedel resonance in form of a *d* impurity which is dissolved in a simple (s,p)-metal. In the absence of a Coulomb exchange interaction at the impurity (and a magnetic field) the behavior of the spin-up and spin-down sub-bands is the same and the spin can be ignored. Then the problem is described by the well-known Friedel Hamiltonian.

$$H_{\mathrm{Fr}} = \sum_i \varepsilon_i c_i^\dagger c_i + \varepsilon_d d^\dagger d + \sum_i V_{sd}(c_i^\dagger d + d^\dagger c_i), \tag{1}$$

where $c_i^\dagger$ and $d^\dagger$ are the creation operators of the (free) conduction electrons and the *d* electron. The *d* level hybridizes with the conduction electrons. An electron injected into the *d* level experiences a finite lifetime which results in a finite half width of the *d* resonance. The half width is given by the golden rule

$$\Delta = \pi \overline{|V_{sd}|^2} \rho_0, \tag{2}$$

where $\overline{|V_{sd}|^2}$ is an average over the *s*-*d*-hopping matrix element and ρ_0 is the density of states. Similar resonances have been investigated by Feshbach[11] and Fano.[12] Beside solid-state physics these resonances play an important role in many other areas of physics, such as nuclear and atomic physics.

As mentioned above for a finite concentration of *d* impurities in a host one generally assumes that their resonances are independent and additive. One obtains a completely different result when the matrix elements for the resonance levels are identical. How one may achieve this condition will be discussed below. To broaden the discussion I introduce two *d* levels with different resonance energies ε_{d_1} and ε_{d_2} into an electron system. Both *d* impurities shall have identical hopping matrix elements with the conduction electrons. A constant electron density of states in the host is assumed (which allows a better comparison of resonances at different energies). In the numerical calculation 200 electron states with the energy $\varepsilon_i = i/2$ for $0 < i \leq 200$ are used so that the band extends from 0 to 100 and has a density of states of $\rho_0 = 2$. The matrix elements are set equal to $V = 1$. This Hamiltonian is numerically diagonalized. In Fig. 1(a) the resulting DOS

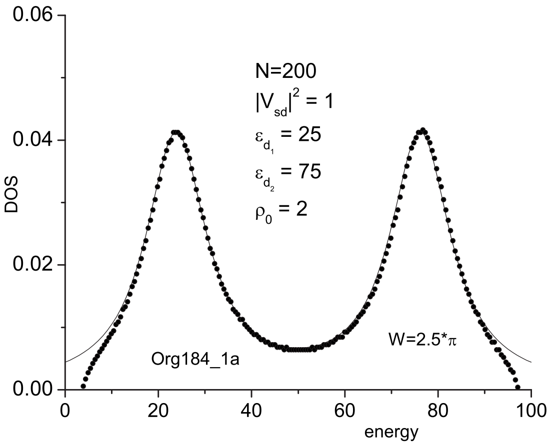

FIG. 1. Two d levels with $\varepsilon_{d_1}=25$ and $\varepsilon_{d_2}=75$ with identical coupling to the conduction band. The fitted resonance widths are $W=2.5\pi$.

of the d electrons is plotted. One obtains two resonances whose resonance energies are well separated at $\varepsilon_{d_1}=25$ and $\varepsilon_{d_2}=75$. The half widths are 2.5π, i.e., 25% larger than the theoretical result for a single Friedel impurity, which is $\Delta=\pi|V_{sd}|^2\rho_0=2\pi$. The full curves are calculated with the half width of 2.5π. The position of the resonances are slightly shifted to $\varepsilon'_{d_1}=23.8$ and $\varepsilon'_{d_2}=76.2$.

The increased value of Δ is an indication of an interference between the two levels. When the two d levels are located at $\varepsilon_{d_1}=45$ and $\varepsilon_{d_2}=55$ one no longer obtains two maxima. The resulting DOS can be described as two resonances with width of $\Delta_1=4\pi$ and $\Delta_2=0.7\pi$, both centered at $\varepsilon'_d=50$.

If one positions both d levels at $\varepsilon_{d_1}=\varepsilon_{d_2}=50$ then figure changes dramatically. This is shown in Fig. 2.

The left figure shows the strong broadening with a needle sharp peek in the center. The broad resonance has a half width of $\Delta_1=5\pi$ and an area of 1.05. In the right figure the vertical scale is compressed by two orders of magnitude. The sharp resonance is very narrow $\Delta_2=0.06\pi\approx 0.19$. However, the level separation $\delta\varepsilon$ of the conduction band is in this calculation only 0.5 which prevents a more narrow resonance. As discussed below the resonance width would approach ideally the value zero.

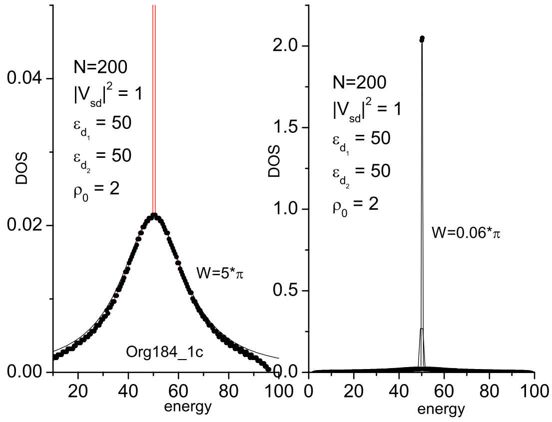

FIG. 2. (Color online) Two identical d levels with $\varepsilon_{d_1}=\varepsilon_{d_2}=50$ with identical coupling to the conduction band. The left figure shows the strong broadening with a needle sharp peek in the center. In the right figure the vertical scale is compressed by two orders of magnitude. The fitted resonance widths are $W=5\pi$ and $W=0.06\pi$.

Since the above result of the simulation is rather surprising and unexpected it shall be derived by means of Green's functions (GF). The GF are defined as $\mathbf{G}=(E+is-H)^{-1}$ or

$$\sum\nolimits_{\lambda}(E+is-H)_{\kappa\lambda}G_{\lambda\mu}=\delta_{\kappa\mu} \tag{3}$$

with the Hamiltonian

$$\begin{aligned} H &= \sum\nolimits_{\nu}\varepsilon_{\nu}c_{\nu}^{\dagger}c_{\nu}+\varepsilon_{d_1}c_{d_1}^{\dagger}c_{d_1}+\sum\nolimits_{\nu}(V_{\nu,1}c_{\nu}^{\dagger}c_{d_1}+V_{\nu,1}^{*}c_{d_1}^{\dagger}c_{\nu}) \\ &\quad+\varepsilon_{d_2}c_{d_2}^{\dagger}c_{d_2}+\sum\nolimits_{\nu}(V_{\nu,2}c_{\nu}^{\dagger}c_{d_2}+V_{\nu,2}^{*}c_{d_2}^{\dagger}c_{\nu}) \\ &= \sum\nolimits_{\kappa,\lambda}c_{\kappa}^{\dagger}H_{\kappa\lambda}c_{\lambda} \end{aligned} \tag{4}$$

Eq. (3) is evaluated for (κ,μ) equal to (d_1,d_1), (d_2,d_1), and (ν,d_1), where ν stands for any conduction-electron state. Together they yield

$$-\sum\nolimits_{\nu}V_{\nu,1}^{*}G_{\nu,d_1}+(E+is-\varepsilon_{d_1})G_{d_1,d_1}=1,$$

$$-\sum\nolimits_{\nu}V_{\nu,2}^{*}G_{\nu,d_1}+(E+is-\varepsilon_{d_2})G_{d_2,d_1}=0,$$

$$(E+is-\varepsilon_{\nu})G_{\nu,d_1}-V_{\nu,1}G_{d_1,d_1}-V_{\nu,2}G_{d_2,d_1}=0.$$

From these equations one can eliminate G_{ν,d_1} and obtain two equations which couple G_{d_1,d_1} and G_{d_2,d_1} (from now on is is included in E).

$$\begin{gathered} \left[E-\varepsilon_{d,1}-\sum\nolimits_{\nu}\frac{V_{1,\nu}V_{1,\nu}^{*}}{(E-\varepsilon_{\nu})}\right]G_{d_1,d_1}-\sum\nolimits_{\nu}\frac{V_{1,\nu}V_{2,\nu}^{*}}{(E-\varepsilon_{\nu})}G_{d_2,d_1}=1 \\ -\sum\nolimits_{\nu}\frac{V_{2,\nu}V_{1,\nu}^{*}}{(E-\varepsilon_{\nu})}G_{d_1,d_1}+\left[(E-\varepsilon_{d,2})-\sum\nolimits_{\nu}\frac{V_{2,\nu}V_{2,\nu}^{*}}{(E-\varepsilon_{\nu})}\right]G_{d_2,d_1}=0 \end{gathered} \tag{5}$$

For identical hopping matrix elements of impurity d_1 and d_2, i.e., $V_{1,\nu}=V_{2,\nu}$, one can set the expression

$$\sum\nolimits_{\nu}\frac{V_{i,\nu}V_{j,\nu}^{*}}{(E-\varepsilon_{\nu})}=X=\Delta_r+i\Delta_i$$

equal to X which consists of a real and an imaginary part.

The denominator of the two GF in Eq. (5) is given by the determinant of the matrix in Eq. (5).

$$(E-\varepsilon_{d,1}-X)(E-\varepsilon_{d,2}-X)-X^2.$$

The zero points of the determinant yield the new energies of the d levels. The imaginary part gives the broadening of the resonance curve. These zero points are

$$E_{1,2}=X+\frac{1}{2}(\varepsilon_{d,1}+\varepsilon_{d,2})\pm\frac{1}{2}\sqrt{4X^2+(\varepsilon_{d,1}-\varepsilon_{d,2})^2}.$$

The Green's function G_{d_1,d_1} has the form

$$G_{d_1,d_1} = \frac{1}{2}\frac{1 + \dfrac{(\varepsilon_{d,1} - \varepsilon_{d,2})}{E_1 - E_2}}{E - E_1} + \frac{1}{2}\frac{1 - \dfrac{(\varepsilon_{d,1} - \varepsilon_{d,2})}{E_1 - E_2}}{E - E_2}.$$

When the two d level energies approach each other, i.e., $|(\varepsilon_{d,1}-\varepsilon_{d,2})| < 2|X|$ then one obtains

$$E_1 \approx 2X + \frac{1}{2}(\varepsilon_{d,1} + \varepsilon_{d,2}) + \frac{(\varepsilon_{d,1} - \varepsilon_{d,2})^2}{8X},$$

$$E_2 \approx + \frac{1}{2}(\varepsilon_{d,1} + \varepsilon_{d,2}) - \frac{(\varepsilon_{d,1} - \varepsilon_{d,2})^2}{8X}.$$

In this case the second term of G_{d_1,d_1} has a denominator with a rather small imaginary part [proportional to $(\varepsilon_{d,1} - \varepsilon_{d,2})^2$]. Its resonance width is strongly reduced.

For $\varepsilon_{d,1} = \varepsilon_{d,2}$ the resonance at $E_2 = \varepsilon_d$ has essentially no imaginary part and therefore represents a δ function. This confirms our observation when diagonalizing the Hamiltonian. It is the result of an interference effect between the two d levels by the coupling through the conduction electrons.

A sharp resonance or density of states is experimentally very desirable. It can be used as a marker in spectroscopy. For example, the sharp horn of the superconducting BCS density of states or the sharp Kondo resonance and others have been used experimentally to trace energy shifts and other phenomena. The question is whether one can fabricate a metal (or any other system) with two resonance level which are not only identical in energy but also in their hopping matrix elements. As one possibility I propose a one-dimensional wire of a material with a Fermi wavelength that is much larger then atomic distances. Such a one-dimensional wire can be a narrow film of a semimetal or a narrow strip of a two-dimensional electron gas where the width is less then the half the Fermi wavelength. This is shown in Fig. 3.

Then the electronic wave functions do not change their phase in the direction perpendicular to the wire, the phase only changes along the wire as sketched in Fig. 3. The two resonance levels are inserted so that they lie symmetrically with the central line of the wire. Then both of them are coupled with the same hopping matrix elements to the conduction band. And both have the same d state energy ε_d. The distance between the two resonance levels must be sufficiently large so that there is no direct overlap of their wave functions.

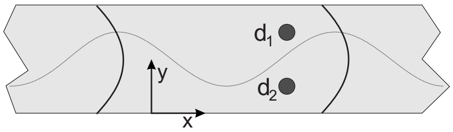

FIG. 3. A short part of a strip which acts as a one-dimensional wire. In y direction there is only one mode with no phase modulation. The two resonance levels are inserted symmetrically with respect to the middle line of the strip.

In summary two noninteracting resonant levels hybridize with a single bath of conduction electrons via a hybridization term. For degenerate levels the spectral density exhibits a broad resonance with a delta function superimposed upon it. The formation of the δ resonance can be intuitively understood if one considers even and odd-parity states $d_+^\dagger = 1/\sqrt{2}(d_1^\dagger + d_2^\dagger)$ and $d_-^\dagger = 1/\sqrt{2}(d_1^\dagger - d_2^\dagger)$. In the degenerate case, the latter decouples from the band, with a Green's function $G_- = 1/(\omega - \varepsilon_d + i\eta)$ giving the observed δ function.

If one introduces single-particle interaction between the d resonances (for example, an overlap of their wave function) the degenerated d-electron energies ε_{d_i} split, changing the δ peak into a finite resonance. Many-body interactions within each impurity yield fascinating complications. One has now two one-channel Friedel-Anderson (FA) impurities which individually form a singlet Kondo ground state at zero temperature. But even if one suppresses the singlet state with an external magnetic field one faces interesting questions. For example, in the magnetic state of the one-channel FA impurity the d resonance width is twice the mean-field value Δ as given by Eq. (2).[2,13] How the δ resonance develops under these circumstances represents a tempting theoretical problem and has the potential for interesting experiments.

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