Delta-Interference of Two Friedel Resonances

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Abstract

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 frequencies one obtains two effective resonances. The effective coupling of one of them to the continuum can be tuned to zero yielding a delta-like resonance.

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 [1], to see the Fermi surface of the host [2] and to measure magnetic energy shifts [3]. In this paper I propose to build a sharp resonance out of two broad resonances. The ability to fine-tune the strength and width of the resonance will be very useful in similar experiments.

A well known example of a broad resonance in solid state physics is the Friedel resonance. It forms when a d-impurity is dissolved in a simple (s,p)-metal [4]. The d-level hybridizes with the conduction electrons. An electron injected into the d-level experiences a finite lifetime which results in a finite finite half-width of the d-state. The latter is given by the golden rule

\[ \Delta = \pi |V_{sd}|^2 \rho_0 \]

where \( |V_{sd}|^2 \) is an average over the s-d-hopping matrix element and \( \rho_0 \) is the density of states. Similar resonances have been investigated by Feshbach [5] and Fano [6]. These resonances play an important role in many areas of physics, such as nuclear and atomic physics as well in solid state.

When a finite concentration of d-impurities is dissolved in the host one generally assumes that their resonances are independent and additive. The main justification is that the matrix
elements $V_{sd}$ have different phases for different positions. Take as a very simple example a one-dimensional wire of length $L$ with periodic boundary conditions. Then the electron wave functions can be expressed as $\varphi_k(x) = \sqrt{1/L} \cos(kx)$ or $\sqrt{2/L} \sin(kx)$. If we put one impurity at $x = 0$ then it has the same s-d-matrix element $V$ with all the $\varphi_k(x) = \sqrt{1/L} \cos(kx)$ electrons because all these states have the same value $\sqrt{2/L}$ at the position of the impurity. The $\sqrt{2/L} \sin(kx)$-states don't couple to the d-impurity. If one puts a second d-impurity at $x = L/2$ then the matrix element alternates between $+V$ and $-V$. Diagonalization of the Hamiltonian shows that the resonances at $x = 0$ and $x = L/2$ just add without distorting each other.

One obtains a completely different result when the matrix elements for the two 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 $\varepsilon_{d_1}$ and $\varepsilon_{d_2}$ into an electron system. Both d-impurities shall have identical hopping matrix elements with the conduction electrons. A constant electron density of states of 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. The matrix elements are set equal to $V = 1$. In Fig.1a the resonance energies are well separated at $\varepsilon_{d_1} = 25$ and $\varepsilon_{d_2} = 75$. One obtains two well separated resonances. The half widths are $2.5\pi$, i.e. 25% larger than the theoretical result for a single Friedel impurity, which is $\Delta = \pi |V_{sd}|^2 \rho_0 = 2\pi$ (in this example the parameters are $|V_{sd}|^2 = 1$ and $\rho_0 = 2$). The full curves are calculated with this half-width. The position of the resonances are slightly shifted to $\varepsilon'_{d_1} = 23.8$ and $\varepsilon'_{d_2} = 76.2$.

![Fig.1: Two d-levels with $\varepsilon_{d_1} = 25$ and $\varepsilon_{d_2} = 75$ with identical coupling to the conduction band](image)

The increased value of $\Delta$ 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 $\varepsilon'_{d} = 50$. 

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

![Diagram](image)

Fig.2: Two identical d-levels with $e_{d_1} = \varepsilon_{d_2} = 50$ with identical coupling to the conduction band. The left figure shows the strong broadening with a needle sharp peak in the center. In the right figure the vertical scale is compressed by two orders of magnitude.

The left figure shows the strong broadening with a needle sharp peak 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.

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

$$
\sum_\lambda (E + is - H)_{\kappa\lambda} G_{\lambda\mu} = \delta_{\kappa\mu}
$$

(1)

with the Hamiltonian

$$
H = \sum_\nu \varepsilon_\nu c_\nu^\dagger c_\nu + \varepsilon_{d_1} c_{d_1}^\dagger c_{d_1} + \sum_\nu \left( V_{\nu,1} c_\nu^\dagger c_{d_1} + V_{\nu,1}^* c_{d_1}^\dagger c_\nu \right) \\
+ \varepsilon_{d_2} c_{d_2}^\dagger c_{d_2} + \sum_\nu \left( V_{\nu,2} c_\nu^\dagger c_{d_2} + V_{\nu,2}^* c_{d_2}^\dagger c_\nu \right) \\
= \sum_{\kappa,\lambda} c_\kappa^\dagger H_{\kappa\lambda} c_\lambda
$$

(2)

Equ. (1) is evaluated for $(\kappa, \mu)$ equal to $(d_1, d_1)$, $(d_2, d_1)$ and $(\nu, d_1)$ where $\nu$ stands for any conduction electron state.
Together they yield

\[-\sum_\nu V_{\nu,1}^* G_{\nu,d_1} + (E + is - \varepsilon_{d_1}) G_{d_1,d_1} = 1\]
\[-\sum_\nu V_{\nu,2}^* G_{\nu,d_1} + (E + is - \varepsilon_{d_2}) G_{d_2,d_1} = 0\]
\[(E + is - \varepsilon_\nu) G_{\nu,d_1} - V_{\nu,1} G_{d_1,d_1} - V_{\nu,2} G_{d_2,d_1} = 0\]

From these equations one can eliminate \(G_{\nu,d_1}\) and obtain two equations which couple \(G_{d_1,d_1}\) and \(G_{d_2,d_1}\):

\[
\begin{align*}
\left( E - \varepsilon_{d,1} - \sum_\nu \frac{V_{1,\nu} V_{1,\nu}^*}{(E - \varepsilon_\nu + is)} \right) G_{d_1,d_1} & - \sum_\nu \frac{V_{1,\nu} V_{2,\nu}^*}{(E - \varepsilon_\nu + is)} G_{d_2,d_1} = 1 \\
- \sum_\nu \frac{V_{2,\nu} V_{1,\nu}^*}{(E - \varepsilon_\nu)} G_{d_1,d_1} & + \left[ (E - \varepsilon_{d,2}) - \sum_\nu \frac{V_{2,\nu} V_{2,\nu}^*}{(E - \varepsilon_\nu)} \right] G_{d_2,d_1} = 0
\end{align*}
\]

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

\[
\sum_\nu \frac{V_{i,\nu} V_{j,\nu}^*}{(E - \varepsilon_\nu + is)} = X = \Delta_r + i\Delta_i
\]
equal to \(X\) which consists of a real and an imaginary part.

The denominator of the two GF in (3) is given by the determinant of the matrix in (3).

\[
(E - \varepsilon_{d,1} - X)(E - \varepsilon_{d,2} - X) - X^2
\]

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

\[
E_{1,2} = X \pm \frac{1}{2} \left( \varepsilon_{d,1} + \varepsilon_{d,2} \right) \pm \frac{1}{2} \sqrt{4X^2 + (\varepsilon_{d,1} - \varepsilon_{d,2})^2}
\]

The Green function \(G_{d_1,d_1}\) has the form

\[
G_{d_1,d_1} = \frac{1}{2} \left[ \frac{1}{E - E_2} + \frac{1}{E - E_1} \right] - \frac{1}{2} \frac{(\varepsilon_{d,1} - \varepsilon_{d,2})}{E_1 - E_2}
\]

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 $\delta$-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 wave length that is much larger then atomic distances. Such a one-dimensional wire can be a narrow film of a semi metal where the width is less then the half the Fermi wave length. This is shown in Fig.3.

![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.](image)

Then the electronic wave functions don’t 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 level 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 $\varepsilon_d$. The distance between the two resonance levels must be sufficiently large so that there is no direct overlap of their wave functions.

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