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Spectral characteristics induced by a single impurity in a two-dimensional system

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Abstract. A single substitutional impurity in a two-dimensional electron system is studied on the basis of the hybrid Anderson model with s - d coupling only between neighbouring sites. Analytic expressions for local densities of states (DOS) for the impurity d orbitals, d_{z^2} and $d_{x^2-y^2}$, and for the s orbitals at the impurity and neighbouring host sites are determined. Special emphasis is put on the appearance of the well-defined resonance states and the antiresonance dips in the spectra, which are discussed in connection with the Fano phenomena. In contrast to the simple s - d Anderson model with the on-site coupling, it is demonstrated that the sharp resonance can be formed by increasing the coupling between the impurity and the host system, and that the resonance energy is shifted towards the band centre where the Van Hove singularity of the host DOS is present.

1. Introduction

The presence of defects significantly influences physical properties of substances [1]. Local characteristics near to the impurity site, such as the local density of states (LDOS), are very different from those of the host crystal. When the number of impurities is not high, the observed change in bulk properties will be proportional to the impurity concentration. Hence the analysis of the single-impurity problem is the first step in exploiting the theoretical description of the disordered system. Localized states formed by the impurity are the most notable change in the LDOS. When the impurity level falls inside the band of a host crystal, the changes are frequently represented by resonance peaks and antiresonance dips in the spectrum.

The localized impurity states are not only interesting in themselves, but also as regards their influence on the subsequent spectrum rearrangement induced by an increase in the impurity concentration [2]. Such spectrum rearrangement has been extensively studied for a wide variety of systems. It has been demonstrated that various types of spectrum rearrangement are realized depending on the type of the localized state. To account for the types of spectrum rearrangement, it is necessary to use a more precise and restricted definition for the resonance state. A sharp peak present in the total or LDOS should not automatically be considered as a resonance: for a resonance state we specify that the damping (width) of the well-defined resonance must be much less than the distance of the impurity level from the nearest Van Hove singularity of the host spectrum. This more precise definition of the resonance state will be used below.

The appearance of resonance states is a well-known feature in the hybrid s - d Anderson model [3]. For the sake of simplicity of the calculations, it is often assumed that the impurity d level is hybridized only with the host s level at the same site [4, 5], so actual symmetries

of wave functions of atomic orbitals are totally neglected. This assumption is supposed to be appropriate when the impurity level is located in the vicinity of the band edge and only long-wavelength excitations are considered. It often occurs that an impurity d_{z^2} level appears inside the host s band. In this case, hopping is allowed from the impurity d_{z^2} level to any s level in surrounding sites but not to the s level located at the impurity site. It will be shown that this slightly more accurate definition of the model has serious consequences. If there is an increase of the s – d coupling strength, the resonance state shifts further from the band edge and the damping of the resonance gradually falls, even though the host density of states does not decrease. These findings are contrary to the results from the simplified model with on-site coupling. This is true not only for the resonance states located deeply in the host s band but also for the ones which are close to the host band edge.

Along with a rapid development of microtechnologies, recently scientific interest has been attracted to low-dimensional systems, such as layered and chain materials. For instance, substances like high- T_c superconductors are essentially impure, and so it is expected that the disorder effect could be significant for their main properties [6]. Also, much attention has been paid recently to the systems of transition metal impurities on the surfaces of s , p metals, such as Fe impurities in Cs films [7]. The underlying physics in this case will be similar to that of the present case for two-dimensional (2D) systems, although the Hamiltonian is more complicated due to the additional electron–electron interaction. Despite some similarities, low-dimensional systems are expected to possess unique features that cannot be reduced to a number of known features of three-dimensional (3D) systems [8]. This common consideration becomes even more valuable for the behaviour of disordered systems, because, as a rule, impurity effects are more pronounced in low-dimensional systems. For instance, impurity effects become most prominent when the parameters describing hopping between the impurity d_{z^2} level and the neighbouring sites are proportional to those describing the corresponding hopping from the s level at the impurity site. This proportionality occurs naturally in low-dimensional systems. The 2D system is more complex than the 1D one, yet still admits a tractable analytical description.

In the present study, we will take a more detailed look at the characteristic features of the LDOS at the impurity and its nearest-neighbour host sites for a 2D single-impurity system. The defect is supposed to be described by the Anderson model with s – d coupling only between neighbouring sites. We have demonstrated the differences in properties of the resonance states between the present model and the common model with on-site coupling. Further, we have also examined the antiresonance dip structure, often referred to as the Fano phenomenon, which is another noticeable feature in the spectrum of the single-impurity system [9].

This paper is organized as follows. In section 2, the model Hamiltonian is introduced, and results for the LDOS of both d_{z^2} and s orbitals at the impurity site, induced by the single-impurity d_{z^2} level, are discussed. In section 3, results for the LDOS of the s orbital at the neighbouring host site are presented. In section 4, The antiresonance dips shown in the LDOS are analysed in connection with the Fano antiresonance. In section 5, the LDOS at the impurity site, induced by the impurity $d_{x^2-y^2}$ level, is determined, and finally conclusions follow in section 6.

2. Spectral features at the impurity site

Let us consider a 2D square lattice and take into account the hopping only between nearest neighbours. If the host band is formed of s -type states and one impurity site has an additional d_{z^2} level, the hopping from the additional d_{z^2} level is allowed only to surrounding sites, in accordance with actual symmetries of wave functions. Thus the model Hamiltonian can be

written in a usual form:

$$\begin{aligned}
 H &= H_s + H_d + H_i \\
 H_s &= t \sum_{n,\delta} s_n^\dagger s_{n+\delta} & H_d &= \varepsilon_z d_z^\dagger d_z \\
 H_i &= \sum_{\delta} (\gamma_z d_z^\dagger s_{0+\delta} + \gamma_z^* d_z s_{0+\delta}^\dagger)
 \end{aligned} \tag{1}$$

where s_n^\dagger and s_n are the creation and annihilation operators for the host s-band electrons at the lattice site n , and d_z^\dagger and d_z are the Fermi operators for the impurity d_{z^2} level, which is assumed to be located at the lattice site 0. Its bare energy is ε_z and the parameter describing the hybridization between the impurity and the host level is γ_z . The parameter t stands for the transfer energy in the unperturbed system, and the index δ runs over all four nearest neighbours.

The Green's function in the single-impurity problem is obtained by suitably partitioning the starting equation in the site representation:

$$\begin{pmatrix} \varepsilon - \varepsilon_z & -\vec{\gamma}_z \\ -\vec{\gamma}_z^\dagger & \varepsilon - \hat{H}_s \end{pmatrix} \begin{pmatrix} G_{dd} & \vec{G}_{ds} \\ \vec{G}_{sd} & \hat{G}_{ss} \end{pmatrix} = \hat{1}. \tag{2}$$

Here it is taken into account that the defect-related space is 1×1 ; that is, G_{dd} is a scalar. From the first two equations in equation (2),

$$\begin{aligned}
 (\varepsilon - \varepsilon_z)G_{dd} - \vec{\gamma}_z \cdot \vec{G}_{sd} &= 1 \\
 -\vec{\gamma}_z^\dagger G_{dd} + (\varepsilon - \hat{H}_s)\vec{G}_{sd} &= 0
 \end{aligned} \tag{3}$$

it is easy to obtain that

$$G_{dd} = (\varepsilon - \varepsilon_z - \vec{\gamma}_z \hat{g} \vec{\gamma}_z^\dagger)^{-1} \tag{4}$$

where $\hat{g} = (\varepsilon - \hat{H}_s)^{-1}$ is the unperturbed Green's function of the host system. Equation (4) can be rewritten in the following form:

$$G_{dd} = \left(\varepsilon - \varepsilon_z - |\gamma_z|^2 \sum_{l,l'} g_{ll'} \right)^{-1} \tag{5}$$

where indices l and l' run over nearest neighbours of the impurity site. The summation in equation (5) can be carried out by utilizing the inversion symmetry of the host system:

$$\sum_{l,l'} g_{ll'} = \frac{1}{N} \sum_{\vec{k}} \sum_{l,l'} \left[e^{-i\vec{k} \cdot (\vec{r}_l - \vec{r}_{l'})} / \left(\varepsilon - t \sum_l e^{i\vec{k} \cdot (\vec{r}_l - \vec{r}_0)} \right) \right] = \frac{\varepsilon^2}{t^2} g_{00}(\varepsilon) - \frac{\varepsilon}{t^2}. \tag{6}$$

The diagonal element of the host Green's function g_{00} for a square lattice can be expressed analytically as

$$g_{00}(\varepsilon) = \frac{\text{sgn}(\varepsilon)}{2\pi t} \text{K}\left(\frac{\varepsilon}{4t}\right) + \frac{i}{2\pi t} \text{K}\left(\sqrt{1 - \left(\frac{\varepsilon}{4t}\right)^2}\right) \tag{7}$$

where K is the complete elliptic integral of the first kind. The LDOS of the d_{z^2} orbital at the impurity site $\rho_z(\varepsilon)$ is obtained by taking the imaginary part of equation (5):

$$\begin{aligned}
 \rho_z(\varepsilon) &= \frac{1}{\pi} \Im G_{dd} = \frac{1}{\pi} \frac{|\gamma_z/t|^2 \varepsilon^2 \Im g_{00}(\varepsilon)}{Z(\varepsilon)} \\
 Z(\varepsilon) &= \left(\varepsilon \left(1 + \left| \frac{\gamma_z}{t} \right|^2 \right) - \varepsilon_z - \left| \frac{\gamma_z}{t} \right|^2 \varepsilon^2 \Re g_{00}(\varepsilon) \right)^2 + \left(\left| \frac{\gamma_z}{t} \right|^2 \varepsilon^2 \Im g_{00}(\varepsilon) \right)^2.
 \end{aligned} \tag{8}$$

These results suggest that a well-defined resonance can appear in the system under consideration. Its energy ε_r is given by the solution of the equation

$$\varepsilon_r = \left(\varepsilon_z + \left| \frac{\gamma_z}{t} \right|^2 \varepsilon_r^2 \Re g_{00}(\varepsilon_r) \right) / \left(1 + \left| \frac{\gamma_z}{t} \right|^2 \right) \quad (9)$$

while the effective damping of the resonance is given by

$$\Gamma_r = \left(\left| \frac{\gamma_z}{t} \right|^2 \varepsilon_r^2 \Im g_{00}(\varepsilon_r) \right) / \left[1 + \left| \frac{\gamma_z}{t} \right|^2 \left(1 - \frac{d}{d\varepsilon} (\varepsilon^2 \Re g_{00}(\varepsilon)) \Big|_{\varepsilon=\varepsilon_r} \right) \right]. \quad (10)$$

It is understood from equation (9) that the resonance is located in between the bare energy of the d_{z^2} level, ε_z , and the band centre, and that, as the s-d coupling is increased, the resonance shifts toward the band centre (see figure 1). It is noteworthy that, in the case of the simplified

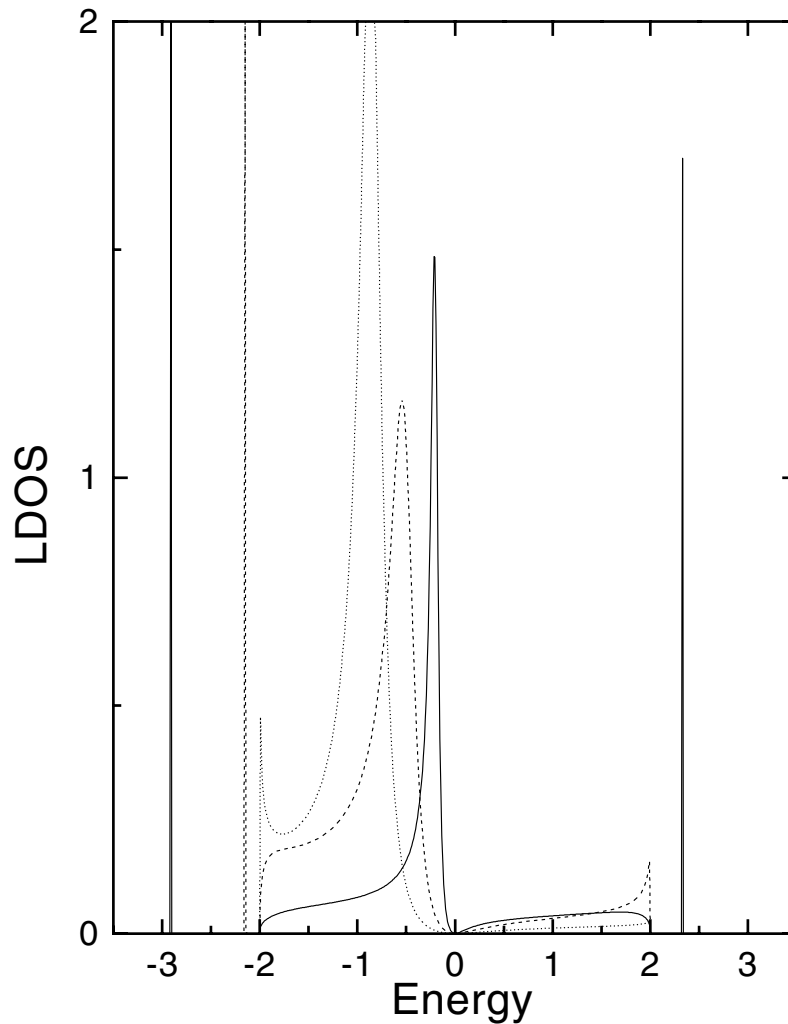


Figure 1. The LDOS of the d_{z^2} orbital at the impurity site for varying strength of the s-d coupling $|\gamma/t|$. Dotted, dashed, and solid lines denote the LDOS for $|\gamma/t| = 0.5, 1.0, 2.0$, respectively. Here the bare energy of the d_{z^2} level is $\varepsilon_z = -1.0$.

model with on-site coupling, the situation is just the opposite. Namely, the resonance is located in between the bare energy of the d_{z^2} level and the band edge, and when the s - d coupling is increased, the resonance shifts toward the band edge. The effective damping of the resonance, equation (10), appears to fall gradually when approaching the band centre, again in contrast to the behaviour in the model with on-site coupling. As a result, the resonance peak in the d_{z^2} LDOS at the impurity site becomes sharper, as the resonance approaches the band centre (see figures 1, 2). Even though the host DOS manifests an inherent 2D logarithmic divergence at the band centre, the region near to the band centre remains favourable to the formation of resonance states. In all cases except that where $\varepsilon_z = 0$, the LDOS for the impurity d_{z^2} level drops to zero at the band centre, i.e. at the position of the bare s level in the host system, as is clearly seen in equation (8). Additional sharp peaks can be present in the LDOS of the

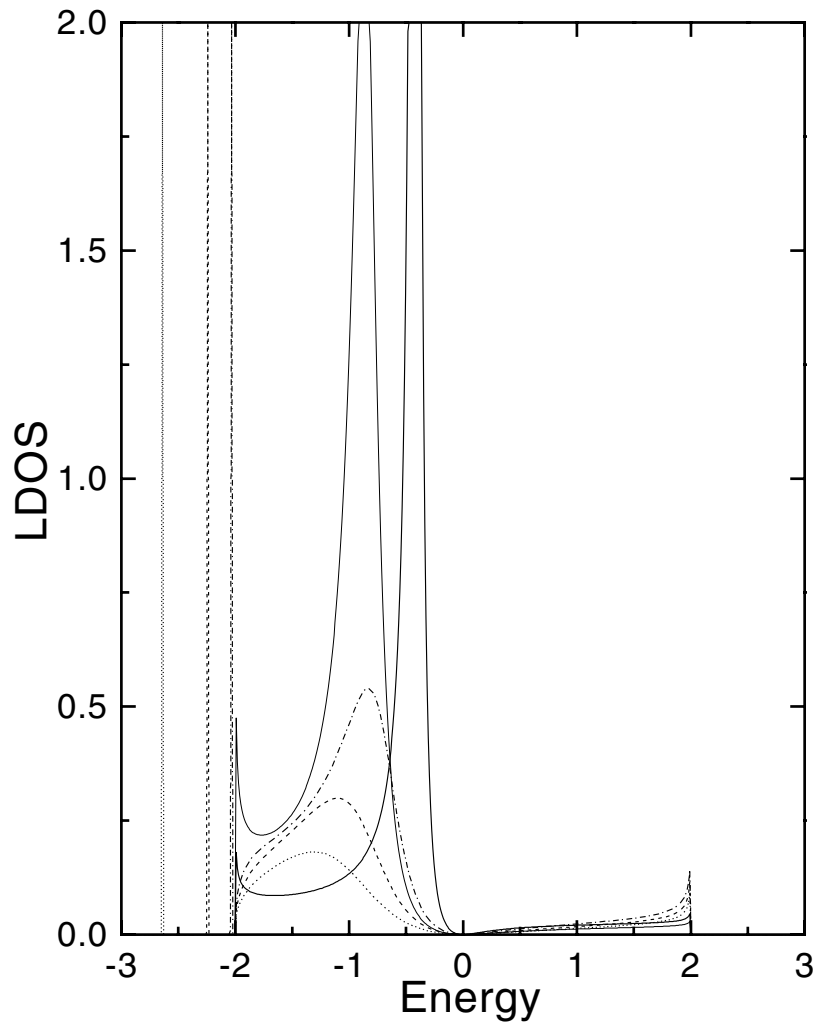


Figure 2. The LDOS of the d_{z^2} orbital at the impurity site for varying bare energy of the d_{z^2} level, ε_z . Dotted, dashed, chain, thin, and solid lines denote the LDOS for $\varepsilon_z = -2.5, -2.0, -1.5, -1.0, -0.5$, respectively. We use the strength of the s - d coupling $|\gamma/t| = 0.5$.

d_{z^2} level near to band edges, but this peak does not correspond to the resonance. Also, it will be seen from later discussion that another sharp peak can appear exactly at the band centre when $\varepsilon_z = 0$.

As the system under consideration is 2D, any small perturbation induced by the defect will also lead to the appearance of split-off local levels. Specifically, when the energy of the impurity d_{z^2} level falls inside the host band, two local levels are always present, above and below the host s band. The positions of the local levels can be obtained from the equation

$$L(\varepsilon_l) = \varepsilon_l \left(1 + \left| \frac{\gamma_z}{t} \right|^2 \right) - \varepsilon_z - \left| \frac{\gamma_z}{t} \right|^2 \varepsilon_l^2 g_{00}(\varepsilon_l) = 0 \quad (11)$$

where $g_{00}(\varepsilon)$ represents the host Green's function for the energy outside the s band:

$$g_{00}(\varepsilon) = \frac{2}{\pi \varepsilon} \text{K} \left(\frac{4t}{\varepsilon} \right). \quad (12)$$

In many cases, these split-off local levels are rather shallow. On increasing the s–d coupling, the local levels move further apart from the host band, and the spectral weights of the local levels become enhanced (see figure 1). It follows from equation (5) that the spectral weights of the local states are given by $|dL(\varepsilon)/d\varepsilon|_{\varepsilon=\varepsilon_l}|^{-1}$.

Now let us consider the s-orbital LDOS at the impurity site. From the two remaining equations in equation (2),

$$\begin{aligned} -\vec{\gamma}_z^\dagger \vec{G}_{ds} + (\varepsilon - \hat{H}_s) \hat{G}_{ss} &= 1 \\ (\varepsilon - \varepsilon_z) \vec{G}_{ds} - \vec{\gamma}_z \hat{G}_{ss} &= 0 \end{aligned} \quad (13)$$

it follows that

$$\hat{G}_{ss} = \hat{g} + \hat{g} \vec{\gamma}_z^\dagger \frac{1}{\varepsilon - \varepsilon_z} \vec{\gamma}_z \hat{g} + \hat{g} \vec{\gamma}_z^\dagger \frac{1}{\varepsilon - \varepsilon_z} \vec{\gamma}_z \hat{g} \vec{\gamma}_z^\dagger \frac{1}{\varepsilon - \varepsilon_z} \vec{\gamma}_z \hat{g} + \dots = \hat{g} + \hat{g} \vec{\gamma}_z^\dagger G_{dd} \vec{\gamma}_z \hat{g}. \quad (14)$$

Hence the diagonal Green's function element of the s level at the impurity site is given by

$$G_{00} = g_{00} + \sum_l g_{0l} \left[|\gamma_z|^2 / \left(\varepsilon - \varepsilon_z - |\gamma_z|^2 \sum_{l,l'} g_{ll'} \right) \right] \sum_l g_{l0}. \quad (15)$$

Using the relation

$$\frac{\varepsilon}{t} \sum_l g_{0l} = \sum_{l,l'} g_{ll'} \quad (16)$$

the last expression can be rewritten as

$$G_{00} = \frac{(\varepsilon - \varepsilon_z) g_{00} + |\gamma_z/t|^2 (1 - \varepsilon g_{00})}{\varepsilon (1 + |\gamma_z/t|^2) - \varepsilon_z - |\gamma_z/t|^2 \varepsilon^2 g_{00}}. \quad (17)$$

Taking the imaginary part of equation (17), we get the LDOS for the s orbital at the impurity site:

$$\rho_0 = \frac{1}{\pi} \Im G_{00} = \frac{1}{\pi} \frac{(\varepsilon - \varepsilon_z)^2 \Im g_{00}(\varepsilon)}{Z(\varepsilon)}. \quad (18)$$

The features of the s-orbital LDOS at the impurity site are similar to those of the d_{z^2} -orbital LDOS. The main feature of the s-orbital LDOS at the impurity site is the existence of a dip located at the bare energy of the d_{z^2} level, ε_z . At this energy, the LDOS goes down to exactly zero, as seen in equation (18). This point will be discussed more in section 4. When the distance between the peak position ε_r given by equation (9) and the bare energy ε_z is larger than the damping of the resonance of equation (10), there is also a peak in the s-orbital LDOS at the impurity site. The peak is located in the vicinity of the resonance peak of the d_{z^2} -orbital

LDOS (see figure 3). The distance between these two peaks does not exceed the smearing of the resonance state and diminishes as the resonance becomes sharper. This always happens when the resonance appears for strong coupling, i.e. $|\gamma_z/t|^2 \gg 1$. In this case, the peak in the s-orbital LDOS will be even more pronounced than that in the d_{z^2} -orbital LDOS, because fewer states are concentrated in the split-off local levels. It is easy to see from equations (11) and (17) that the spectral weights of the local levels in the s-orbital LDOS differ from those in the d_{z^2} -orbital LDOS by the factor

$$\frac{1}{|\gamma_z/t|^2} \left(\frac{\varepsilon_l - \varepsilon_z}{\varepsilon_l} \right)^2. \quad (19)$$

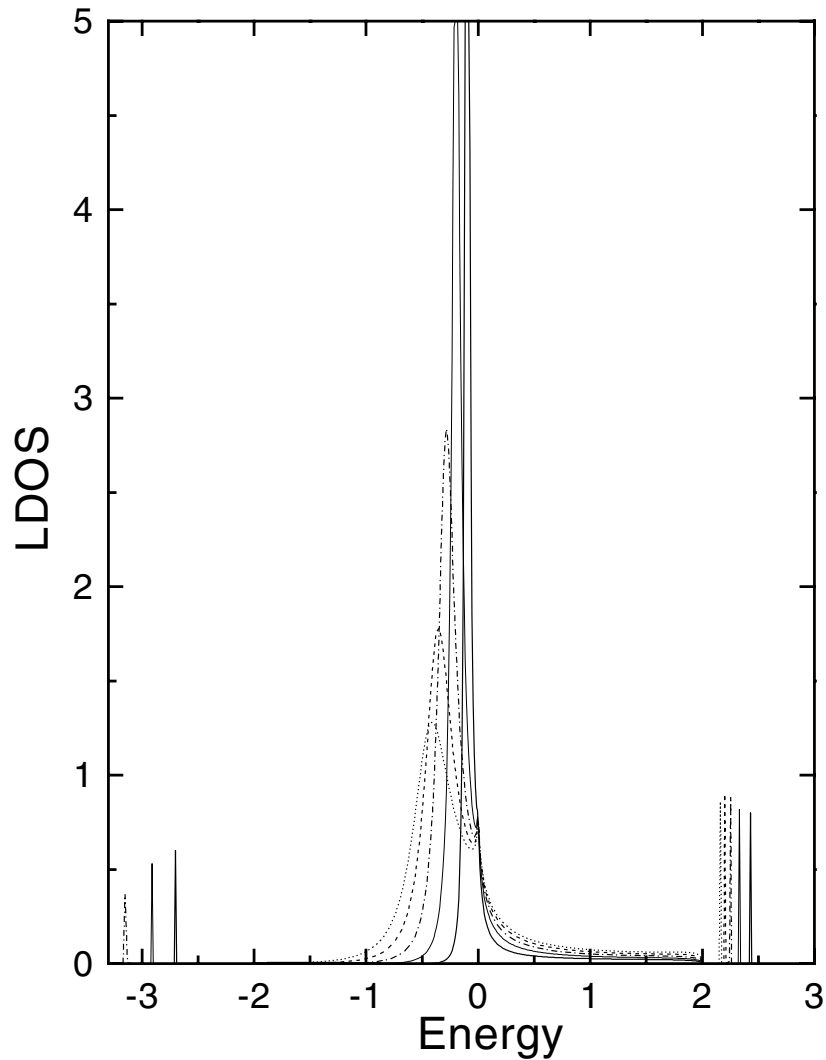


Figure 3. The LDOS of the s orbital at the impurity site for varying bare energy of the d_{z^2} level, ε_z . Dotted, dashed, chain, thin, and solid lines denote the LDOS for $\varepsilon_z = -2.5, -2.0, -1.5, -1.0, -0.5$, respectively. We use $|\gamma/t| = 2.0$.

However, for weak coupling, the resonance peak in the s-orbital LDOS is not so prominent and becomes smeared out when the resonance appears near to the band edge (see figure 4). In this case, there is only a dip rather than a peak in the vicinity of the resonance energy of the d_{z^2} orbital.

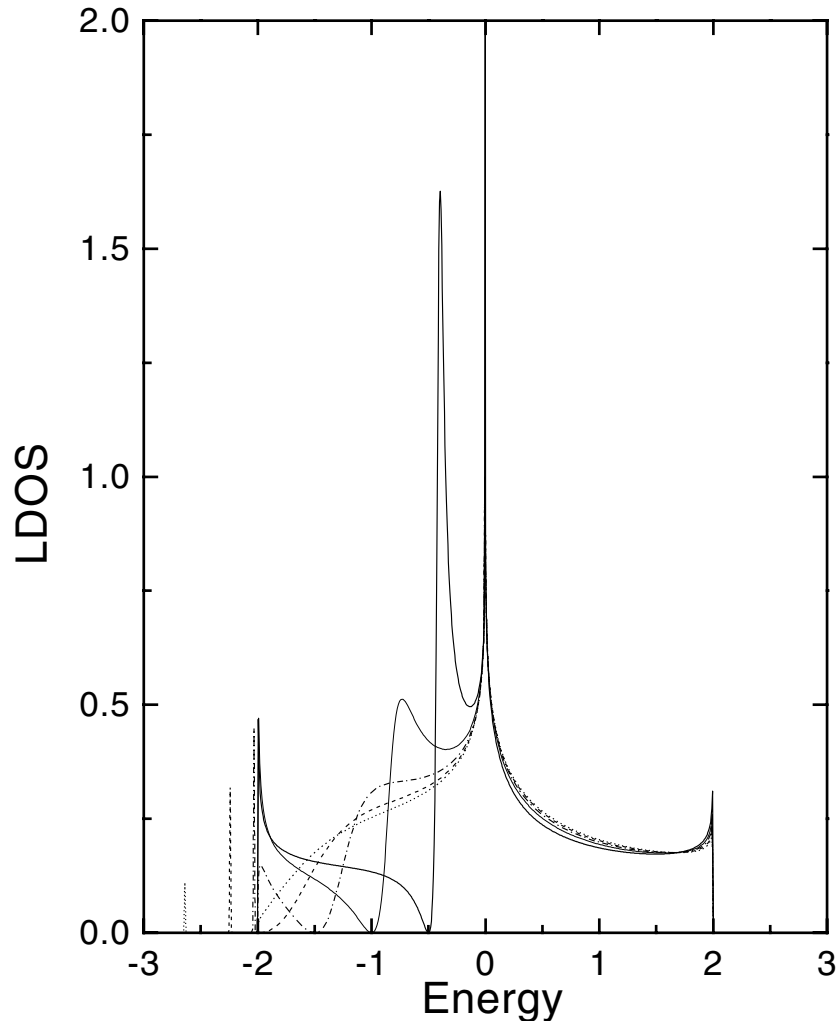


Figure 4. The LDOS of the s orbital at the impurity site for varying bare energy of the d_{z^2} level, ε_z . Dotted, dashed, chain, thin, and solid lines denote the LDOS for $\varepsilon_z = -2.5, -2.0, -1.5, -1.0, -0.5$, respectively. We use $|\gamma/t| = 0.5$.

It is generally understood that the resonance state becomes well defined as the coupling is reduced. Note, however, that in the present study the well-defined resonance state can be formed not only through the weakening of the coupling but also through the strengthening of it. As the coupling is strengthened, the resonance is shifted towards the band centre—that is, to the domain of low damping. Then, a well-defined resonance state, which has mainly impurity s character, is formed.

To support the obvious correspondence between the two LDOSs of the s and d_{z^2} orbitals, let us calculate the off-diagonal element of the Green's function. From the second equation of

equations (3), we have

$$G_{0d} = \hat{g}\tilde{\gamma}_z^\dagger G_{dd} = \gamma_z^* G_{dd} \sum_l g_{0l} = \gamma_z^* G_{dd} \frac{t}{\varepsilon} \sum_{l,l'} g_{ll'} = \frac{t}{\gamma_z \varepsilon} ((\varepsilon - \varepsilon_z)G_{dd} - 1) \quad (20)$$

where equations (5) and (16) were used. The imaginary part of this off-diagonal element of the Green's function:

$$\Im G_{0d} = \left(\frac{\varepsilon - \varepsilon_z}{\varepsilon} \right) \left(\frac{t}{\gamma_z} \right) \Im G_{dd} \quad (21)$$

gives rise to the bond order [10]:

$$\theta_{0d} = \frac{\Im G_{0d}}{\sqrt{\Im G_{00} \Im G_{dd}}} = \text{sgn} \left(\frac{\varepsilon - \varepsilon_z}{\varepsilon \gamma_z} \right). \quad (22)$$

The bond order changes its sign at dip positions—at the bare energies of the s and d_{z^2} level. Such an abrupt change in the bond order is usually related to the presence of antiresonance states [11]. We will come back to this point in section 3.

There still remains one exceptional case where the bare energies of the s and d_{z^2} levels have the same value: i.e. $\varepsilon_z = 0$. In this case, equations (8) and (18) give rise to smooth parts of the LDOS in the vicinity of the band centre ($|\varepsilon| \ll zt$):

$$\begin{aligned} \rho_z &\approx \frac{1}{\pi} \frac{|\gamma_z/t|^2}{(1 + |\gamma_z/t|^2)^2} \Im g_{00} \\ \rho_0 &\approx \frac{1}{\pi} \frac{1}{(1 + |\gamma_z/t|^2)^2} \Im g_{00}. \end{aligned} \quad (23)$$

However, a more careful look at the original expressions (5) and (17) reveals the presence of poles at the zero energy. The poles yield δ -function peaks at the band centre with the spectral weight of $(1 + |\gamma_z/t|^2)^{-1}$ for the d_{z^2} -orbital LDOS and with the weight of $|\gamma_z/t|^2/(1 + |\gamma_z/t|^2)$ for the s-orbital LDOS, respectively. Interestingly, the spectral weights of these peaks vary in the opposite way to those of the smooth parts, which reflects a proper normalization.

As was stated before, resonance states inside the domain of the host band are accompanied by the split-off local levels. In all cases with symmetric DOS, one can expand the host Green's function into a series for the energy lying far beyond the band, i.e., $|\varepsilon| \gg zt$:

$$g_{00} = \frac{1}{\varepsilon} \left(1 + \left(\frac{\lambda_2}{\varepsilon} \right)^2 + \left(\frac{\lambda_4}{\varepsilon} \right)^4 + \dots \right) \quad (24)$$

where the coefficients λ_2 and λ_4 are of the order of the bandwidth. As the positions of the local levels ε_l are determined by equation (11), and their spectral weights are inversely proportional to the derivative of the left-hand side of equation (11), we have, in the case of strong coupling, i.e. $|\gamma_z/t| \gg 1$, two local levels for the d_{z^2} -orbital LDOS at $\varepsilon_l \approx \pm |\gamma_z/t| \lambda_2$ with the spectral weights of approximately $(2(1 + (\lambda_4^2/(\lambda_2 \varepsilon_l))^2))^{-1}$, mirrored about the band centre. On the other hand, the spectral weight of the s-orbital LDOS is less by the factor $|\gamma_z/t|^2$. Hence, for strong coupling, $|\gamma_z/t| \gg 1$, the contribution of the δ -function at the band centre to the d_{z^2} -orbital LDOS is insignificant, and nearly all states are focused in two distant symmetric local levels. As for s-orbital LDOS, states are gathered in the δ -function at the band centre, while the rest of the host band domain is nearly empty and local levels have vanishing spectral weights. For weak coupling, $|\gamma_z/t| \ll 1$, the d_{z^2} -orbital LDOS is small throughout the whole domain of the host band, spectral weights of shallow local levels are low, and most of the states are concentrated in the δ -function at the band centre. In contrast, as for the s-orbital LDOS, the contribution from the pole at the band centre is small, and the spectrum shape is almost unchanged except at the band edges.

3. Spectral features at the neighbouring host sites

The LDOS of the s orbital at neighbouring host sites can be obtained straightforwardly from equation (14):

$$G_{ll} = g_{00} + \sum_{l'} g_{ll'} \left[|\gamma_z|^2 / \left(\varepsilon - \varepsilon_z - |\gamma_z|^2 \sum_{l,l'} g_{ll'} \right) \right] \sum_{l''} g_{l'l''}. \quad (25)$$

Considering the symmetry of the system, it is evident that

$$\sum_{l'} g_{ll'} = \frac{1}{z} \sum_{l,l'} g_{ll'} \quad (26)$$

where $z = 4$ stands for the number of nearest neighbours. By the use of equation (26), equation (25) can be simplified as follows:

$$\begin{aligned} G_{ll} &= g_{00} + \frac{1}{z^2} \left(\left[|\gamma_z|^2 \left(\sum_{l,l'} g_{ll'} \right)^2 \right] / \left[\varepsilon - \varepsilon_z - |\gamma_z|^2 \sum_{l,l'} g_{ll'} \right] + \sum_{l,l'} g_{ll'} - \sum_{l,l'} g_{ll'} \right) \\ &= g_{00} - \frac{1}{z^2} \sum_{l,l'} g_{ll'} + \frac{1}{z^2} \left(\left[(\varepsilon - \varepsilon_z) \sum_{l,l'} g_{ll'} \right] / \left[\varepsilon - \varepsilon_z - |\gamma_z|^2 \sum_{l,l'} g_{ll'} \right] \right. \\ &\quad \left. + \frac{(\varepsilon - \varepsilon_z)}{|\gamma_z|^2} - \frac{(\varepsilon - \varepsilon_z)}{|\gamma_z|^2} \right) \\ &= g_{00} - \frac{1}{z^2} \sum_{l,l'} g_{ll'} - \frac{(\varepsilon - \varepsilon_z)}{z^2 |\gamma_z|^2} + \left(\frac{\varepsilon - \varepsilon_z}{z |\gamma_z|} \right)^2 G_{dd}. \end{aligned} \quad (27)$$

Then, using equation (6), the LDOS at the nearest-neighbour host sites ρ_l is given by

$$\rho_l = \frac{1}{\pi} \Im G_{ll} = \frac{1}{\pi} \left(\left(1 - \left(\frac{\varepsilon}{tz} \right)^2 \right) \Im g_{00} + \left(\frac{\varepsilon - \varepsilon_z}{z |\gamma_z|} \right)^2 \Im G_{dd} \right). \quad (28)$$

This relation can be expressed in another way:

$$\rho_l = \frac{1}{\pi} \left(\left(1 - \left(\frac{\varepsilon}{tz} \right)^2 \right) \Im g_{00} + \left(\frac{\varepsilon}{tz} \right)^2 \Im G_{00} \right). \quad (29)$$

When the resonance energy is close to the band centre, the LDOS at the neighbouring host sites is not so much affected by the presence of the resonance state. The first term in equation (28) or in equation (29) represents the unperturbed DOS with smooth cut-offs at the band edges. As seen in figure 5, states near the band edges are depleted. This is a usual feature of the LDOS at sites located close to the impurity. The second term is in many cases relatively small as compared to the first. However, when the well-defined resonance state is located close to the band edge, the second term gives rise to an antiresonance dip in the spectrum. To see this, it is convenient to rewrite equation (28) in a different manner:

$$\rho_l = \rho_0 + \frac{1}{\pi} \left(1 - \left(\frac{\varepsilon}{tz} \right)^2 \right) \left(1 - \frac{(\varepsilon - \varepsilon_z)^2}{Z(\varepsilon)} \right) \Im g_{00}. \quad (30)$$

The first multiplier in the second term of equation (30) increases from zero at the band edge to unity at the band centre. Meanwhile, the second multiplier becomes extremely small when the well-defined resonance is formed, especially when the resonance emerges due to the weak coupling. Then the LDOS at the neighbouring site ρ_l will be very close in appearance to the s-orbital LDOS ρ_0 at the impurity site (see figure 6). The main difference is that the dip in the LDOS does not go down to zero in the case of ρ_l .

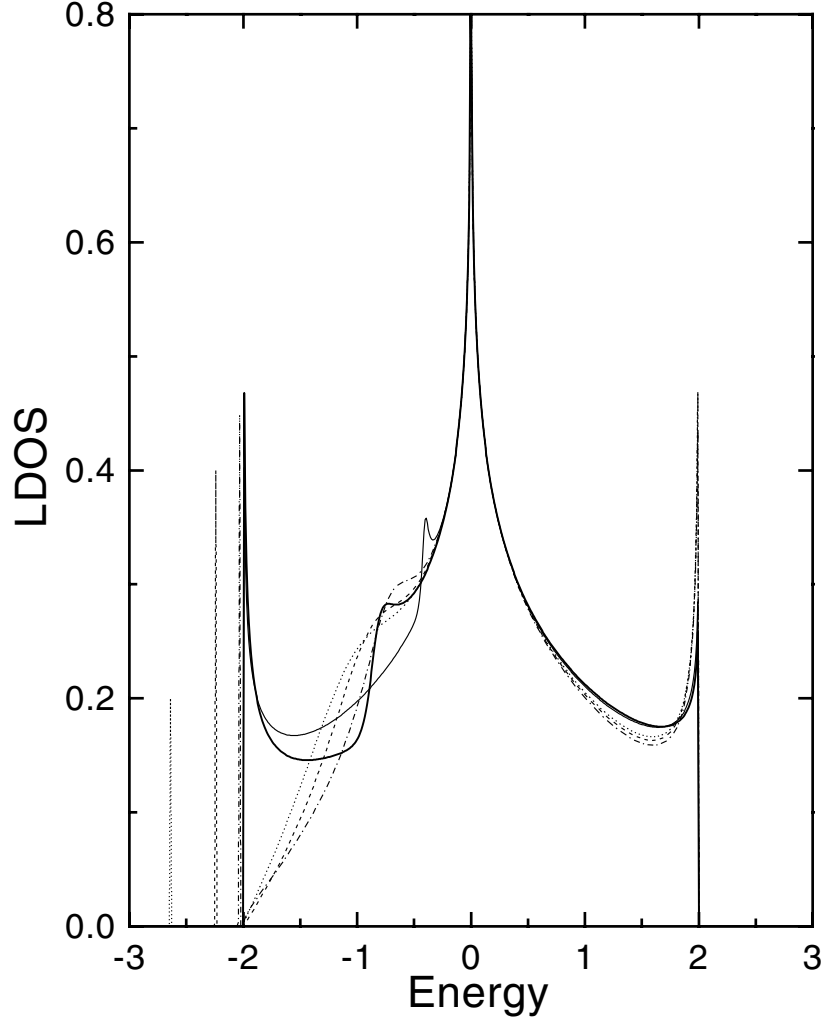


Figure 5. The LDOS of the s orbital at the neighbouring host site for varying bare energy of the d_{z^2} level, ε_z . Dotted, dashed, chain, thin, and solid lines denote the LDOS for $\varepsilon_z = -2.5, -2.0, -1.5, -1.0, -0.5$, respectively. We use $|\gamma/t| = 0.5$.

The bond order can be obtained from the corresponding off-diagonal Green's function element:

$$G_{ld} = \hat{g} \vec{\gamma}_z^\dagger G_{dd} = \frac{\gamma_z^*}{z} G_{dd} \sum_{l,l'} g_{ll'} = \frac{1}{z\gamma_z} ((\varepsilon - \varepsilon_z)G_{dd} - 1) \quad (31)$$

$$\Im G_{ld} = \frac{\varepsilon - \varepsilon_z}{z\gamma_z} \Im G_{dd} \quad (32)$$

$$\theta_{ld} = \frac{\varepsilon - \varepsilon_z}{z\gamma_z} \sqrt{\frac{\Im G_{dd}}{\Im G_{ll}}} = \text{sgn}\left(\frac{\varepsilon - \varepsilon_z}{\gamma_z}\right) / \sqrt{1 + \frac{t^2 z^2 - \varepsilon^2}{(\varepsilon - \varepsilon_z)^2 \varepsilon^2} Z(\varepsilon)}. \quad (33)$$

As mentioned previously, the bond order becomes exactly zero at the band centre and changes its sign at the bare energy of the d_{z^2} level. The presence of the antiresonance dip in the

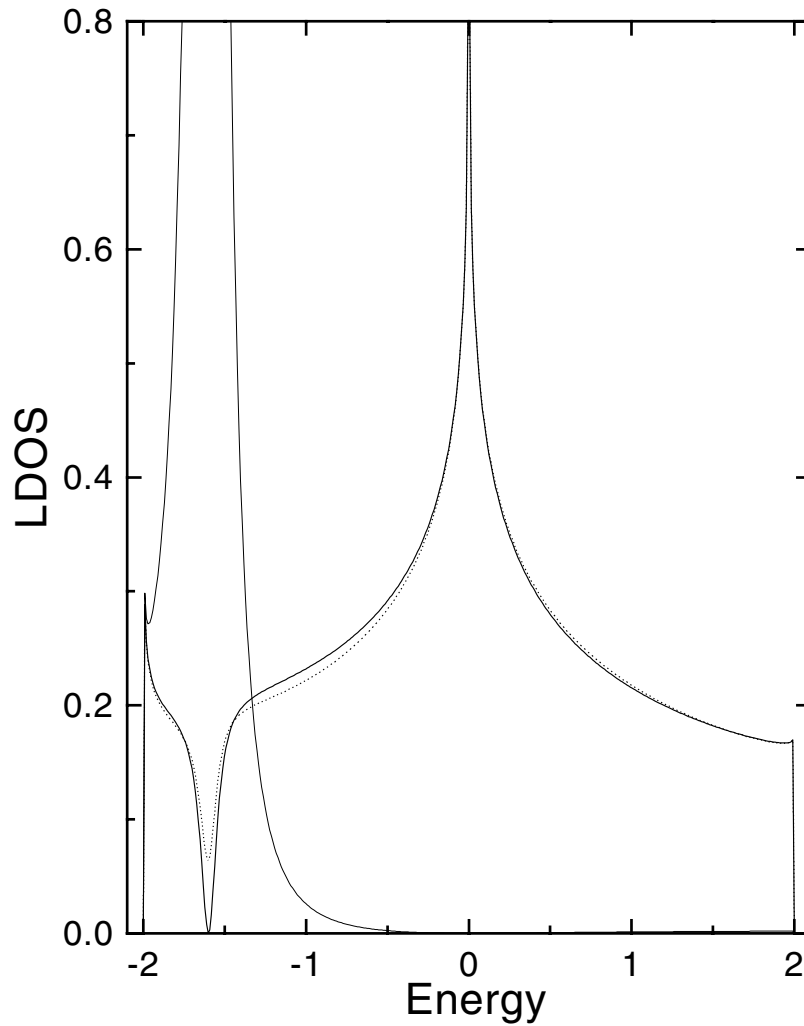


Figure 6. The LDOS for $|\gamma/t| = 0.2$ and $\varepsilon_z = -1.6$. Dotted, thin, and solid lines denote the LDOS of the s orbital at neighbouring host site, the d_{z^2} orbital at the impurity site, and the s orbital at the impurity site, respectively.

spectrum is connected with the variation of the bond order. Because $Z(\varepsilon)$ has only a logarithmic singularity at the band edges due to the singularity of the host Green's function, the bond order is exactly equal to ± 1 at the band edges, as is easily seen from equation (33). The same rule holds for 3D systems, but is not valid for 1D systems with stronger singularity.

4. Fano antiresonance

Diagonal elements of the Green's functions relating to the s levels at both the impurity and its neighbours (equation (15) and equation (25)) can be expressed in the following form:

$$G_{ii} = g_{00} + (A + iB) \frac{1}{\varepsilon - \varepsilon_z - \Delta - i\Gamma} (A + iB) \quad (34)$$

which is reminiscent of the form of the generalized Fano effect [11]. Taking the imaginary part of equation (34), we have

$$\frac{\Im G_{ii}}{\Im g_{00}} = 1 - U + U \frac{(E + q)^2}{E^2 + 1} \tag{35}$$

$$E = \frac{\varepsilon - \varepsilon_z - \Delta}{\Gamma} \quad q = \frac{A}{B} \quad U = \frac{B^2}{\Gamma \Im g_{00}}$$

where the usual parameters of the Fano line shape are introduced. Comparison of equation (15) with equations (34) and (35) gives directly for the s-orbital LDOS at the impurity site

$$A = \frac{|\gamma_z|}{t} (\varepsilon \Re g_{00} - 1) \quad B = \frac{|\gamma_z|}{t} \varepsilon \Im g_{00}$$

$$\Gamma = \left(\frac{|\gamma_z|}{t} \right)^2 \varepsilon^2 \Im g_{00} \quad \Delta = \left(\frac{|\gamma_z|}{t} \right)^2 (\varepsilon^2 \Re g_{00} - \varepsilon) \tag{36}$$

$$q = \frac{\Re g_{00} - 1/\varepsilon}{\Im g_{00}} \quad U = 1.$$

For the nearest-neighbour sites, only the following parameters are different:

$$A = \frac{|\gamma_z|}{zt^2} (\varepsilon^2 \Re g_{00} - \varepsilon) \quad B = \frac{|\gamma_z|}{zt^2} \varepsilon^2 \Im g_{00} \tag{37}$$

$$U = \left(\frac{\varepsilon}{zt} \right)^2.$$

The antiresonance dip is located at the energy

$$\varepsilon_a = \varepsilon_z + \Delta - q\Gamma \tag{38}$$

which in both cases is actually equal to ε_z . Compensation occurs because of the coincidence of the symmetry of the impurity and that of the host system, as is manifested in equation (16). This kind of compensation is known to give some preference to the existence of sharp antiresonance dips in the spectra [12]. The parameter U becomes largest (unity) for the s level at the impurity site, whereas, for nearest neighbours, it reaches unity only at the band edges in accordance with the previous description of the spectra.

The physical origin of dips in the spectra is more easily understood from the following basic equations. Let us denote the wave-function components of the s levels and the d_{z^2} level by ψ_i and ϕ , respectively, in the site representation. Then, ψ_i and ϕ satisfy

$$\varepsilon \phi = \varepsilon_z \phi + \gamma_z \sum_l \psi_l$$

$$\varepsilon \psi_0 = t \sum_l \psi_l. \tag{39}$$

Hence,

$$(\varepsilon - \varepsilon_z) \phi = \frac{\gamma_z}{t} \varepsilon \psi_0. \tag{40}$$

Since the LDOS is just the density of the squared modulus of the wave-function component at a given energy, the interrelation between the LDOS for d_{z^2} and that for the s orbital at the impurity site is obvious from the above equations. It turns out that spectral features can be described on the basis of the problem of coupled oscillators. By analogy, as long as the bare energy of the d_{z^2} level ε_z is not equal to zero, i.e. does not coincide with the bare energy of the s level, the s-level wave-function component ψ_0 must be zero at ε_z and vice versa, which clarifies the origin of the dips in the corresponding LDOS.

In the vicinity of the host band centre, which corresponds to the energy of the s levels of the host system, the additional d_{z^2} level sees the same environment as the host levels, with the hopping to the neighbouring sites scaled only by some coefficient. Thus, because of the phase cancellation between the amplitudes of the wave function at the neighbouring sites, the additional level weakly interacts with the states of the host system in the vicinity of the band centre, and this spectral region appears to be favourable for the appearance of the resonance states. In turn, the s level at the impurity site is linked to the additional level by the hopping to the same neighbours. Both levels at the impurity site form a system of coupled oscillators, and the transfer between them drastically changes the shape of the LDOS of the s orbital. As a result, the resonance behaviour of the LDOS is also transferred to the s orbital at the impurity site, and sharp resonances can emerge not only in the usual case of a weakly coupled d level, but also for the strongly coupled d level. These considerations also clarify the shift of the resonance position towards the band centre when there is an increase of the hopping strength between the additional level and neighbouring sites.

5. Effects of the impurity $d_{x^2-y^2}$ level on the spectra

Besides the d_{z^2} impurity level, the $d_{x^2-y^2}$ impurity level will also interact with the s levels on a square lattice. The analysis is quite similar to the former one. One must note, however, that the transfer integral in this case changes its sign depending on the direction of the hopping. Thus components of the corresponding hybridization vector $\vec{\gamma}_x$ also change their signs, and so the diagonal element of the Green's function for the single-impurity $d_{x^2-y^2}$ level is given by

$$G_{dd} = \left(\varepsilon - \varepsilon_x - |\gamma_x|^2 \sum'_{l,l'} g_{ll'} \right)^{-1}. \quad (41)$$

Here the subscript x represents the $d_{x^2-y^2}$ level, and the prime in the sum denotes that elements of the Green's function connecting second neighbours are taken with the negative sign. The summation can be changed into the following integral:

$$\sum'_{l,l'} g_{ll'} = \frac{4}{\pi^2} \int_0^\pi \int_0^\pi dx dy \frac{(\cos x - \cos y)^2}{\varepsilon - 2t(\cos x + \cos y)}. \quad (42)$$

After some transformations, equation (42) can be expressed as

$$\begin{aligned} \sum'_{l,l'} g_{ll'} = & \left(16 - \left(\frac{\varepsilon}{t} \right)^2 \right) g_{00}(\varepsilon) - 3 \frac{\varepsilon}{t^2} \\ & + \frac{8}{\pi t} \left(\text{sgn}(\varepsilon) \int_0^{\arccos(\varepsilon/(2t)+1)} dx \sqrt{\left(\frac{\varepsilon}{2t} - \cos x \right)^2 - 1} \right) \\ & - i \frac{8}{\pi t} \left(\int_0^{\arccos(\varepsilon/(2t)-1)} dx \sqrt{1 - \left(\frac{\varepsilon}{2t} - \cos x \right)^2} \right). \end{aligned} \quad (43)$$

Since the integrands are smooth, the integration can be performed numerically.

It follows from equation (43) that the effective damping retains the singularity of the host at the band centre and reduces to zero on approaching the band edges. Hence, resonance states can be easily formed near the band edges, whereas it is hard to obtain a well-defined resonance in the vicinity of the band centre. These features are in contrast to the case of the impurity d_{z^2} level. The $d_{x^2-y^2}$ -orbital LDOS is zero at the band centre, since the effective damping becomes infinity. However, this dip is very sharp. The real part of equation (43) suggests that

the well-defined resonance located near the band edges is not accompanied by local split-off levels, but by a second resonance state located above the band centre which is usually smeared out (see figure 7).

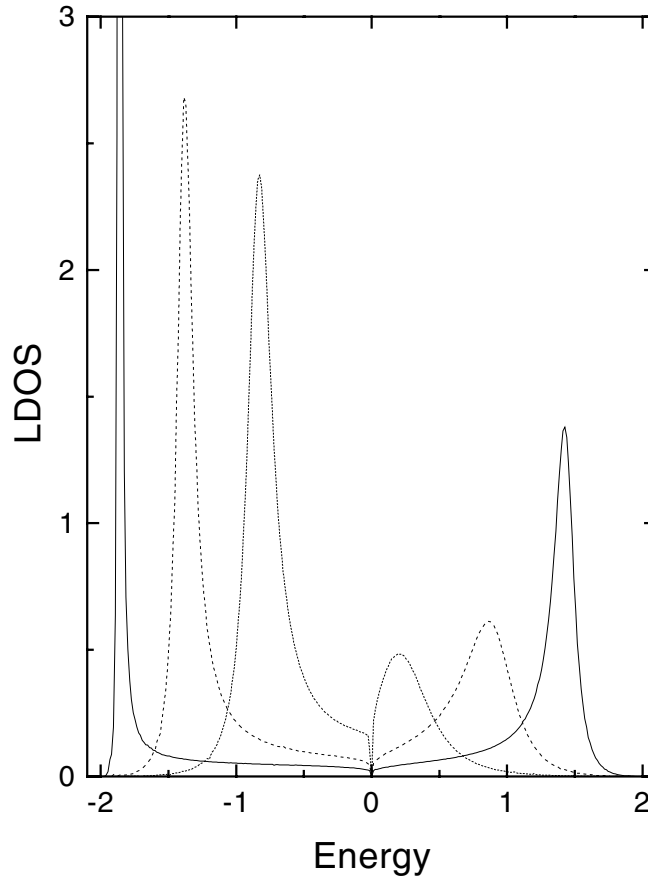


Figure 7. The LDOS of the $d_{x^2-y^2}$ orbital at the impurity site for varying strength of the s - d coupling $|\gamma/t|$. Dotted, dashed, and solid lines denote the LDOS for $|\gamma/t| = 0.5, 1.0, 1.5$, respectively. Here the bare d_{z^2} energy level is $\varepsilon_z = -0.5$.

It is evident that, because of the sign alternation in the hopping parameter, the s -orbital LDOS at the impurity site remains unperturbed. At neighbouring host sites, the diagonal element of the Green's function can be expressed in a form similar to equation (27). Just the sum with the prime, i.e., $\sum'_{l,l'} g_{ll'}$, and the subscripts in ε_x, γ_x are to be replaced. The first two terms produce a rather smooth background in the LDOS, because the logarithmic singularities in the two terms are mutually cancelled. To this background, distinct $d_{x^2-y^2}$ resonance peaks are added (see figure 8). As indicated in equation (27), the contribution from $d_{x^2-y^2}$ resonances has a factor $((\varepsilon - \varepsilon_x)/(z|\gamma_x|))^2$. This contribution will be relatively small for large $|\gamma_x|$. The main resonance peak near ε_x is suppressed to some extent due to the term $(\varepsilon - \varepsilon_x)^2$, and so the second resonance above the band centre becomes more pronounced. On the other hand, for small $|\gamma_x|$, the contribution from the main resonance peak becomes significant, because the cut-off effect of the factor $(\varepsilon - \varepsilon_x)$ is compensated by the small $|\gamma_x|$.

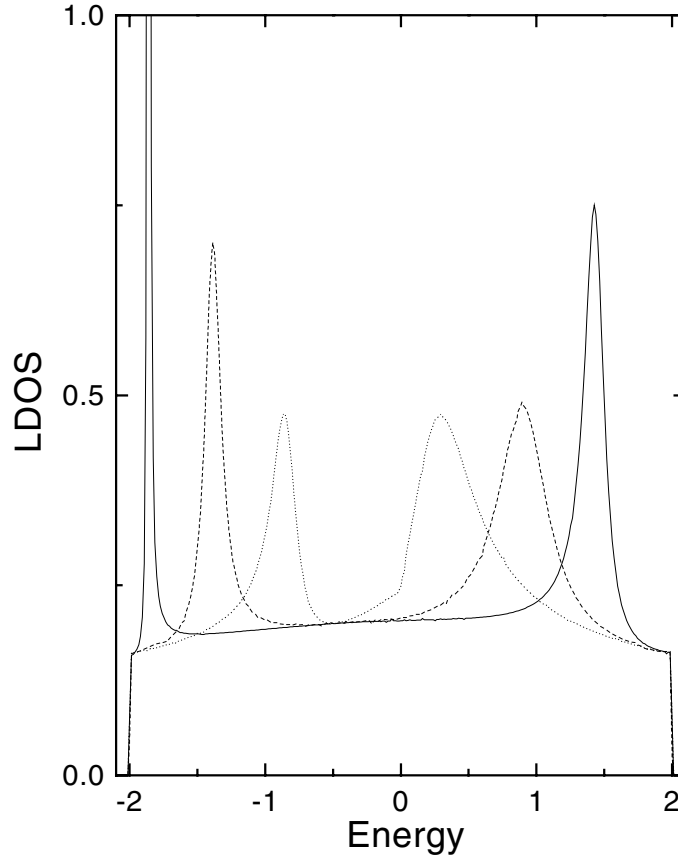


Figure 8. The LDOS of the s orbital at the neighbouring host site with varying $|\gamma/t|$. Dotted, dashed, and solid lines denote the LDOS for $|\gamma/t| = 0.5, 1.0, 1.5$, respectively. We use the bare energy of the $d_{x^2-y^2}$ level $\varepsilon_x = -0.5$.

The bond order between the $d_{x^2-y^2}$ level and the neighbouring s level changes sign at ε_x . It is zero inside the sharp dip at the band centre and at the band edges. Near to every resonance, it shows an extremum. The parameter in the Fano formula

$$U = \sum_{l,l'} g_{ll'}/z^2 \mathfrak{R}g_{00}$$

is equal to zero at the band edges and to unity at the band centre. Again we have the compensation $\Delta = q\Gamma$. The parameter q gains its maximum magnitudes at the band edges, and changes sign passing through the band centre.

So far we have analysed separately the effects of the impurity d_{z^2} and $d_{x^2-y^2}$ levels. This is valid if the difference between the bare energies of these levels is larger than the width of the host s band. But such an assumption has no physical justification. Therefore, let us consider two levels simultaneously as in the following equation:

$$\begin{pmatrix} \varepsilon - \varepsilon_z & 0 & -\vec{\gamma}_z \\ 0 & \varepsilon - \varepsilon_x & -\vec{\gamma}_x \\ -\vec{\gamma}_z^\dagger & -\vec{\gamma}_x^\dagger & \varepsilon - \hat{H}_s \end{pmatrix} \begin{pmatrix} \vec{G}_{zz} & G_{zx} & \vec{G}_{zs} \\ \vec{G}_{xz} & G_{xx} & \vec{G}_{xs} \\ \vec{G}_{sz} & \vec{G}_{sx} & \hat{G}_{ss} \end{pmatrix} = \hat{1}. \quad (44)$$

Since these two states have different symmetries, their contributions can be separated. Solving the above equation for G_{zz} , we have

$$(\varepsilon - \varepsilon_z)G_{zz} - \vec{\gamma}_z \left(\hat{g} + \hat{g} \vec{\gamma}_x^\dagger \frac{1}{\varepsilon - \varepsilon_x} \vec{\gamma}_x \hat{g} + \dots \right) \vec{\gamma}_z^\dagger G_{zz} = 1. \quad (45)$$

Because the symmetry of the impurity is the same as the symmetry of the host system and $\vec{\gamma}_z$ is orthogonal to $\vec{\gamma}_x^\dagger$, the combination $\vec{\gamma}_z \hat{g} \vec{\gamma}_x^\dagger$ becomes zero. Hence we obtain again the expression given as equation (4), which means that the presence of the $d_{x^2-y^2}$ level does not affect the diagonal element of the Green's function for the d_{z^2} level. It is easy to see that the same is true for the $d_{x^2-y^2}$ level. Analogously, we have

$$\vec{G}_{sz} = \left(\hat{g} + \hat{g} \vec{\gamma}_x^\dagger \frac{1}{\varepsilon - \varepsilon_x} \vec{\gamma}_x \hat{g} + \dots \right) \vec{\gamma}_z^\dagger G_{zz} = \hat{g} \vec{\gamma}_z^\dagger G_{zz} \quad (46)$$

confirming the previous result for \vec{G}_{sz} , and

$$G_{xz} = \frac{1}{\varepsilon - \varepsilon_x} \vec{\gamma}_x \vec{G}_{sz} = 0 \quad (47)$$

because the components of $\vec{\gamma}_x$ alternate their signs and all elements G_{Iz} are equal. Also from the following relations:

$$\begin{aligned} \vec{G}_{zs} &= \vec{G}_{sz}^\dagger = G_{zz} \vec{\gamma}_z \hat{g} \\ \vec{G}_{xs} &= \vec{G}_{sx}^\dagger = G_{xx} \vec{\gamma}_x \hat{g} \end{aligned} \quad (48)$$

it follows that

$$\hat{G}_{ss} = \hat{g} + \hat{g} \frac{\vec{\gamma}_z^\dagger \vec{\gamma}_z}{\varepsilon - \varepsilon_z - \vec{\gamma}_z \hat{g} \vec{\gamma}_z^\dagger} \hat{g} + \hat{g} \frac{\vec{\gamma}_x^\dagger \vec{\gamma}_x}{\varepsilon - \varepsilon_x - \vec{\gamma}_x \hat{g} \vec{\gamma}_x^\dagger} \hat{g}. \quad (49)$$

Thus, the two d levels make their own independent contributions to the Green's function element connecting s levels. It is also evident from equation (49) that only the d_{z^2} level influences the s-level diagonal Green's function element at the impurity site.

6. Conclusions

We have examined the spectral nature of a model 2D disordered system with a single impurity. The effects of the impurity d levels, d_{z^2} and $d_{x^2-y^2}$, on the LDOS at the impurity and neighbouring host sites are investigated. It is shown that the symmetry matching between the host and the impurity d_{z^2} level in low-dimensional systems produces interesting features. Namely, with increasing the s–d coupling, the resonance shifts toward the band centre, becomes sharper, and changes its character from d to s character, whereas the split-off local levels move further apart from the host band. Complementary antiresonance dips in both LDOS at the impurity site fall to exactly zero at the bare energies of the s and d levels, manifesting a special case of the Fano effect. Further, it is found that, for an impurity with a $d_{x^2-y^2}$ level, a phase cancellation leads to low damping of the resonance at the band edges, in contrast to the case for d_{z^2} impurity.

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