Self-consistent localization theory in the two-band model

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Abstract. This paper deals with calculations within the self-consistent localization theory of the conductivity, critical disorder, and the localization radius for the two-band model with Gaussian disorder. It demonstrates that at the Fermi level the localized states corresponding to the narrow band cannot coexist with the delocalized states in the wide band. Hybridization of the states of the narrow and wide bands leads to the delocalization of the system. The critical disorder corresponding to localization exceeds the values characteristic of an unhybridized wide band. Within a certain range of parameters of the system the behaviour of the conductivity may be nonmonotonic; for instance, it can increase with disorder owing to the evolution of the hybridization pseudogap in the density of states.

We study the Anderson localization of electrons in the two-band model with hybridization. Such a statement of the problem is of interest both from the viewpoint of possible applications to real disordered systems, such as alloys and compounds of transition metals and systems with heavy fermions, and for solving some questions of principal importance. Of greatest interest here, obviously, is the case of a relatively narrow (d) band that is near the Fermi level and inside a broad (s) band. This situation is not at all exotic from the experimenter's viewpoint, while from the theoretician's viewpoint it is interesting because for unhybridized bands the critical disorder corresponding to the localization of electronic states varies considerably—it is easier to localize a narrow band [1]. At times, especially when discussing experiments, some researchers assume that at the Fermi level the localized states, corresponding to the narrow band, 'coexist' with the delocalized states. The fact that this is impossible in principle has generally been known for a long time: hybridization with states of the broad band is certain to transform the localized states of the narrow band into delocalized states [2, 3].

At the same time the question of localization and the specific properties of localization in the two-band model have not, to our knowledge, received special attention. Below we consider this problem within the framework of the self-consistent localization theory [5–8], which makes it possible to carry out all calculations to the final result. We show that localization in the two-band model does indeed possess a number of features that can manifest themselves in experiments. For one thing, no 'coexistence' of localized and delocalized states is possible in the above sense, and the Anderson transition may occur only when a value of critical disorder exceeding that corresponding to localization of the electronic states of the unhybridized broad band is reached.

Our approach is based on the generalized Anderson model [1] with diagonal disorder, whose Hamiltonian in the momentum representation has the following form:

$$H = \sum_{\mathbf{k},\mathbf{q}} h_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{\mu\nu} a_{\mathbf{k}+\mathbf{q}}^{\dagger\mu} a_{\mathbf{k}}^{\nu} \qquad h_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{\mu\nu} = \left[\varepsilon_{\mathbf{k}}^{\mu} \delta^{\mu\nu} + \gamma (1 - \delta^{\mu\nu}) \right] \delta_{\mathbf{q},0} + V_{\mathbf{q}}^{\mu} \delta^{\mu\nu}$$
(1)

with μ and ν the band indices. Here and in what follows we assume (if the opposite is not obvious) the summation convention over repeated indices valid, $a_k^{\dagger\mu}$ and a_k^{μ} are operators of creation and annihilation of a ' μ '-electron with momentum k, ε_k^{μ} is the spectrum of the ' μ '-electron in the tight binding approximation, and γ is the hybridization constant. The scattering potentials V_q^{μ} are assumed distributed according to the Gaussian delta-correlated law

$$\langle V_{\mathbf{q}}^{\mu} V_{\mathbf{q}'}^{\nu} \rangle = \delta^{\mu\nu} \delta_{\mathbf{q}, -\mathbf{q}'} W^2 \tag{2}$$

with W the width of the disorder. Here we have ignored the off-diagonal correlations in the scattering potential, which simplifies calculations considerably.

We define the one-particle Green function averaged over the realizations of the random potential,

$$\mathcal{G}_{\mathbf{k}}^{\mu\alpha}(\mathcal{E}^{\pm})\delta_{\mathbf{k},\mathbf{k}'} = \left\langle G^{\mu\alpha}(\mathbf{k},\mathbf{k}',\mathcal{E}^{\pm}) \right\rangle \tag{3}$$

with $\mathcal{E}^{\pm} = \mathcal{E} \pm i\delta$, as the solution of the equation

$$\left[\left(\mathcal{E}^{\pm} - \varepsilon_{\mathbf{k}}^{\mu} \right) \delta^{\mu\sigma} - \gamma (1 - \delta^{\mu\sigma}) - \Sigma_{\mathbf{k}}^{\mu\sigma} (\mathcal{E}^{\pm}) \right] \mathcal{G}_{\mathbf{k}}^{\sigma\alpha} (\mathcal{E}^{\pm}) = \delta^{\mu\alpha} \tag{4}$$

where we have introduced $\Sigma_{\mathbf{k}}^{\mu\alpha}(\mathcal{E}^{\pm})$, the self-energy part. The contributions of the sand d-states to the density of states of the system, $\rho(\mathcal{E}) = \rho^{s}(\mathcal{E}) + \rho^{d}(\mathcal{E})$, have the following form:

$$\rho^{\mathrm{s(d)}}(\mathcal{E}) = -\frac{1}{\pi} \operatorname{Im} \sum_{\mathbf{k}} \mathcal{G}_{\mathbf{k}}^{\mathrm{ss(dd)}}(\mathcal{E}^{+}). \tag{5}$$

The dynamical conductivity of the system is [4, 8]

$$\sigma_{\mathcal{E}_{\mathrm{F}}}(\omega) = \frac{2e^2}{\hbar\Omega^0} \lim_{q \to 0} \left(-\frac{\mathrm{i}\omega}{q^2} \right) \chi_{\rho\rho}^{\mathcal{E}_{\mathrm{F}}}(q;\omega)$$

where $\chi_{\rho\rho}^{\mathcal{E}_{F}}(q;\omega)$ is the density response function, and Ω^{0} is the volume per lattice site. For q and ω small we have

$$\chi_{\rho\rho}^{\mathcal{E}_{F}}(q;\omega) \simeq \omega \Phi_{\rho\rho}(q;\mathcal{E}_{F}^{+} + \omega, \mathcal{E}_{F}^{-}) + \rho(\mathcal{E}_{F}) + O(\omega, q^{2})$$
(6)

where

$$\Phi_{\rho\rho}\left(q;\mathcal{E}_{F}^{+}+\omega,\mathcal{E}_{F}^{-}\right) = \delta^{\mu\nu}\delta^{\alpha\beta}\sum_{\mathbf{k},\mathbf{k}'}\Psi_{\mathbf{k}\mathbf{k}'}^{\mu\nu\alpha\beta}\left(q;\mathcal{E}_{F}^{+}+\omega,\mathcal{E}_{F}^{-}\right)$$

$$\Psi_{\mathbf{k}\mathbf{k}'}^{\mu\nu\alpha\beta}\left(q;\mathcal{E}_{F}^{+}+\omega,\mathcal{E}_{F}^{-}\right) = -\frac{1}{2\pi\mathrm{i}}\left\langle G^{\mu\alpha}(\mathbf{k}+,\mathbf{k}'+;\mathcal{E}_{F}^{+}+\omega)G^{\nu\beta}(\mathbf{k}'-,\mathbf{k}-;\mathcal{E}_{F}^{-})\right\rangle$$
(7)

is the two-particle Green function averaged over the realizations of the random potential and satisfies the Bethe-Salpeter equation

$$\Psi_{\mathbf{k}\mathbf{k}'}^{\mu\nu\alpha\beta}(q;\mathcal{E}_{F}^{+}+\omega,\mathcal{E}_{F}^{-}) = \mathcal{G}_{\mathbf{k}+}^{\mu\sigma}(\mathcal{E}_{F}^{+}+\omega)\mathcal{G}_{\mathbf{k}-}^{\nu\delta}(\mathcal{E}_{F}^{-}) \left[-\frac{1}{2\pi i} \delta_{\mathbf{k}\mathbf{k}'} \delta^{\sigma\alpha} \delta^{\delta\beta} + \sum_{\mathbf{k}''} U_{\mathbf{k}\mathbf{k}''}^{\sigma\delta\eta\lambda}(q;\mathcal{E}_{F}^{+}+\omega,\mathcal{E}_{F}^{-}) \Psi_{\mathbf{k}''\mathbf{k}'}^{\eta\lambda\alpha\beta}(q;\mathcal{E}_{F}^{+}+\omega,\mathcal{E}_{F}^{-}) \right]$$
(8)

with $U_{kk'}^{\mu\nu\alpha\beta}(q;\mathcal{E}_{\mathrm{F}}^{+}+\omega,\mathcal{E}_{\mathrm{F}}^{-})$ the irreducible vertex part. Here $k\pm = k\pm q/2$. In the self-consistent Born approximation with q and ω small

$$\Sigma_{\mathbf{k}}^{\mu\alpha}(\mathcal{E}_{F}^{\pm}) \simeq \mp i\Delta_{\mathcal{E}_{F}}^{\mu}\delta^{\mu}\alpha \qquad \Delta_{\mathcal{E}_{F}}^{s(d)} = \pi\rho^{s(d)}(\mathcal{E}_{F})W^{2}$$

$$U_{\mathbf{k}\mathbf{k}'}^{\mu\nu\alpha\beta}\alpha\beta(q;\mathcal{E}_{F}^{+} + \omega,\mathcal{E}_{F}^{-}) \simeq \delta^{\mu\nu}\delta^{\mu\alpha}\delta^{\nu\beta}U_{\mathcal{E}_{F}}^{\nu} \qquad U_{\mathcal{E}_{F}}^{s(d)} = \frac{\Delta_{\mathcal{E}_{F}}^{s(d)}}{\pi\rho_{(\mathcal{E}_{F})}^{s(d)}}$$

$$\Phi_{\rho\rho}(q;\mathcal{E}_{F}^{+} + \omega,\mathcal{E}_{F}^{-}) \simeq \rho(\mathcal{E}_{F}) \frac{i}{-i\omega + D_{\mathcal{E}_{F}}q^{2}}$$
(9)

with $D_{\mathcal{E}_{\mathrm{F}}}$ the Born diffusion coefficient of the system,

$$\rho(\mathcal{E}_{F})D_{\mathcal{E}_{F}} = \rho^{s}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{s} + \rho^{d}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{d}$$

$$D_{\mathcal{E}_{F}}^{s} = \frac{1}{d\pi\rho^{s}(\mathcal{E}_{F})} \sum_{\mathbf{k}} \left\{ \left[\operatorname{Im} \mathcal{G}^{ss}(\mathcal{E}_{F}^{+}) \right] \left(\nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}}^{s} \right)^{2} + \left[\operatorname{Im} \mathcal{G}^{sd}(\mathcal{E}_{F}^{+}) \right]^{2} \left(\nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}}^{s} \nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}}^{d} \right) \right\}.$$

$$(10)$$

Here d is the dimensionality of the space, and $D_{\mathcal{E}_F}^d$ is obtained from $D_{\mathcal{E}_F}^s$ by interchanging the band indices s and d.

Combining the calculation of the two-particle Green function with the self-consistent approach to localization theory in the spirit of [5-10] yields

$$\Phi_{\rho\rho}(q; \mathcal{E}_{F}^{+} + \omega, \mathcal{E}_{F}^{-}) \simeq \rho(\mathcal{E}_{F}) \frac{i}{-i\omega + D_{\mathcal{E}_{F}}(\omega)q^{2}}$$
(11)

where we have introduced $D_{\mathcal{E}_{F}}(\omega)$, the generalized diffusion coefficient of the system, which can be found by solving the following self-consistent system of equations:

$$\rho(\mathcal{E}_{F})D_{\mathcal{E}_{F}}(\omega) = \rho^{s}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{s}(\omega) + \rho^{d}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{d}(\omega) \tag{12}$$

$$\rho^{s}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{s}(\omega) = \rho^{s}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{s} - \frac{\Theta_{\mathcal{E}_{F}}^{ss}}{\pi\rho(\mathcal{E}_{F})} \sum_{q} \frac{\rho^{s}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{s}(\omega)}{-i\omega + D_{\mathcal{E}_{F}}(\omega)q^{2}}$$

$$- \frac{\Theta_{\mathcal{E}_{F}}^{sd}}{\pi\rho(\mathcal{E}_{F})} \sum_{q} \frac{\rho^{d}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{d}(\omega)}{-i\omega + D_{\mathcal{E}_{F}}(\omega)q^{2}}$$

$$\rho^{d}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{d}(\omega) = \rho^{d}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{d} - \frac{\Theta_{\mathcal{E}_{F}}^{dd}}{\pi\rho(\mathcal{E}_{F})} \sum_{q} \frac{\rho^{d}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{d}(\omega)}{-i\omega + D_{\mathcal{E}_{F}}(\omega)q^{2}}$$

$$- \frac{\Theta_{\mathcal{E}_{F}}^{ds}}{\pi\rho(\mathcal{E}_{F})} \sum_{q} \frac{\rho^{s}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{s}(\omega)}{-i\omega + D_{\mathcal{E}_{F}}(\omega)q^{2}}$$

where

$$\Theta_{\mathcal{E}_{F}}^{ss} = \frac{2\Delta_{\mathcal{E}_{F}}^{s}}{d\pi\rho^{s}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{s}} \sum_{\mathbf{k}} \left\{ \Delta_{\mathcal{E}_{F}}^{s} \mathcal{G}_{\mathbf{k}}^{ss}(\mathcal{E}_{F}^{+}) \mathcal{G}_{\mathbf{k}}^{ss}(\mathcal{E}_{F}^{-}) \right\} \\
\times \left\{ \left[\operatorname{Im} \mathcal{G}_{\mathbf{k}}^{ss}(\mathcal{E}_{F}^{+}) \right]^{2} \left(\nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}}^{s} \right)^{2} + \operatorname{Im} \mathcal{G}_{\mathbf{k}}^{sd}(\mathcal{E}_{F}^{+}) \right]^{2} \left(\nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}}^{s} \nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}}^{d} \right) \right\} \\
\Theta_{\mathcal{E}_{F}}^{sd} = \frac{2\Delta_{\mathcal{E}_{F}}^{d}}{d\pi\rho^{d}(\mathcal{E}_{F})D_{\mathcal{E}_{F}}^{d}} \sum_{\mathbf{k}} \left\{ \Delta_{\mathcal{E}_{F}}^{d} \mathcal{G}_{\mathbf{k}}^{sd}(\mathcal{E}_{F}^{+}) \mathcal{G}_{\mathbf{k}}^{sd}(\mathcal{E}_{F}^{-}) \right\} \\
\times \left\{ \left[\operatorname{Im} \mathcal{G}_{\mathbf{k}}^{dd}(\mathcal{E}_{F}^{+}) \right]^{2} \left(\nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}}^{d} \right)^{2} + \operatorname{Im} \mathcal{G}_{\mathbf{k}}^{ds}(\mathcal{E}_{F}^{+}) \right]^{2} \left(\nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}}^{d} \nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}}^{s} \right) \right\}.$$

The coefficients $\Theta_{\mathcal{E}_F}^{ds}$ and $\Theta_{\mathcal{E}_F}^{dd}$ can be obtained from the corresponding relations by interchanging s and d.

Equation (11)-(14) formulate of the self-consistent localization theory for the two-band model with hybridization. If in the first equation in (13) we put $\rho^{d}(\mathcal{E}) \equiv 0$ and in the second $\rho^{s}(\mathcal{E}) \equiv 0$, the two transform, as $\gamma \to 0$, into the appropriate equations for the unhybridized s- and d-bands.

In the metallic region, equations (6) and (11)-(13) yield the following expression for the DC conductivity: $\sigma = \sigma_{\rm Born} - \sigma_{\rm corr}$, where $\sigma_{\rm Born} = \sigma_{\rm B}^{\rm s} + \sigma_{\rm B}^{\rm d}$, and

$$\sigma_{\text{corr}} = \frac{1}{2} \left[\left(\sigma_{\text{B}}^{\text{s}} + \vartheta^{\text{ss}} \right) + \left(\sigma_{\text{B}}^{\text{d}} + \vartheta^{\text{dd}} \right) \right. \\
\left. - \left\{ \left[\left(\sigma_{\text{B}}^{\text{s}} - \vartheta^{\text{ss}} \right) + \left(\sigma_{\text{B}}^{\text{d}} - \vartheta^{\text{dd}} \right) \right]^{2} \right. \\
\left. + 4 \left[\sigma_{\text{B}}^{\text{s}} \left(\vartheta^{\text{dd}} - \vartheta^{\text{ds}} \right) + \sigma_{\text{B}}^{\text{d}} \left(\vartheta^{\text{ss}} - \vartheta^{\text{sd}} \right) - \left(\vartheta^{\text{ss}} \vartheta^{\text{dd}} - \vartheta^{\text{ss}} \vartheta^{\text{dd}} \right) \right] \right\}^{1/2} \right]. \tag{15}$$

Here

$$\sigma_{\rm B}^{\rm s(d)} = \frac{2e^2}{\hbar\Omega^0} \rho^{\rm s(d)}(\mathcal{E}_{\rm F}) D_{\mathcal{E}_{\rm F}}^{\rm s(d)} \qquad \vartheta^{\mu\nu} = \frac{2e^2}{\pi\hbar\vartheta^0} I\Theta_{\mathcal{E}_{\rm F}}^{\mu\nu}$$

$$I_{\mathcal{E}_{\rm F}}(\omega) = \int_{|q| \le k_0} \frac{\delta^d q}{(2\pi)^d} \frac{1}{-\mathrm{i}\omega/D_{\mathcal{E}_{\rm F}}(\omega) + q^2}$$

$$(16)$$

with k_0 the cut-off momentum. In the metallic region, as $\omega \to 0$, we have $-\mathrm{i}\omega/D_{\mathcal{E}_{\mathrm{F}}}(\omega) \to 0$ and

$$I \equiv I_{\mathcal{E}_{\mathbf{F}}}(\omega)\big|_{\omega \to 0} \simeq \frac{\pi^{d/2} k_0^{d-2} \Gamma(d/2-1)}{(2\pi)^d \Gamma(d/2)} \qquad \text{for } d > 2.$$

We define the critical disorder W_c corresponding to the localization of the electronic states of the system for \mathcal{E}_{F} fixed by the condition $\sigma_{\mathcal{E}_{\mathrm{F}}}[W_c]=0$, which yields

$$\frac{\sigma_{\rm B}^{\rm s}(\vartheta^{\rm dd} - \vartheta^{\rm ds}) + \sigma_{\rm B}^{\rm d}(\vartheta^{\rm ss} - \vartheta^{\rm sd})}{\vartheta^{\rm ss}\vartheta^{\rm dd} - \vartheta^{\rm ds}\vartheta^{\rm sd}} = 1. \tag{17}$$

For γ small,

$$\left(\frac{\sigma^{\rm s}}{\vartheta^{\rm ss}}\right)_{\gamma\equiv 0} + \left(\frac{\sigma^{\rm d}}{\vartheta^{\rm dd}}\right)_{\gamma\equiv 0} + O(\gamma^2) = 1$$

which shows that the critical disorder W_c is greater than $\max\{W_c^s, W_c^d\}$ and increases with γ .

In the region of localized states, $\sigma_{\rm Born} < \sigma_{\rm corr}$, we define the localization radius ξ by the following relation [6, 7]:

$$\lim_{\omega \to 0} \left(-\frac{\mathrm{i}\omega}{D_{\mathcal{E}_{\mathbf{p}}}(\omega)} \right) = \frac{1}{\xi^2}.$$
 (18)

At d=3, combining equations (12) and (13), we arrive at an equation determining the localization radius for different sets of the system parameters:

$$\frac{1}{\xi k_0} \tanh^{-1}(\xi k_0) = 1 - \frac{\sigma_{\rm B}^{\rm s} (\vartheta^{\rm dd} - \vartheta^{\rm ds}) + \sigma_{\rm B}^{\rm d} (\vartheta^{\rm ss} - \vartheta^{\rm sd})}{\vartheta^{\rm ss} \vartheta^{\rm dd} - \vartheta^{\rm ds} \vartheta^{\rm sd}}.$$
 (19)

Numerical calculations are done for a simple cubic lattice with a half-filled band. We introduce the following model density of states [11]:

$$\rho_{0}(\mathcal{E}) = \sum_{\mathbf{k}} \delta(\mathcal{E} - \varepsilon_{\mathbf{k}})$$

$$= \frac{2}{\pi w} \left[1 - \left(\frac{\mathcal{E}}{w} \right)^{2} \right]^{1/2} \theta(w - |\mathcal{E}|)$$

$$\sum_{\mathbf{k}} \delta(\mathcal{E} - \varepsilon_{\mathbf{k}}) (\nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}})^{2} = \frac{2V_{\text{max}}^{2}}{\pi w} \left[1 - \left(\frac{\mathcal{E}}{w} \right)^{2} \right]^{3/2} \theta(w - |\mathcal{E}|)$$
(20)

where w is the band halfwidth, $-w < \varepsilon_{\mathbf{k}} < w$, $V_{\max} = aw/\sqrt{3}$ is the maximum velocity in the semielliptical band, and a the lattice parameter. We also assume that for unperturbed bands $\varepsilon_{\mathbf{k}}^{\mathbf{s}} \equiv \varepsilon_{\mathbf{k}}$ and $\varepsilon_{\mathbf{k}}^{\mathbf{d}} \equiv \alpha \varepsilon_{\mathbf{k}}$, $0 < \alpha < 1$, with α the scaling parameter.

For a fixed set of system parameters $\{\alpha, \gamma, W, \mathcal{E}\}$ we calculate the 'Born damping' $\Delta_{\mathcal{E}}^{\mu}$ as the solution of the self-consistent system of equations (9) with the initial approximation

$$\rho^{\mathrm{s}}(\mathcal{E}) = \rho_0(\mathcal{E}) \qquad \rho^{\mathrm{d}}(\mathcal{E}) = \frac{\rho_0(\mathcal{E}/\alpha)}{\alpha}.$$

Equations (16), (14) and (10) can now be used to calculate the contributions to the Born conductivity σ_B^{μ} and the coefficients $\vartheta^{\mu\nu}$. For the cut-off momentum one usually takes $k_0 = \kappa \pi/a$, with $\kappa \simeq 1, \ldots, 2$ a parameter. In our calculations $\kappa = \pi^2/9$.

The results of numerical calculations with $\alpha=0.1$ are presented in figures 1-5, where $\rho(\mathcal{E})$ is given in units of $(\pi w)^{-1}$; \mathcal{E} , γ , and W are in units of w; σ in units of $\sigma_0 \equiv e^2/9\pi\hbar a$; and ξ in units of a.

Figure 1 demonstrates the behaviour of the density of states $\rho(\mathcal{E})$ for various values of the hybridization constant γ . When hybridization occurs, the curve of ρ plotted

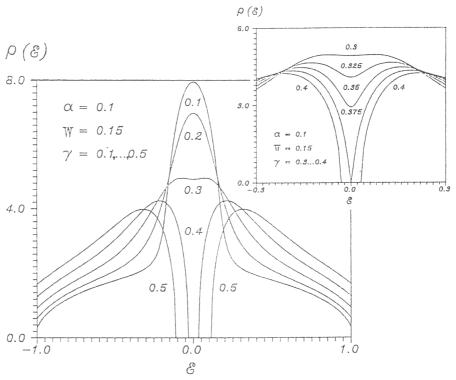


Figure 1. Density of states $\rho(\mathcal{E})$ for various values of the hybridization constant γ .

against \mathcal{E} acquires what is known as a pseudogap, whose depth increases with γ for W fixed. For $\gamma \geq \alpha^{1/2}w$, in the limit of $W \to 0$, the density of states $\rho(\mathcal{E})$ at the middle of the band vanishes and a hybridization gap forms. A further increase in γ causes the hybridization gap to broaden. As W grows with γ fixed, the hybridization gap closes and the depth of the pseudogap decreases owing to the increase in $\rho(\mathcal{E})$.

Figure 2 depicts the curves for the system's DC conductivity σ plotted against the disorder width W for different values of the hybridization constant γ . For $\gamma < \alpha^{1/2}w$, the conductivity decreases as W grows and vanishes at $W = W_c(\gamma)$, which corresponds to an Anderson transition. The nonmonotonicity of σ for small values of W, due to the hybridization pseudogap, increases with γ , and for $\gamma \geq \alpha^{1/2}w$ a metal-insulator transition caused by the formation of a hybridization gap may occur. In this event in the region of small values of W a rather exotic increase in σ with W is observed at a fixed value of γ , an increase is due to the evolution of the hybridization pseudogap in the density of states. A further increase in W at a fixed γ brings about an increase in the localization correction. This leads to growth saturation and a rapid decrease in σ , with σ vanishing at $W = W_c(\gamma)$.

The dependence of the critical disorder W_c on the hybridization constant γ is depicted in figure 3. We see that W_c increases with γ .

Figure 4 depicts the curves for σ , DC conductivity, plotted against the hybridization constant γ for different values of the disorder width W.

The system is in the localized states region, for $W > W_c^0$, where $W_c^0 \gtrsim W_c^s$, with

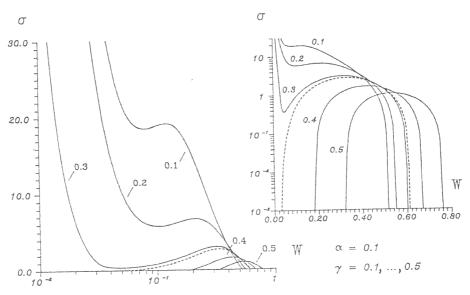


Figure 2. DC conductivity σ of the system as the function of the disorder width W for different values of the hybridization constant γ . The broken curves correspond to $\gamma = \alpha^{1/2}w$.

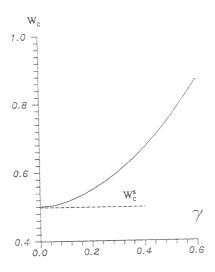


Figure 3. Critical disorder W_c as a function of the hybridization constant γ . The broken horizontal line depicts W_c^s , the critical disorder of the unhybridized s-band.

 W_c^0 the critical disorder of the system as $\gamma \to 0$, and for $\gamma < \gamma_c$, where γ_c is determined from the condition $W_c(\gamma_c) = W$. As γ increases at a fixed W, the system may become

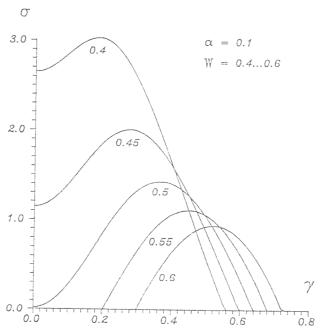


Figure 4. The DC conductivity of the system, σ , as a function of the hybridization constant γ for different values of the disorder width W.

delocalized for $\gamma \geq \gamma_c$. A further increase in γ at a fixed W leads to an increase in σ owing, apparently, to the contribution of band-to-band transitions. The value of σ rapidly becomes saturated and, later, decreases because of the widening of the hybridization pseudogap in the density of states.

For $W < W_c^0$, an increase in γ in the region of small values of γ also leads to an increase in σ owing to the contribution of band-to-band transitions, and again the value of σ becomes rapidly saturated and then falls off owing to the evolution of the hybridization pseudogap in the density of states.

The curves in figure 5 for the localization radius ξ as the function of the disorder width W at different values of the hybridization constant γ demonstrate the divergence of ξ as $W \to W_c$, with the critical disorder W_c obviously depending on γ .

Our results show that an Anderson transition in the two-band model possesses a number of features setting it apart from the standard case. Hybridization of states of the narrow and wide bands leads to delocalization in the system, and the critical disorder corresponding to localization exceeds the value characteristic of an unhybridized wide band. This indicates that at the Fermi level the localized states corresponding to the narrow band cannot coexist with the delocalized states corresponding to the wide band. From the experimenter's viewpoint, the most interesting is the nonmonotonic behaviour of conductivity (for one thing, the increase in conductivity with disorder).

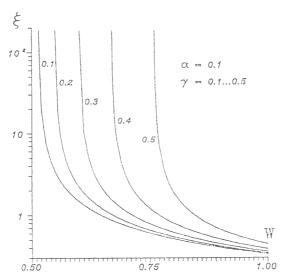


Figure 5. The localization radius ξ of the system plotted against the disorder width W for different values of the hybridization constant γ .

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