Interference of resonant and electron-phonon scattering in conductors with quasilocalized impurity states

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The interaction of a quasilocalized electron with vibrational degrees of freedom of an impurity atom is considered within the framework of standard perturbation theory. It is shown that the resonance shape changes substantially even in the case of weak electron-phonon coupling. The temperature dependence of the band-carrier mobility is discussed.

1. INTRODUCTION

Along with the diligent study of metallic systems with variable valency, as well as of IV-VI semiconductors doped with group-III elements, much attention is paid of late to the problem of local impurity states located in the allowed band of a conductor.[1,2] The presence of such states in the immediate vicinity of the system's Fermi level alters greatly the transport and thermodynamic properties of the considered compounds. The extremely strong (resonant) dependence of the scattering cross section on the energy points to the importance of taking into account various factors capable of altering the location of the resonance level relative to the Fermi level, as well as the shape of the resonance curve. One such factor is inhomogeneity of the sample (inhomogeneous broadening). The impurity-level scatter due to this inhomogeneity can decrease noticeably the average scattering cross section (if the scatter exceeds the "natural" resonance width due to hybridization of the band and impurity states).

It is important, at the same time, to examine the mechanisms that lead to "homogeneous broadening" of a level. Much interest is attached in this connection to effects of interaction of a localized electron with vibrational degrees of freedom of an impurity atom (or of its crystalline environment). In fact, vibration of an impurity ion about the equilibrium position lead to modulation of the potential in which the electron localized on the impurity moves. This interaction gives rise to an additional uncertainty in the energy of the electron at the center (on top of the uncertainty due to hybridization). The shape of the resonance curve is consequently altered, and its changes depend substantially on the temperature. Clearly, if the local level is close to a Fermi level, all these changes are strongly manifested in the kinetic properties of the system.

The aim of the present paper is a detailed analysis of the influence of local electron-phonon interaction on the overall picture of the resonant scattering. It should be noted that Refs. 3 and 4 dealt with scattering of one electron (or hole) by a resonant center with local electron-phonon coupling. The single-electron treatment yielded an exact expression for the scattering cross section. Such a formulation of the problem, however, has patently no connection with the situation of importance from the standpoint of measuring the transport properties. "Single-electron" scattering corresponds to the case when the local level is far from the Fermi surface (when the Pauli principle imposes no noticeable constraints on the scattering of a test particle). It is clear, however, that in this case resonant scattering makes altogether no noticeable contribution to the mobility. We shall show below that the Fermi-statistics influence is substantial in a situation when the local level is close to the Fermi level. We shall therefore be unable to carry out calculations for arbitrary electron-phonon coupling constants. Nonetheless, perturbation theory in terms of the coupling constants make it possible to draw some qualitative conclusions regarding the system in question.

2. FORMULATION OF MODEL, LOCAL DENSITY OF STATES AND RELAXATION TIME AT NEAR-ZERO TEMPERATURES

We wish to consider the interaction between a quasilocalized electron and the vibrations of an impurity atom. Strictly speaking, such oscillations set also in motion the surrounding crystal atoms. We can therefore consider either quasilocal models that exist against the background of the crystal phonon continuum, or the true local vibrations occurring in the band gap of this crystal. We shall treat all these vibrations in a unified manner, introducing a set of discrete frequencies Ω_m and neglecting the finite lifetimes of some of these modes. We describe the interaction of the electrons with the vibrations by a term linear in the displacements of the impurity ion from an equilibrium position.

The Hamiltonian takes then in second-quantization representation the form

$$H=H_e+H_{ph}+H_{int}, \tag{1}$$

where

$$H_e=\sum_{\mathbf{k},\sigma}\varepsilon(k)c_{\mathbf{k}\sigma}^{+}c_{\mathbf{k}\sigma}+\varepsilon_0\sum_{\sigma}d_\sigma^{+}d_\sigma+\frac{t_0}{N^{1/2}}\sum_{\mathbf{k},\sigma}(c_{\mathbf{k}\sigma}^{+}d_\sigma+d_\sigma^{+}c_{\mathbf{k}\sigma}),$$

$$H_{ph}=\sum_{m}\hbar\Omega_m(b_m^{+}b_m+{}^1/_2).$$

$$H_{int}=\sum_{m,\sigma}g_m(b_m+b_m^{+})d_\sigma^{+}d_\sigma,$$

while $c_{\mathbf{k}\sigma}$, d_σ, and b_m are respectively the annihilation operators of the band and impurity electrons and of the local phonons, $\varepsilon(\mathbf{k})$ and ε_0 are the band and electron-impurity energies measured from the Fermi level of the system, Ω_m are the frequencies of the local oscillations, g_m are the electron-phonon coupling constants, and t_0 is the hybridization matrix element.

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We consider the case of zero temperature ($T=0$). In this case the system properties are determined by a set of causal Green's functions:

$$G_{dd}(t)=-i\langle Td_{\sigma}(t)d_{\sigma}^{+}(0)\rangle,\quad G_{\mathbf{kk}'}(t)=-i\langle Tc_{\mathbf{k}\sigma}(t)c_{\mathbf{k}\sigma}^{+}(0)\rangle,$$
$$D_m(t)=-i\langle T[b_m(t)+b_m^{+}(t)][b_m(0)+b_m^{+}(0)]\rangle.$$

All the operators are chosen here in the Heisenberg representation, T is the chronological-product symbol, and the averaging is over the ground state of the system.

It is known that the Fourier transform $G_{dd}(t)$ of the Green's function at the center determines the local density of states of the d electron:

$$\rho_{dd}(E)=-\frac{1}{\pi}\operatorname{sign}E\cdot\operatorname{Im}G_{dd}(E),\tag{2}$$

where E is the energy reckoned from the Fermi level. It is easy to show (using, e.g., the method of equations of motion) that in the absence of interaction

$$G_{dd}^{0}(\omega)=\frac{1}{\omega-\varepsilon_0'+i\Gamma\operatorname{sign}\omega},\tag{3}$$

where $\varepsilon_0'=\varepsilon_0+\Delta\varepsilon$, $\Delta\varepsilon$ is the energy correction due to the asymmetry of the band density of states with respect to ε_0, $\Gamma(\omega)=t_0^2\pi\rho(\omega)$, and $\rho(\omega)$ is the band density of st which, if a smooth function of the energy, can be set equ $\rho(\omega)=\rho(\varepsilon_0)=\text{const}$. We have then ($\hbar\equiv1$)

$$\rho_{dd}^{0}(E)=\frac{1}{\pi}\frac{\Gamma}{(E-\varepsilon_0')^2+\Gamma^2},\tag{4}$$

i.e., we obtain the known Lorentz distribution, $G_{dd}(\omega)$ is in general a complicated function of ω.

If the exact function $G_{dd}(\omega)$ is known for one impurity we can determine in the case of low impurity-center densities the relaxation times of the band carriers. Indeed, as follows from analysis of various orders of perturbation theory (within the framework of the cross and boson techniques^5), in the linear approximation in the impurity density we have

$$\frac{1}{\tau(\omega)}=-n_c t_0^2\operatorname{sign}\omega\cdot\operatorname{Im}\langle G_{dd}(\omega)\rangle,\tag{5}$$

where $n_c=N_{\text{imp}}/N$ is the density of the impurity atoms, and the angle brackets denote averaging over the possible scatter of the local levels.

Note the important circumstance that Eq. (5) contains the exact function $G_{dd}(\omega)$ in which account is taken of all the electron-phonon interaction and tunneling processes. Thus, the damping of the band carrier is determined by a complicated interference between the resonant and electron-phonon scatterings.

We now calculate G_{dd}. It is known that this function can be represented in the form

$$G_{dd}(\omega)=\frac{1}{(G_{dd}^{0}(\omega))^{-1}-\Sigma(\omega)},\tag{6}$$

where $\Sigma(\omega)$ is called the irreducible self-energy part.

We calculate Σ in the lowest order in the electron-phonon coupling (note that the formal parameter of the expansion is $g^2/\max\{\Gamma^2,\Omega^2\}$). In this case Σ is represented by the diagram of Fig. 1 and is equal to

$$\Sigma(\omega)=-n_0\sum_m\frac{g_m^2}{\Omega_m}+i\sum_m g_m^2\int\frac{d\omega'}{2\pi}D_m^{0}(\omega-\omega')G_{dd}^{0}(\omega').\tag{7}$$

Here

$$D_m^{0}(\omega)=\frac{2\Omega_m}{\omega^2-(\Omega_m-i\delta)^2}$$

is the phonon unperturbed Green's function. G_{dd}^{0} is given by expression (3), and $n_0=n_{0\uparrow}+n_{0\downarrow}$ is the unperturbed local density.

The first term in (7) correspond simply to a static polaron energy shift. This shift is the result of displacement of an impurity ion from equilibrium into a new position that minimizes the electron-phonon system energy. Note that in the diagram technique describing the interaction of the Bloch electrons with longitudinal ion oscillations (see, e.g., Ref. 5) there are no diagrams corresponding to a static shift, since the matrix element in them is $g(\mathbf{k}=0)=0$ (a reflection of the fact that displacement of the lattice as a whole does not change the state of the electron).

Evaluation of the integral in (7) yield

$$\operatorname{Im}\Sigma(\omega)=-\operatorname{sign}\omega\cdot\sum_m g_m^2\left\{\frac{\Gamma}{[\omega-(\varepsilon_0'+\Omega_m)]^2+\Gamma^2}\theta(\omega-\Omega_m)\right.$$
$$\left.+\frac{\Gamma}{[\omega-(\varepsilon_0'-\Omega_m)]^2+\Gamma^2}\theta(-(\omega+\Omega_m))\right\},\tag{8a}$$

$$\operatorname{Re}\Sigma(\omega)=-2n_\sigma^0\sum_m\frac{g_m^2}{\Omega_m}$$
$$+\sum_m g_m^2\left\{\frac{\Gamma}{2\pi}\left(\frac{1}{[\omega-(\varepsilon_0'+\Omega_m)]^2+\Gamma^2}\ln\frac{(\omega-\Omega_m)^2}{\varepsilon_0'^2+\Gamma^2}\right.\right.$$
$$\left.-\frac{1}{[\omega-(\varepsilon_0'-\Omega_m)]^2+\Gamma^2}\ln\frac{(\omega+\Omega_m)^2}{\varepsilon_0'^2+\Gamma^2}\right)$$
$$+n_\sigma^0\frac{\omega-(\varepsilon_0'-\Omega_m)}{[\omega-(\varepsilon_0'-\Omega_m)]^2+\Gamma^2}$$
$$\left.+(1-n_\sigma^0)\frac{\omega-(\varepsilon_0'+\Omega_m)}{[\omega-(\varepsilon_0'+\Omega_m)]^2+\Gamma^2}\right\}.\tag{8b}$$

Here $n_\sigma^0=1/2-(1/\pi)\operatorname{arctg}(\varepsilon_0'/\Gamma)$ is the unperturbed density of the d-electrons with spin σ.

The local density of states takes the form

$$\rho_{dd}(\omega)=\frac{1}{\pi}\frac{\Gamma-\operatorname{sign}\omega\cdot\operatorname{Im}\Sigma(\omega)}{[\omega-\varepsilon_0'-\operatorname{Re}\Sigma(\omega)]^2+[\Gamma-\operatorname{sign}\omega\cdot\operatorname{Im}\Sigma(\omega)]^2}.\tag{9}$$

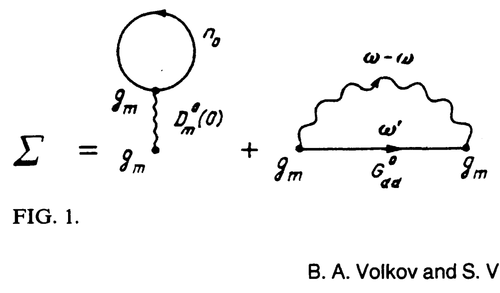

FIG. 1.

Note some features of the function ρ_{dd}.

1. The logarithmic divergences at the frequencies $\omega = \pm\Omega_m$ lead to $\rho_{dd}(\pm\Omega_m)\to 0$. These divergences are due both to the presence of a Fermi step at $\omega = 0$ and to neglect of the phonon linewidths. Allowance for finite temperature as well as for phonon-mode damping effects smooths out the logarithmic singularities, but the dips in the local density of states at the frequencies Ω_m remain.

2. For $|\omega| < \min\{\Omega_m\}$ we have $\operatorname{Im}\Sigma = 0$. The reason is that an electron with energy $\sigma < \varepsilon < \min\{\Omega_m\}$ (ε is reckoned from the Fermi energy) cannot be scattered and emit a phonon, for in this case it would have to go over into a state with $\varepsilon < 0$, which is forbidden at $T = 0$ by the Pauli principle. The same pertains to a hole with energy $-\min\{\Omega_m\} < \varepsilon < 0$. We have thus at $|\omega| < \min\{\Omega_m\}$.

$$\rho_{dd}(\omega) = \frac{1}{\pi}\frac{\Gamma}{(\omega-\varepsilon_0'-\operatorname{Re}\Sigma)^2+\Gamma^2}. \tag{10}$$

It follows from (10) that the root of the equation $\omega - \varepsilon_0' \operatorname{Re}\Sigma(\omega) = 0$ in the interval $|\omega| < \min\{\Omega_m\}$ determines the position of the maximum of the function ρ_{dd}. Owing to the polaron effect, the maximum shifts towards negative ω and this in turn increases the electron density at the center. On the other hand, the value of ρ_{dd} at the center does not change and is equal to $1/\pi\Gamma$.

In the general case the shape of the resonance curve depends strongly on the location of ε_0'. Thus, if $\varepsilon_0' \approx \Omega_m$, two equal maxima appear on the $\rho_{dd}(\omega)$ plot. An approximate form of ρ_{dd} in the case $\varepsilon_0' = 0 (n_\sigma^0 = \frac{1}{2})$, $\Gamma = \Omega(m = 1)$, $g^2/\Gamma^2 = 0.5$ is shown in Fig. 2.

To conclude this section, we consider the case $\varepsilon_0' \gg \Omega_m, \Gamma$. It follows then from (8) and (9) that $\rho_{\max} < 1/\pi\Gamma$ (i.e., the resonance broadens). Although the static polaron increment tends in this limit to zero. Since $n^0 \to 0$, nonetheless the maximum of the resonance is shifted away from ε_0' by dynamic effects. Note also that in this limiting case the problem can be solved exactly, since the Green's function G_{dd} has patently a single-electron character (it is analytic in the upper ω half-plane). It is easily seen that calculation of G_{dd} with the aid of diagrams is equivalent to averaging over an electron vacuum with a Hamiltonian

$$H = (\varepsilon_0' - i\Gamma)\, d^+d + g d^+d(b+b^+) + \Omega b^+b.$$

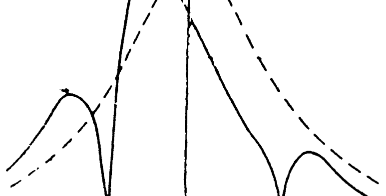

FIG. 2. Approximate form of $\rho_{dd}(\omega)$ in the case $\varepsilon_0' = 0$, $\Gamma = \Omega(m = 1)$, $g^2/\Gamma^2 = 0.5$. The unperturbed density ρ_{dd}^0 is shown dashed.

This averaging is easily effected because the interaction operator commutes with the electron-number operator (this procedure was in fact used in Refs. 3 and 4).

3. FINITE TEMPERATURE. TEMPERATURE DEPENDENCE OF MOBILITY

To study the temperature dependence of the system it is convenient to use the retarded Green's function G_{dd}^R:

$$G_{dd}^R(t) = \begin{cases} -i\,\mathrm{Sp}\Big\{\exp\Big(-\dfrac{\Omega+\mu\hat{N}-\hat{H}}{T}\Big)(d_\sigma(t)d_\sigma^+(0) \\ \quad +d_\sigma^+(0)d_\sigma(t))\Big\}, \quad t>0, \\ \qquad 0, \qquad t<0. \end{cases} \tag{11}$$

Then

$$\rho_{dd}(E,T) = \frac{1}{\pi}\operatorname{Im} G_{dd}^R(E,T),$$

$$\frac{1}{\tau(\omega,T)} = t_0^2 n_c \operatorname{Im} G_{dd}^R(\omega,T). \tag{12}$$

It is known that determination of $G^R(\omega)$ by perturbation theory reduces to finding a Matsubara function $G(\omega_n)$ (which can be determined by standard diagram technique) and continuing it into the upper half-plane ($\omega_n > 0$). The Matsubara self-energy part has the form

$$\Sigma(\omega_n) = -n_0(T)\sum_m \frac{g_m^2}{\Omega_m} - \frac{1}{\beta}\sum_m g_m^2 \sum_{n'=-\infty}^{\infty} \frac{2\Omega_m}{(i\omega_{n'}-i\omega_n)^2-\Omega_m^2}$$
$$\times\frac{1}{i\omega_{n'}-\varepsilon_0'+i\Gamma\,\mathrm{sign}\,\omega_{n'}}, \tag{13}$$

where $n_0(T)$ is the unperturbed charge density in the center at the temperature T, $\beta = 1/T$, $\omega_n = \pi(2n+1)T$. Since the electron function has a sign $\omega_{n'}$ singularity, it is convenient to break up the sum over n' into two parts with $n' \geqslant 0$ and $n' < 0$. We can then go over from the sum to integrals along the countours c_1 and c_2 enclosing the upper and lower imaginary axes, respectively. Next, extending the contours to infinity and taking into account the poles encountered along the way, as well replacing $i\omega_n$ by $\omega + i\delta (\delta > 0)$ in the last expression, we obtain the function $\Sigma^R(\omega)$, which is analytic in the upper half-plane. Thus, after separating the real and imaginary parts of the function $\Sigma^R(\omega)$, we obtain

$$\operatorname{Re}\Sigma^R(\omega,T) = -n_0(T)\sum_m \frac{g_m^2}{\Omega_m}$$
$$+\sum_m g_m^2\Big\{\frac{n(\Omega_m)[\omega-(\varepsilon_0'-\Omega_m)]}{[\omega-(\varepsilon_0'-\Omega_m)]^2+\Gamma^2}$$
$$+\frac{[1+n(\Omega_m)][\omega-(\varepsilon_0'+\Omega_m)]}{[\omega-(\varepsilon_0'+\Omega_m)]^2+\Gamma^2}$$
$$-\frac{1}{\pi}\int^{\infty} d\omega' f(\omega')\Big[\frac{\Gamma}{\omega'-(\Omega_m+\omega)}$$
$$-\frac{\Gamma}{\omega'-(\Omega_m-\omega)}\Big]\frac{\Gamma}{(\omega'-\varepsilon_0')^2+\Gamma^2}\Big\}, \tag{14a}$$

$$\operatorname{Im}\Sigma^R(\omega,T)=-\sum_m g_m{}^2\left\{\frac{\Gamma}{[\omega-(\varepsilon_0{}'-\Omega_m)]^2+\Gamma^2}[n(\Omega_m)+f(\omega+\Omega_m)]+\frac{\Gamma}{[\omega-(\varepsilon_0{}'-\Omega_m)]^2+\Gamma^2}\times[1+n(\Omega_m)-f(\omega-\Omega_m)]\right\}. \qquad (14b)$$

where

$$f(\omega)=1/(e^{\beta\omega}+1)$$

is the fermion distribution function, and

$$n(\Omega_m)=1/(e^{\beta\Omega_m}-1)$$

is the phonon distribution function.

We note now some peculiarities of the function $\rho_{dd}(\omega,T)$.

1. The logarithmic divergences at the points $\omega=\pm\Omega_m$ drop out. However, the value of Re Σ^R at these points is

$$\frac{g^2}{\Gamma}\ln\frac{T^2}{\varepsilon_0{}'^2+\Gamma^2}$$

and remains large so long as $T\ll(\varepsilon_0'^2+\Gamma^2)^{1/2}$. Thus, the resonance curve $\rho_{dd}(\omega)$ has dips at the points $\omega=\pm\Omega_m$, which decrease with increase of T and drop out completely at $T\sim(\varepsilon_0'^2+\Gamma^2)^{1/2}$.

2. At temperatures other than zero, Im Σ^R is not zero in the interval $|\omega|<\min\{\Omega_m\}$. This is due both to the smearing of the Fermi step and to the presence of real phonons at $T>0$. In addition, the damping due to the scattering of the d electrons by phonons increases with increase of T. Thus, at $\omega=0$ we have

$$\operatorname{Im}\Sigma^R(0)\approx-2\sum_m g_m{}^2\left[\frac{\Gamma}{(\Omega_m-\varepsilon_0{}')^2+\Gamma^2}+\frac{\Gamma}{(\Omega_m+\varepsilon_0{}')^2+\Gamma^2}\right]e^{-\Omega_m/T},\qquad T\ll\Omega_m,$$

$$\operatorname{Im}\Sigma^R(0)\approx-2\sum_m g_m{}^2\left[\frac{\Gamma}{(\Omega_m-\varepsilon_0{}')^2+\Gamma^2}+\frac{\Gamma}{(\Omega_m+\varepsilon_0{}')^2+\Gamma^2}\right]\frac{T}{\Omega_m},\qquad T\gg\Omega_m. \qquad (15)$$

3. $\rho_{dd}^{\max}<1/\pi\Gamma$, and the value at the maximum decreases with increase of T. Thus, the resonance broadens—the value of ρ_{dd} decreases near the maximum and the level density in the peripheral region increases correspondingly.

We discuss now the temperature dependence of the mobility of the band electrons. This dependence is given by the integral

$$\int_{-\infty}^{\infty}\tau(\omega)\frac{\partial f_0}{\partial\omega}d\omega,$$

where $f_0(\omega)$ is the equilibrium distribution function of the band carriers. As follows from the preceding analysis in (12), $\tau(\omega,T)$ increases with increase of temperature at frequencies ω near the maximum of the local density of states; it decreases, conversely, at frequencies corresponding to the periphery of the resonance curve. A substantial contribution to the integral is made at low temperatures by the energy regions close to the Fermi energy. Therefore, if the Fermi level is located near the maximum of the function ρ_{dd}, the mobility increases with increase of T. From Eqs. (14) we obtain that at $T\ll\Omega_m$ the mobility μ takes the form

$$\mu\approx\mu_0+\sum_m\mu_m\frac{\Gamma^2-E_0{}^2}{\Gamma^2}e^{-\Omega_m/T}, \qquad (16)$$

where μ_0 and μ_m are certain constant quantities, and E_0 is the location of the maximum of the resonance curve (reckoned from the Fermi level). If $E_0<\Gamma$ the mobility (along with the static electric conductivity) increases exponentially with temperature. In the case $T\gg\Omega_m$ the exponential growth becomes linear. The interaction between a polarized electron and vibrations of an impurity atom weakens thus the resonant scattering of the band carriers.

To consider a real situation, however, it is necessary to bear in mind that τ contains contributions from direct scattering of band electrons by the lattice vibrations. Therefore the total value of τ must be calculated using the Mathiessen rule

$$\frac{1}{\tau}=\frac{1}{\tau_{\text{band}}}+\frac{1}{\tau_{\text{imp}}}.$$

Here $1/\tau_{\text{band}}$ increases with temperature (obeying a power-law if the phonons are acoustic and an exponentially if optical). The two effects are thus in competition. At not too low a density of the resonant centers, and also in the presence of a relatively soft mode in the spectrum of the local oscillations, the contribution ot $1/\tau$ from the impurity scattering (its temperature part) can exceed $1/\tau_{\text{band}}$. The $\mu(T)$ dependence is then nonmonotonic.

Thus, in the case of scattering by acoustic vibrations of ions we have

$$\frac{1}{\tau_{\text{band}}}\propto\frac{T}{\hbar}\left(\frac{T}{\Theta}\right)^3$$

(T is lower than the Debye temperature Θ) and the condition for the onset of a minimum of the function $\mu(T)$ is

$$n_c\varepsilon_F\left(\frac{g}{\Gamma}\right)^2e^{-\Omega/T}\gtrsim\frac{T^2}{\Omega}\left(\frac{T}{\Theta}\right)^3.$$

Note also that an additional contribution is made to $1/\tau$ by the interference between the band-carrier scattering by lattice vibrations and by impurities; the damping due to this interference, however, is small. In fact, the perturbation of the band-carrier state densities by the presence of resonance centers is equal to $\rho^2_{\text{band}}(\varepsilon_F)[n_c/\rho_{\text{band}}(\varepsilon_F)]$ so that the damping due to phonons changes by an amount

$$\Delta(1/\tau_{\text{band}}) \sim g^2_{\text{band}}\,\rho_{\text{band}}(\varepsilon_F)\,n_c$$

(optical vibrations). Then

$$\Delta\left(\frac{1}{\tau_{\text{imp}}}\right)\Big/\Delta\left(\frac{1}{\tau_{\text{band}}}\right)\sim\left(\frac{g_{\text{imp}}}{g_{\text{band}}}\right)^2\left(\frac{\varepsilon_F}{\Gamma}\right)^2.$$

The origin of the factor $(\varepsilon_F\Gamma)^2$ is easy to understand. If $\Gamma = 0$, the entire electron density connected with the resonance is concentrated on the impurity center. If $\Gamma \neq 0$ this density spreads out over the band states (over the neighboring atoms of the principal lattice of the semiconductor) like $(\Gamma/\varepsilon_F)^2$. The exponent 2 is entered here because we are dealing with density and not with amplitude. Obviously, the phonon modes of the crystal "affect" only the wings of the electron resonance density, i.e., only the electrons that tunnel from the center into the band. The electron-phonon interaction with the resonance is therefore suppressed like $(\Gamma/\varepsilon_F)^2$.

4. DISCUSSION OF RESULTS

The results reported in the preceding sections show that even weak electron-phonon interaction at a center can alter strongly the pattern of resonant scattering.

1. At energies corresponding to local-vibration quanta, the density of state of *d*-electrons has abrupt dips that become smeared out when the temperature is increased. The form of the resonance changes particularly substantially when the local-level energy ε_0' (reckoned from the Fermi level) is close to one of the frequencies Ω_m. Two equal state-density maxima appear then. Observation and analysis of such singularities have yielded valuable information both on the characer of the local vibrations of the impurity ion and on the properties of the localized electrons. It appears that these singularities can be observed in experiments on tunnel spectroscopy of compounds containing resonance centers.

2. The local polaron effect shifts the maximum of the resonance curve into the region of lower energies. This means that the charge density on the impurity increases. The density change is substantial ($\Delta n \sim 1$) if the polaron shift is comparable with the resonance width. A correct description of such a situation, however, requires inclusion of higher-orders of perturbation theory. Note also that the expression that specifies the energy shift of an electron with a given spin in Eqs. (7) and (13) contains the total charge density ($n_0 = n^0_\uparrow + n^0_\downarrow$). Account is therefore taken here of both the "self-action" effect and the effect of interaction with an electron with opposite spin (bipolaron effect).

3. The resonance broadens at finite temperatures. The scattering of band electrons having an energy close to the resonance maximum becomes weaker and, conversely, the scattering cross sections of electrons with energies far from the maximum of the function ρ_{dd} increase. All this can be the cause of the nonmonotonic temperature dependence of the mobility. We note in this connection a study[6] of the temperature dependence of the conductivity of PbTe compounds doped with thallium. The authors observed a nonmonotonic $\sigma(T)$ variation, where the initial section of the conductivity growth was exponential and its temperature was $\lesssim 100$ K. It is possible that this behavior of the conductivity is due to the local electron-phonon interaction effects considered above. It must be assumed in this case that the frequency of the local mode is $\Omega \sim 100$ K, and the initial decrease of the conductivity is due to scattering of band carriers by lattice vibrations.

We conclude by discussing briefly the influence of inhomogeneous broadening on the transport properties of the system. Formal allowance for the scatter of the impurity levels reduces to integration of the function $G_{dd}(\omega)$ in expression (5) over the position of ε_0 with a certain weight function $f(\varepsilon_0)$ (the distribution function of the impurity levels). It is easily seen that if the width W of the spread exceeds the width Γ of the resonance, then the average time of flight τ is increased by the ratio W/Γ. At the same time, the temperature-induced increment to τ, due to the homogeneous broadening, decreases in the ratio Γ/W. It is therefore hardly possible to observe in strongly inhomogeneous samples a substantial temperature dependence brought about by the effects considered above.

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