Auger recombination in direct-gap semiconductors: Effect of anisotropy and warping

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(Received 30 July 1986; revised manuscript received 17 December 1987)

We show that the temperature dependence of the Auger lifetime for direct-gap semiconductors depends on the symmetry of the band structure. For a complete three-dimensional anisotropy such as the warping of the valence band, one finds that the usual Beattie and Landsberg result, $\tau^{-1} \sim (k_B T/E_g)^{3/2} \exp(-\lambda E_g/k_B T)$, has to be multiplied by $k_B T/E_g$, while for a dispersion relation having the shape of an ellipsoid of revolution (or more generally for a symmetry of revolution around some axis), it has to be multiplied by $k_B T/E_g$ or $(k_B T/E_g)^{1/2}$, depending on whether the direction for the threshold energy of the Auger process is or is not parallel to the symmetry axis.

The Auger recombination of an electron-hole (e-h) pair in a semiconductor is an old subject. In 1950, Fröhlich and O'Dwyer¹ used, in the e-h recombination rate, an exponential term $\exp(-E_g/k_BT)$ coming from the e-h minimum energy which they assumed to be the band gap E_g . In 1958, Beattie and Landsberg² showed that energy and momentum conservation during an Auger process imply nonzero kinetic energies for the electron and the hole which recombine, so that the threshold energy for the Auger recombination has to be larger than E_g . More precisely, they have shown that, for nondegenerate e-h plasma, in the limit of large E_g/k_BT , the temperature dependence of the Auger life-time is

$$\frac{1}{\tau} \sim \left[\frac{k_B T}{E_g}\right]^{3/2} \exp\left[-\frac{1+2\rho}{1+\rho}\frac{E_g}{k_B T}\right],$$

$$\rho = \inf\left[\frac{m_e}{m_h}, \frac{m_h}{m_e}\right].$$
(1)

 m_e and m_h are the *e* and *h* masses, the band structure being assumed isotropic. Inf(x, y) is the smaller of *x* and *y*. Twenty years later, Haug, Kerkhoff, and Lochmann³ made an exact calculation of the Auger coefficient at any value of E_g/k_BT for a nondegenerate plasma, but still with an isotropic band structure. Their result, of course, agrees with Eq. (1) for large E_g/k_BT .

In Auger-effect theory for direct-gap semiconductors, there are mathematical difficulties coming from the restrictions due to energy and momentum conservation. It is indeed much simpler to consider the Auger effect in indirect-gap materials as the phonon required in the recombination process reduces these constraints. In a previous work,⁴ we used a very convenient device to deal with the conservation laws for the case of a degenerate e-h plasma. This consists of replacing the δ functions of the conservation laws by their standard integral representations in terms of the exponential. Although the order of the integral appearing in the recombination rate is increased, this approach greatly simplifies the calculation as it decouples the integrations over each particle. In this paper we use the same procedure. It allows one to get

very simply the exact result of Haug et al. in the case of nondegenerate e-h plasma with isotropic band structure. More interesting is the fact that this procedure allows one to take into account anisotropy of the band structure. Considering first the case of an ellipsoidal dispersion relation as for CdS or CdSe, we show that the appropriate effective mass which enters in ρ differs from the densityof-states mass; but surprisingly, we also show that the temperature dependence in the prefactor term of $1/\tau$ is changed. The power of $(k_B T/E_g)$ in front of the exponential is linked to the degeneracy of the threshold for Auger recombination, which is itself, in general, related to the dimensionality of the band-structure symmetry. If the energy threshold for Auger recombination is degenerate for a set of wave vectors, the extremities of which cover a surface, as in the case of spherical symmetry, one finds the temperature dependence of Eq. (1). But if the energy threshold corresponds to a finite number of wave vectors as in the case of the two extremities of an ellipsoidal symmetry, one finds a prefactor in $(k_B T/E_g)^{5/2}$. In between, a prefactor $(k_B T/E_g)^2$ is found if the degeneracy of the wave vectors at threshold is one dimensional (which means that the extremities of these wave vectors are along a line).

We have also been able to include explicitly the valence-band warping. Along the same lines, we find that the effective mass that appears in ρ is different from the usual heavy- or light-hole mass, and also that the temperature dependence of the recombination rate is different from that in Eq. (1), the energy threshold corresponding to a finite number of wave vectors. Naturally the effective-mass approximation is only valid for low-energy electrons and holes. But our study of warping allows one to see quite explicitly the effect of anisotropy, besides its direct interest whenever it is applicable.

In Sec. I, we write the basic equations for the Auger recombination rate. As is usually done, we do not take into account the problem coming from the uncertainties on the e-e interaction and consider the matrix element as a constant. In Sec. II, we calculate the threshold energy for an ellipsoidal conduction band and for a warped valence band. We consider both Auger effects, between two electrons and one hole, and between two holes and

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one electron. In Sec. III, we consider the case of spherical symmetry and recover the exact result of Haug et al. In Sec. IV, we take an ellipsoidal band structure and show how the temperature dependence of the Auger lifetime varies with symmetry. In Sec. V, we include the valence-band warping and calculate the Auger effect for two electrons and one hole. In Sec. VI, we do the same for two holes and one electron. In Sec. VII we present a complete account of our method previously reported in Ref. 5 in abbreviated form. In this section we show how a stationary phase method may be used to solve for the temperature dependence of Auger recombination in a semiconductor whose band gap is much larger than $k_B T$. This result is both powerful and general as it does not require explicit knowledge of the $\varepsilon(k)$ energy-momentum relationship.

I. BASIC EQUATIONS

The recombination probability of the Auger processes of Fig. 1 is given by

$$W = 4(2\pi)^{-12} 2\pi \hbar^{-1} \int d^3 k_{i=1,4} |M|^2 P$$

× $\delta(E_1 + E_2 + E'_3 - E_4)$
× $\delta(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4)$. (2)

An electron (hole) with momentum \mathbf{k}_1 and energy E_1 recombines with a hole (electron) with momentum \mathbf{k}_3 and energy E'_3 , while an electron (hole) with momentum \mathbf{k}_2 and energy E_2 is excited in the state (\mathbf{k}_4, E_4), see Fig. 1. The energies will be counted from the bottom of the conduction band (top of the valence band). We assume that |M|, the matrix element for such a collision, remains constant as is usually done. We will review this assumption at the end of Sec. VII. P is a statistical term which accounts for the occupation probabilities of the different states:

$$P = f_{1}f_{2}f'_{3}(1-f_{4}) - (1-f_{1})(1-f_{2})(1-f'_{3})f_{4}$$

$$\sim \exp\left[\frac{2\mu + \mu' - (E_{1} + E_{2} + E'_{3})}{k_{B}T}\right] - \exp\left[\frac{\mu - E_{4}}{k_{B}T}\right],$$
(3)

for a nondegenerate e-h plasma, μ and μ' being the e and h chemical potentials.

Let us introduce dimensionless momenta $\mathbf{K} = \mathbf{k}/K_0$ where K_0 has the dimension of a momentum and is such that $A_0K_0^2 = k_BT$, A_0 being an arbitrary temperatureindependent constant. We will assume that the dependence of the dispersion relations $\varepsilon(\mathbf{k})$ on the modulus of the wave vector \mathbf{k} is quadratic, i.e., $\varepsilon(K_0\mathbf{K}) = K_0^2\varepsilon(\mathbf{K})$. Expressing the chemical potential $\mu(\mu')$ in terms of the particles density n(n'),

$$n = 2(2\pi)^{-3} e^{\mu/k_B T} K_0^3 \int d^3 K \ e^{-\varepsilon(K)/A_0} \ , \qquad (4)$$

and using the energy conservation one can rewrite the statistical factor P [Eq. (3)] as



FIG. 1. Auger effect where the e-h pair energy is given (a) to an electron or (b) to a hole.

$$P = \frac{n}{\alpha K_0^3} \left[\frac{nn'}{n_0^2(T)} - 1 \right] e^{-E_4/k_B T}, \qquad (5)$$

where $n_0(T)$ is the equilibrium plasma density (obtained for $\mu + \mu' = 0$) at temperature T and α is a T-independent constant.

Using Eq. (5), one can rewrite the recombination probability [Eq. (2)] as

$$W = \frac{n}{\tau_0(T)} \left[\frac{nn'}{n_0^2(T)} - 1 \right] G \left[\frac{E_g - \tilde{\Delta}}{k_B T} \right] e^{-\tilde{\Delta}/k_B T} .$$
 (6)

The parameter $\tau_0(T)$ has the dimension of time and varies with temperature as $K_0^{-12+3+3}(k_BT) \sim T^{-2}$. The dimensionless function $G(\gamma)$ is a 12th-order integral containing the two δ functions coming from conservation laws:

$$G(\gamma) = \int d^{3}K_{i=1,4} \delta(\mathbf{K}_{1} + \mathbf{K}_{2} + \mathbf{K}_{3} + \mathbf{K}_{4})$$

$$\times \delta \left[\gamma + \frac{\varepsilon(\mathbf{K}_{1}) + \varepsilon(\mathbf{K}_{2}) + \varepsilon'(\mathbf{K}_{3}) - \varepsilon(\mathbf{K}_{4})}{A_{0}} \right]$$

$$\times \exp \left[-\frac{\varepsilon(\mathbf{K}_{4})}{A_{0}} \right]$$
(7)

(we have changed \mathbf{K}_4 into $-\mathbf{K}_4$). For an *h*-*h*-*e* Auger process $E_4 = \Delta + \varepsilon(\mathbf{K}_4)$ [see Fig. 1(b)], so that $\tilde{\Delta} = \Delta$ the valence-band splitting, while for an *e*-*e*-*h* process $\tilde{\Delta} = 0$.

The $\varepsilon(\mathbf{K}_i)$ are quadratic functions of **K**. For an ellipsoidal band structure, the dispersion relation is

$$\varepsilon(\mathbf{K}) = A_x K_x^2 + A_y K_y^2 + A_z K_z^2 .$$
 (8)

This band structure is encountered in II-VI semiconductors such as CdS and CdSe, but also in materials under uniaxial stress; the spherical case would correspond to $A_x = A_y = A_z = A.$

For low-energy holes, the $\mathbf{k} \cdot \mathbf{p}$ theory gives a warped form for the two upper valence-band energies, usually written as

$$\varepsilon(\mathbf{K}) = A'K^{2} \pm [B'^{2}K^{4} + C'^{2}(K_{x}^{2}K_{y}^{2} + K_{y}^{2}K_{z}^{2} + K_{z}^{2}K_{x}^{2})]^{1/2}$$

$$\equiv A'[K^{2} + e\Phi(\mathbf{K})] = A'K^{2}\Psi(\Omega) . \qquad (9)$$

Equation (9) is a definition for $\Phi(\mathbf{K})$ and $\Psi(\Omega)$; $\Psi(\Omega)$ depends only on the direction Ω of \mathbf{K} , $e = \pm 1$. The usual heavy- and light-hole masses are related to the coefficients A', B', C' by

$$\frac{\hbar^2}{2m_{H,L}} = A' \mp \left[B'^2 + \frac{C'^2}{6} \right]^{1/2}.$$
 (10)

The warping of the third valence band is smaller and for simplicity we will assume it is spherical, $\varepsilon(\mathbf{K}) = A'' K^2$.

The problem is to calculate $G(\gamma)$. One keeps the symmetry between the four particles and decouples the integration over the K_i 's if one uses

$$\delta(\mathbf{K}) = (2\pi)^{-3} \int d^3 r \, e^{i\mathbf{K} \cdot \mathbf{r}} \,, \qquad (11a)$$

$$\delta(E) = (2\pi)^{-1} \int_{-\infty}^{+\infty} dt \ e^{iEt} \ . \tag{11b}$$

This leads to

$$G(\gamma) = (2\pi)^{-4} \int \int dt \, d^3r \, e^{i\gamma t} g_1(\mathbf{r}, t) g_2(\mathbf{r}, t)$$
$$\times g_3(\mathbf{r}, t) g_4(\mathbf{r}, i - t) \, . \tag{12}$$

The functions g_i are defined in terms of the energy ε_i of the *i*th particle as

$$g_i(\mathbf{r},t) = \int d^3 K \exp\left[i\left[\mathbf{K}\cdot\mathbf{r} + \frac{\varepsilon_i(\mathbf{K})}{A_0}t\right]\right].$$
 (13)

In the case of an *e-e-h* Auger effect, g_1 , g_2 , and g_4 are identical, while $g_1 = g_2 \neq g_4$ for an *h-h-e* process, as the excited hole is going in a different valence band.

We will see that $g_i(\mathbf{r}, t)$ is singular for t = 0. In order to avoid this singularity we can, since $\exp(iEt)$ is analytical, push the contour of integration in Eq. (11b) slightly into the upper complex half-plane. This gives t a positive and infinitesimally small imaginary part. In this way the defining integral equation (13) for g_i is always convergent for large k on our t contour (it is divergent if t is in the lower complex half-plane). In the same way the integral giving $g_4(\mathbf{r}, i - t)$ will be convergent.

II. THRESHOLD ENERGY

Before going further into the calculation of g and G, let us find first the lowest possible value of E_4 taking into account the conservation laws. From Eqs. (2) and (5), this threshold energy gives the principal exponential term of the Auger lifetime for small T (i.e., large E_g/k_BT). This threshold energy has already been calculated in the case of spherical symmetry,⁶ or evaluated⁷ by numerical methods for other symmetries. We give here an analytical method that we apply to ellipsoidal symmetry as well as to the case of the warping of the valence band.

We look for the smallest $E_4 = \tilde{\Delta} + K_0^2 \varepsilon(\mathbf{K}_4)$, i.e., the smallest positive value of $\varepsilon(\mathbf{K}_4)$, with the constraints

$$K_1 + K_2 + K_3 + K_4 = 0$$
, (14a)

$$\gamma + \frac{\varepsilon(\mathbf{K}_1) + \varepsilon(\mathbf{K}_2) + \varepsilon'(\mathbf{K}_3) - \varepsilon(\mathbf{K}_4)}{A_0} = 0 , \qquad (14b)$$

where $\gamma = (E_g - \tilde{\Delta})/k_B T$. The simplest way is to use Lagrange multipliers *a* and **u** and look for the extremum of

$$\varepsilon(\mathbf{K}_4) + \mathbf{u} \cdot (\mathbf{K}_1 + \mathbf{K}_2 + \mathbf{K}_3 + \mathbf{K}_4) + a \left[\gamma + \frac{\varepsilon(\mathbf{K}_1) + \varepsilon(\mathbf{K}_2) + \varepsilon'(\mathbf{K}_3) - \varepsilon(\mathbf{K}_4)}{A_0} \right],$$

or to introduce $\mathbf{V} = A_0 a^{-1} \mathbf{u}$ and $b = A_0 a^{-1} - 1$, and to look for the extremum of the quantity S defined as

$$S = \mathbf{V} \cdot (\mathbf{K}_1 + \mathbf{K}_2 + \mathbf{K}_3 + \mathbf{K}_4) + \gamma A_0 + \varepsilon(\mathbf{K}_1) + \varepsilon(\mathbf{K}_2) + \varepsilon'(\mathbf{K}_3) + b\varepsilon(\mathbf{K}_4) .$$
(15)

The fact that S has to be extremum versus the \mathbf{K}_i 's leads to

$$\frac{\partial S}{\partial \mathbf{K}_{1,2}} = \mathbf{V} + \frac{\partial \varepsilon(\mathbf{K}_{1,2})}{\partial \mathbf{K}_{1,2}} = \mathbf{0} , \qquad (16a)$$

$$\frac{\partial S}{\partial \mathbf{K}_3} = \mathbf{V} + \frac{\partial \varepsilon'(\mathbf{K}_3)}{\partial \mathbf{K}_3} = \mathbf{0} , \qquad (16b)$$

$$\frac{\partial S}{\partial \mathbf{K}_4} = \mathbf{V} + b \frac{\partial \varepsilon(\mathbf{K}_4)}{\partial \mathbf{K}_4} = \mathbf{0} .$$
 (16c)

Equations (14) and (16) form a set of 16 equations with 16 unknowns (the K_i 's, V and b).

(a) e-e-h, spherical symmetry: $\varepsilon_{1,2,4}(\mathbf{K}) = AK^2$, $\varepsilon'_3(\mathbf{K}) = A'K^2$. Equations (16) give immediately

$$\mathbf{K}_{1,2} = -\frac{\mathbf{V}}{2A}, \quad \mathbf{K}_3 = -\frac{\mathbf{V}}{2A'}, \quad \mathbf{K}_4 = -\frac{\mathbf{V}}{2Ab}.$$
 (17)

One gets b from Eq. (14a), then V from Eq. (14b), and finally the lowest $\varepsilon(\mathbf{K}_4)$ and the threshold energy $E_{\rm th} = K_0^2 \varepsilon_{\rm min}(\mathbf{K}_4)$ are

$$\varepsilon_{\min}(\mathbf{K}_4) = \frac{A+2A'}{A+A'} \gamma A_0, \text{ i.e., } E_{\text{th}} = \frac{A+2A'}{A+A'} E_g .$$
(18)

This is, with the usual notations, $E_{th} = E_g(m_h + 2m_e)/(m_h + m_e)$, in agreement with the result of Eq. (1) for the *e-e-h* process.

(b) *h-h-e, spherical symmetry*: $\varepsilon_{1,2,4}(\mathbf{k}) = A'k^2$ and $\varepsilon'_3(\mathbf{k}) = Ak^2$. A procedure similar to the above case gives

$$\varepsilon_{\min}(\mathbf{K}_{4}) = \gamma A_{0} \{ (A'+2A) / [A'+A(2-A'/A'')] \}$$

if γ is positive, but $\varepsilon_{\min}(\mathbf{K}_4) = 0$ if γ is negative, so that the threshold energy is

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$$E_{\rm th} = \Delta + \frac{A' + 2A}{A' + 2A - AA'/A''} \sup(0, E_g - \Delta) , \quad (19)$$

where $\sup(x, y)$ is the larger of x and y.

(c) Ellipsoidal symmetry: $\varepsilon(\mathbf{K}) = A_x K_x^2 + A_y K_y^2 + A_z K_z^2$ and similarly for ε' . Equation (16) gives $(K_{1,2})_i = -V_i/2A_i$, and similarly for \mathbf{K}_3 and \mathbf{K}_4 . Replacing the K_i 's by their above values into the momentum conservation Eq. (14a), one finds that two components of V must be zero, and one obtains the coefficient b from the equation for the third component. Then the calculation goes on as in case (a) and one finds for the threshold

$$E_{\rm th} = \frac{A_x + 2A'_x}{A_x + A'_x} E_g , \qquad (20)$$

the direction x being the one giving the lowest value of $(A_i + 2A'_i)/(A_i + A'_i)$.

(d) e-e-h, warping: $\varepsilon_{1,2,4}(\mathbf{K}) = AK^2$, $\varepsilon'(\mathbf{K}) = A'K^2 + e\Phi(\mathbf{K})$, where $\Phi(\mathbf{K})$ is defined in Eq. (9). Equation (15a) gives $\mathbf{K}_{1,2} = -\mathbf{V}/2A$, while Eq. (15c) gives $\mathbf{K}_4 = -\mathbf{V}/2Ab$. From momentum conservation one deduces

$$\mathbf{K}_3 = \mathbf{V}(2 + b^{-1})/2A \quad . \tag{21}$$

For a quadratic function $\varepsilon'(\alpha \mathbf{V}) = \alpha^2 \varepsilon'(\mathbf{V})$ and Eq. (16b) gives

$$V_{i}\left[\frac{A}{2+b^{-1}}+A'+e\frac{B'^{2}+\frac{C'^{2}}{2}}{\Phi(\mathbf{V})}V^{2}-e\frac{C'^{2}V_{i}^{2}}{2\Phi(\mathbf{V})}\right]=0,$$
(22)

for i = x, y, z. Equation (22) implies that zero, one, or two V_i must be zero, and that the nonzero V_i are equal. The first solution of Eq. (22) is $V_x = V_y = V_z \neq 0$: in that case $V_x^2 = V^2/3$, and $\Phi(\mathbf{V}) = V^2(B'^2 + C'^2/3)^{1/2}$. From Eqs. (14b) and (22), one obtains V^2 and b, and finally the threshold energy for that direction is found to be $\gamma kT/(b+1)$, i.e.,

$$E_{\rm th}^{[111]} = \frac{A + 2A' + 2e(B'^2 + C'^2/3)^{1/2}}{A + A' + e(B'^2 + C'^2/3)^{1/2}}E_g .$$
(23)

The next solution is $V_x \neq 0$, $V_y = V_z = 0$; then $\Phi(\mathbf{V}) = B'V^2$ and the corresponding threshold is

$$E_{\rm th}^{[100]} = \frac{A + 2A' + 2eB'}{A + A' + eB'} E_g . \qquad (24)$$

Finally for the third kind of extremum, with all the K in the direction [110], for example, one replaces B' by $(B'^2 + C'^2/4)^{1/2}$ in Eq. (24).

The direction of the lowest threshold depends on whether the Auger recombination is with a heavy or a light hole. From Eqs. (23) and (24), the threshold corresponds to $[2-A/(A+A'+e\overline{\Phi})]E_g$, with $\overline{\Phi}=B'$,

 $(B'^2+C'^2/4)^{1/2}$, or $(B'^2+C'^2/3)^{1/2}$, depending on the direction. For a heavy hole, e = -1, and the lowest threshold is for the largest $\overline{\Phi}$, i.e., in the [111] direction. For light hole, e = +1, and the lowest threshold is for the smallest $\overline{\Phi}$, i.e., in the [100] (or [010], or [001]) direction. But in both cases $\overline{\Phi}$ differs from $(B'^2+C'^2/6)^{1/2}$, the value appearing in the usual light- and heavy-hole masses.

(e) e-h-h, warping: $\varepsilon_{1,2}(\mathbf{K}) = A'K^2 + \Phi(\mathbf{K})$, $\varepsilon_3 = AK^2$, $\varepsilon_4 = A''K^2$. Equations (16b) and (16c) give $\mathbf{K}_3 = -\mathbf{V}/2A$ and $\mathbf{K}_4 = -\mathbf{V}/2A''b$. As Eq. (16a) leads in general to $\mathbf{K}_1 = \mathbf{K}_2$, one deduces from the momentum conservation

$$\mathbf{K}_1 = \mathbf{V}(1/4A + 1/4A''b) \ . \tag{25}$$

Using Eq. (25) into Eq. (16a), V should be such that

$$V_{i}\left[\frac{2AA''}{A''+b^{-1}A}+A'+\frac{B'^{2}+C'^{2}/2}{\Phi(\mathbf{V})}V^{2}-\frac{C'^{2}V_{i}^{2}}{2\Phi(\mathbf{V})}\right]=0,$$
(26)

for i = x, y, z. The calculation goes on as in case (d), and one finds for the threshold

$$E_{\rm th} = \Delta + \frac{A' + e\overline{\Phi} + 2A}{A' + e\overline{\Phi} + 2A - \frac{A(A' + e\overline{\Phi})}{A''}} \sup(0, E_g - \Delta) .$$
(27)

We have set $\overline{\Phi} = (B'^2 + \beta C'^2)^{1/2}$ with $\beta = 0$, $\frac{1}{4}$, or $\frac{1}{3}$ depending on the directions ([100], [110], and [111], respectively). For heavy holes (e = -1), the lowest threshold is for the largest $\overline{\Phi}$, i.e., $\overline{\Phi} = (B'^2 + C'^2/3)^{1/2}$, in the [111] direction, while for light holes (e = +1) the lowest threshold is for $\overline{\Phi} = B'$, in the [100] direction. The conclusions are identical to the ones for an Auger effect between two electrons and one hole. But this was not a *priori* obvious: in particular, if the excited hole stays in the same valence band, one has to replace A'' by $A' + e\Phi$ in Eq. (27) and in that case, one finds the reverse: the threshold for heavy holes is in the [100] direction, while the one for light holes is in the [111] direction.

(f) Numerical estimate. If we define the threshold energy as λE_g , for an *e-e-h* Auger process the factor λ is of the form A + 2A'/A + A' where A depends on the effective mass as m^{-1} .

For a conduction band with ellipsoidal symmetry, the usual electron effective mass is $m_e = (m_{\parallel}m_{\perp}^2)^{1/3}$, while from Eq. (20) the threshold corresponds to the smallest of m_{\parallel} and m_{\perp} . For germanium $m_{\parallel} = 1.59$, $m_{\perp} = 0.082$: using the hole effective mass $m_h = 0.30$, one finds $\lambda = 1.42$ (taking $m_e = 0.22$) while $\lambda = 1.21$ if one uses m_{\perp} .

For a valence band with warping, the usual hole effective mass is given by Eq. (10) while from Eq. (23) the real threshold corresponds to use $B'^2 + C'^2/3$ instead of $B'^2 + C'^2/6$. For GaAs, A = 14.9, A' = 7.65, B' = 4.82, and C' = 7.71. This gives $\lambda = 1.07$ instead of $\lambda = 1.11$.

III. SPHERICAL SYMMETRY

Let us return to the explicit calculation of the g's and $G(\gamma)$ defined in Eqs. (12) and (13). For $\varepsilon(\mathbf{K}) = AK^2$, $g(\mathbf{r},t)$ is easily found as

$$g(\mathbf{r},t) = \left[\frac{i\pi A_0}{At}\right]^{3/2} \exp\left[-i\frac{A_0r^2}{4At}\right].$$
 (28)

We recall that t has a small positive imaginary part. Replacing these values of g's into Eq. (12), one finds

$$G(\gamma) = (2\pi)^{-4} (i\pi)^6 \frac{A_0^6}{A^{9/2} A'^{3/2}} \int dt \frac{e^{i\gamma t}}{t^{9/2} (i-t)^{3/2}} \int d^3 r \exp\left[i \frac{r^2 A_0 [t(A+A') - i(A+2A')]}{4t(i-t)AA'}\right],$$
(29)

which gives after an easy integration over r

$$G(\gamma) = (2\pi)^{-4} (i\pi)^{6} (4\pi)^{3/2} \frac{A_0^{9/2}}{A^3 (A+A')^{3/2}} I(\gamma) , \qquad (30)$$

with

$$I(\gamma) = i^{3/2} \int_{-\infty + i\varepsilon}^{+\infty + i\varepsilon} dt \frac{e^{i\gamma t}}{t^3 (t - i\lambda)^{3/2}} , \qquad (31)$$

$$\lambda = \frac{A + 2A'}{A + A'} . \tag{32}$$

In order to calculate $I(\gamma)$, we deform the integration path, see Fig. 2.

For $\gamma < 0$, we can push it to infinity in the lower complex half-plane. The only nonzero contribution comes from the pole at t = 0 which gives

$$I(\gamma < 0) = \frac{\pi}{\lambda^{7/2}} \left[(\lambda \gamma)^2 - 3\lambda \gamma + \frac{15}{4} \right].$$
(33)

For $\gamma > 0$, we push the contour toward infinity in the upper complex half-plane. The nonzero contribution comes from the cut starting at the branch point $t = i\lambda$ and going to $+i\infty$ along the imaginary axis. We make the change of variables t = ix so that

$$I(\gamma) = \int_{C} dx \frac{e^{-\gamma x}}{x^{3}(x-\lambda)^{3/2}} , \qquad (34)$$



FIG. 2. Integral path used for the calculation of the integrals $I(\gamma)$ for $\gamma > 0$ and $\gamma < 0$.

with an integration path C around the cut $[\lambda, +\infty]$ (see Fig. 2) and a determination for $(x - \lambda)^{3/2}$ real positive below the cut, and real negative above it. The calculation of $I(\gamma)$ goes on in the following way: one integrates $(x - \lambda)^{-3/2}$ by parts in order to have at $x = \lambda$ a convergent function behaving as $(x - \lambda)^{-1/2}$. Then the function jump over the cut gives a factor 2 and one obtains two real integrals, the integration over x going from λ to ∞ . The integrals can be identified⁸ as two Whittaker functions $W_{-5/4, -5/4}$ and $W_{-7/4, -7/4}$. Using⁸ the identity $W_{\lambda,\mu} = W_{\lambda,-\mu}$, one can finally rewrite the result in terms of only one Whittaker function:

$$I(\gamma > 0) = 4\pi^{1/2} \lambda^{-7/2} (\lambda \gamma)^{5/4} e^{-\lambda \gamma/2} W_{-3/4,7/4}(\lambda \gamma) .$$
(35)

One can check that the three incomplete Γ functions appearing in the exact result of Haug *et al.* form simply $W_{-3/4,7/4}$.

As for large z, $W_{\lambda,\mu}(z) \sim z^{\lambda} e^{-z/2}$, one finds that

$$\lim_{\sigma \to +\infty} I(\gamma) = 4\pi^{1/2} \lambda^{-3} \gamma^{1/2} e^{-\lambda \gamma} , \qquad (36)$$

as easily obtained directly from Eq. (34). This gives for the Auger rate a temperature variation in the case of $E_g > \tilde{\Delta}$

$$\frac{1}{\tau} \sim \left[\frac{k_B T}{E_g}\right]^2 \left[\frac{E_g - \tilde{\Delta}}{k_B T}\right]^{1/2} \exp\left[-\frac{\tilde{\Delta}}{k_B T}\right] \times \exp\left[-\frac{A + 2A'}{A + A'} \frac{E_g - \tilde{\Delta}}{k_B T}\right], \quad (37)$$

in agreement with Eq. (1) for $\tilde{\Delta} = 0$. (The additional E_g^2 term comes from dimensional argument.)

IV. ELLIPSOIDAL SYMMETRY

We consider now the case $\varepsilon(\mathbf{K}) = A_x K_x^2 + A_y K_y^2 + A_z K_z^2$ and $\varepsilon'(\mathbf{K}) = A'_x K_x^2 + A'_y K_y^2 + A'_z K_z^2$. The calculation of the g's gives a result similar to Eq. (28),

$$g(\mathbf{r},t) = \left[\frac{i\pi}{t}\right]^{3/2} \left[\frac{A_0^3}{A_x A_y A_z}\right]^{1/2}$$
$$\times \exp\left[-i\frac{A_0}{4t}\left[\frac{x^2}{A_x} + \frac{y^2}{A_y} + \frac{z^2}{A_z}\right]\right]. \quad (38)$$

Using these g's into $G(\gamma)$, one can easily perform the Gaussian integral over x, y, and z, so that

$$G(\gamma) = (2\pi)^{-4} (i\pi)^{6} (4\pi)^{3/2} \frac{A_{0}^{9/2}}{A_{x} A_{y} A_{z} (A_{x} + A_{x}')^{1/2} (A_{y} + A_{y}')^{1/2} (A_{z} + A_{z}')^{1/2}} I(\gamma) ,$$

$$I(\gamma) = i^{3/2} \int_{-\infty + i\varepsilon}^{+\infty + i\varepsilon} dt \frac{e^{i\gamma t}}{t^{3} (t - i\lambda_{x})^{1/2} (t - i\lambda_{z})^{1/2}} ,$$
(39)

with $\lambda_x = (A_x + 2A'_x)/(A_x + A'_x)$. Equation (39) reduces to the spherical expression (31) if $\lambda_x = \lambda_y = \lambda_z$.

The calculation of $I(\gamma)$ is very simple for $\gamma < 0$ as the contribution of the t = 0 pole gives again a second-order polynomial in γ :

$$I(\gamma < 0) = \frac{\pi}{(\lambda_x \lambda_y \lambda_z)^{1/2}} \left[\gamma^2 - \gamma \left[\frac{1}{\lambda_x} + \frac{1}{\lambda_y} + \frac{1}{\lambda_z} \right] + \frac{3}{4} \left[\frac{1}{\lambda_x^2} + \frac{1}{\lambda_y^2} + \frac{1}{\lambda_z^2} \right] + \frac{1}{2} \left[\frac{1}{\lambda_x \lambda_y} + \frac{1}{\lambda_y \lambda_z} + \frac{1}{\lambda_z \lambda_x} \right] \right].$$
(40)

For $\gamma > 0$, one has now four "poles," t = 0, λ_x , λ_y , and λ_z , and our expression does not reduce to a Whittaker function.

If $\lambda_x < \lambda_y < \lambda_z$, one is left with a first-order integral

$$I(\gamma) = 2 \int_{\lambda_x}^{\lambda_y} dx \frac{e^{-\gamma x}}{x^{3}(x - \lambda_x)^{1/2}(x - \lambda_y)^{1/2}(x - \lambda_z)^{1/2}} + 2 \int_{\lambda_z}^{\infty} dx \frac{e^{-\gamma x}}{x^{3}(x - \lambda_x)^{1/2}(x - \lambda_y)^{1/2}(x - \lambda_z)^{1/2}},$$
(41)

which has to be calculated numerically. However, in the limit of large positive γ , the result is controlled by the lowest pole λ_x and one easily finds that

$$\lim_{\gamma \to +\infty} I(\gamma) = \frac{2}{\lambda_x^3 (\lambda_y - \lambda_x)^{1/2} (\lambda_z - \lambda_x)^{1/2}} \left(\frac{\pi}{\gamma}\right)^{1/2} e^{-\gamma \lambda_x} .$$
(42)

One sees that the exponential term of the Auger rate is controlled by the lowest $(A_i + 2A'_i)/(A_i + A'_i)$ as previously found in the threshold calculation, but most of all that the prefactor of $I(\gamma)$ goes now as $\gamma^{-1/2}$ instead of $\gamma^{1/2}$, so that

$$\frac{1}{\tau} \sim \left(\frac{k_B T}{E_g}\right)^2 \left(\frac{k_B T}{E_g}\right)^{1/2} \exp\left(-\lambda_x \frac{E_g}{k_B T}\right), \qquad (43)$$

i.e., $1/\tau$ goes as $T^{5/2}$ and is smaller than the well-known result of Eq. (1) by a factor $k_B T/E_g$.

If two of the λ_i are equal, as encountered in most physical situations, one has to consider two cases:

(i) If $\lambda_y = \lambda_z > \lambda_x$, the preceding result applies, and one finds a prefactor temperature dependence going as $T^{5/2}$. (ii) If $\lambda_x = \lambda_y < \lambda_z$, then

$$I(\gamma) = 2\pi \frac{e^{-\lambda_x \gamma}}{\lambda_x^{3/2} (\lambda_z - \lambda_x)^{1/2}} + 2 \int_{\lambda_z}^{\infty} dx \frac{e^{-\gamma x}}{x^3 (x - \lambda_x) (x - \lambda_z)^{1/2}} .$$
(44)

The first term comes from the contribution of the pole at λ_x . For large γ , it is the dominant factor of the result, and one finds in that case for the temperature dependence of the Auger rate,

$$\frac{1}{\tau} \sim \left[\frac{k_B T}{E_g}\right]^2 \exp\left[-\lambda_x \frac{E_g}{k_B T}\right]. \tag{45}$$

If $\lambda_x = \lambda_y = \lambda_z$, the result is that of Sec. III.

One can relate these behaviors to the symmetry of the band structure. When all the λ_i are distinct, the threshold corresponds to only two points on the energy surface because we have only a discrete symmetry: in that case $G(\gamma)$ behaves as $\gamma^{-1/2}$. This is also the case if one has an ellipsoid of revolution, and if the threshold corresponds to the direction parallel to the symmetry axis: in that case also only two points contribute at threshold. On the contrary, if the threshold is in the direction perpendicular to the symmetry axis, because of the symmetry of revolution, there is a degeneracy for the threshold which corresponds to an equatorial circle and in that case $G(\gamma)$ behaves as γ^0 . Finally, for a spherical symmetry, there is again degeneracy and the threshold corresponds to a spherical surface which gives $G(\gamma) \sim \gamma^{1/2}$.

V. WARPING, e-e-h AUGER EFFECT

We have now $\varepsilon_{1,2,4}(\mathbf{K}) = AK^2$ and $\varepsilon_3(\mathbf{K}) = A'\Psi(\Omega)K^2$, where $\Psi(\Omega)$ depends only on the momentum direction [see Eq. (9)]. The $g_{1,2,4}$'s are simply given by Eq. (28), but, due to the complexity of $\Psi(\Omega)$, we leave for the moment the integral of g_3 uncalculated. $G(\gamma)$ can be written as

$$G(\gamma) = (2\pi)^{-4} (i\pi)^{9/2} \left[\frac{A_0}{A} \right]^{9/2} \int dt \frac{e^{i\gamma t}}{t^3 (i-t)^{3/2}} \int d^3 K \exp\left[i \frac{A'}{A_0} \Psi(\Omega) K^2 t \right] \\ \times \int d^3 r \exp\left[-i \frac{A_0}{4A} r^2 \left[\frac{2}{t} + \frac{1}{i-t} \right] + i \mathbf{K} \cdot \mathbf{r} \right].$$
(46)

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The Gaussian integral over r is then easily calculated, so that $G(\gamma)$ becomes

$$G(\gamma) = (2\pi)^{-4} (i\pi)^{9/2} (4i\pi)^{3/2} \left[\frac{A_0}{A}\right]^3 J(\gamma) ,$$

$$J(\gamma) = \int dt \frac{e^{i\gamma t}}{t^{3/2} (t-2i)^{3/2}} \int d\Omega \frac{1}{4\pi} \int_0^\infty dK \, 4\pi K^2 \exp\left[i\frac{t}{A_0} \left[A'\Psi(\Omega) + A\frac{i-t}{2i-t}\right] K^2\right] .$$
(47)

Performing the Gaussian integration over K, one is left with a third-order integral

$$J(\gamma) = (i\pi A_0)^{3/2} \int d\Omega \frac{1}{4\pi [A + A'\Psi(\Omega)]^{3/2}} \int_{-\infty + i\varepsilon}^{+\infty + i\varepsilon} dt \frac{e^{i\gamma t}}{t^3 \left[t - i\frac{A + 2A'\Psi(\Omega)}{A + A'\Psi(\Omega)}\right]^{3/2}}$$
(48)

One can check that for $\Psi(\Omega) = 1$, Eqs. (47) and (48) give the spherical case, Eqs. (30) and (31). The next step is to perform the integration over t. This is done as for the spherical case (Sec. III), where λ is replaced by $\lambda(\Omega)$ with

$$\lambda(\Omega) = \frac{A + 2A'\Psi(\Omega)}{A + A'\Psi(\Omega)} .$$
(49)

The result depends if γ is positive or negative.

For $\gamma < 0$, the contribution of the t = 0 pole gives, as for Eq. (33),

$$J(\gamma < 0) = \frac{\pi^{3/2}}{4} \int d\Omega \left[\frac{A_0}{A + 2A'\Psi(\Omega)} \right]^{3/2} \\ \times \left[\gamma^2 - \frac{3\gamma}{\lambda(\Omega)} + \frac{15}{4\lambda^2(\Omega)} \right]. \quad (50)$$

One concludes that the temperature dependence is the same as for the spherical case, with only some different combinations of A', B', C' than the ones appearing in the usual heavy and light holes.

For $\gamma > 0$, the integration over t gives a Whittaker function, as in Eq. (35), so that

$$J(\gamma > 0) = \pi \int d\Omega \left[\frac{A_0}{A + A'\Psi(\Omega)} \right]^{3/2} \\ \times \frac{[\gamma\lambda(\Omega)]^{5/4}}{\lambda(\Omega)^{7/2}} \exp\left[-\frac{\gamma\lambda(\Omega)}{2} \right] \\ \times W_{-3/4,7/4}(\gamma\lambda(\Omega)) .$$
(51)

There is of course no hope to do this last integral analytically for any γ . Nevertheless one can find simply, from Eq. (51), its behavior for large γ . Using the asymptotic expansion of the Whittaker function, one rewrites $J(\gamma)$ as

$$J(\gamma \to +\infty) = \pi \gamma^{1/2} \int d\Omega \left[\frac{A_0}{A + A' \Psi(\Omega)} \right]^{3/2} \frac{e^{-\gamma \lambda(\Omega)}}{\lambda^3(\Omega)} ,$$
(52)

for which the dominant contribution comes from the directions where $\lambda(\Omega)$ is minimum. These directions have already been found in Sec. II, and they vary depending whether the recombination is with a heavy or a light hole. Noting $\Omega_0(\theta_0, \varphi_0)$ as such a direction, one expands the function to be integrated around Ω_0 so that

$$J(\gamma \to +\infty) = \pi \left[\frac{A_0}{A + A'\Psi(\Omega_0)} \right]^{3/2} \frac{\gamma^{1/2} \exp[-\gamma \lambda(\Omega_0)]}{\lambda^3(\Omega_0)} \times \int_0^{\pi} d\theta \sin\theta_0 \int_0^{2\pi} d\varphi \exp\left[-\frac{\gamma}{2} \left[\frac{\partial^2 \lambda(\Omega)}{\partial \theta^2} (\theta - \theta_0)^2 + \frac{\partial^2 \lambda(\Omega)}{\partial \varphi^2} (\varphi - \varphi_0)^2 \right] \right].$$
(53)

Each of the integrations over θ and φ gives a factor $\gamma^{-1/2}$ so that finally we have

$$J(\gamma \to +\infty) \sim \gamma^{-1/2} \exp[-\gamma \lambda(\Omega_0)] .$$
 (54)

Besides the main exponential term already discussed in Sec. II, one notes a prefactor temperature dependence similar to the ellipsoidal case when $\lambda_x \neq \lambda_y \neq \lambda_z$: in both cases the threshold comes from a finite number of points on the energy surface and not, for example, from a whole

surface as in spherical case. One concludes that if the warping is taken into account, the temperature dependence of the Auger rate is not the one of the standard Eq. (1), but instead,

$$\frac{1}{\tau} \sim \left(\frac{k_B T}{E_g}\right)^{5/2} \exp\left[-E_g \frac{A + 2A'\Psi(\Omega_0)}{A + A'\Psi(\Omega_0)}\right].$$
 (55)

As this T dependence is linked to the distance between

the poles $\lambda_x, \lambda_y, \lambda_z$, or in the case of warping, the distance between $\Psi_{max}(\Omega)$ and $\Psi_{min}(\Omega)$, one expects that the temperature range for which such a new behavior is predicted depends on the importance of the warping. The behavior depicted in Eq. (55) will be found for temperature low enough so that the exponential term found for Ψ_{min} is much larger than the one found for Ψ_{max} . When the temperature is raised one has a crossover to the spherical symmetry case obtained when the two exponential terms are of the same order.

VI. WARPING, h-h-e AUGER EFFECT

For a recombination of an *e*-*h* pair associated with the excitation of a hole in the lowest valence band, the four energies are, respectively, $\varepsilon(\mathbf{K}_{1,2}) = A'\Psi(\Omega_{1,2})K_{1,2}^2$, $\varepsilon(\mathbf{K}_3) = AK_3^2$, and $\varepsilon(\mathbf{K}_4) = A''K_4^2$. g_3 and g_4 are then simply given by Eq. (28). For $g_{1,2}$ we perform the integration over K, and leave the angular part. Setting $\mathbf{K}_1 \cdot \mathbf{r} = K_1 rh(\Omega_1, \Omega)$, where Ω is the direction of **r** within the cubic axis, one finds

$$g_{1}(\mathbf{r},t) = \int \frac{d\Omega_{1}}{4\pi} \int_{0}^{\infty} 4\pi K_{1}^{2} dK_{1} \exp\left[i\frac{A'\Psi_{1}K_{1}^{2}}{A_{0}}t\right]^{\frac{1}{2}} \cos(rK_{1}K_{2})$$

$$= \left[\frac{i\pi A_{0}}{tA'}\right]^{3/2} \int \frac{d\Omega_{1}}{4\pi\Psi_{1}^{3/2}} \exp\left[-i\frac{A_{0}\nu_{1}r^{2}}{4A't}\right] \left[1-i\frac{A_{0}\nu_{1}r^{2}}{2A't}\right],$$
(56)

with $v_1 = h_1^2 / \Psi_1$. Replacing these g's into Eq. (12) one finds

$$G(\gamma) = (2\pi)^{-4} \left[\frac{i\pi A_0}{A'} \right]^3 \left[\frac{i\pi A_0}{A} \right]^{3/2} \left[\frac{i\pi A_0}{A''} \right]^{3/2} \int d\Omega_1 \frac{1}{4\pi} \int d\Omega_2 \frac{1}{4\pi} \int d\Omega_2 \frac{1}{4\pi} \int d\Omega_2 \frac{1}{4\pi} \frac{H(\gamma, \Omega_1, \Omega_2, \Omega)}{\Psi_1^{3/2} \Psi_2^{3/2}} , \qquad (57)$$

$$H(\gamma, \Omega_1, \Omega_2, \Omega) = \int_{-\infty + i\varepsilon}^{+\infty + i\varepsilon} dt \frac{e^{i\gamma t}}{t^{9/2} (i-t)^{3/2}} \int_0^\infty dr \, 4\pi r^2 \left[1 - \frac{iA_0 r^2 v_1}{2A' t} \right] \left[1 - \frac{iA_0 r^2 v_2}{2A' t} \right] \exp \left[-\frac{iA_0 \tilde{\mu}(t-i\tilde{\lambda})r^2}{4A' t(i-t)} \right] ,$$

where

$$\tilde{\lambda} = \frac{\nu_1 + \nu_2 + A'/A}{\nu_1 + \nu_2 + (A'/A) - (A'/A'')} \equiv \frac{\nu_1 + \nu_2 + A'/A}{\tilde{\mu}} .$$
(58)

After an easy integration over r of a Gaussian function, one is left with

$$H = \left[\frac{4\pi A'i}{A_0\tilde{\mu}}\right]^{3/2} \int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon} dt \frac{e^{i\gamma t}}{t^{3}(t-i\tilde{\lambda})^{3/2}} \left[1 + 3\frac{\nu_1 + \nu_2}{\tilde{\mu}}\frac{i-t}{t-i\tilde{\lambda}} + \frac{15\nu_1\nu_2}{\tilde{\mu}^2} \left[\frac{i-t}{t-i\tilde{\lambda}}\right]^2\right].$$
(59)

The result of this integral depends if γ is positive or negative.

For $\gamma < 0$, the contribution of the t = 0 pole gives for $H(\gamma < 0)$ a second-order polynomial in γ , i.e., for $G(\gamma)$ a result similar to the one of Eq. (40), with some more complicated angular averages.

For $\gamma > 0$, one changes the integration path as done in Fig. 2. One then integrates by parts in order to have only $(t - \lambda)^{1/2}$. The resulting integrals can be expressed in terms of Whittaker functions. If one looks only for the leading term of H at large γ , one finds easily from Eq. (59) that

$$H(\gamma \to +\infty) \simeq 2 \left[\frac{4\pi A'i}{A_0 \tilde{\mu}} \right]^{3/2} \times \frac{15\nu_1\nu_2}{\tilde{\mu}^2} \frac{2^3}{1\times 3\times 5} \frac{(1-\tilde{\lambda})^2}{\tilde{\lambda}^3} \gamma^{5/2} e^{-\gamma \tilde{\lambda}} .$$
(60)

As the main contribution in $G(\gamma)$ comes from the directions $\Omega_1, \Omega_2, \Omega$ for which $\tilde{\lambda}$ is minimum, as in Sec. V, one expands $\tilde{\lambda}$ around these directions. We have to integrate over six angles. As in Eq. (53), each integration gives a factor $\gamma^{-1/2}$. One finally gets for G

$$G(\gamma \rightarrow \infty) \sim \gamma^{-1/2} \exp(-\gamma \lambda_{\min})$$
,

i.e., again a temperature dependence of the Auger rate prefactor as $T^{5/2}$, as could have been expected using the same preceding dimensional arguments.

VII. GENERAL BAND STRUCTURE: THE STATIONARY PHASE METHOD

We present here a general method to obtain directly from Eq. (12) the behavior of $G(\gamma)$ at large $\gamma = E_g/k_B T$ for any complicated dispersion relation: This method is extremely powerful as the calculation is performed without using an explicit form for $\varepsilon(k)$. Of course, the result reduces to the ones which have already been obtained, in the case of ellipsoidal symmetry and warping, but it also applies for any more realistic band structure provided it satisfies $\varepsilon(\mathbf{k}) = k^2 \varepsilon(\hat{\mathbf{k}})$, where $\mathbf{k} = k\hat{\mathbf{k}}$.

Let us set

$$K(t) = (2\pi)^{-4} \int d^3r \, g_1(\mathbf{r}, t) g_2(\mathbf{r}, t) g_3(\mathbf{r}, t) g_4(\mathbf{r}, i - t) ;$$
(61)

then

$$G(\gamma) = \int_{-\infty + i\varepsilon}^{+\infty + i\varepsilon} dt K(t) e^{i\gamma t} .$$
(62)

If we push the contour of integration over t toward infinity in the upper complex half-plane, we see easily that for large γ , the dominant contribution comes from the singularity of K(t) nearest to the real t axis. This is also clear from all the preceding examples which we have explicitly investigated. Now since all the g's are regular functions of t and r, the singularities of K(t) arise because the defining integral equation (61) diverges for large r.

The behavior of $g(\mathbf{r},t)$ for large r is easily obtained from the stationary phase method:⁹ when r is large the exponential in Eq. (13) oscillates very rapidly as a function of \mathbf{k} , which leads to an almost complete cancellation in the integral. The dominant contribution comes from the region in \mathbf{k} space where this rapid oscillation does not occur. It is obtained by writing that the phase in the exponential, namely $\mathbf{k} \cdot \mathbf{r} + \varepsilon(\mathbf{K})t / A_0$, is almost constant in this region, which means that its \mathbf{k} gradient is almost zero. Let us call \mathbf{K}_s the wave vector for which this gradient is zero,

$$\nabla_{K} \varepsilon(\mathbf{K}) \mid_{\mathbf{K}_{s}} = -A_{0} \frac{\mathbf{r}}{t} , \qquad (63)$$

where t has to be replaced by i-t for g_4 . We see that these equations for the stationary wave vectors \mathbf{K}_s are exactly the same as Eq. (16) for the threshold wave vectors. The role of V is played by $A_0\mathbf{r}/t$ and the role of b by t/i - t.

Now we expand the phase up to second order around the stationary wave vector,

$$\mathbf{K}_{i} \cdot \mathbf{r} + \frac{\varepsilon(\mathbf{K})t}{A_{0}} \simeq \mathbf{K}_{s} \cdot \mathbf{r} + \frac{\varepsilon(\mathbf{K}_{s})t}{A_{0}} + \frac{t}{2A_{0}}K_{i}K_{j}\frac{\partial^{2}\varepsilon}{\partial K_{i}\partial K_{j}}\Big|_{K_{s}}$$
(64)

After performing the Gaussian integrals over K_i for i = x, y, z, one gets for the behavior of $g(\mathbf{r}, t)$

$$g(\mathbf{r},t) = (2i\pi A_0)^{3/2} \exp\left[i\left[K_s \cdot \mathbf{r} + t\frac{\varepsilon(\mathbf{K}_s)}{A_0}\right]\right] D(\mathbf{K}_s),$$
(65)

where we have set

$$D(\mathbf{K}_s) = \left[\det \frac{\partial^2 \varepsilon}{\partial K_i \partial K_j}\right]^{1/2}$$

In order to be able to investigate the r dependence we now make use of the assumption that $\varepsilon(\mathbf{K})$ depends quadratically on $|\mathbf{K}|$. Let us introduce the vector $\mathbf{q}(\mathbf{u})$ such that

$$\nabla_{\mathbf{K}} \varepsilon \mid_{\mathbf{K}=\mathbf{q}} = -A_0 \mathbf{u} , \qquad (66)$$

where **u** is an unit vector. Since $\varepsilon(\mathbf{K})$ is a quadratic function of $|\mathbf{K}|$, one deduces from Eq. (63) that the vector \mathbf{K}_s associated to $\mathbf{r}=r\mathbf{u}$ is simply $\mathbf{K}_s=r\mathbf{q}/t$ and consequently $\varepsilon(\mathbf{K}_s)=r^2\varepsilon(\mathbf{q})/t^2$, while $D(\mathbf{K}_s)=D(\mathbf{q})$ does not depend on *r*. One can then note that

$$\mathbf{K}_{s} \cdot \mathbf{r} + \frac{t}{A_{0}} \varepsilon(\mathbf{K}_{s}) = \frac{r^{2}}{t} \left[\mathbf{q} \cdot \mathbf{u} + \frac{\varepsilon(\mathbf{q})}{A_{0}} \right] \equiv \frac{r^{2}}{t} R(\mathbf{u}) .$$
(67)

The function $R(\mathbf{u})$ depends only on the direction of \mathbf{r} , but not on its modulus.

Doing the same for g', one finds that the exponential term of the product $g^{2}(\mathbf{r},t)g'(\mathbf{r},t)g(\mathbf{r},i-t)$ is

$$\exp\left[-ir^2\frac{t(R+R')-i(2R+R')}{t(i-t)}\right],\qquad(68)$$

where R and R' mean $R(\mathbf{u})$ and $R'(\mathbf{u})$. One can then easily perform the integration over r without still knowing the explicit forms of ε and ε' , i.e., of R and R', leaving apart the r angular variables Ω . Using Eqs. (65) and (67), one rewrites $G(\gamma)$ as

$$G(\gamma) = (2\pi)^{-4} \int d\Omega \frac{1}{4\pi} D^3(\mathbf{q}) D'(\mathbf{q}')(i\pi)^6 \pi^{3/2} \int dt \frac{e^{i\gamma t}}{t^3} \left[\frac{1}{t(R+R')-i(2R+R')} \right]^{3/2}.$$
(69)

One easily sees that the function to be integrated over t has the same form as the one found previously, namely $t^{-3}[t-i\tilde{\lambda}(\Omega)]^{-3/2}e^{i\gamma t}$ with $\tilde{\lambda}(\Omega)=(2R+R')/(R+R')$. $\tilde{\lambda}$ is an unexplicited function that depends only on the direction of **r**, and as we will see we do not need to know its explicit form to get the behavior of $G(\gamma)$ at large γ . Nevertheless, one can check that within the specific form of ϵ and ϵ' used in Secs. III-VI, $\tilde{\lambda}$ reduces to the λ 's used earlier.

The integration over t in Eq. (69) is performed as before, and one finds in the limit of large $\gamma > 0$, $\gamma^{1/2} \exp[-\gamma \tilde{\lambda}(\Omega)]$. One is then left with the integration over the **r** directions.

If there is a spherical symmetry for *all* the $\varepsilon(\mathbf{K})$, $\tilde{\lambda}$ will not depend explicitly on any angular variable, and

$$G(\gamma) \sim \gamma^{1/2} e^{-\gamma \bar{\lambda}} . \tag{70}$$

If there is a complete anisotropy for any one of the ε 's, $\tilde{\lambda}$ will depend on two angular variables. For large γ , the behavior of $G(\gamma)$ is controlled by the direction Ω_{\min} which gives the smallest $\tilde{\lambda}$; one expands $\tilde{\lambda}(\Omega)$ around this direction,

$$\begin{split} \widetilde{\lambda}(\Omega) = & \widetilde{\lambda}(\Omega_{\min}) + \frac{1}{2}(\theta - \theta_m)^2 (\partial^2 \widetilde{\lambda} / \partial \theta^2) \\ & + \frac{1}{2}(\varphi - \varphi_m)^2 (\partial^2 \widetilde{\lambda} / \partial \varphi^2) \; . \end{split}$$

Noting that each of the integrations over θ and φ for large γ gives a factor $\gamma^{-1/2}$, one finds in that case

$$G(\gamma) \sim \gamma^{-1/2} \exp[-\gamma \tilde{\lambda}(\Omega_{\min})] .$$
(71)

If in the direction of the minimum of $\overline{\lambda}$ there is a symmetry of revolution, $\overline{\lambda}$ around that minimum will depend only on one angular variable, the integration over which gives only one factor $\gamma^{-1/2}$, so that

$$G(\gamma) \sim \exp[-\gamma \tilde{\lambda}(\Omega_{\min})] .$$
(72)

As we see, the power of the prefactor depends only on the dimensionality of the dispersion relation symmetry (or more precisely of the dimensionality of the threshold degeneracy that results directly from symmetry), and not at all on its detailed form, as it can be obtained formally without even writing any explicit form for $\varepsilon(\mathbf{K})$.

A simple way to understand physically the T dependence of the Auger prefactor is to say that only a restricted region, in **k** space, of size $(k_BT)^{1/2}$ around the threshold, contributes to the Auger rate. For spherical symmetry this region is not limited in some directions because of the degeneracy due to the symmetry. Further limitation appears for this region if there is anisotropy, which produces reducing factors $(k_BT/E_g)^{1/2}$ or k_BT/E_g . One can also say that this anisotropy is expected to play some role if the anisotropy energy is larger than k_BT . For k_BT larger than this anisotropy energy, one finds again the spherical symmetry situation.

As the dominant terms in the Auger rate come from a

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restricted region in \mathbf{k} space, only the matrix element M of the recombination in that small region is important, i.e., M is roughly a constant in the dominant part; so that our result also holds for a general matrix element M, different from a constant.

Numerical estimate: In the case of full anisotropy, the usual prefactor of the Auger rate is decreased by an extra term in $k_B T/E_g$, which gives 2 or 3 orders of magnitude at room temperature depending on the band gap. For GaAs, $E_g \simeq 1.4$ eV so that $k_B T/E_g \simeq 1.8 \times 10^{-2}$ for T = 300 K. The corresponding change in the exponential term due to the proper value $\lambda = 1.07$ of the threshold energy, instead of 1.11, gives an increase of the exponential of 8.9 which partly compensates the prefactor change.

VIII. CONCLUSION

We have shown that the temperature dependence of the Auger lifetime is related to the symmetry of the electron and hole dispersion relations. We find that in the limit of large E_g/k_BT ,

$$\frac{1}{\tau} \sim \left[\frac{k_B T}{E_g}\right]^{(5-p)/2} \exp\left[\frac{-\lambda E_g}{k_B T}\right], \qquad (73)$$

with p = 2, 1, or 0, respectively, for a spherical symmetry, a one-dimensional symmetry, or a complete anisotropy. λE_g is the threshold energy for the Auger process, λ being related to the ratio ρ of the electron and hole effective masses. The well-known Beattie and Landsberg result, which corresponds to p = 2, does not hold if, in particular, a warping of the valence band is present.

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