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Evaluation of the stimulated emission rate of semiconductors with no k selection rule

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Introduction

For the case of high impurity concentration in semiconductors the k selection rule will not be valid any longer. Lasher and Stern (LS) [1] have given an integral expression for the stimulated emission rate in a direct semiconductor when (i) the transitions occur between parabolic bands, (ii) the k selection is not valid, and (iii) the optical matrix element can be taken as independent from energy. These assumptions seem to be justified if the semiconductor has a high concentration of shallow impurities, merging with the adjacent band, and for moderate carrier densities, which are in the order of some 10^{18} cm^{-3} for GaAs. Further papers of Hwang [2] and Casey and Stern [3] take into consideration the influence of band edge tailing and energy dependent matrix elements, the first of which dominates for low band filling and the second dominates for very high band filling. Marinelli (M) [4] and Unger [5] have given analytical approximation formulae for the LS stimulated emission rate.

In this paper we give the exact solution of the LS integral by expanding the difference between the LS- and M-integrals into a series which is rapidly converging for the room temperature case. Constant transition probabilities between parabolic bands and no k selection rule are assumed. Finally is given a brief discussion of how the incorporation of an energy dependent transition probability could be possible.

1. Method

After LS [1] the stimulated emission rate per unit volume (for unit frequency interval and per stimulating photon) is given by the integral

$$r_{\text{st}}(\Delta E)=C\int_0^{\Delta E} E^{\frac{1}{2}}(\Delta E-E)^{\frac{1}{2}}(f_{\text{c}}-f_{\text{v}})\,\mathrm{d}E \tag{1}$$

ΔE is the photon energy minus the band gap energy; the Fermi distributions in the conduction band and valence band are

$$f_{\text{c}}=\frac{1}{1+\exp\left[(E-F_{\text{n}}')/kT\right]} \tag{2}$$

$$f_{\text{v}}=\frac{1}{1+\exp\left[(E+F_{\text{p}}'-\Delta E)/kT\right]} \tag{3}$$

F_{n}' is the quasi-Fermi level in the conduction band minus the conduction band edge energy, F_{p}' is the valence band edge energy minus the quasi-Fermi level in the valence band. C is a constant, which for Zn acceptors in GaAs has the value

$C=2{,}6\times10^{23}$ cm^{-3} s^{-1} meV^{-3} [1].

To evaluate the integral (1) we use the substitution

$$x=\frac{2E}{\Delta E}-1 \tag{4}$$

and obtain

$$C^{-1}r_{\text{st}}(\Delta E)=\frac{1}{4}\Delta E^2\int_{-1}^{+1}\sqrt{1-x^2}\,g(x)\,\mathrm{d}x \tag{5}$$

with

$$g(x)=\frac{\sinh a}{\cosh a+\cosh(bx+c)} \tag{6}$$

$$a=(F_{\text{n}}'+F_{\text{p}}'-\Delta E)/2kT \tag{7}$$

$$b=\Delta E/2kT \tag{8}$$

$$c=(F_{\text{p}}'-F_{\text{n}}')/2kT \tag{9}$$

Now we proceed in the following way: First we expand the function g in a series and then, after an interchange of the summation sign and the integration sign, we integrate term by term and consequently obtain a series expansion of the integral solution. The two functions $\sqrt{1-x^2}$ and $g(x)$ constituting the integrand are defined in the whole z-plane and have analytic properties which allow the evaluation of the integral by contour integration [6].

The function $g(z)$ is meromorphic. It's only singularities (except at infinity) are simple poles at

$$z_{\mu,\nu}=[\mu a-c+(2\nu+1)\pi\mathrm{i}]/b\begin{cases}\mu=-1;\ +1\\ \nu=\ldots-2;\ -1;\ 0;\ 1;\ 2\ldots\end{cases} \tag{10}$$

By Mittag-Leffler's Theorem [7] we can expand the function $g(z)$ in a series, each term of which corresponds to one of the poles $z_{\mu,\nu}$ in the finite part of the z-plane, and obtain

$$g(z)=\frac{\sinh a}{\cosh a-\cosh c}-\sum_{\mu=\pm1}\sum_{\nu=-\infty}^{+\infty}\frac{1}{\mu b}\left(\frac{1}{z-z_{\mu,\nu}}+\frac{1}{z_{\mu,\nu}}\right) \tag{11}$$

Introducing this series expansion into eq. (5) and interchanging summation and integration we obtain

$$C^{-1}r_{\text{st}}(\Delta E)=A+\sum_{\mu=\pm1}\sum_{\nu=-\infty}^{+\infty}(B_{\mu,\nu}+C_{\mu,\nu}) \tag{12}$$

with

$$A=\frac{1}{4}\Delta E^2\frac{\sinh a}{\cosh a+\cosh c}\int_{-1}^{+1}\sqrt{1-x^2}\,\mathrm{d}x =\frac{\pi}{8}\Delta E^2\frac{\sinh a}{\cosh a+\cosh c} \tag{13}$$

$$B_{\mu,\nu}=-\frac{1}{4}\Delta E^2\frac{1}{\mu b}\int_{-1}^{+1}\frac{\sqrt{1-x^2}}{x-z_{\mu,\nu}}\,\mathrm{d}x \tag{14}$$

$$C_{\mu,\nu}=-\frac{1}{4}\Delta E^2\frac{1}{\mu b z_{\mu,\nu}}\int_{-1}^{+1}\sqrt{1-x^2}\,\mathrm{d}x =-\frac{\pi}{8}\Delta E^2\frac{1}{\mu b z_{\mu,\nu}} \tag{15}$$

The term A is identical to the approximation for $C^{-1}r_{\text{st}}(\Delta E)$ of Marinelli [4]. This approximation is allowed when $g(x)$ can be approximated by $g(0)$ in the interval $[-1,+1]$. The physical condition for the validity of the approximation is $\Delta E\ll 2kT$.

Now we compute the $B_{\mu,\nu}$ by contour integration in the complex z-plane. First of all we consider the function $\sqrt{1-z^2}$ which is multivalued and has branch points at $z=-1$ and at $z=+1$. For the intended contour integration it is useful to cut the z-plane by a branch line from $z=-1$ to $z=+1$ along the real axis. For $|x|<1$ and y approaching zero $\sqrt{1-z^2}$ is real and has opposite sign above and below the real axis. We introduce the function

$$w(z)=\sqrt{1-z^2} \tag{16}$$

by making the additional convention that for $|x|<1$ just above the branch cut the positive sign of the square root is valid. From this choice it follows that the real part of $w(z)$ has the same sign as the imaginary part of z, whereas the imaginary part of $w(z)$ and the real part of z have opposite sign. Furthermore we note the useful relations

$$w(-z)=-w(z) \quad \text{and} \quad w(z^*)=-w^*(z)$$

Let us now determine the contour of integration. Figure 1 shows the z-plane, cut between the branch points -1 and $+1$ of $w(z)$, the pole $z_{\mu,\nu}$ and the contour of integration, involving an infinitesimal small semicircle around $z=-1$, a line along the real axis from $z=-1$ to $z=R$ (between $z=-1$ and $z=+1$ above the branch cut), a circle with radius R and a line going back from $z=R$ to $z=-1$ (between $z=+1$ and $z=-1$ below the branch cut). Since in eq. (13) the positive sign of the square root has to be choosen, the interval of integration in eq. (13) corresponds to the integration from $z=-1$ to $z=+1$ above the branch cut (or in the opposite direction below the branch cut). Hence the part of the contour integral from $z=+1$ to $z=-1$ below the branch cut, then along the semicircle around $z=-1$ and back to $z=+1$ above the branch cut, yields twice the value of the real integral from $x=-1$ to $x=+1$. That part of the contour integral which is along the real axis from $z=+1$ to $z=R$ is cancelled out by the integral along the same line but in the opposite direction. The rest of the contour integral is performed along the circle with the radius R. To make this part vanishing when R goes to infinity, we use the following procedure: We multiply the integrand by the function $\kappa^2/(\kappa^2+z^2)$. Then we let go R to infinity, and with this contour we calculate the integral. Afterwards, by a subsequent limiting process, we let go κ to infinity, too. In this way we get from eq. (13)

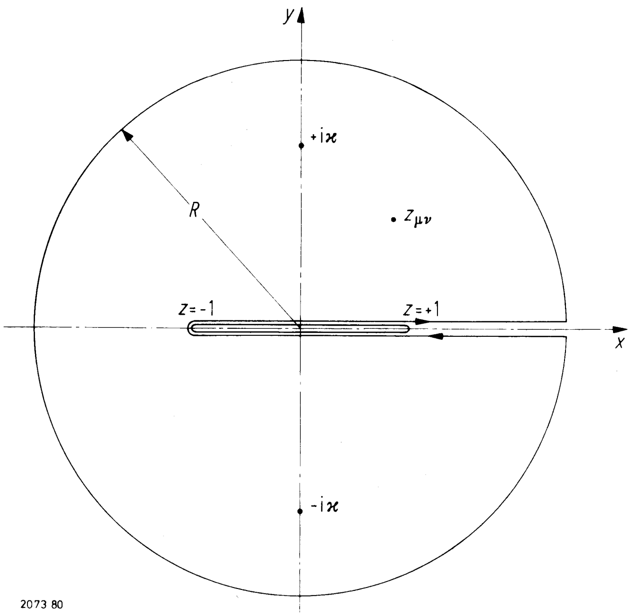

Figure 1:
Contour for evaluation of $B_{\mu,\nu}$

$$B_{\mu,\nu}=-\frac{\Delta E^2}{8\mu b}\lim_{\kappa\to\infty}\oint\frac{\kappa^2}{\kappa^2+z^2}\,\frac{w(z)}{z-z_{\mu,\nu}}\,dz \tag{17}$$

The integral is easily computed by Cauchy's integral formula and yields

$$B_{\mu,\nu}=\frac{\pi\Delta E^2}{4\mu b}\lim_{\kappa\to\infty}\frac{z_{\mu,\nu}\kappa w(i\kappa)-i\kappa^2 w(z_{\mu,\nu})}{\kappa^2+z_{\mu,\nu}^2} \tag{18}$$

We let $\kappa\to\infty$ and obtain

$$B_{\mu,\nu}=\frac{\pi\Delta E^2}{4\mu b}\,(z_{\mu,\nu}-iw(z_{\mu,\nu})) \tag{19}$$

We now sum the terms $B_{\mu,\nu}$ and $C_{\mu,\nu}$; and since according to eq. (10)

$$z_{\mu,-\nu-1}=z_{\mu,\nu}^*$$

it is also useful to combine the terms with the indices ν and $-\nu-1$. We obtain

$$C^{-1}r_{st}(\Delta E)=\frac{\pi\Delta E^2}{8}\,\frac{\sinh a}{\cosh a+\cosh c}-\frac{\Delta E^2}{4b}\sum_{\nu=0}^{\infty}(S(z_{1,\nu})-S(z_{-1,\nu})) \tag{20}$$

with

$$S(z)=\pi\left[\left(\frac{1}{|z^2|}-2\right)\mathrm{Re}\,\{z\}-2\,\mathrm{Im}\,\{\sqrt{1-z^2}\}\right] \tag{21}$$

The square root in eq. (20) obeys the convention

$$\mathrm{sign}\,\mathrm{Im}\,\{\sqrt{1-z^2}\}=-\mathrm{sign}\,\mathrm{Re}\,\{z\} \tag{22}$$

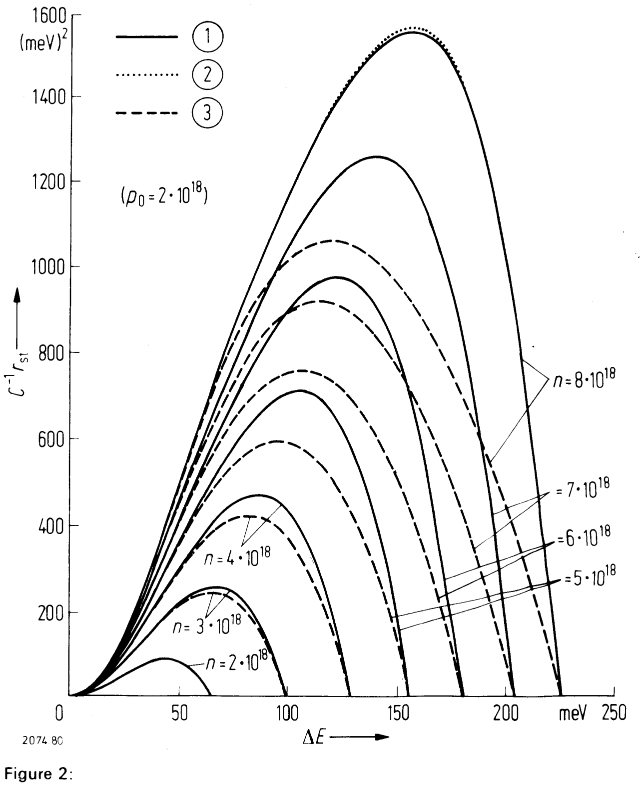

Figure 2:
Spectral dependence of the stimulated emission rate for 2×10^{18} cm^{-3} p-doped GaAs after eq. (20) with sum extended to $\nu=10$ (1), containing only the $\nu=0$ term (2) and calculated from Marinelli's approximation [4] (3).

2. Discussion

The series expansion eq. (20) gives the exact solution of the integral in eq. (1). At room temperature a very good approximation is obtained even when the series expansion is broken off after a few steps. Figure 2 shows the spectral dependence of the stimulated emission rate for p-doped material with net hole concentration $p_0=2\times10^{18}$ cm^{-3} and different electron densities n. The result for summing up to $\nu=10$ is exact within four digits. For comparison the result of Marinelli's approximation is plotted as well as for $n=8\times10^{18}$ cm^{-3} the result obtained by breaking the summation in eq. (20) after $\nu=0$.

The incorporation of an energy dependent transition probability according to [2, 3] could be possible as follows: Such energy dependence yields an additional factor in the integral (5) which is a sum of terms of the form $P(x)\cdot(x-z_i)^{-m}$ where $P(x)$ is a polynomial with the order "equal or less m". The way of computation is now straighforward when in eqs. (11) to (15) the m-fold poles at z_i are considered as well.

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