Derivation of analytical expressions for optical gain coefficient in bulk semiconductors

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An analytical model is proposed to determine expressions of the semiconductor optical gain coefficient by using special functions. These expressions differ from standard numerical calculation approaches and they involve sums of polylogarithm and incomplete gamma functions. The new formula obtained here provides a sufficient method to calculate the semiconductor optical gain for total carrier density and temperature in semiconductor lasers. The obtained analytical expression gives an accurate and precise evaluation of the semiconductor gain function. The performance of the proposed formula is confirmed by its implementation for the different parameter values. The sufficiency of the obtained results using this approach is confirmed by other data from the literature.

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1. Introduction

An important problem in physics is to investigate the physical and chemical properties of semiconductor lasers. It is well known that, semiconductor lasers-which have complex multi-layer structures requiring nanometer-scale precision and attentive design-play an important role in electronic communications, especially as a natural transmitter of digital data and an interface for fiber optic cables [1-4]. Theoretical and experimental studies on semiconductor lasers have been conducted for years by many researchers. Many effective and useful pieces of knowledge have been obtained from suggested theoretical and experimental studies. Kaftroudi and Mazandarani investigated a new asymmetric waveguide structure with an InP-based laser diode with InGaAsP in nano dimensional structures that are used in the semiconductor laser industry [5]. Elamathi et al studied different dielectric environment matrices of InP/ZnS core/shell quantum dot on the optical gain coefficient in nano-hetero-structures [6]. Karaliunas et al are analyzed the optical gain coefficient for MBE-grown ZnO in nanostructures [7]. Suemune et al. studied a photopumped ZnSe/ZnSSe blue semiconductor and theoretically calculated optical gain [8]. Liau et al. investigated microlens in GaAs and GaP for integrating with diode laser [9]. Also, Liu conducted work on the masstransport production of effective microlenses, mirrors, and monolithic integrated diode lasers [10]. Gavrielides et al. analytically suggested the stability boundaries of a semiconductor laser [11]. Mukai et al. experimentally investigated semiconductor laser diodes [12]. Duarte et al. studied the monochromatic solutions of a semiconductor laser and its stability [13]. Zhang et al. proposed a new method to drive semiconductor lasers for optical frequency standard based on constant voltage source [14]. Bao et al. WDM-based bidirectional suggested chaotic communication for a semiconductor laser system [15]. Mahmoud et al. presented a theoretical work on the effect of intermodal asymmetric gain suppression on the dynamics and output of multimode semiconductor lasers [16]. Semiconductor laser theoretical definition is significant not only from a general point of view, but also to generate new and advanced designs. A theoretical analysis and prediction of laser action based on a semiconductor diode was proposed for the first time in [17, 18]. As is well known, the notion of a semiconductor laser was introduced by Basov et al. [17]. Basov et al. presented a work on quantum mechanical semiconductors [17]. Basov et al. conducted a study on the production of negative-temperature cases in P-N junctions of degenerate semiconductors [18]. When compared with other lasers, the main advantage of a semiconductor laser is a high optic gain and variation in the refractive index of the medium brings a change in the gain [19, 20]. Optical gain, which defines optical amplification in the semiconductor material, is the most significant requirement for the realization of a semiconductor laser. Therefore, an efficient calculation method is important to calculate semiconductor gain for total carrier density and temperature in semiconductor lasers. To our knowledge, there is only one study related to analytical evaluation of the semiconductor optical gain coefficient in the literature [21]. As can be seen from [21], the semiconductor optical gain coefficient can be evaluated fully analytically with the help of a binomial expansion theorem in the case of q > p and s < 0. We note that numerical methods including integral forms [21-26] have been applied for approximate evaluation of the semiconductor optical gain coefficient [27-31]. It is well known that numerical integration methods give correct results for a restricted range of parameters and are not convenient for most circuit designers because they are time-consuming [32-37]. Researchers have used various numerical processes to handle these insufficiencies. However, these integrals cannot be solved completely due to some limitations. The numerical processes avoid parameter limits but cannot be applied to a

wide range of parameters [38]. Therefore, numerical integration methods give accurate results for a limited range of parameters. Further, the numerical processes do not offer complete solutions. Therefore, computational accuracy and sensitivity of the evaluation of semiconductor optical gain coefficient is a very significant piece of this kind of work.

This study presents a new analytical method for calculating the semiconductor optical gain coefficient for cases of arbitrary values of parameters. By using series expansion formulas, the calculation of the semiconductor optical gain coefficient was reduced to basic special evaluation functions. The obtained formulas seem to be easy to use when making the numerical calculation and, in this sense, the results would be useful for application in a realistic system. As an application, the optical gain of GaAs that is used in microlens fabrication has calculated using the semiconductor gain functions.

2. Analytical expression for the semiconductor optical gain coefficient

The theoretical definition of semiconductor laser properties has been investigated according to the Free-Carrier theory and Fermi–Dirac distributions. By using the Free-Carrier theory and Fermi–Dirac distributions, the authors of [39, 40] presented the following significant relation for the optical gain coefficient:

$$g = \frac{v \left|\mu_{k}\right|^{2} h\gamma}{4\pi^{2} \varepsilon_{0} nc} \left(\frac{2m_{r}}{h^{2}}\right)^{3/2} \int_{0}^{\infty} \frac{f_{e}(x) - f_{v}(x)}{\left(h\gamma\right)^{2} + \left(x - h\delta\right)^{2}} \sqrt{x} dx \qquad (1)$$

where h is the Planck constant, γ is the homogeneous line width factor, n is the refractive index, m_r is the reduced mass, and f_{α} is the electrons and valance band Fermi-Dirac distribution, defined as:

$$f_{\alpha}(x) = \frac{1}{\exp\left[\beta\left(\frac{m_{r}}{m_{\alpha}}x - \mu_{\alpha}\right)\right] + 1}$$
(2)

where μ_{α} is the carrier quasi-chemical potential, $\beta = 1/kT$, $\alpha \equiv v$, and *e* corresponds to the electrons and valance band. The optical gain coefficient, considering Eq. (2) in Eq. (1), can be expressed as:

$$g = \frac{v |\mu_k|^2 h\gamma}{4\pi^2 \varepsilon_0 nc} \left(\frac{2m_r}{h^2}\right)^{3/2} \left[e^{\beta \mu_e} Q(h\gamma, h\delta, \beta m_r / m_e, \beta \mu_e) + e^{\beta \mu_r} Q(h\gamma, h\delta, \beta m_r / m_h, \beta \mu_e) \right]$$
(3)

where Q is the semiconductor gain function, which can be written as:

$$Q = (p, q, r, s) = \int_{0}^{\infty} \frac{\sqrt{x}}{\left[p^{2} + (x - q)^{2}\right] \left(e^{rx} + e^{s}\right)} dx \qquad (4)$$

In the quantum statistical theory of semiconductor gain, the correct assessment of the semiconductor gain function is of major significance because they are very susceptible to little errors [21, 39-42]. Also, it is important to note that the accurate assessment of the semiconductor optical gain coefficient is dependent on the evaluation of Q functions. Therefore, the choice of reliable expressions for the semiconductor gain function is of major significance for accurate and precise calculations of the optical gain coefficient. To evaluate the semiconductor optical gain in Eq. (4), we use the exponential series expansion and binomial expansion theorems, according to [43], as follows:

$$e^{\pm x} = \sum_{k=0}^{\infty} (\pm 1)^k \, \frac{x^k}{k!},\tag{5}$$

$$(x \pm y)^{n} = \sum_{m=0}^{n} (\pm 1)^{m} F_{m}(n) x^{n-m} y^{m}$$
(6)

where $F_m(n)$ is the binomial coefficients, described by

$$F_m(n) = \begin{cases} \frac{n(n-1)\dots(n-m+1)}{m!} & \text{for integer n} \\ \frac{(-1)^m \Gamma(m-n)}{m! \Gamma(-n)} & \text{for noninterger n} \end{cases}$$
(7)

The analytical expressions for the semiconductor optical gain coefficient were derived using the series expansion as follow:

$$Q(p,q,r,s) = \lim_{N \to \infty} \sum_{i=0}^{N} \sum_{j=0}^{N^{i}} (-1)^{i+j} F_{j}(i) (2q)^{j}$$

$$\left(p^{2} + q^{2}\right)^{-(1+i)} T_{2i-j+1/2}(r,s)$$
(8)

where $F_j(i)$ is the binomial coefficient and $T_m(r,s)$ is the auxiliary function defined as:

$$T_m(r,s) = \int_0^\infty \frac{x^m}{e^{rx} + e^s} dx.$$
 (9)

The auxiliary functions $T_m(r, s)$ can be expressed as:

$$T_m(r,s) = -\frac{\Gamma(m+1)Li_{m+1}(-e^s)}{e^s r^{m+1}}$$
(10)

for s > -1

$$T_{m}(r,s) = \frac{1}{r^{m+1}} \left[\frac{s^{m+1}}{m+1} + \lim_{N \to \infty} \sum_{l=0}^{N} (-1)^{l+m} e^{-s(1+l)} \right]$$
$$\frac{\gamma(m+1,-ls)}{l^{m+1}} + \lim_{N' \to \infty} \sum_{k=0}^{N'} (-1)^{k} e^{ks} \frac{\Gamma(m+1,(k+1)s)}{(k+1)^{m+1}} \right] (11)$$

The special functions $Li_n(x)$, $\Gamma(\alpha, x)$, and $\gamma(\alpha, x)$ occurring in Eqs. (10) and (11) are the incomplete polylogarithm and incomplete gamma functions and are defined as, respectively, [43]:

$$Li_n(x) = \frac{1}{\Gamma(n)} \int_0^\infty \frac{t^{n-1}}{e^t/x - 1} dt$$
(12)

$$\Gamma(\alpha, x) = \int_{x}^{\infty} t^{\alpha - 1} e^{-t} dt$$
 (13)

$$\gamma(\alpha, x) = \int_{0}^{x} t^{\alpha - 1} e^{-t} dt$$
 (14)

3. Numerical results and discussion

It is most important to evaluate the semiconductor gain coefficient for semiconductor lasers. Therefore, we have presented efficient methods for the analytical evaluation of the integral semiconductor gain function. An approximation of the analytical assessment of optic gain function has been derived and applied. The analytical formula was evaluated by the solution of Eq. (4) that was calculated quickly using series expansion theorems. The method is based on exponential and binomial expansion series formulas that establish an analytical solution in the form of a convergent series. The application of the semiconductor gain function is performed mostly using a numerical approach to calculation of important parameters and ensures the required results. In order to compare correctness and precision, numerical integration, available literature data [21], and the suggested analytical formulas were applied in Mathematica Software 7.0. To show the precision and accuracy of the analytical expression, we have presented several calculations of semiconductor gain function. The precision of the proposed method is admissible and can be propounded for the evaluation of the optical gain coefficient. By comparing the results of calculation with numerical integration and literature data [21], we demonstrate the validity of the given results. The obtained results are given in Tables 1-2. As seen in Table 1-2, the analytical expression is correct within a range of wide

parameters. The results in Tables 1-2 indicate that the method is extremely accurate and suitable for comparison purposes. As seen from Tables 1-2, the results obtained from the semiconductor gain function are in very good agreement with numerical integration results and theoretical data [21]. As seen from Table 2, the results of the calculation of the analytical expression are in very good agreement with the numerical integral calculation. Good agreement with analytical, theoretical, and numerical values has raised the reliability of our obtained analytical formula. Table 3 shows that the convergence properties of Eq. (8) and [21] are considered to change widely. As seen from Table 3, Eq. (8) shows more rapid convergence to the numerical results than [21] results for various values of parameters. Iim demonstrates the upper limit of the series.

Given that we achieved the requested correctness, the upper limit of the infinite series was adjusted to that value. As seen from Table 3, the upper limit values N = N' = 60 of summations of the analytical expressions provide the most suitable convergence for arbitrary values of parameters. Also, Table 3 displays the most rapid convergence to the numerical result, with seventeen digits stable and correct by the fiftieth term for infinite summations. The CPU times of Eq. (8) cannot be illustrated in the tables due to the use of various computers in the literature for the assessments. The analytical formula gives convincing CPU times. As an example, in the case of the analytical formula for semiconductor optical gain, numerical integration and [21] are about 7.550, 0.016, and 17.566 ms, respectively. All computations were made using Eq. (8) for N = 60, the upper limits of the series. To demonstrate application in physics, optical gain for GaAs was calculated using the analytical formula obtained for semiconductor gain functions. As an application, the energy dependence on the optical gain coefficient for GaAs was demonstrated in Fig. 1 and compared with numerical results and [21]. Also, Fig. 1 shows that the optical gain changes exponentially as the energy increases. As seen from Figure 1, the analytical expression gives values closer to numerical calculations in from -0.0194 to 0.04 range of energy. However, with increasing values of energy, the agreement with the numerical results decreases. The optical gain of different values of γ is plotted and shown in Fig. 2. As seen in Fig. 2, the peak gain reduces with increasing γ . As seen in Fig. 2, the desired curve for the optical gain coefficient was obtained for different values of γ using Eq. (8). The parameter values are $v = 10^9 s^{-1}$, $h = 6.58.10^{-16} eVs$, $\gamma = 10^{12} s^{-1}$, n = 3.6, $c = 10^{18} A s^{-1}$, $m_a = 0.066 m_0$, $m_r = 0.056m_0$, $m_h = 0.52m_0$, $\mu_e = -1.17eV$, $\mu_v = -0.27eV$, and kT = 0.025 eV [44]. The different values of γ give different curves for gain coefficient. γ is defined homogeneously and in the homogeneously broadened limit where the gain spectrum is the product of the density of state. For example, curves is shown inhomogeneously broadened limit for $\gamma \rightarrow 0$. The curves shown that $\gamma \rightarrow 10^{12}$ and $\gamma \rightarrow 10^{13}$ is much closed to inhomogeneously

broadened limit and gives a importantly different curve from that at inhomogeneously broadened limit in Fig. 2, respectively. As seen from Fig. 2, the peak optical gain decreases generally as γ increases.

Table 1. Comparative calculation results of Qig(p,q,r,sig) semiconductor gain function

р	q	r	S	Eq.(8)	Ref.[21]	Mathematica Numerical Results
5.2	2.6	4.5	-0.2	2.3057694655302776672 ×10 ⁻³	2.3057521070563379×10 ⁻³	2.305752106867286450×10 ⁻³
8.5	2.4	3.5	-0.6	$1.5097886900053914664 \times 10^{-3}$	1.5097886898999967×10 ⁻³	1.509788689899996769×10 ⁻³
12	11	10	-0.6	9.10083926566079244 ×10 ⁻⁵	9.10083926534021059×10 ⁻⁵	9.1008392653402108×10 ⁻⁵
18.5	12.4	13.5	-0.8	3.1574477043853786 ×10 ⁻⁵	3.157447704385142307×10 ⁻⁵	3.1574477043851413×10 ⁻⁵
23.8	15.2	15.6	-0.9	1.5961348806248191 ×10 ⁻⁵	1.596134880624276426×10 ⁻⁵	1.5961348806242761×10 ⁻⁵
25.2	22.6	21.5	-0.95	6.8970202955913217×10 ⁻⁶	6.897020295591316584×10 ⁻⁶	6.897020295591307273×10 ⁶
31.8	22.6	14.5	-0.4	8.7174752921092952533384×10-6	8.164666180471492413×10 ⁻⁶	8.717475145766489230×10 ⁶
43.1	32.2	24.1	-0.45	$2.1522973513670842630927 \times 10^{-6}$	2.1522973435973320475×10 ⁻⁶	2.152297343597333768×10 ⁻⁶

Table 2. Comparative calculation results of Qig(p,q,r,sig) semiconductor gain function

р	q	r	S	Eq.(8)	Mathematica Numerical Results
6.2	3.6	4.3	-0.2	1.62182136204011×10 ⁻³	1.62180917327795×10 ⁻³
7.2	2.6	5.3	-0.5	1.0638314441811×10 ⁻³	1.06383144337586×10 ⁻³
12.5	11.5	10	-0.55	8.29608538287100×10 ⁻⁵	8.29608538163736×10 ⁻⁵
17.2	15.3	13	-0.8	3.13123019536×10 ⁻⁵	3.13123019536565×10 ⁻⁵
21.3	17.6	16	-0.25	1.46370748786195×10 ⁻⁵	1.46370501167247×10 ⁻⁵
28.7	25.6	21	-0.6	5.3004263127510×10 ⁻⁶	5.30042631256278×10 ⁻⁶
33.2	28	18	-0.9	5.43779648898374×10 ⁻⁶	5.43779648898101×10 ⁻⁶
46.1	40.9	20.5	-0.7	2.16703097270170891×10 ⁻⁶	2.16703097269828×10 ⁻⁶
50	45	42	-0.75	6.2362583941772714×10 ⁻⁷	6.23625839417505×10 ⁻⁷
56	48	53	-0.85	3.702850248778548×10 ⁻⁷	3.70285024877852×10 ⁻⁷
63.5	42.5	56	-0.65	3.09772040337034×10 ⁻⁷	3.0977204033940×10 ⁻⁷

Table 3. Convergence of expressions Eq. (8) and Ref.[21] for Q(p,q,r,s) as functions summation limits N and N

	p=41.8; q=33.4; r=26.1; s=-0.6				
N = N [']	Eq.(8)	Ref.[21]			
10	1.974012757269492427E-6	1.987636228528209097E-6			
20	1.973961647286595178E-6	1.974109572306391665E-6			
30	1.973961597207667714E-6	1.973963204675267484E-6			
40	1.973961597137428482E-6	1.973961614618339203E-6			
50	1.973961597137313157E-6	1.973961597327549767E-6			
60	1.973961597137312950E-6	1.973961597139384618E-6			
70	1.973961597137312950E-6	1.973961597137335525E-6			



Fig. 1. Optical gain change according to energy $(h\delta)$ for GaAs (color online)



Fig. 2. Optical gain of GaAs. $\gamma = 10^{12}$ (green line) and $\gamma = 10^{13}$ (blue line) (color online)

In consequence, a new analytical expression for the computation of optical gain in semiconductor lasers is presented in this work. The novelty of this work is that it is more efficient and computes accurately the semiconductor gain function in arbitrary parameter values. The newly obtained analytical formula for the semiconductor optical gain coefficient adequately prevents calculation challenges.

4. Conclusions

In this work, we derived an explicit and efficient analytical formula for the semiconductor gain function. The results from the analytical formula for arbitrary values of parameters are in good agreement with numerical results and literature data. These calculations are widely used for semiconductor lasers. In conclusion, for arbitrary values of parameters, the analytical formula offers the advantage of direct and precise calculation of the semiconductor gain function.

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