Fully analytical evaluation of optical gain coefficient in bulk semiconductors in quasi-equilibrium free-carrier approximation

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In this letter, a new analytical method is presented to calculate of the semiconductor optical gain coefficient. This method is particularly suitable for theoretical analyses to determine the dependence of semiconductor gain on the total carrier density and temperature in the semiconductor lasers. Also, the optical gain functions for semiconductor optical gain coefficient are presented analytically. The analytical evaluation is verified with numerical methods, which illustrates the accuracy of these obtained analytical expressions.

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The Free-Carrier theory and the Fermi-Dirac distribution played a significant role in the investigation of optical gain in semiconductor lasers. It is well known, the concept of a semiconductor laser was introduced by Basov et al.^[1] who suggested that stimulated emission of radiation could occur in semiconductors by the recombination of carriers injected across a p - n junction^[2,3]. The semiconductor lasers have a wide range of applications in the optical-fiber communication and the optical memory (audio and video discs) industry^[4-9]. Evaluating theoretically the semiconductor gain coefficient is significant for semiconductor laser. In studies^[3-5] the authors have discussed the main properties of the semiconductor laser and provided the background for constructing useful theoretical models. Therefore, accurate evaluation of semiconductor gain is important in different areas of science. For evaluating the semiconductor gain, a generalized optical gain coefficient is obtained, which may be written in terms of the optical gain functions. Although the theoretically evaluation of optical gain coefficient has been in literature^[10-26] for a long time, there has been no actual analytical evaluation attempt so far.

In this letter, we will deduce the analytical expression of the semiconductor laser optical gain function. The results allow a direct evaluation of the dependence of semiconductor gain on the total carrier density and temperature. Moreover, the formulas can be easily implemented with an algebraic computer language. The results are compared with those obtained according to one of the Mathematica numerical integration results. As an example of the effectiveness of the method we present the calculation results of the optical gain of the GaAs.

The theoretically evaluation of semiconductor lasers properties have been analyzed based on the Free-Carrier theory and the Fermi-Dirac distributions^[3-5]. The use of the Free-Carrier theory and the Fermi-Dirac distributions gives the following relation for the optical gain coefficient^[2,4]:

$$g = \frac{\nu \left|\mu_k\right|^2 \hbar\gamma}{4\pi^2 \varepsilon_0 nc} \left(\frac{2m_{\rm r}}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{f_e(x) - f_v(x)}{(\hbar\gamma)^2 + (x - \hbar\delta)^2} \sqrt{x} \,\mathrm{d}x, \quad (1)$$

where n is refractive index, γ is homogeneous line width factor, $m_{\rm r}$ is the reduced mass, and the energy-dependent Fermi-Dirac distribution is given by

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

where $\beta = \frac{1}{kT}$, μ_{α} is the carrier quasi-chemical potential, where $\alpha \equiv v$ and e for the electrons and valance band. Taking into account Eq. (2) in Eq. (1), generally we can rewrite Eq. (1) in the following form:

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

The quantity Q occurring in Eq. (3) are semiconductor gain function generally defined as

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

Quantum statistical theory of semiconductor gain requires the more accurate evaluation of semiconductor gain function because they are very sensitive to the minor errors. In order to establish expressions for the semiconductor gain functions we shall first consider the well known binomial expansion theorems as follows $(x \ge y)^{[27,28]}$:

$$(x \pm y)^n = \lim_{N \to \infty} \sum_{m=0}^N (\pm 1)^m F_m(n) x^{n-m} y^m, \quad (5)$$

where $F_m(n)$ are binomial coefficients defined by

$$F_m(n) = \begin{cases} \frac{n(n-1)\dots(n-m+1)}{m!} & \text{for integer } n\\ \frac{(-1)^m \Gamma(m-n)}{m! \Gamma(-n)} & \text{for noninteger } n \end{cases}$$
(6)

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Inserting Eq. (5) into Eq. (4) we obtain the series expansion formulae for the semiconductor gain functions in terms of binomial coefficients: for q > p > 0

 $Q(p,q,r,s) = \lim_{\substack{L \to \infty \\ M \to \infty}} \sum_{i=0}^{L} F_i(-1)e^{is} \sum_{j=0}^{M} \frac{F_j(-1)}{p^{2j+1}} \sum_{k=0}^{2j} \frac{F_k(2j)q^k \Gamma(2j-k+3/2)}{[(i+1)r]^{2j-k+3/2}},$ (7)

for p = 0 and q = 0

$$Q(p,q,r,s) = \lim_{L' \to \infty} \sum_{i=0}^{L'} F_i(-1)e^{is}\sqrt{(i+1)r}\,\Gamma(-1/2), \quad (8)$$

$$Q(p,q,r,s) = \lim_{L \to \infty} \sum_{n=0}^{L} F_n(-1)e^{is} \operatorname{Re}[K_{n+1}(p,q,r)]. \quad (9)$$

The quantities $K_m(p,q,r)$ in Eq. (9) determined by the relation

$$K_m(p,q,r) = \int_0^\infty \frac{\sqrt{x} e^{-mrx}}{p^2 + (x-q)^2} dx.$$
 (10)

For particular values of parameters for which the Q(p,q,0,0) and $K_m(p,q,r)$ functions exists in Eqs. (3) and (9), the program Mathematica gives the following results, respectively:

$$Q(p,q,0,0) = -\frac{i}{4p} \Big\{ 2\pi \sqrt{ip-q} + \sqrt{q+ip} \Big[\ln \Big(-\frac{1}{\sqrt{q+ip}} \Big) + \ln(q+ip) \Big] \Big\},$$
(11)

$$K_{m}(p,q,r) = -\frac{i\pi e^{-(m+1)(q+ip)r}}{2p} \Big[e^{2i(m+1)rp} \sqrt{ip-q} \\ \operatorname{Erfc} \Big[\sqrt{(m+1)(ip-q)r} \Big) - \sqrt{-q-ip} \\ \operatorname{Erfc} \Big(\sqrt{-(m+1)(q+ip)r} \Big) \Big],$$
(12)

where $i = \sqrt{-1}$. The quantities $\Gamma(\alpha)$ and $\operatorname{Erfc}(x)$ in Eqs. (7) and (12) are well known familiar functions defined by^[27]

$$\Gamma(\alpha) = \int_{0}^{\infty} t^{\alpha - 1} e^{-t} \mathrm{d}t, \qquad (13)$$

$$\operatorname{Erfc}(x) = \frac{2}{\sqrt{\pi}} \int_{x}^{\infty} e^{-t^2} \mathrm{d}t.$$
 (14)

In Eqs. (5), (7), (8), and (9) the indices N, L, L', and M are the upper limits of summations.

An approach for the analytical evaluation of optic gain function has been derived and implemented. By using the binomial expansion theorem, we obtained an exact closed-form expression of the optic gain functions and the expression is written in terms of the binomial coefficients and incomplete Gamma functions. All calculations were performed on Mathematica 7.0 supporting programming. The desktop computer with typical configuration, Pentium, Intel (R), 2.20 GHz, 1.0 GB RAM, was utilized. The results are listed in Table 1. To verify the representations that we obtained for various cases, we compared the results of the new formulations with the results of a direct Mathematica numerical integration technique. As can be seen in Table 1, the values of the optic gain function calculated with these two analytical and numerical methods are in very good agreement. Using the new decomposition the obtained results are presented in Table 2 to demonstrate the improvements in convergence rates. Greater accuracy is attainable by the use of more terms in expansions of Eqs. (7) and (9). Thus, the performance of the present formulations for optic gain functions is satisfactory for s < 0. In this letter, for the first time to our knowledge, we calculate the semiconductor optical gain coefficient analytically for all parameters satisfying Eqs. (7) and (9).

As an application, the results of the optical gain calculation are shown in Fig. 1 for GaAs semiconductor. The best fitting procedure is performed at room temperature and the curve obtained with the parameters values

Table 1. Comparative Values of Q(p,q,r,s) Semiconductor Gain Functions for L = M = 80

p	q	r	s	Eqs. (9) and (11)	Mathematica Numerical Integration Results
5.2	2.6	4.5	-0.2	$2.3057521070563379\ \times 10^{-3}$	$2.305752106867286\ \times 10^{-3}$
8.5	2.4	3.5	-0.6	$1.5097886898999967\ \times 10^{-3}$	$1.5097886898999967\ \times 10^{-3}$
12	11	10	-0.6	$9.10083926534021059\ \times 10^{-5}$	$9.10083926534021059\ \times 10^{-5}$
18.5	12.4	13.5	-0.8	$3.157447704385142307 \times 10^{-5}$	$3.157447704385142307\ \times 10^{-5}$
23.8	15.2	15.6	-0.9	$1.596134880624276426\ \times 10^{-5}$	$1.596134880624276426\ \times 10^{-5}$
25.2	22.6	21.5	-0.95	$6.897020295591316584\ \times 10^{-6}$	$6.897020295591316584\ \times 10^{-6}$
8.5	6.7	0.0	0.0	1.09401105037167612	1.0940110503716761
18.5	16.7	0.0	0.0	0.77469039032834205	0.7746903903283421
31.8	41.6	0.0	0.0	0.67714915904714389	0.6771491590471439
31.8	22.6	14.5	-0.4	$8.164666180471492413\ \times 10^{-6}$	$8.164666180471492413\ \times 10^{-6}$
43.1	32.2	24.1	-0.45	$2.1522973435973320475\ \times 10^{-6}$	$2.1522973435973320479\ \times 10^{-6}$

Table 2. Convergence of Derived Expressions Eqs. (7) and (9) for Q(p,q,r,s) as a Function of Summation Limits L = M

L = M	p = 41.8; q = 33.4; r = 26.1; s = -0.6 Eq. (9)	p = 18.4; q = 13.6; r = 11.8; s = -0.06 Eq.(7)
10	$1.987636228528209097\ \times 10^{-6}$	$3.37136295616455221\ \times 10^{-5}$
20	$1.974109572306391665\ \times 10^{-6}$	$3.36684346718376754\ \times 10^{-5}$
30	$1.973963204675267484\ \times 10^{-6}$	$3.366666840550732733\ \times 10^{-5}$
40	$1.973961614618339203\ \times 10^{-6}$	$3.36665859387207483\ \times 10^{-5}$
50	$1.973961597327549767\ \times 10^{-6}$	$3.36665794716173479\ \times 10^{-5}$
60	$1.973961597139384618\ \times 10^{-6}$	$3.36665790045493919\ \times 10^{-5}$
70	$1.973961597137335525\ \times 10^{-6}$	$3.36665789687768251\ \times 10^{-5}$
80	$1.973961597137313196\ \times 10^{-6}$	$3.36665789659226324\ \times 10^{-5}$

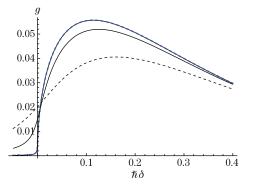


Fig. 1. (Color online) Optical gain (g) dependence of the energy ($\hbar\delta$). The solid line represents the numerical results, and the thick dashed line is the fitting line by the analytical method for $\gamma = 10^{12} \text{ s}^{-1}$. The curves are for homogeneous line width factors $\gamma = 2 \times 10^{12}$ (black solid) and 10^{13} s^{-1} (black dashed).

 $\nu = 10^9 \text{ s}^{-1}$; $\hbar = 6.58.10^{-16} \text{ eVs}$; $\gamma = 10^{12} \text{ s}^{-1}$; n = 3.6; $c = 10^{18} \text{ As}^{-1}$; $m_e = 0.066m_0$; $m_r = 0.056m_0$; $m_h = 0.52m_0$; $\mu_e = -1.17 \text{ eV}$; $\mu_v = -0.27 \text{ eV}$; $E_g = -1.43 \text{ eV}$; kT = 0.025 eV. Figure 1 show that the peak optical gain decreases with the increasing of γ homogeneous line width factors value. The close agreement between analytical and numerical values seems to give rise to more reliability of our obtained formulae.

In conclusion, we introduce a new analytical formula for calculation of the optical gain in semiconductor lasers. The newly derived analytical expression for the semiconductor optical gain coefficient well avoids the computational difficulties.

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