

Kinetic theory of quantum cascade lasers

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The kinetics of the behavior of nonequilibrium electrons in a quantum cascade laser, which take into account the strong interaction of the electrons with optical phonons, is investigated. A system of kinetic equations for the distribution functions of the electrons and nonequilibrium phonons is obtained, and its exact solution is found. It is shown that optical phonons accumulate and are reabsorbed with resultant smearing of the electron energy distribution and an additional increase in the threshold current, which is already very high due to the interband emission of optical phonons in a quantum cascade laser. The possibility of lowering the threshold current by increasing the effective lifetime of the electrons in the upper subband as a result of the reabsorption of phonons and the buildup of electrons in the lower subband at energies which are multiples of the phonon energy is demonstrated. The threshold lasing conditions are also found with consideration of the nonparabolicity of the subbands. © 1995 American Institute of Physics.

1. INTRODUCTION

Semiconductor lasers (including diode lasers and *QW* lasers) operate on electron transitions between the valence band and the conduction band. The emission wavelength is determined by the width of the band gap. Although injected nonequilibrium electrons (or holes) fill a fairly large energy range, the radiative transitions occur in a narrow energy region near Fermi quasilevels. This is attributed to the different signs of the effective masses of the bands and restrictions imposed by the energy and momentum conservation laws.

A new type of semiconductor laser, which differs in a fundamental way from those mentioned above, was recently demonstrated in Ref. 1. The laser, which was called a quantum cascade laser by the authors, operates on electronic transitions between subbands in the conduction band (i.e., they use one type of carrier), which appear as a result of size quantization in the semiconductor heterostructure.

The work on the creation of such lasers began with the pioneering theoretical paper by Kazarinov and Suris,² and an appropriate review was presented in Ref. 1. The advantage of quantum cascade lasers stems from the possibility of tuning the emission wavelength from the infrared range to the submillimeter range. Quantum cascade lasers¹ were prepared by molecular epitaxy and consist of a set of quantum wells with approximately parallel energy subbands. As a result, the electrons undergoing radiative transitions between subbands (for example, $n=2$ and 1) emit photons of the same frequency Ω with an energy $\hbar\Omega = \varepsilon_{2p} - \varepsilon_{1p}$ (Fig. 1). Injected electrons accumulate in upper working level 2 and are rapidly emptied from lower working level 1 by resonant tunneling in an electric field (which is achieved by appropriately selecting the parameters of the quantum wells).

Despite some obvious merits, quantum cascade lasers are plagued by some significant shortcomings, primarily the

high values of the threshold current J_{th} (in Ref. 1 $J_{th} \approx 10^4$ A/cm²). They are due to the absence of a prohibition against intersubband electron transitions with phonon emission, as well as impurity and electron–electron scattering. In fact, the parallel character of the subbands (the identical sign of the mass) actually means that there is no band gap. The greatest contribution to these radiationless transitions is made by optical phonons (the corresponding lifetimes are $\tau_0 \approx 10^{-12} - 10^{-13}$ s). Therefore, the lifetime of an electron in the upper working level is very short (approximately two orders of magnitude shorter than in a semiconductor laser), and therefore large threshold injection currents are required to create the necessary population inversion. The short lifetime is responsible for another special feature of quantum cascade lasers, viz., the highly nonequilibrium state of the electrons. We recall that in interband semiconductor lasers the lifetime in the bands is large compared with the energy relaxation times. Hence follows the need for a kinetic approach to describe the energy relaxation of electrons in quantum cascade lasers.

The purpose of the present work is to investigate the kinetics of the behavior of nonequilibrium electrons in a quantum cascade laser with consideration of the strong interaction of the electrons with optical phonons. A system of kinetic equations for the distribution functions of the electrons and nonequilibrium phonons is obtained, and an exact solution is found. It is shown that optical phonons accumulate and are reabsorbed with resultant smearing of the electron energy distribution and an additional increase in the threshold current, which is already very high due to the interband emission of optical phonons.

At the same time, the possibility of lowering the threshold current by increasing the effective lifetime of the electrons in the upper subband as a result of the reabsorption of phonons and the buildup of electrons in the lower subband at

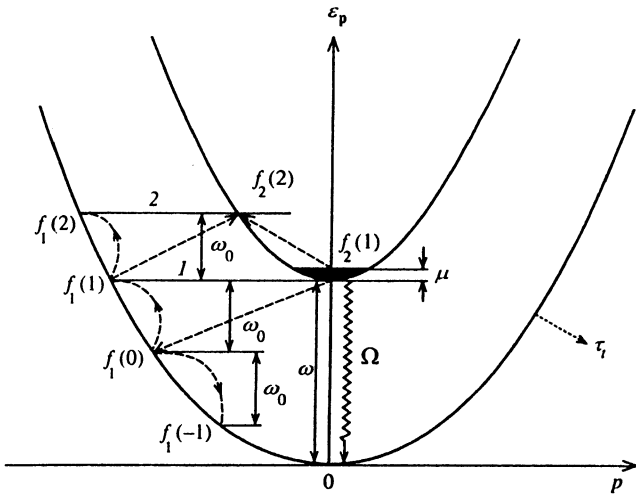


FIG. 1. Dependence of the energy of the subbands on the quasimomentum. The dashed lines correspond to transitions with the emission of an optical phonon, and the wavy lines correspond to transitions with the emission of a photon.

energies which are multiples of the optical phonon energy is demonstrated. This can be achieved by increasing the tunneling escape time τ_t of the electrons from the lower subband, for example, by increasing the thickness of the barrier.

The format of this paper is as follows. The model considered is described in Sec. 2, where the kinetic equations for the electrons and phonons, as well as expressions for the gain coefficient are derived. Sec. 3 is devoted to finding the threshold conditions for lasing in quantum cascade lasers with consideration of the nonparabolicity of the subbands. The transition is made from the integral kinetic equations to a system of coupled equations, and a solution is found for them in the absence of phonons in Sec. 4. An exact solution of the linearized system of equations is obtained in Sec. 5. The limiting values of the nonequilibrium phonon number and the distribution functions, as well as the threshold currents, are calculated in Sec. 6. In Sec. 7 the results are generalized to any lasing frequency. The electron-electron relaxation time is estimated in Conclusions.

2. FORMULATION OF THE PROBLEM AND BASIC EQUATIONS

The real scheme of a quantum cascade laser¹ is quite complex. To study only the kinetics of the energy relaxation between the two working subbands in the conduction band, we consider the following simplified model (see Fig. 1). Let there be two subbands with the energies ε_{2p} and ε_{1p} , between which transitions occur with the emission of photons having an energy $\hbar\Omega$. The subbands can belong to either one or several quantum wells (as for example, in Ref. 1). Electrons are injected into band 2 at a rate Q , which is much greater than the rate of the direct transition to a neighboring well. At the same time, the transition from band 1 (due to resonant tunneling) takes place with a fairly high probability τ_t^{-1} . Such conditions are achieved by appropriately select-

ing the parameters of the heterostructure (see Ref. 1). The injection rate is related to the injection current J by the expression

$$J = Q\mu\rho, \quad (1)$$

The interaction of electrons with phonons and electrons results in intraband and interband scattering. In $A^{III}B^V$ semiconductors the main contribution is made by the interaction with the optical phonons ($\tau_0 \approx 10^{-12} - 10^{13}$ s), so that the acoustic phonons can be neglected. As for electron-electron collisions, we shall discuss their contribution later on.

The Hamiltonian which describes the present model and takes into account the interaction of electrons with the resonant electromagnetic field $\mathbf{E}(t) = \mathbf{E} \cos \Omega t$ has the form (see, for example, Refs. 3 and 4)

$$H(t) = H_0(t) + H_{ph}, \quad (2)$$

where

$$H_0(t) = \sum_{\mathbf{p}} (\varepsilon_{2p} a_{2p}^+ a_{2p} + \varepsilon_{1p} a_{1p}^+ a_{1p} + \lambda a_{2p}^+ a_{1p} e^{-i\Omega t} + \lambda^* a_{1p}^+ a_{2p} e^{i\Omega t}),$$

$$H_{ph} = \sum_{n_1 n_2 \mathbf{p}_1 \mathbf{p}_2 \mathbf{q}} a_{n_1 \mathbf{p}_1}^+ a_{n_2 \mathbf{p}_2} [c_{\mathbf{q}} \Phi_{n_1 n_2}(\mathbf{p}_1 \mathbf{p}_2 \mathbf{q}) + c_{\mathbf{q}}^+ \Phi_{n_1 n_2}(\mathbf{p}_2 \mathbf{p}_1 \mathbf{q})] + \sum_{\mathbf{q}} \omega_{\mathbf{q}} c_{\mathbf{q}}^+ c_{\mathbf{q}},$$

$$n_{1,2} = 1, 2, \quad \hbar = c = 1, \quad (3)$$

where a_{1p}^+ , a_{2p}^+ , and $c_{\mathbf{q}}^+$ are, respectively, the creation operators of electrons in subbands 1 and 2 and of phonons, ε_{1p} and ε_{2p} are the energy spectra of the electrons in the first and second subbands,

$$\lambda = \frac{eE\mathbf{V}_{12}}{\Omega}, \quad \mathbf{V}_{1,2} = \frac{1}{m_0} \int \psi_{1p}^*(r) (-i\nabla) \psi_{2p}(r) d^3r \quad (4)$$

is the matrix element of the transition between subbands with the wave functions ψ_{1p} and ψ_{2p} , and m_0 is the free electron mass.

The Hamiltonian H_{ph} describes the interaction with phonons, $\Phi_{n_1 n_2}$ being the matrix elements for scattering within a band ($n_1 = n_2$) and between subbands ($n_1 \neq n_2$):

$$\Phi_{n_1 n_2}(\mathbf{p}_1 \mathbf{p}_2 \mathbf{q}) = G_{n_1 n_2}(q) \delta(\mathbf{p}_1 - \mathbf{p}_2 - \mathbf{q}). \quad (5)$$

According to Refs. 3 and 4, it is convenient to use the unitary transformation

$$U(t) = \exp \left[-\frac{i\Omega t}{2} \sum_{\mathbf{p}} (a_{2p}^+ a_{2p} - a_{1p}^+ a_{1p}) \right] \quad (6)$$

to make the transition to a representation in which H_0 does not depend explicitly on the time:

$$H_0 = U^+ H_0(t) U - iU^+ \frac{\partial U}{\partial t} = \sum_{\mathbf{p}} (a_{2p}^+ a_{2p} \xi_{2p} + a_{1p}^+ a_{1p} \xi_{1p} + \lambda a_{2p}^+ a_{1p} + \lambda^* a_{1p}^+ a_{2p}), \quad (7)$$

$$\xi_{2p} = \varepsilon_{2p} - \frac{\Omega}{c}, \quad \xi_{1p} = \varepsilon_{1p} + \frac{\Omega}{c}. \quad (8)$$

As we know, the output of a laser is determined by the gain coefficient (see, for example, Refs. 4 and 5)

$$\alpha(\Omega) = \frac{2\pi\Omega}{E^2} \sum_{\mathbf{p}} [\lambda^* \rho_{12}(\mathbf{p}) - \lambda \rho_{12}^*(\mathbf{p})], \quad (9)$$

where $\rho_{12}(\mathbf{p})$ is an off-diagonal element of the density matrix

$$\rho_{12}(\mathbf{p}) = \langle a_{2p}^+ a_{1p} \rangle,$$

which obeys the equation^{4,5}

$$\left(i \frac{\partial}{\partial t} + \xi_{2p} - \xi_{1p} \right) \rho_{12}(\mathbf{p}) = \lambda (f_{2p} - f_{1p}) - i \gamma(\mathbf{p}) \rho_{12}(\mathbf{p}). \quad (10)$$

Here $\gamma(\mathbf{p})$ is the damping of the off-diagonal density matrix, and the f_{ip} are the distribution functions of the electrons in subbands 1 and 2:

$$f_{1p} = \langle a_{1p}^+ a_{1p} \rangle, \quad f_{2p} = \langle a_{2p}^+ a_{2p} \rangle.$$

Equation (10) and the equations for f_{1p} and f_{2p} can be obtained by Bogolyubov's method.^{6,5} Here we shall not present the explicit form of the function $\gamma(\mathbf{p})$, which depends on the interaction matrix element and the electron distribution function. The magnitude of γ does not exceed (and can be smaller than) τ_0^{-1} and τ_i^{-1} and will henceforth be assumed not to depend on \mathbf{p} .

It is seen from (9) and (10) that the gain coefficient $\alpha(\Omega)$ depends on the supersaturation $f_{2p} - f_{1p}$. We shall find f_{ip} from the solution of the kinetic equations. Following Refs. 4 and 5, we obtain a system of equations for f_{1p} , f_{2p} , and $N_q = \langle c_q^+ c_q \rangle$:

$$\begin{aligned} \frac{\partial f_{1p}}{\partial t} = & -\frac{f_{1p}}{\tau_i} - \frac{1}{\tau_0 \rho} \sum_{\mathbf{p}'} \{ \delta(\varepsilon_{1p} - \varepsilon_{1p'} - \omega_q) [f_{1p}(1 - f_{1p'}) + N_q(f_{1p} - f_{1p'})] - \delta(\varepsilon_{1p'} - \varepsilon_{1p} - \omega_q) \\ & \times [f_{1p'}(1 - f_{1p}) + N_q(f_{1p'} - f_{1p})] + \delta(\varepsilon_{2p'} - \varepsilon_{1p} + \omega_q) [f_{1p}(1 - f_{1p'}) + N_q(f_{1p} - f_{2p'})] - \delta(\varepsilon_{2p'} \\ & - \varepsilon_{1p} - \omega_q) [f_{2p'}(1 - f_{1p}) + N_q(f_{2p'} - f_{1p})] \}, \end{aligned} \quad (11)$$

$$\begin{aligned} \frac{\partial f_{2p}}{\partial t} = & Q(\mathbf{p})(1 - f_{2p}) - \frac{1}{\tau_0 \rho} \sum_{\mathbf{p}'} \{ \delta(\varepsilon_{2p} - \varepsilon_{2p'} - \omega_q) \\ & \times [f_{2p}(1 - f_{2p'}) + N_q(f_{2p} - f_{2p'})] - \delta(\varepsilon_{2p'} - \varepsilon_{2p} - \omega_q) [f_{2p'}(1 - f_{2p}) + N_q(f_{2p'} - f_{2p})] + \delta(\varepsilon_{2p} \\ & - \varepsilon_{1p'} - \omega_q) [f_{2p}(1 - f_{1p'}) + N_q(f_{2p} - f_{1p'})] \\ & - \delta(\varepsilon_{1p'} - \varepsilon_{2p} - \omega_q) [f_{1p'}(1 - f_{2p}) + N_q(f_{1p'} - f_{2p})] \}, \end{aligned} \quad (12)$$

$$\begin{aligned} \frac{\partial N_q}{\partial t} = & -\frac{N_q - N_q(T)}{\tau_{\text{esc}}} + \frac{1}{\tau_0 \rho^2 \mu} \sum_{\mathbf{p}, \mathbf{p}'} \{ \delta(\varepsilon_{2p} \varepsilon_{2p'} - \omega_q) [f_{2p}(1 - f_{2p'}) + N_q(f_{2p} - f_{2p'})] + \delta(\varepsilon_{1p} \\ & - \varepsilon_{1p'} - \omega_q) [f_{1p}(1 - f_{1p'}) + N_q(f_{1p} - f_{1p'})] + \delta(\varepsilon_{2p} - \varepsilon_{1p'} - \omega_q) [f_{2p}(1 - f_{1p'}) + N_q(f_{2p} - f_{1p'})] + \delta(\varepsilon_{1p'} - \varepsilon_{2p} - \omega_q) \\ & \times [f_{1p'}(1 - f_{2p}) + N_q(f_{1p'} - f_{2p})] \}, \end{aligned} \quad (13)$$

$$\frac{1}{\tau_{\text{esc}}} = \frac{s}{4\nu d},$$

where $N_q(T)$ is the thermal phonon number, τ_{esc} is the phonon escape time from a region with the dimension d , s is the velocity of the phonons, ν is the coefficient of their penetrability through the barrier, τ_i is the escape time of the electrons (by means of resonant tunneling) from subband 1, Q is the rate of injection of electrons into subband 2, $\rho = m/2\pi$ is the density of states, m is the electron effective mass, $q = |\mathbf{p} - \mathbf{p}'|$, and $1/\tau_0$ is the probability of scattering on optical phonons:

$$\frac{1}{\tau_0} = \rho |G|^2, \quad G_{11} = G_{22} = G_{12} = G_{21} \equiv G, \quad (14)$$

which is assumed not to depend on the energy.

The terms that depend on the field \mathbf{E} , which is small near the threshold, were omitted in Eqs. (11) and (12). Equation (13) is needed to describe the intensity of the emission of the optical phonons, which can accumulate and play a significant role in the kinetics even at low temperatures.

The particle number and energy conservation laws can be obtained in the usual manner from Eqs. (11)–(13). In a stationary state they have the form

$$\tau_i \sum_{\mathbf{p}} Q(\mathbf{p})(1 - f_{2p}) = \sum_{\mathbf{p}} f_{1p}, \quad (15)$$

$$\sum_{\mathbf{p}} \varepsilon_{2p} Q(\mathbf{p})(1 - f_{2p}) = \sum_{\mathbf{p}} \frac{\varepsilon_{1p} f_{1p}}{\tau_i} + \frac{N\omega_0}{\tau_{\text{esc}}}. \quad (16)$$

Here we utilized the fact that the spectrum of optical phonons does not depend on q , i.e., $\omega_q = \omega_0$, and $N_q = N(\omega_0) \equiv N$.

3. LASING THRESHOLD

Solving Eq. (10) and substituting $\rho_{12}(\mathbf{p})$ into (9), we find the gain (absorption) coefficient $\alpha(\Omega)$ (per well):⁴

$$\frac{\alpha(\Omega)}{\alpha_0} = \frac{1}{\rho} \sum_{\mathbf{p}} \frac{\gamma(f_{2p} - f_{1p})}{(\xi_{2p} - \xi_{1p})^2 + \gamma^2}, \quad \alpha_0 = \frac{e^2 |V_{12}|^2}{\Omega \kappa}, \quad (17)$$

where κ is the dielectric constant.

Amplification ($\alpha > 0$) in a certain range of frequencies Ω becomes possible, if population inversion appears as a result of injection in a certain energy range, i.e., if

$$f_{2p} > f_{1p}, \quad 0 < \varepsilon < \mu, \quad \varepsilon = \frac{p^2}{2m}. \quad (18)$$

Lasing begins when $\alpha(\Omega)$ achieves a value of $1/\tau$, where τ is the lifetime of photon in the cavity (which is determined by the total losses). This first occurs at the frequency Ω_0 corresponding to the maximum of $\alpha(\Omega)$:

$$\left. \frac{\partial \alpha(\Omega)}{\partial \Omega} \right|_{\Omega=\Omega_0} = 0, \quad \alpha(\Omega_0, f_{th}) = \frac{1}{\tau}. \quad (19)$$

Conditions (19) determine the lasing frequency Ω_0 , the threshold gain coefficient, the threshold functions f_{2th} and f_{1th} , and, therefore, the threshold current $J_{th}(Q_{th})$.

Since the integrand in (17) depends only on ε , we rewrite $\alpha(\Omega)$ in the following form

$$\frac{\alpha(\Omega)}{\alpha_0} = \int_0^\infty \frac{d\varepsilon \gamma [f_2(\xi) - f_1(\varepsilon)]}{[\xi_2(\varepsilon) - \xi_1(\varepsilon)]^2 + \gamma^2}. \quad (20)$$

If we neglect the nonparabolicity of the subbands, the energies of the subbands in the effective mass approximation equal

$$\xi_2(\varepsilon) = \varepsilon + \omega - \frac{\Omega}{2}, \quad \xi_1(\varepsilon) = \varepsilon + \frac{\Omega}{2}, \quad (21)$$

where ω is the size-quantization energy between the subbands when $p=0$. The difference $\xi_2 - \xi_1 = \omega - \Omega \equiv \delta$ does not depend on the momentum. This means that photons are emitted over the entire population-inversion region, and expression (20) takes the form

$$\frac{\alpha(\Omega)}{\alpha_0} = \frac{\gamma}{\delta^2 + \gamma^2} \int_0^\infty d\varepsilon [f_2(\varepsilon) - f_1(\varepsilon)] = \frac{\gamma \mu}{\delta^2 + \gamma^2} \Delta f, \quad (22)$$

if it is assumed that

$$f_2 - f_1 = \begin{cases} \Delta f, & 0 < \varepsilon < \mu, \\ 0, & \mu < \varepsilon. \end{cases} \quad (23)$$

The gain coefficient maximum is achieved when $\delta=0$, $\Omega_0 = \omega$, and the value of

$$\frac{\alpha(\Omega)}{\alpha_0} = \frac{\Delta f \mu}{\gamma} \quad (24)$$

increases in proportion to μ/γ .

From threshold conditions (19) and (24) it is not difficult to determine the threshold value Δf_{th} :

$$\Delta f_{th} = \frac{\gamma}{\mu \tau \alpha_0}. \quad (25)$$

The nonparabolicity of the subbands restricts the lasing region. To illustrate this, we used the simplest approximation for the spectrum \mathcal{E} near the bottom of the conduction band in GaAs⁷

$$\mathcal{E} \left(1 + \frac{\mathcal{E}}{\mathcal{E}_g} \right) = \frac{p^2}{2m}, \quad (26)$$

where \mathcal{E}_g is the width of the band gap. Then, assuming that ε_{2p} and ε_{1p} correspond to the two lowest subbands of a deep quantum well, we find the difference

$$\xi_{2p} - \xi_{1p} = \delta - \frac{\beta p^2}{2m}, \quad \beta = \frac{2\omega}{\mathcal{E}_g}. \quad (27)$$

Assuming that equality (23) is again satisfied, for $\alpha(\Omega)$ we obtain

$$\frac{\alpha(\Omega)}{\alpha_0} = \frac{\Delta f}{\beta} \left(\arctan \frac{\delta}{\gamma} - \arctan \frac{\delta - \beta \mu}{\gamma} \right). \quad (28)$$

It is not difficult to see from (28) that the lasing frequency corresponding to the maximum of $\alpha(\Omega)$ equals

$$\Omega_0 = \omega - \frac{\mu \beta}{2}, \quad \delta_0 = \frac{\mu \beta}{2}, \quad (29)$$

i.e., it is shifted by $\mu\beta/2$.

The gain coefficient at Ω_0 ,

$$\frac{\alpha(\Omega_0)}{\alpha_0} = \frac{2\Delta f}{\beta} \arctan \frac{\mu \beta}{2\gamma}, \quad (30)$$

increases with increasing μ/γ , but at $\mu\beta > 2\gamma$ it subsequently reaches a limiting value

$$\frac{\alpha(\Omega_0)}{\alpha_0} = \frac{\Delta f \pi}{\beta}. \quad (31)$$

Using (31), we find the threshold value Δf_{th} with consideration of the nonparabolicity

$$\Delta f_{th} = \frac{\beta}{\pi \tau \alpha_0}. \quad (32)$$

The fact that the nonparabolicity restricts the range of energies from which lasing takes place is responsible for the insensitivity of $\alpha(\Omega_0)$ to the form of the electron distribution function at high energies.

In fact, let $f_{2p} - f_{1p} = \widetilde{\Delta f}$ be nonzero (and have either sign) when $\varepsilon = \omega_0$ in a range of width μ . We evaluate the contribution to $\alpha(\Omega_0)$, which we denote by $\widetilde{\alpha}(\Omega_0)$:

$$\begin{aligned} \frac{\widetilde{\alpha}(\Omega_0)}{\alpha_0} &= \widetilde{\Delta f} \int_{\omega_0 - \mu/2}^{\omega_0 + \mu/2} \frac{\gamma d\varepsilon}{(\delta_0 - \beta \varepsilon)^2 + \gamma^2} \\ &\approx \frac{\widetilde{\Delta f}}{\beta} \arctan \frac{\gamma \mu \beta}{\gamma^2 + \beta^2 \omega_0^2}. \end{aligned} \quad (33)$$

If $\omega_0 \beta / \gamma \gg 1$ and $\omega_0 \gg \mu$, for the ratio $\widetilde{\alpha}/\alpha$ we obtain (when $\widetilde{\Delta f} \sim \Delta f$)

$$\frac{\widetilde{\alpha}(\Omega_0)}{\alpha(\Omega_0)} \approx \frac{\widetilde{\Delta f} \mu \gamma}{\Delta f \omega_0^2 \beta} \ll 1. \quad (34)$$

The insensitivity of $\alpha(\Omega_0)$ to $\widetilde{\Delta f}$ at $\varepsilon \sim \omega_0$ is an important circumstance, since it is no longer necessary to rapidly remove the electrons from all of subband 1. If the case of "resonance," in which $\omega = n\omega_0$, $n=2, 3, \dots$, is ignored, the electrons do not fall into the "dangerous" range $0 < \varepsilon < \mu$ at the bottom of subband 1 when optical phonons are emitted, and consequently $f_{1p} = 0$ in that range. There-

fore, there is a possibility to increase τ_i and, as we shall see below, to significantly lower the threshold current.

4. ELECTRON DISTRIBUTION FUNCTIONS IN THE ABSENCE OF NONEQUILIBRIUM PHONONS

Relations (25) and (32) give us the threshold values Δf_{th} . To relate them to the threshold current $J_{th} \propto Q_{th}$, the solution of the system of kinetic equations (11)–(13) must be found. The influence of the interaction of the electrons with the equilibrium optical phonons on the threshold current was previously studied in Ref. 8.

If it is taken into account that the energy of an optical phonon and the matrix element of the electron–phonon interaction do not depend on the momentum (and if the small contribution of the nonparabolicity of the subbands is ignored here), the integral equations (11) and (12) can be reduced to a system of coupled equations. In addition, we shall assume that the source Q creates electrons in subband 2 in the energy range $\mu \ll \omega_0$:

$$Q(\varepsilon) = \begin{cases} Q, & \omega < \varepsilon < \omega + \mu, \\ 0, & \text{elsewhere.} \end{cases} \quad (35)$$

Then the electrons will concentrate in a range of width μ at the energies $\varepsilon = \omega \pm n\omega_0$, where n is an integer. For simplicity, we restrict ourselves to the situation in which $\omega_0 < \omega < 2\omega_0$ (the general case in Sec. 7). It is convenient to introduce the discrete variable n in the distribution functions:

$$f_1(\varepsilon) = f_1(\omega + (n-1)\omega_0) \equiv f_1(n), \\ f_2(\varepsilon) = f_2(\omega + n\omega_0) \equiv f_2(n), \quad n = 0, 1, 2, \dots \quad (36)$$

With consideration of the foregoing, the system (11) and (12) takes the form

$$f_1(0)[\xi + 2N + f_2(1) + f_1(1)] = (1+N)[f_1(1) + f_2(2)], \quad (37)$$

$$f_1(1)[\xi + 1 + 3N - f_1(0) + f_1(2) + f_2(2)] = Nf_1(0) + (1+N)[f_1(2) + f_2(2)], \quad (38)$$

$$f_1(n)[\xi + 2 + 4N - f_1(n-1) - f_2(n-1) + f_1(n+1) + f_2(n+1)] = N[f_1(n-1) + f_2(n-1)] + (1+N) \times [f_1(n+1) + f_2(n+1)], \quad (39)$$

$$f_2(1)[1 + 3N - f_1(0) + f_1(2) + f_2(2)] = Nf_1(0) + (1+N)[f_1(2) + f_2(2)] + \bar{Q}\xi[1 - f_2(1)], \quad (40)$$

$$f_2(n)[2 + 4N - f_1(n-1) - f_2(n-1) + f_1(n+1) + f_2(n+1)] = N[f_1(n-1) + f_2(n-1)] + (1+N)[f_1(n+1) + f_2(n+1)], \quad (41)$$

where $\bar{Q} = Q\tau_i$ and $\xi = \tau_0/\tau_i$. One more equation for N (13) should be added to this system. However, it is more convenient to use the equivalent equation (16) instead. Thus, we have a closed system of equations for $f_1(n)$, $f_2(n)$, and N .

Here and in the following we shall consider the case of $T=0$ and $N_q(T)=0$. The generalization to $T \neq 0$ presents no difficulty.

We first study the simplest situation, in which the non-equilibrium phonon number is small. As follows from (16), this is realized, if the phonon escape time τ_{esc} is small (exact criteria are presented below). Then the system (37)–(41) becomes simplified and reduces to two equations

$$f_1(0)[\xi + f_2(1)] = f_2(1), \\ f_2(1)[1 - f_1(0)] = \bar{Q}\xi[1 - f_2(1)], \quad (42)$$

$$f_1(1) = f_1(2) = \dots = f_1(n) = 0, \quad f_2(2) = \dots = f_2(n) = 0,$$

whose solution has the form

$$f_2(1) = \frac{1}{2} \left[- \left(\frac{1}{\bar{Q}} + \xi - 1 \right) + \sqrt{\left(\frac{1}{\bar{Q}} + \xi - 1 \right)^2 + 4\xi} \right], \quad (43) \\ f_1(0) = \frac{1}{2} \bar{Q} \left[\left(\frac{1}{\bar{Q}} + \xi + 1 \right) - \sqrt{\left(\frac{1}{\bar{Q}} + \xi - 1 \right)^2 + 4\xi} \right]. \quad (44)$$

Let us consider the limiting cases of weak and intense injection. For weak injection ($\bar{Q} \ll 1$), from (43) and (44) it is not difficult to find

$$f_2(1) \approx \bar{Q}\xi = Q\tau_0, \quad f_1(0) \approx \bar{Q}. \quad (45)$$

We see that the electron distribution function $f_2(1)$ is determined by the very short time τ_0 for the emission of an optical phonon. The corresponding threshold current

$$Q_{th} = \frac{1}{\tau_0} \begin{cases} \gamma/\mu\tau\alpha_0, & \beta\mu \ll \gamma, \\ \beta/\pi\tau\alpha_0, & \beta\mu \gg \gamma \end{cases} \quad (46)$$

is proportional to the probability of the emission of an optical phonon $1/\tau_0$, which accounts for its large value.

We note that in semiconductor lasers operating on interband transitions (see, for example, Ref. 4) the role of τ_0 is played by the interband recombination time, which is two orders of magnitude greater than τ_0 . We also note that in quantum cascade lasers¹ the ratio $\tau_0/\tau_i = \xi$ is great (~ 10), so that $f_1(0) \ll f_2(1)$. Such a ratio was chosen to ensure the rapid removal of electrons from subband 1 and, therefore, population inversion over the entire band.

However, it is apparently not necessary, since owing to the nonparabolicity of the subbands, $\alpha(\Omega_0)$ is insensitive to the form of the distribution function with $\varepsilon \geq \omega_0$ (see Sec. 2 above). Therefore, the presence of electrons with energies $\varepsilon \geq \omega_0$ makes a small contribution to the absorption and does not alter the population inversion in the crucial energy range.

In the limiting case of intense injection ($\bar{Q} \gg 1$) the expressions (43) and (44) give

$$f_2(1) \approx 1 - \frac{1}{\bar{Q}(\xi + 1)}, \quad f_1(0) \approx \frac{1}{\xi + 1}, \quad (47)$$

i.e., in the situation in Ref. 1, in which $\xi \gg 1$, the values $f_2(1) \approx 1 - 1/Q\tau_0$ and $f_1(0) \approx 1/\xi$ are achieved when $Q\tau_0 > 1$. If $\xi \ll 1$, the relations

$$f_2(1) \approx 1 - 1/\bar{Q}, \quad f_1(0) \approx 1 \quad (48)$$

hold when $\bar{Q} > 1$, i.e., at a value of Q which is τ_i/τ_0 times smaller. Therefore, it is possible to lower Q_{th} by a factor of $1/\xi$ by accumulating electrons in band 1 at $\varepsilon \approx \omega - \omega_0$.

5. ELECTRON DISTRIBUTION FUNCTIONS IN THE PRESENCE OF NONEQUILIBRIUM PHONONS

As we shall see below, the real phonon escape times τ_{esc} are such that nonequilibrium phonons accumulate in the system, the limiting value of the phonon number for the situation under consideration ($\omega_0 < \omega < 2C_0$) being approximately equal to unity. Electrons which reabsorb phonons increase their energy again, and, in particular, return from subband 1 to 2. Thus, their effective lifetime in subband 2 increases. The increase becomes especially marked, if the residence time of the electrons in subband 1, i.e., τ_i , increases. Therefore, it is possible to lower the threshold current by means of phonon reabsorption, of course, provided the subbands are nonparabolic.

Phonon reabsorption also results in "smearing" of the electron energy distribution, so that the values of $f_i(n)$ remain small compared with, for example, $1 + 3N$ even when $\bar{Q} \sim 1$. (This approximation actually "works" when $\bar{Q} \sim N$.)

For this reason we can neglect the nonlinear terms in Eqs. (37)–(41), (15), and (16). Passing to the new functions

$$f_i(n) = \bar{Q} \xi \psi_i(n), \quad (49)$$

instead of (37)–(41), (15), and (16) we obtain the following system of equations:

$$\psi_1(0)(\xi + 2N) = (1 + N)[\psi_1(1) + \psi_2(1)], \quad (50)$$

$$\psi_1(1)(\xi + 1 + 3N) = N\psi_1(0) + (1 + N)[\psi_1(2) + \psi_2(2)], \quad (51)$$

$$\psi_1(n)(\xi + 2 + 4N) = N[\psi_1(n-1) + \psi_2(n-1)] + (1 + N) \times [\psi_1(n+1) + \psi_2(n+1)], \quad (52)$$

$$\psi_2(1)(1 + 3N) = 1 + N\psi_1(0) + (1 + N)[\psi_1(2) + \psi_2(2)], \quad (53)$$

$$\psi_2(n)(2 + 4N) = N[\psi_1(n-1) + \psi_2(n-1)] + (1 + N) \times [\psi_1(n+1) + \psi_2(n+1)],$$

$$n = 0, 1, 2, \dots, \quad (54)$$

$$\frac{1}{\xi} = \sum_{n=0}^{\infty} \psi_1(n), \quad (55)$$

$$\frac{N\eta}{\xi^2} = \psi_1(0) - \sum_{n=2}^{\infty} (n-1)\psi_1(n), \quad \eta = \frac{\tau_0}{\tau_i Q \tau_{esc}}. \quad (56)$$

The parameter η in (56) specifies the concentration of nonequilibrium phonons. Setting $\nu = 1$, $s = 10^5$ cm/s (the velocity for optical phonons is small), and $d \approx 10^{-4}$ cm, we obtain $\tau_{esc} \approx 10^{-8} - 10^{-9}$ s. Even when $d \approx 10^{-4}$ cm and $\tau_0 \approx 10^{-12} - 10^{-13}$ s, we have $\eta \approx 10^{-3}$.

The system (50)–(55) has an exact solution. We seek the functions $\psi_i(n)$ for $n \geq 1$ in the form

$$\psi_1(n) = A_1 e^{\alpha n}, \quad \psi_2(n) = A_2 e^{\alpha n}. \quad (57)$$

Substituting (57) into (52) and (54), we obtain the system of homogeneous equations

$$\begin{aligned} A_1(\xi + b - C) - A_2 C &= 0, \\ A_1 C - A_2(b - c) &= 0, \end{aligned} \quad (58)$$

where

$$b = 2(1 + 2N), \quad C = (1 + N)e^{\alpha} + Ne^{-\alpha},$$

whence follows the equation for α :

$$e^{2\alpha} - \frac{b(\xi + b)e^{\alpha}}{(1 + N)(\xi + 2b)} + \frac{N}{1 + N} = 0. \quad (59)$$

The solution of Eq. (59) satisfying the conditions

$$\psi_i(n) \rightarrow 0, \quad n \rightarrow \infty,$$

has the form

$$\begin{aligned} e^{\alpha} &= \frac{b(\xi + b)}{2(1 + N)(\xi + 2b)} \\ &\quad - \sqrt{\left[\frac{b(\xi + b)}{2(1 + N)(\xi + 2b)} \right]^2 - \frac{N}{1 + N}}. \end{aligned} \quad (60)$$

Substituting $\psi_1(1)$ and $\psi_2(1)$, as well as $\psi_1(0)$ from (50), into (51) and (53), we arrive at a system of equations for A_1 and A_2 :

$$\begin{aligned} \bar{A}_1(\xi + 1 + 3N - y) - \bar{A}_2 y &= 0, \\ -\bar{A}_1 y + \bar{A}_2(1 + 3N - y) &= 1, \end{aligned} \quad (61)$$

whose solution is written in the form

$$\bar{A}_1 \equiv A_1 e^{\alpha} = \frac{y}{\Delta}, \quad \bar{A}_2 \equiv A_2 e^{\alpha} = \frac{\xi + 1 + 3N - y}{\Delta}, \quad (62)$$

where

$$\begin{aligned} \Delta &= (1 + 3N)(\xi + 1 + 3N) - y(\xi + 2 + 6N), \\ y &= (1 + N)e^{\alpha} + \frac{N(1 + N)}{\xi + 2N}. \end{aligned} \quad (63)$$

Solution (62) gives the useful exact relation

$$\bar{A}_1 + \bar{A}_2 = \frac{\xi + 1 + 3N}{\Delta}, \quad (64)$$

which can be used together with (50) to find

$$\psi_1(0) = \frac{(1 + N)(\xi + 1 + 3N)}{\Delta(\xi + 2N)}. \quad (65)$$

The nonequilibrium phonon number can be found from Eq. (56). Summing the series, we bring (56) into the form

$$\frac{N\eta}{\xi^2} = \psi_1(0) - \psi_1(1) \frac{e^{\alpha}}{(1 - e^{\alpha})^2}. \quad (66)$$

Using (55), we can write Eq. (66) in an even more convenient form:

$$\frac{N\eta}{\xi^2} = \frac{\psi_1(0) - e^{\alpha}/\xi}{1 - e^{\alpha}}. \quad (67)$$

Thus, Eqs. (57), (60), (62), and (65) together with the equation for N (67) give us the complete solution of the problem.

6. LIMITING VALUES OF THE NONEQUILIBRIUM PHONON NUMBER AND THE ELECTRON DISTRIBUTION FUNCTIONS

Let us first consider the situation in which $\xi \gg 1$ and $\xi \gg N$, which is characteristic of quantum cascade lasers.¹ Performing the expansion in $1/\xi$ in (62) and (63), we find the expression for $\psi_2(1)$

$$\psi_2(1) \approx \frac{1}{1 + 3N - (1 + N)e^\alpha}, \quad (68)$$

where

$$e^\alpha \approx \frac{2(1 + 4\bar{N}) - \sqrt{3 + 16\bar{N}}}{1 + 8\bar{N}},$$

and the equation for the phonon number $\bar{N} = N/\xi$

$$\bar{N}\eta = \frac{\varphi(\bar{N}) - e^\alpha}{1 - e^\alpha}, \quad (69)$$

where

$$\varphi(\bar{N}) = \left\{ (1 + 2\bar{N}) \left[3 - \frac{1 + 6\bar{N}}{1 + 3\bar{N}} \left(e^\alpha + \frac{\bar{N}}{1 + 2\bar{N}} \right) \right] \right\}^{-1}.$$

If $\eta \ll 1$, expanding (69) in small \bar{N} , we obtain the limiting value N_0 :

$$N_0 \approx \frac{\xi\sqrt{3}}{(1 + \sqrt{3})8}, \quad (70)$$

which becomes equal to $N_0 \approx 1$ when $\xi \approx 10$.

Substituting e^α and N_0 into (68), we have

$$\psi_1(1) \approx 0.3, \quad f_2(1) \approx 0.3Q\tau_0, \quad (71)$$

i.e., the reabsorption of nonequilibrium phonons decreases $f_2(1)$ and increases Q_{th} approximately three fold in comparison with (45) and (46) for the relation between the times $\tau_0 \gg \tau_r$, which was adopted in Ref. 1.

Let us now consider the reverse situation, in which $\xi \ll 1$. It is achieved, if τ_r is increased at a fixed value of τ_0 by varying, for example, the thickness of the barrier. Of course, τ_r must remain smaller than the relaxation times on acoustic phonons and electrons.

Performing the expansion in $\xi \ll 1$ ($\xi \ll N$) in (60), (62), and (63), after some cumbersome calculations we find

$$\psi_1(0) \approx \frac{1}{\xi(1 + N)}, \quad \psi_1(1) \approx \frac{N}{\xi(1 + N)^2}, \quad (72)$$

$$\psi_2(1) \approx \frac{N}{\xi(1 + N)^2}, \quad f_2(1) \approx \frac{Q\tau_0 N}{\xi(1 + N)^2}. \quad (73)$$

The function $\psi_1(0)$ decreases monotonically with increasing N owing to the phenomenon of reabsorption [compare with (45)], while $\psi_2(1)$ and $\psi_1(1)$ each exhibit a maximum at $N = 1$. In fact, as N increases, the electrons which have accumulated in the lowest level of subband 1 [$f_1(0)$] pass into subband 2 [$f_2(1)$] and into subband 1 [$f_1(1)$], so that

$\psi_2(1)$ and $\psi_1(1)$ increase sharply. Then, when $N > 1$, electrons begin to go to higher levels, and the functions $\psi_2(1)$ and $\psi_1(1)$ decrease.

Substituting the values of $\psi_2(N)$ from (72) and (73) into the equation for N and solving it, we obtain

$$N \approx \frac{\xi}{\eta + \xi}. \quad (74)$$

The limiting value N_0 , which is achieved when $\eta \ll \xi$, equals $N_0 = 1$, and accordingly

$$\psi_1(0) \approx \frac{1}{2\xi}, \quad \psi_2(1) \approx \frac{1}{4\xi}, \quad f_2(1) \approx \frac{Q\tau_r}{4}. \quad (75)$$

Comparing the values of $\psi_2(1)$ from (75) and (71) (for fixed τ_0), we obtain

$$\frac{\psi_2(1, \xi \ll 1)}{\psi_2(1, \xi \gg 1)} \approx \frac{1}{\xi} \gg 1. \quad (76)$$

Therefore, an improvement in the threshold current by a factor of $1/\xi$ is possible. As the evaluations show (see below), the value $\xi \approx 0.1$ ($\tau_r \approx 3 \times 10^{-12}$ s) is perfectly permissible, and, accordingly, the expected decrease in the threshold current amounts to approximately one to two orders.

7. ELECTRON ENERGY DISTRIBUTION AND LIMITING PHONON NUMBER FOR ANY ω

The foregoing analysis can be generalized to the case of $\omega \sim k\omega_0$, in which k optical phonons fall within ω (for example, in Ref. 1 $k = 7-8$). It is not difficult to show that Eqs. (51)–(54) for $f_i(n)$ with $n \geq 1$ remain unchanged, while Eq. (50) takes the form

$$\psi_1(0)(\xi + 1 + 3N) = N\psi_1(-1) + (1 + N)[\psi_1(1) + \psi_2(1)], \quad (77)$$

and the following equations must be added for the new functions $\psi_1(-n)$:

$$\begin{aligned} \psi_1(-n)(\xi + 1 + 2N) &= N\psi_1(-n-1) \\ &+ (1 + N)\psi_1(-n+1), \quad 1 \leq n \leq k, \end{aligned} \quad (78)$$

$$\psi_1(-k)(\xi + N) = (1 + N)\psi_1(-k+1), \quad n = k. \quad (79)$$

Relations (55) and (56) are also modified:

$$\frac{1}{\xi} = \sum_{n=-k}^{\infty} \psi_1(n), \quad (80)$$

$$\frac{N\eta}{\xi^2} = \sum_{n=1}^k n\psi_1(-n+1) - \sum_{n=1}^{\infty} n\psi_1(n+1). \quad (81)$$

It is easy to see that the results for the limit $\xi \gg 1$ remain practically unchanged. In fact, as follows from Eqs. (78) and (79), all the new functions $f_1(-n)$ are small compared with $f_2(1)$ and $f_1(0)$ with respect to the parameter ξ^{-n} . Therefore, the system of equations [including (56)] remains unchanged, as do, consequently, the values of N_0 and $\psi_2(1)$ [see (68) and (70)].

Let us analyze the limit $\xi \ll 1$. The new system of equations can again be solved exactly in the general case. To avoid cumbersome expressions, we restrict ourselves to consideration of the limit of large k . In this case the limiting phonon number is large, being $N_0 \approx k/\sqrt{2}$ [see (85)]. This makes it possible to simplify Eqs. (78) and (79) and to easily obtain

$$\psi_1(-k) \approx \psi_1(-k+1) = \dots = \psi_1(-1) = \psi_1(0). \quad (82)$$

When relation (82) is taken into account, Eq. (77) is transformed back into its former form (50), and Eq. (81) for the phonons takes a different form:

$$\frac{N\eta}{\xi^2} \approx \psi_1(0) \frac{k(k+1)}{2} - \frac{\psi_1(1)e^\alpha}{(1-e^\alpha)^2}, \quad (83)$$

[when $k=1$, it transforms into (56)].

Therefore, we have the former system of equations for the $\psi_i(n)$ with a different phonon number, and thus the former expressions (72) and (73) can be used. Substituting them into (83) we arrive at the following equation for N :

$$N^2 \left(1 + \frac{\eta}{\xi} \right) + \frac{N\eta}{\xi} - \frac{k(k+1)}{2} = 0. \quad (84)$$

When $\eta \ll \xi$, the limiting value of N_0 equals

$$N_0 \approx \sqrt{\frac{k(k+1)}{2}} \approx \frac{k}{\sqrt{2}}. \quad (85)$$

Accordingly, the functions $\psi_2(1)$ and $\psi_1(0)$ can be written in the form

$$\psi_2(1) \approx \frac{k}{\sqrt{2}\xi(1+k/\sqrt{2})^2} \approx \frac{\sqrt{2}}{\xi k}, \quad (86)$$

$$\psi_1(0) \approx \frac{1}{\xi(1+k/\sqrt{2})} \approx \frac{\sqrt{2}}{\xi k}. \quad (87)$$

Setting $\omega = 0.295$ eV (Ref. 1), $\omega_0 = 0.036$ eV, and $k=7$, we find

$$N_0 \approx 5, \quad \psi_2(1) = \psi_1(0) \approx \frac{1}{5\xi}. \quad (88)$$

Comparing (87) with (75), we see a modest (20%) decrease in $\psi_2(1)$.

Thus, the conclusion regarding the possibility of significantly lowering the threshold current remains valid for any k .

8. CONCLUSIONS

The treatment of the kinetics of the relaxation of the nonequilibrium electrons in quantum cascade lasers showed that its important features are the emission and accumulation

of nonequilibrium optical phonons. Reabsorption of the nonequilibrium phonons results in smearing of the electron energy distribution and an additional increase in the threshold current.

The fundamental possibility of decreasing the threshold current J_{th} by increasing the time for the removal of electrons from the lower working subband was also demonstrated in this work. The decrease in J_{th} is attributed to an increase in the effective lifetime of the electrons in the upper subband due to the reabsorption of nonequilibrium phonons and the accumulation of electrons in the lower subband at energies equal to the multiples $n\omega_0$. There are two necessary conditions here: the absence of a dependence of the energy of an optical phonon on the momentum and the nonparabolicity of the subbands. The improvement in the threshold current is limited by the minimal electron-electron relaxation time, which can be evaluated approximately in the two-dimensional case using the expression

$$\frac{1}{\tau_{esc}} \approx \frac{e^4 m \mu \pi \zeta}{16 \hbar^2 \kappa^2 \omega_0}, \quad \zeta \sim 1.$$

Taking $m/m_0 = 0.07$, a dielectric constant $\kappa = 13.3$, and $\mu/\omega_0 = 0.2-0.1$, we obtain $\tau_{esc} \approx 3 \times 10^{-12}$ to 6×10^{-12} s, and, therefore, $\xi \leq 0.1$.

It must be stressed that the evaluations performed in this work have an approximate character, since knowledge of the matrix elements of the radiative phonon and electron-electron transitions with consideration of the concrete parameters of the nanostructures is needed for rigorous quantitative results. Such calculations are beyond the scope of this paper. However, the qualitative results obtained make it possible to outline the procedure for optimizing the structure of quantum cascade lasers and to significantly lower the threshold current in these certainly promising lasers.

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