Nonequilibrium electron-phonon scattering in semiconductor heterojunctions

W. Cai and M. C. Marchetti*
Department of Physics, City College of the City University of New York, New York, New York 10031

M. Lax
Department of Physics, City College and Graduate School, City University of New York, New York, New York 10031
and AT&T Bell Laboratories, Murray Hill, New Jersey 07974-2070

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We calculate the energy-loss rate of a quasi-two-dimensional (2D) hot-electron gas at a semiconductor heterojunction due to the emission and reabsorption of nonequilibrium optical phonons. A kinetic equation for the nonequilibrium lattice excitations (hot phonons) in the spatially inhomogeneous field created by the quasi-2D electrons is obtained. The equation is solved by a transformation that introduces the occupation number for wave packets of phonons that are "localized" in a spatial region near the electron layer. Our result does not contain the spurious dependence on the size of the sample that results when the nonequilibrium phonons are represented in terms of decoupled 3D plane waves. We apply our results to electrons in a GaAs-$Ga_xAl_{1-x}As$ heterojunction. We find that the reabsorption of the emitted hot phonons reduces considerably the electron cooling rate if the optical-phonon lifetime $\tau_{op} \geq 5$ psec. Furthermore, the electron-energy relaxation rate, $1/\tau$, changes from a weakly decreasing function of the electron temperature, T_e, when $\tau_{op}=0$ to a increasing function of T_e, as τ_{op} increases. This result compares favorably with recent experimental data.

I. INTRODUCTION

Recently there has been much interest in the relaxation of quasi-two-dimensional hot electrons at the interface of semiconductor heterojunctions.[1-5] In these systems the carriers are dynamically two-dimensional (2D) since they have quantized energy levels in the direction normal to the junction plane, while are essentially free in the other two dimensions.[6] The carriers can be displaced from equilibrium (heated) either ohmically or optically and relax via inelastic scattering with the lattice excitations. The relaxation rates reported in some recent experiments[1,3,4] are much slower than those predicted theoretically.[7] Photoluminescence experiments of steady state[1-3] and the time-dependent distribution[4] of hot electrons in GaAs-$Ga_xAl_{1-x}As$ devices show that the distribution function of the hot electrons is well described by a single electron temperature, T_e. Also, for $T_e > 50$ K the dominant energy-loss mechanism from the electrons to the lattice is the emission of longitudinal-optical (LO) phonons. The relaxation rates reported in Refs. 1, 3, and 4 are, however, one order of magnitude smaller than those of Ref. 2. The latter is in agreement with theoretical estimates.

It has been suggested that the bottleneck effect due to the presence of a population of nonequilibrium LO phonons (hot phonons) might be responsible for slowing down the electron cooling.[1,8] It is well known, in fact, that mutual heating effects of the coupled nonequilibrium electron-phonon system are important in bulk semiconductors.[9] The description of the coupled nonequilibrium electron-phonon system in quantum wells is, however, not straightforward. The theoretical analysis of the interaction between the quasi-2D electrons and the phonons is usually based on the assumption that the lattice modes are those of the bulk and are unaffected by the presence of the electron layer. It was, however, pointed out by Price[8] that a naive estimate of the nonequilibrium LO phonon population in a model where the lattice modes are described in terms of decoupled 3D plane waves leads to an artificial dependence of the result on the size of the sample. This is because this model does not recognize that the coupled (quasi-2D) electron-phonon system is not spatially homogeneous in the direction normal to the electron-layer plane (z direction). The nonequilibrium "physical" phonons are not plane-wave states and the corresponding nonequilibrium one-body density matrix is not diagonal in the plane-wave representation. Furthermore, its off-diagonal elements are not negligible compared to the diagonal ones—i.e., the familiar occupation number for 3D plane-wave phonon states—which are of order $1/L$, with L the size of the crystal in the z direction.

In this paper we present a description of the nonequilibrium electron-phonon system where the inhomogeneity is properly incorporated. We derive a kinetic equation for the phonon one-body density matrix in the spatially inhomogeneous external field created by the quasi-2D electrons. As mentioned, the one-body density matrix is not diagonal in the plane-wave representation, and the kinetic equation, even though linear, is an integral equation and cannot easily be solved in this representation. On the other hand, both physical considerations and the mathematical structure of the equation suggest a change of representation that considerably simplifies the problem. In the scattering between the quasi-2D electrons and the lattice excitations there is no conservation law for the z component of the momentum. The emitted phonons have no

well-defined z component of the momentum and are better described in terms of lattice excitations that are localized near the layer in the z direction, rather than in terms of extended plane waves.[10] This is achieved in a natural way by constructing "wave packets" of phonons with weights that are directly related to the electronic wave functions in the z direction. If the LO phonons are assumed to be dispersionless, the phonon kinetic equation reduces from an integral equation to a finite set of coupled algebraic equations labeled by the electronic subband indices, in the "wave-packet representation." Such equations can easily be solved for the nonequilibrium phonon distribution.

This approach is used here to calculate the energy-loss rate of steady-state hot electrons in a GaAs-$Ga_xAl_{1-x}As$ heterojunction. We assume that the electron distribution function is a Fermi-Dirac distribution at the temperature T_e and that the electron-LO—phonon interaction is described by the Fröhlich Hamiltonian. The power emitted per electron can then be written as

$$P_e=\frac{\hbar\omega_L}{\tau}\exp(-\hbar\omega_L/k_BT_e)\ , \tag{1.1}$$

where $\hbar\omega_L$ is the energy of the LO phonons. Equation (1.1) defines the "energy-loss rate" $1/\tau$.

We find that the power-loss rate $1/\tau$ is reduced considerably by phonon reabsorption (see Fig. 1) if the optical-phonon lifetime $\tau_{op}\geq 5$ psec. Furthermore, we observe a qualitative change in the functional dependence $1/\tau$ on T_e as τ_{op} increases. When $\tau_{op}=0$, corresponding to an equilibrium phonon distribution, $1/\tau$ is a weakly decreasing function of T_e. For $\tau_{op}>5$ psec, $1/\tau$ is always an increasing function of T_e since the bottleneck effect due to the presence of the nonequilibrium hot-phonon population becomes weaker as the electron temperature increases. In GaAs $\tau_{op}=7$ psec and phonon reabsorption should be important. In fact we notice from Fig. 1 of Ref. 1 that the electron cooling rate, $1/\tau$, is a weakly increasing function of the electron temperature. Our theoretical results compare favorably with the measurements reported in Refs. 1 and 3, as will be discussed below. The origin of the discrepancy between the results of Ref. 2 where "hot-phonon" effects seem to be negligible, and those of Refs. 1, 3, and 4 are at present unclear.

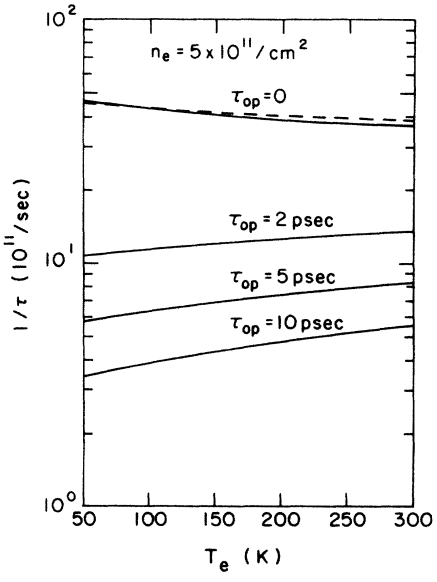

FIG. 1. $1/\tau$ as a function of the electron temperature T_e, for $\tau=0$, 2, 5, and 10 psec and lowest subband ($n=0$) occupation. Dynamical screening is included (solid curves). $1/\tau$ for $\tau_{op}=0$ without dynamical screening is also shown (dashed curve).

In Sec. II we briefly discuss the derivation of a generalized Boltzmann equation for the lattice excitations in a inhomogeneous system. In Sec. III we introduce the change of representation and obtain a kinetic equation for the "physical" phonon occupation number. The solution of this equation is used to evaluate the cooling rate of hot electrons in a GaAs-$Ga_xAl_{1-x}As$ heterojunction. The results are compared with recent experiments. The paper is concluded with a brief discussion.

II. PHONON KINETIC EQUATION

The Hamiltonian of the coupled electron-phonon system is given by

$$\hat{H}=\hat{H}_e+\hat{H}_p+\hat{V}_{ep}+\hat{V}_{pp} \tag{2.1}$$

Where $\hat{H}_e$ and $\hat{H}_p$ are the electron and phonon Hamiltonians, respectively, and $\hat{V}_{ep}$ and $\hat{V}_{pp}$ denote the electron-phonon and the phonon-phonon interactions.

The states of the quasi-2D electrons at the interface of semiconductor heterojunctions have been studied extensively.[6] Due to the confining potential in the direction normal to the interface, the 3D conduction band is split in 2D subbands. The wave function of a single electron in the nth subband with 2D wave vector $\mathbf{k}$ is

$$\Psi_{n,\mathbf{k}}(\mathbf{r},z)=A^{-1/2}\zeta_n(z)\exp(i\mathbf{k}\cdot\mathbf{r})\ ,$$

where A is the layer area and $\zeta_n(z)$ is the envelope function in the z direction. Its explicit form depends on the confining potential. It can be generally represented in terms of variational functions[11] as $\zeta_n(z)=\sum_{i=1}^{n+1}\alpha_{i,n}z^ie^{-\beta_nz}$, for $z\geq 0$ and $\zeta_n=0$ for $z<0$. The parameters $\alpha_{i,n}$ and β_n, together with the subband energy levels E_n, for $n=0$ and $n=1$, have been given elsewhere[12] for a GaAs-$Ga_xAl_{1-x}As$ heterojunction. In the representation of second quantization the electron Hamiltonian is then written as

$$\hat{H}_e=\sum_{n,\mathbf{k}}E_{n\mathbf{k}}\hat{a}^{\dagger}_{n\mathbf{k}}\hat{a}_{n\mathbf{k}}+\hat{V}_{ee}\ , \tag{2.2}$$

where $E_{n\mathbf{k}}=E_n+\hbar^2k^2/2m$, with m the electron effective mass. Here $\hat{a}^{\dagger}_{n\mathbf{k}}$ and $\hat{a}_{n\mathbf{k}}$ are the electron creation and annihilation operators; spin indices have been omitted. Finally, $\hat{V}_{ee}$ is the Coulomb interaction between the electrons. We do not specify it here, since we are not concerned with the kinetic equation for the electrons. The latter has been obtained previously.[13]

In the occupation number representation of 3D plane-wave phonon states, the longitudinal optical-phonon Hamiltonian is given by

$$\hat{H}_p=\sum_{\mathbf{Q}}\hbar\omega_L\hat{b}^{\dagger}_{\mathbf{Q}}\hat{b}_{\mathbf{Q}}\ , \tag{2.3}$$

where $\mathbf{Q}=(\mathbf{q},q_z)$ is the 3D phonon quasimomentum and $\hat{b}^{\dagger}_{\mathbf{Q}}$ and $\hat{b}_{\mathbf{Q}}$ are the phonon creation and annihilation operators.

For the electron-phonon interaction we use the Fröhlich continuum model,[14]

$$\hat{V}_{ep}=\frac{1}{4\pi}\int d\mathbf{R}\int d\mathbf{R}'\,e\hat{\rho}(\mathbf{R})\frac{1}{|\mathbf{R}-\mathbf{R}'|}[-4\pi\nabla'\cdot\hat{\mathbf{P}}(\mathbf{R}')]\ , \tag{2.4a}$$

where $\hat{\rho}(\mathbf{R})$ is the electron density operator and $[-4\pi\nabla\cdot\mathbf{P}(\mathbf{R})]$ is the charge density due to the polarization of the medium. It is related to the relative displacement of positively and negatively charged ions, $\hat{\mathbf{u}}(\mathbf{R})=\hat{\mathbf{u}}_+(\mathbf{R})-\hat{\mathbf{u}}_-(\mathbf{R})$, by $\nabla\cdot\hat{\mathbf{P}}=(e^*/v_c)\nabla\cdot\hat{\mathbf{u}}$, with v_c the volume of a unit cell. Here e^* is an effective charge given by

$$e^*=[(\mu v_c/4\pi)\omega_L^2(1/\epsilon_\infty-1/\epsilon_0)]^{1/2}\ ,$$

with μ the atomic reduced mass and ϵ_∞ and ϵ_0 are the high frequency and the static dielectric constants. The relative displacement can be represented in terms of plane waves as

$$\hat{\mathbf{u}}(\mathbf{R})=\left[\frac{\hbar}{2\omega_L\mu N}\right]^{1/2}\sum_{\mathbf{Q}}\frac{\mathbf{Q}}{Q}(\hat{b}_{\mathbf{Q}}e^{i\mathbf{Q}\cdot\mathbf{R}}+\hat{b}^{\dagger}_{\mathbf{Q}}e^{-i\mathbf{Q}\cdot\mathbf{R}})\ , \tag{2.4b}$$

where N is the number of unit cells. In second-quantized representation $\hat{V}_{ep}$ becomes then

$$\hat{V}_{ep}=\frac{i\alpha}{\sqrt{A}}\sum_{n,\mathbf{k}}\sum_{n',\mathbf{k}}\sum_{\mathbf{Q}}[\hat{b}_{\mathbf{Q}}\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}G_{n'n}(q,q_z)-\hat{b}^{\dagger}_{\mathbf{Q}}\delta_{\mathbf{k}',\mathbf{k}-\mathbf{q}}G^*_{n'n}(q,q_z)]\hat{a}^{\dagger}_{n'\mathbf{k}}\hat{a}_{n\mathbf{k}}\ , \tag{2.5a}$$

where α is the Fröhlich electrons-LO—phonons coupling constant $\alpha=[2\pi e^2\hbar\omega_L(1/\epsilon_\infty-1/\epsilon_0)]^{1/2}$, and

$$G_{n'n}(q,q_z)=\frac{1}{Q\sqrt{L}}\int_{-\infty}^{+\infty}dz\,\xi^*_{n'}(z)\exp(iq_zz)\xi_n(z)\ . \tag{2.5b}$$

Finally, $\hat{V}_{pp}$ denotes the phonon-phonon interaction that leads to the decay of the LO phonons into acoustic phonons and to their thermalization with the equilibrium lattice. We do not specify this interaction here because we will use a single relaxation time approximation for the corresponding contribution to the phonon kinetic equation and treat the relaxation time as a constant, i.e., wave vector independent, parameter.

The nonequilibrium state of the electron-phonon system is described by the density matrix $\hat{\rho}(t)$, whose time evolution is governed by the quantum-mechanical Liouville equation,

$$i\hbar\frac{\partial\hat{\rho}(t)}{\partial t}=[\hat{H},\hat{\rho}(t)]\ . \tag{2.6}$$

To derive the quantum kinetic equation for the phonons we use here the idea first introduced by Bogoliubov for classical systems that, after an initial transient, the nonequilibrium state of the system is well described in terms of the expectation values of a reduced number of macroscopic observables, denoted here by the components of a vector $\boldsymbol{\gamma}(t)=\{\gamma_i(t)\}$,[15] defined by the expectation value of a set of operators $\{\hat{\gamma}_i\}$,

$$\gamma_i(t)=\mathrm{Tr}[\hat{\rho}(t)\hat{\gamma}_i]\ . \tag{2.7}$$

The choice of the set $\boldsymbol{\gamma}(t)$ depends on the time scale of interest. Here we are concerned with the description of the kinetic stage of the relaxation. The $\boldsymbol{\gamma}(t)$ are then identified with the reduced one-body density matrices of the electron and phonon gas.[15,16] The one-body density matrix of a phonon gas that is spatially inhomogeneous in the z direction is nondiagonal in the z component of the momentum in the plane-wave representation. It is defined as

$$n_q(q_z,q_z',t)=\mathrm{Tr}[\hat{b}^{\dagger}_{qq_z}\hat{b}_{qq_z'}\hat{\rho}(t)]\ . \tag{2.8}$$

The average values of all phonon one-body observables can be expressed in terms of this one-body density matrix. In particular, the average energy of the phonon gas at time t is

$$E_p(t)=\mathrm{Tr}[\hat{H}_p\hat{\rho}(t)]=\sum_{\mathbf{Q}}\hbar\omega_L n_q(q_z,q_z,t)\ . \tag{2.9}$$

The diagonal element, $n_q(q_z,q_z,t)$, is the familiar phonon occupation number. Similarly, the electron one-body reduced density matrix is

$$f_{n\mathbf{k}}(t)=\mathrm{Tr}[\hat{a}^{\dagger}_{n\mathbf{k}}\hat{a}_{n\mathbf{k}}\hat{\rho}(t)]\ . \tag{2.10}$$

It is diagonal in the chosen representation and is the familiar electron distribution function. Therefore we choose $\boldsymbol{\gamma}(t)=[n_q(q_z,q_z',t),f_{n\mathbf{k}}(t)]$, for the present problem.

The rate of change of any function of $\boldsymbol{\gamma}(t)$, denoted by $F(\boldsymbol{\gamma}(t))$ is given by

$$i\hbar\frac{\partial F(\boldsymbol{\gamma}(t))}{\partial t}=\mathrm{Tr}\{[F(\hat{\boldsymbol{\gamma}}),\hat{H}]\hat{\rho}(t)\}\ . \tag{2.11}$$

The central assumption is that for times longer than a microscopic collision time, t_0, the nonequilibrium density matrix depends on time only via the time dependence of the macroscopic observable, i.e.,

$$\hat{\rho}(t)=\hat{\rho}(\boldsymbol{\gamma}(t)),\quad \text{for } t\gg t_0\ . \tag{2.12}$$

For $t\gg t_0$ the time evolution of the nonequilibrium state is then described by a set of coupled kinetic equations for the components of $\boldsymbol{\gamma}(t)$. A closed kinetic equation is obtained from Eq. (2.11) when the nonequilibrium density

matrix $\hat{\rho}(\gamma(t))$ is inserted on the right-hand side of the equation. To determine $\hat{\rho}(\gamma(t))$ one needs, in addition to Eqs. (2.6) and (2.12), an appropriate boundary condition, chosen in such a way to guarantee the irreversible character of the time evolution of $\gamma(t)$. The question of the choice of the boundary condition and its meaning has been discussed extensively in the literature and will not be addressed here. We refer the reader to Refs. 15 and 16 for a discussion of this point. The kinetic equation can be obtained following closely the method of Ref. 16. Only the result is given here. To second order in the interaction potential $\hat{V}=\hat{V}_{ee}+\hat{V}_{ep}+\hat{V}_{pp}$, one obtains

$$\frac{\partial F(\gamma(t))}{\partial t}=\frac{i}{\hbar}\mathrm{Tr}[\hat{H}_p,F(\hat{\gamma})]\hat{\rho}_0(t)+\left[\frac{i}{\hbar}\right]^2\lim_{\epsilon\to 0^+}\int_{-\infty}^{0}d\tau e^{\epsilon\tau}\mathrm{Tr}\{[\hat{V}(\tau),[\hat{V},F(\hat{\gamma})]]\hat{\rho}_0(t)\} \tag{2.13a}$$

where

$$\hat{V}(\tau)=\exp[i(\hat{H}_e+\hat{H}_p)\tau/\hbar]\hat{V}\exp[-i(\hat{H}_e+\hat{H}_p)\tau/\hbar] \tag{2.13b}$$

and $\hat{\rho}_0(t)=\hat{\rho}_0(\gamma(t))$ is a Gibbsian or quasiequilibrium distribution, given by

$$\hat{\rho}_0(t)=\frac{1}{\Xi}\exp\left[-\sum_i B_i(\gamma(t))\hat{\gamma}_i\right], \tag{2.14a}$$

where Ξ is a normalization constant and the functions B_i are determined by the requirement

$$\gamma_i(t)=\mathrm{Tr}(\hat{\gamma}_i\hat{\rho}_0(t)) . \tag{2.14b}$$

Equation (2.13) is the desired kinetic equation. The first term on the right-hand side is the streaming term, the second is the collision term.

The phonon kinetic equation can be obtained from Eqs. (2.5), (2.8), and (2.13) in a straightforward way. Due to the assumption of dispersionless lattice excitations, the streaming term vanishes and one obtains

$$\frac{\partial n_q(q_z,q_z',t)}{\partial t}=\left[\frac{\partial n_q(q_z,q_z',t)}{\partial t}\right]_{ep}+\left[\frac{\partial n_q(q_z,q_z',t)}{\partial t}\right]_{pp} . \tag{2.15}$$

The first term, representing the contribution from electron-phonon collisions, is given by,

$$\begin{aligned}\left[\frac{\partial n_q(q_z,q_z',t)}{\partial t}\right]_{ep}=&\lim_{\epsilon\to 0^+}\frac{2\alpha^2}{\hbar A}\sum_{n,\mathbf{k}}\sum_{n',\mathbf{k}'}\sum_{q_z''}f_{n\mathbf{k}}(t)[1-f_{n'\mathbf{k}'}(t)]\\ &\times\left[\delta_{\mathbf{k}',\mathbf{k}-\mathbf{q}}\frac{G_{n'n}(q,q_z)G^*_{n'n}(q,q_z'')}{\varepsilon-i[E_{n\mathbf{k}}-E_{n'\mathbf{k}'}-\hbar\omega_L]}[\delta_{q_z'',q_z'}+n_q(q_z'',q_z',t)]\right.\\ &+\delta_{\mathbf{k}',\mathbf{k}-\mathbf{q}}\frac{G^*_{n'n}(q,q_z')G_{n'n}(q,q_z'')}{\varepsilon+i[E_{n\mathbf{k}}-E_{n'\mathbf{k}'}-\hbar\omega_L]}[\delta_{q_z'',q_z}+n_q(q_z,q_z'',t)]\\ &-\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\frac{G_{n'n}(q,q_z)G^*_{n'n}(q,q_z'')}{\varepsilon+i[E_{n\mathbf{k}}-E_{n'\mathbf{k}'}+\hbar\omega_L]}n_q(q_z'',q_z',t)\\ &\left.-\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\frac{G^*_{n'n}(q,q_z')G_{n'n}(q,q_z'')}{\varepsilon-i[E_{n\mathbf{k}}-E_{n'\mathbf{k}'}+\hbar\omega_L]}n_q(q_z,q_z'',t)\right],\end{aligned} \tag{2.16}$$

where $G_{n'n}(q,q_z)$ is defined in Eq. (2.5b). For the contribution from phonon-phonon scattering we use a single relaxation time approximation,

$$\left[\frac{\partial n_q(q_z,q_z',t)}{\partial t}\right]_{pp}=-\frac{n_q(q_z,q_z',t)-\delta_{q_z,q_z'}n_L}{\tau_{\mathrm{op}}} , \tag{2.17}$$

where n_L is the equilibrium LO phonon distribution at lattice temperature T_L. In the following we will choose $T_L=0$. The relaxation time τ_{op} is in general wave vector and temperature dependent. Some theoretical calculations and experimental measurements of LO phonon lifetimes in bulk semiconductors (specifically, GaAs) are available.[9,17] There is, however, little knowledge of phonon lifetimes in semiconductor heterojunctions. A microscopic calculation of τ_{op} requires a detailed analysis of the anharmonic effects leading to phonon-phonon scattering and is beyond the scope of the present work. We therefore assume here that τ_{op} is a constant independent of wave vector and treat it as a parameter. This assumption considerably simplifies the discussion of Sec. III.

Finally, a set of kinetic equations for the electron distribution functions, $f_{n\mathbf{k}}(t)$, for $n=0,1,\ldots,$ can be obtained in the same way. They are given by

$$\frac{\partial f_{n\mathbf{k}}(t)}{\partial t}=\left[\frac{\partial f_{n\mathbf{k}}(t)}{\partial t}\right]_{ep}+\left[\frac{\partial f_{n\mathbf{k}}(t)}{\partial t}\right]_{ee} , \tag{2.18}$$

with

$$\left[\frac{\partial f_{n\mathbf{k}}(t)}{\partial t}\right]_{ep}=\frac{2\alpha^2}{\hbar A}2\pi\sum_{\mathbf{q}}\sum_{q_z q_z'}\sum_{n',\mathbf{k}'}G^*_{nn'}(q,q_z)G_{nn'}(q,q_z')$$

$$\times(\{f_{n'\mathbf{k}'}(t)[1-f_{n\mathbf{k}}(t)]\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\delta(E_{n'\mathbf{k}'}-E_{n\mathbf{k}}-\hbar\omega_L)$$

$$-f_{n\mathbf{k}}(t)[1-f_{n'\mathbf{k}'}(t)]\delta_{\mathbf{k}',\mathbf{k}-\mathbf{q}}\delta(E_{n\mathbf{k}}-E_{n'\mathbf{k}'}-\hbar\omega_L)\}[\delta_{q_z q_z'}+n_q(q_z,q_z',t)]$$

$$+\{f_{n'\mathbf{k}'}(t)[1-f_{n\mathbf{k}}(t)]\delta_{\mathbf{k}',\mathbf{k}-\mathbf{q}}\delta(E_{n'\mathbf{k}'}-E_{n\mathbf{k}}+\hbar\omega_L)$$

$$-f_{n\mathbf{k}}(t)[1-f_{n'\mathbf{k}'}(t)]\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\delta(E_{n\mathbf{k}}-E_{n'\mathbf{k}'}+\hbar\omega_L)\}n_q(q_z,q_z',t))\ . \tag{2.19}$$

The term arising from the electron-electron collision $[\partial f_{n\mathbf{k}}(t)/\partial t]_{ee}$ is not specified here, it has been derived before by other methods and can be found for instance in Ref. 13.

III. ELECTRON COOLING RATE

The objective of the present paper is to evaluate the rate at which the electrons lose energy by inelastic scattering with the LO phonons. The energy-loss rate per electron, $P_e(t)$, is given by

$$P_e(t)=\frac{\hbar\omega_L}{N_e}\sum_{\mathbf{Q}}\left[\frac{\partial n_q(q_z,q_z,t)}{\partial t}\right]_{ep}, \tag{3.1}$$

where N_e is the total number of electrons in the 2D layer. Inserting Eq. (2.12) for $q_z=q_z'$ on the right-hand side of Eq. (3.1), we obtain

$$P_e(t)=\frac{2\pi\alpha^2}{N_e\hbar A}\hbar\omega_L 2\sum_{n\mathbf{k}}\sum_{n'\mathbf{k}'}f_{n\mathbf{k}}(t)[1-f_{n'\mathbf{k}'}(t)]$$

$$\times\sum_{\mathbf{q}}\sum_{q_z}\sum_{q_z'}G^*_{n'n}(q,q_z)G_{n'n}(q,q_z')$$

$$\times\{\delta_{\mathbf{k}',\mathbf{k}-\mathbf{q}}\delta(E_{n\mathbf{k}}-E_{n'\mathbf{k}'}-\hbar\omega_L)[\delta_{q_z,q_z'}+n_q(q_z,q_z',t)]$$

$$-\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\delta(E_{n\mathbf{k}}-E_{n'\mathbf{k}'}+\hbar\omega_L)n_q(q_z,q_z',t)\}\ . \tag{3.2}$$

The evaluation of $P_e(t)$ requires the solution of both the phonon and the electron kinetic equations. Even when the electron distribution function is given, the equation for $n_q(q_z,q_z',t)$ is an integral equation and cannot be solved easily. We can, however, perform a simple change of representation by introducing new phonon states as superpositions of plane-wave states weighted with the electronic subband wave functions, $\zeta_n(z)$. We define

$$N_{n'n,m'm}(q,t)=\frac{\sum_{q_z}\sum_{q_z'}G^*_{n'n}(q,q_z)n_q(q_z,q_z',t)G_{m'm}(q,q_z')}{F_{n'n,m'm}(q)/2q}\ , \tag{3.3a}$$

where $F_{n'n,m'm}(q)$ is the electronic form factor, given by

$$F_{n'n,m'm}(q)=2q\sum_{q_z}G^*_{n'n}(q,q_z)G_{m'm}(q,q_z)\ . \tag{3.3b}$$

It is easy to see that the definition of Eq. (3.3b) is identical to the familiar one, given by

$$F_{m'm,n'n}(q)=\int dz_1\int dz_2\,\zeta^*_{m'}(z_1)\zeta_m(z_1)\zeta^*_{n'}(z_2)\zeta_n(z_2)e^{-q|z_1-z_2|}\ . \tag{3.3c}$$

In terms of this effective or physical phonon occupation number, Eq. (3.2) becomes

$$P_e(t)=\frac{2\pi\alpha^2}{\hbar N_e}\hbar\omega_L\sum_{n,n'}\sum_{q}\frac{1}{2q}F_{n'n,n'n}(q)\{I^{(+)}_{nn'}(q)[1+N_{nn',nn'}(q,t)]-I^{(-)}_{nn'}(q)N_{nn'nn'}(q,t)\} \tag{3.4}$$

with

$$I^{(\pm)}_{nn'}(q,t)=\frac{2}{A}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}f_{n\mathbf{k}}(t)[1-f_{n'\mathbf{k}'}(t)]\delta_{\mathbf{k}',\mathbf{k}\mp\mathbf{q}}\delta(E_{nk}-E_{n'k'}\mp\hbar\omega_L)\ . \tag{3.5}$$

The rate of change of $N_{n'n,m'm}(q)$ due to electron-phonon collisions can be obtained by multiplying Eq. (2.12) with $G^*_{n'n}(q,q_z)G_{m'm}(q,q'_z)$, summing over q_z and q'_z, and dividing with the same normalization factor used in Eq. (3.3a), with the result,

$$\left[\frac{\partial N_{n'n,m'm}(q,t)}{\partial t}\right]_{ep}=\frac{\alpha^2}{\hbar}\sum_{l,l'}\frac{1}{2q}\frac{F_{n'n,l'l}(q)F_{l'l,m'm}(q)}{F_{n'n,m'm}(q)}$$
$$\times\{\pi I^{(+)}_{l'l}(q,t)[2+N_{n'n,l'l}(q,t)+N_{l'l,m'm}(q,t)]-\pi I^{(-)}_{ll'}(q,t)[N_{n'n,l'l}(q,t)+N_{l'l,m'm}(q,t)]$$
$$-i[J^{(+)}_{l'l}(q,t)+J^{(-)}_{ll'}(q,t)][N_{n'n,l'l}(q,t)-N_{l'l,m'm}(q,t)]\}\ . \tag{3.6}$$

where $I^{(\pm)}_{ll'}$ is given by Eq. (3.5) and

$$J^{(\pm)}_{ll'}(q,t)=\frac{2}{A}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}f_{l\mathbf{k}}(t)[1-f_{l'\mathbf{k}'}(t)]$$
$$\times\delta_{\mathbf{k}',\mathbf{k}\mp\mathbf{q}}P\frac{1}{E_{lk}-E_{l'k'}\mp\hbar\omega_L}\ . \tag{3.7}$$

In Eq. (3.6) we have made use of the symmetry of $F_{n'n,l'l}(q)$ and $N_{n'n,l'l}(q)$ under the interchange of $n'n$ and $l'l$. The transformation has reduced the integral on the right-hand side of Eq. (2.12) to a finite sum.[18] This occurs because the kernel of the q''_z sum on the right-hand side of Eq. (2.12) is degenerate. The first term on the right-hand side of Eq. (3.4) is the contribution from phonon emission, the second that from phonon absorption. Finally, using the same transformation, Eq. (2.13) becomes,

$$\left[\frac{\partial N_{n'n,m'm}(q,t)}{\partial t}\right]_{pp}=-\frac{N_{n'n,m'm}(q,t)-n_L}{\tau_{\rm op}}\ . \tag{3.8}$$

The phonon kinetic equation is then given by

$$\frac{\partial N_{nn',mm'}(q,t)}{\partial t}=\left[\frac{\partial N_{nn',mm'}(q,t)}{\partial t}\right]_{ep}+\left[\frac{\partial N_{nn',mm'}(q,t)}{\partial t}\right]_{pp}\ . \tag{3.9}$$

The set of Eqs. (3.4), (3.6), and (3.8) can now be solved easily once the electron distribution is known.

As suggested by experiments, we assume here that due to the frequent electron-electron collisions, the electron distribution function is a Fermi-Dirac distribution at the temperature $T_e(t)$, or $f_{n\mathbf{k}}(t)=f(E_{nk},t)$, with

$$f(E,t)=\{\exp[(E-E_f)/k_BT_e(t)]+1\}^{-1}\ .$$

Here E_f is the Fermi energy at T_e, which is related to the 2D density of electrons $n_e=N_e/A$ by $(2/A)\sum_{n,\mathbf{k}}f(E_{n\mathbf{k}},t)=n_e$. The functions $I^{(\pm)}_{n'n}$ and $J^{(\pm)}_{n'n}$ can then be evaluated explicitely, with the result,

$$I^{(+)}_{nn'}(q,t)=\frac{m}{\pi^2\hbar^2q}\int_{|q/2+m\tilde{\omega}_{n'n}/\hbar q|}^{\infty}dk\,k\frac{1}{[k^2-(q/2+m\tilde{\omega}_{n'n}/\hbar q)^2]^{1/2}}f(E_{nk},t)[1-f(E_{nk}-\hbar\omega_L,t)] \tag{3.10a}$$

and

$$J^{(+)}_{n'n}(q,t)+J^{(-)}_{nn'}(q,t)=\frac{m}{\pi\hbar^2q}\int_0^{m\tilde{\omega}_{n'n}/\hbar q-q/2}dk'\,k'\frac{f(E_{n'k'},t)}{[(m\tilde{\omega}_{n'n}/\hbar q-q/2)^2-k'^2]^{1/2}}$$
$$-\frac{m}{\pi\hbar^2q}\int_0^{m\tilde{\omega}_{n'n}/\hbar q+q/2}dk\,k\frac{f(E_{nk},t)}{[(m\tilde{\omega}_{n'n}/\hbar q+q/2)^2-k^2]^{1/2}}\ , \tag{3.10b}$$

where $\tilde{\omega}_{n'n}=(E_{n'}-E_n)/\hbar+\omega_L$. As expected from the detailed balance condition, one also finds

$$I^{(-)}_{nn'}(q,t)=I^{(+)}_{n'n}(q,t)\exp[\hbar\omega_L/k_BT_e(t)]\ . \tag{3.10c}$$

Finally, we will only consider here the steady-state situation. The nonequilibrium phonon distribution is then obtained by equating to zero the right-hand side of Eq. (3.9). For simplicity, we also restrict ourselves to the case where the electrons occupy only the lowest subband, $n=0$. In this case, letting for simplicity $N_{00,00}(q)=N_0(q)$, we obtain

$$\frac{1}{\tau}=\frac{1}{2\pi n_e}e^{\hbar\omega_L/k_BT_e}\int_0^{\infty}dq\,q\left[\frac{N_0(q)+1}{\tau_e(q)}-\frac{N_0(q)}{\tau_a(q)}\right]\ , \tag{3.11}$$

where $1/\tau$ is defined by Eq. (1.1), and

$$\left[\frac{\partial N_0(q)}{\partial t}\right]_{ep}+\left[\frac{\partial N_0(q)}{\partial t}\right]_{pp} =\frac{N_0(q)+1}{\tau_e(q)}-\frac{N_0(q)}{\tau_a(q)}-\frac{N_0(q)}{\tau_{\rm op}}=0\ , \quad (3.12)$$

with

$$\frac{1}{\tau_e(q)}=\frac{\pi\alpha^2}{\hbar}\frac{1}{q}F_{00,00}(q)I_{00}^{(+)}(q)\ , \quad (3.13a)$$

$$\frac{1}{\tau_a(q)}=\exp(\hbar\omega_L/k_BT_e)\frac{1}{\tau_e(q)}\ . \quad (3.13b)$$

We have evaluated Eq. (3.11) for a GaAs-$Ga_xAl_{1-x}As$ heterojunction. We used the following values for the parameters: $n_e=5\times10^{11}/\text{cm}^2$, $\hbar\omega_L=36.8$ meV, $m=0.072m_0$, with m_0 the electron mass, $\epsilon_\infty=10.91$, and $\epsilon_0=12.91$. We have included the effect of dynamical screening in the random-phase approximation in the single subband calculation. The corresponding equations are given by Eqs. (3.11)—(3.13) with $F_{00,00}(q)$ replaced by $F_{00,00}(q)/|\epsilon_{00,00}(q,\omega_L)|^2$, where $\epsilon_{00,00}(q,\omega_L)$ is the element of the inverse dielectric matrix corresponding to lowest subband occupation. Its expression can be found for instance in Ref. 6, Eqs. (4.67) and (4.68). The calculated $1/\tau$ is shown in Fig. 1 as a function of the electron temperature T_e. The results for $\tau_{\rm op}=0$, 2, 5, and 10 psec are displayed. We notice that the presence of a population of nonequilibrium LO phonons not only reduces considerably the electron cooling rate, but also changes qualitatively its functional dependence on the electron temperature. For $\tau_{\rm op}=0$, $1/\tau$ is a decreasing function of T_e. For $\tau_{\rm op}=5$ psec the value of $1/\tau$ is reduced about 8 times and $1/\tau$ is an increasing function of T_e. This can be understood by describing the nonequilibrium distribution of LO phonons by the "phonon temperature" $T(q)$, defined by

$$N_0(q)=1/\{\exp[\hbar\omega_L/k_BT(q)]-1\}\ .$$

The electron energy-loss rate decreases with the difference $[T_e-T(q)]/T_e$. In Fig. 2, we show $T(q)$ as a function of

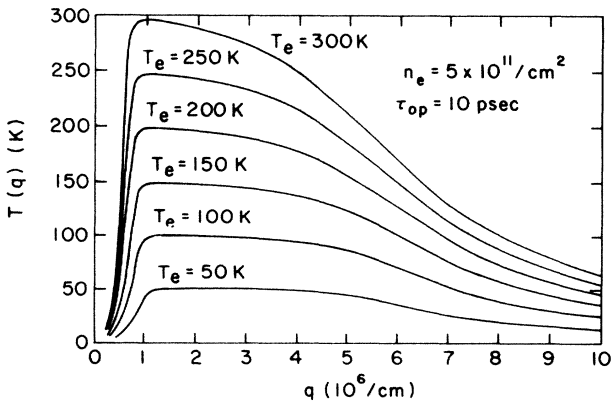

FIG. 2. "Phonon temperature" $T(q)$ as a function of q for 50 K $\le T_e \le$ 300 K and lowest-subband occupation.

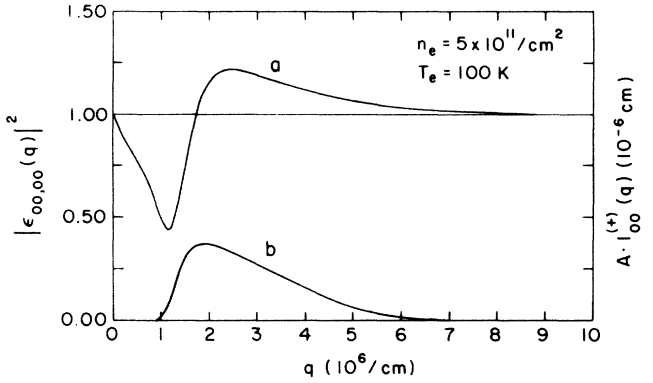

FIG. 3. $|\epsilon_{00,00}(q)|^2$ (curve a) and $A\cdot I_{00}^{(+)}(q)$, with $A=(\pi^2\hbar^2)/(mk_F)e^{\hbar\omega_L/k_BT_e}$ (curve b) as functions of q for $T_e=100$ K.

q for different values of T_e, with $\tau_{\rm op}=10$ psec. The difference $[T_e-T(q)]/T_e$ is particularly small in the region of q where $I_{00}^{(+)}$ and $I_{00}^{(-)}$ are nonvanishing. This leads to an appreciable decrease of the cooling rate. Furthermore, $[T_e-T(q)]/T_e$ increases as T_e increases; at higher electron temperature the hot-phonon mechanism becomes less effective in reducing the cooling rate. Finally, the dynamical screening effect is not very important. In Fig. 3 we show $|\epsilon_{00,00}(q,\omega_L)|^2$ and $I_{00}^{(+)}(q)$ as functions of q for $T_e=100$ K. The behavior of the dynamical dielectric function is qualitatively different from that of the static one. In particular $|\epsilon_{00,00}(q,\omega_L)|^2$ is smaller than 1 in the region of small q: this corresponds to an antiscreening effect.[5,19] Figure 1 also shows $1/\tau$ as a function of T_e for $\tau_{\rm op}=0$ without (dashed curve) dynamical screening. We see that antiscreening dominates in the lower T_e region where it slightly increases the cooling rate. At higher T_c the screening effect dominates and leads to a small decrease in the cooling rate. The contribution to the dielectric function from the plasmon pole is important only over a very narrow q region where $I_{00}^{(\pm)}(q)\approx0$.

We now compare our results with the experiments reported in Ref. 1. If the T_e dependence of $1/\tau$ can be neglected, a plot of $1/T_c$ versus $\ln P_c$ gives a straight line with slope $-\hbar\omega_L/k_B$. In analyzing experiments an "average", i.e., T_e-independent, relaxation rate, $1/\tau_{\rm avg}$ is usually defined by the intercept on the $\ln P_e$ axis of a linear fit to the data. From Fig. 1 of Ref. 1 one obtains $\tau_{\rm avg}\approx1.2$ psec. This value is about 8 times longer than the value obtained when the emitted phonons thermalize instantaneously with the lattice. Furthermore, the relaxation rate $1/\tau$ increases with increasing T_e. Our results are in quantitative agreement with these measurements and attributes the slowing down of electron cooling to the presence of an appreciable population of nonequilibrium phonons.

IV. DISCUSSION

We conclude this paper with a few remarks.

(1) An appreciable population of nonequilibrium pho-

nons can be maintained only if the time scale for the relaxation of the emitted phonons into the heat bath of the thermal phonons is longer than that characterizing electron-phonon scattering. In other words when hot-phonon effects are important the "physical" nonequilibrium phonons are mostly determined by the electron-phonon interaction. The phonon-phonon scattering is only a small perturbation. This is the central assumption of our calculation. As discussed in the Introduction, the LO lattice excitations emitted by electrons confined in a quantum well are localized in the z direction in a spatial region of the order of the mean width of the electron layer. This observation naturally leads to the description of the nonequilibrium lattice excitations in terms of phonon wave packets and to the introduction of an occupation number for phonon wave packets as defined in Eqs. (3.3). The choice of weighting the plane-wave states with functions directly proportional to the electronic subband wave functions is a natural one for this problem and provides an exact solution of the phonon kinetic equation (2.12).

(2) The reduction of the phonon kinetic equation from an integral equation to a finite set of coupled algebraic equations only occurs if (a) the LO phonons are assumed to be dispersionless and (b) the wave-vector dependence of the LO phonons lifetime, τ_{op}, is neglected. When either of these two assumptions is relaxed, the phonon kinetic equation cannot be solved easily. The introduction of phonon wave packets that represent the nonequilibrium physical phonons more closely than plane-wave states may, however, still be useful. In the plane-wave representation in fact all off-diagonal elements of the one-body reduced density matrix have to be retained to adequately describe the nonequilibrium lattice excitations and Eq. (2.12) cannot be decoupled. On the contrary, after representing the lattice excitations in terms of localized phonon wave packets one can argue on physical grounds that in this representation the off-diagonal elements of the one-body density matrix are negligible compared to the diagonal ones. The accuracy of the resulting approximation can then be verified in detail. Even when a transformation of the type given in Eqs. (3.3) does not lead to an exact solution, in this new representation one may therefore still be able to approximately describe the dynamics of the nonequilibrium lattice excitations by a transport equation of the familiar (Boltzmann) form for the occupation number of a suitably constructed phonon wave packet. Work in this direction is in progress. The description of the relaxation of the nonequilibrium lattice modes by a Boltzmann equation for the occupation number of decoupled 3D plane-wave phonon states is, however, simply incorrect because the system is spatially inhomogeneous.

(3) The phonon kinetic equation (3.5) contains no assumptions regarding the electron distribution function. In particular, it is not restricted to the use of an electron temperature model. No analytic solution of the electron equation is, however, available when electron degeneracy and scattering with LO phonons are included. Furthermore, the electron temperature model appears to describe well the experimental results of interest here. Within this model it is straightforward to consider the time-dependent situation that is probed in picosecond time development experiments. This work is currently in progress. As expected from previous 3D calculations, preliminary results indicate that in a time-dependent situation the bottleneck effect due to the nonequilibrium phonons is even more effective than in the steady-state case in slowing down the hot carrier cooling.

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*Present address: University of Illinois at Chicago, Chicago, IL 60680.

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