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Nonlinear response of a superlattice

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Abstract— In this work we study the nonlinear dc and ac response of a superlattice. We develop asymptotic theories for the I-V curve and ac gain valid in both the very low frequency quasistatic limit, the intermediate frequency limit and high frequency limit. We also explore the I-V curve and ac gain for a quite extensive parameter regime. Parameter regimes which have gain and positive differential conductivity are identified for sufficiently high ac amplitudes. These parameter regimes will be important to understand the nonlinear state of solid state sources in the THz range.

I. INTRODUCTION

We will in this work report on nonlinear ac and dc conductivities in a superlattice favorable for a THz source [1]. Esaki and Tsu [1] proposed to use a semiconductor superlattice to to achieve a device with a currentvoltage characteristic with negative differential conductivity (NDC) above a certain critical dc-bias proportional to the geometric mean collision frequency (ν_q) . Subsequently, Ktiterov et al.[2] gave a simple model for the miniband electron distribution function for a superlattice including both momentum and energy relaxation. They showed that for dc-bias in the NDC-regime and linear ac-drive that there was ac-gain for frequencies slightly below the resonant Bloch frequency. We will further investigate Ktiterov's theory into the nonlinear ac-drive regime. It turns out that the problem of calculating currents in Ktiterov's Boltzmann model, can be reduced to studying the momentum equation and energy equation[3, 4] . The electron density equation for homogenous E-field is simply $\rho_0=const$.

The model we will concentrate on is based on the fluid moments of the Ktiterov's Boltzmann equation, but in a nondimensional form where the essential parameters of the theory is stressed from the beginning. This emphasis has simplifying implications for scaling of theoretical, simulation and experimental results and parameters. Our goal is to find conditions under which a dcbiased and nonlinearly ac-driven superlattice can have both gain and positive differential conductivity. The coincidence of the regime of gain of small amplitude oscillations and negative differential conductivity imply that domain formation is an obstacle to the construction of a superlattice THz source. The ac E-field is assumed to give rise to such high electric fields in the medium that the dc and ac conductivities in the superlattice is nonlinearly modified . We want to explore conditions under which the dc conductivity is locally of the positive differential type and at the same time that the nonlinear conductivity give rise to gain. The model we choose to investigate is the momentum $ho_0 v$ and energy $ho_0 arepsilon$ fluid moments of a Boltzmann equation with a simple energy and momentum collision operator. We find the following equations in agreement with several earlier works :

$$(\frac{\partial}{\partial t} + \nu_p)v + \frac{ed^2E}{\hbar^2}(\varepsilon - \frac{\Delta_1}{2}) = 0,$$

$$\frac{\partial}{\partial t}\varepsilon + \nu_{\varepsilon}(\varepsilon - \varepsilon_{T0}) - eEv = 0,$$
 (1)
$$\varepsilon_{T0} \equiv \frac{\Delta_1}{2}(1 - \frac{I_1(\frac{\Delta_1}{2k_BT_0})}{I_0(\frac{\Delta_1}{2k_BT_0})})$$

By introducing new variables $v_{\varepsilon} = (\varepsilon - \varepsilon_{T0})d/\hbar$, $v_{\varepsilon}^{0} \equiv (\frac{\Delta_{1}}{2} - \varepsilon_{T0})d/\hbar = (\Delta_{1}d/2\hbar)\frac{I_{1}(\frac{\Delta_{1}}{2k_{B}T_{0}})}{I_{0}(\frac{\Delta_{1}}{2k_{B}T_{0}})}$ and defining the Bloch frequency $\omega_{B} = edE/\hbar$, we find the alternative description

$$(\frac{\partial}{\partial t} + \nu_p)v_p + \omega_B v_\varepsilon = \omega_B v_\varepsilon^0, \qquad (2)$$

$$\frac{(\partial}{\partial t} + \nu_{\varepsilon})v_{\varepsilon} - \omega_B v = 0 \tag{3}$$

These equations can now be put into a nondimensional

form by scaling the velocities by v_{ε}^{0} (alternatively by $d\omega_{B0}$ or $d\omega$) and time and frequency by the background Blochfrequency $\omega_{B0} = \frac{edE_{0}}{\hbar}$ (alternatively ω or the the geometric mean collision frequency which we also will discuss below). We then find the following nondimensional form of the equations with frequencies and time scaled with respect to the dc Bloch frequency. Here we have by abuse of notation used the same symbols for the variables $\omega_{B} \rightarrow \omega_{B}/\omega_{B0}, \nu_{\varepsilon,p} \rightarrow \nu_{\varepsilon,p}/\omega_{B0}, t \rightarrow t\omega_{B0}, (v_{\varepsilon}, v) \rightarrow (v_{\varepsilon}, v)/v_{\varepsilon 0}$

$$(\frac{\partial}{\partial t} + \nu_p)v + \omega_B v_\varepsilon = \omega_B, \tag{4}$$

$$\left(\frac{\partial}{\partial t} + \nu_{\varepsilon}\right)v_{\varepsilon} - \omega_B v = 0.$$
 (5)

An alternative useful scaling of frequencies and times of this equation are given in terms of units of the geometric mean collision frequency (c.f. discussion below) $\nu_g = (\nu_{\varepsilon}\nu_g)^{0.5}$ which means $t \to \bar{t} = t\nu_g$; $\nu_{\varepsilon,p} \to \kappa_{\varepsilon p}, \frac{1}{\kappa_{\varepsilon p}}; \omega_{B0} \to \omega_0 = \frac{\omega_{B0}}{\nu_g}; \omega_B \to \bar{\omega}_B = \frac{\omega_B}{\nu_g}$; $\omega \to \bar{\omega} = \frac{\omega}{\nu_g}. \kappa_{\varepsilon p} = (\frac{\nu_{\varepsilon}}{\nu_p})^{0.5}.$ The dc-solutions of these equations for a given con-

The dc-solutions of these equations for a given constant E-field $E_0 = V_0/L$ corresponding to a constant Bloch frequency ω_{B0} is given in these scaled variables by

$$v_0 = \kappa_{ep} \omega_0 / (1 + \omega_0^2) = \sigma_0 \omega_0; \ v_{e0} = \omega_0^2 / (1 + \omega_0^2)$$
(6)

Here we have introduced the scaled dc conductivity σ_0 . We have also introduced the relative Bloch frequency in units of the geometric mean collision frequency ω_0 which is normalized to 1 at the maximum of the I-V curve. Another quantity we will be interested in is the linear response of the velocity and energy due to a harmonic perturbation in the E-field drive corresponding to $\omega_B = 1 + \epsilon \omega_{B1}(t), \ \omega_{B1}(t) = -\omega_1 \cos(\omega t) = -\frac{\omega_1}{2} \exp(-i\omega t) + c.c. \ \varepsilon$ is just an ordering parameter. We now find the $O(\varepsilon)$ scaled ac-response (the dc and ac response for a nonlinear ac drive is too long to be included explicitly) in agreement with Khiterov's model ac-conductivity

$$\hat{\mathbf{v}}_1 = \begin{pmatrix} \hat{v}_1 \\ \hat{v}_{\varepsilon 1} \end{pmatrix} = -\frac{\omega_1 \omega_0}{2} \begin{pmatrix} \sigma_1(\omega) \\ \sigma_{\varepsilon 1}(\omega) \end{pmatrix}$$
(7)

$$\begin{pmatrix} \sigma_l \\ \sigma_{\varepsilon l} \end{pmatrix} = \frac{\sigma_0}{\omega_0^2 + 1 - (\omega\omega_0)^2 - i\omega\omega_0(\kappa_{\varepsilon p} + 1/\kappa_{\varepsilon p})} (\$) \\ \begin{pmatrix} 1 - \omega_0^2 - i\omega\omega_0/\kappa_{\varepsilon p} \\ \omega_0(2/\kappa_{\varepsilon p} - i\omega\omega_0) \end{pmatrix}.$$
(9)

$$\hat{\omega}^2 = \frac{1}{\hat{\nu}_{\varepsilon}\hat{\nu}_p}, \quad \hat{\nu}_{\varepsilon} = \nu_{\varepsilon} - i\omega, \quad \hat{\nu}_p = \nu_p - i\omega \quad (10)$$

We immediately see that there is a resonance in the ac-conductivity at frequency $\omega_r = \pm (1 - \nu_d^2)^{1/2}$

 $(\nu_d = (\nu_p - \nu_{\epsilon})/2 = \hat{\nu}_d/\omega_0, \hat{\nu}_d = (1/\kappa_{\epsilon p} - \nu_{\epsilon})/2$ $(\kappa_{ep})/2 \approx 0.35$) which for high enough ω_0 is close to the normalized Bloch frequency 1. For fixed Bloch frequency (ω_0) or fixed frequency $(\bar{\omega})$ this resonance translate to $\bar{\omega}_r = \pm (\omega_0^2 - \hat{\nu}_d^2)^{0.5}$ or $\omega_{0r} = \pm (\bar{\omega}^2 - \hat{\nu}_d^2)^{0.5}$ respectively. A short calculation will show that there is linear gain, i.e. $\sigma_1 = \operatorname{Re}(\sigma_l) < 0$ only if $\omega_0 > 1$ and in the frequency regime $\omega < \omega_z < \omega_{0c} = 1$. Here ω_z (near to ω_r) is the crossover frequency from gain to no gain. Consequently there is no coincidence between gain and PDC in the linear limit $\bar{\omega}_1 \rightarrow 0$ We remark that no resonance is found for $u_d(\simeq .35/\omega_0) > 1$, i.e. $\omega_0 < \hat{\nu}_d$ or $\bar{\omega} < \hat{\nu}_d$ respectively. If we assume that the ratio of the collision frequencies are reasonably fixed, we see that the description of the dc and ac response can be given in terms of the three nondimensional parameters $\bar{\omega}_1 = \omega_1 \omega_0$, $\bar{\omega} = \omega \omega_0$ and ω_0 which is nothing but the ac-drive amplitude, frequency and Bloch frequency measured in units of the geometric mean collision frequency. These three variables are also reasonable to use since for given geometric mean collision frequency they correspond to fixed frequency and ac-amplitude as we vary the dc bias.

II. AC AND DC CONDUCTIVITIES WITH A NONLINEAR AC-DRIVE

We summarize our theoretical (there is no space to give the theory) and numerical investigation below(see some of the results of I-V curves and ac response in Fig. 2a,b) This has eventually to be substantiated by experimental results.

1. The solution of our model in the high frequency limit approaches a limit cycle with a timescale $\tau = O(1/\bar{\nu})$ and with leading order oscillation frequency and renormalized resonance given as $\omega_l = (1 - \bar{\nu}_d)^{1/2}$ if $\bar{\nu}_d = \nu_d J_0(2\omega_1/\omega) < 1$. For $\bar{\omega}_1 \ge O(1)$ there is a narrow layer of PDC and gain in the domain $\omega_0 \in [\bar{\omega} - \delta, \bar{\omega}]$ where $\delta = o(1)$ and similar indications near the second resonance $\precsim 2\bar{\omega}$ for $\bar{\omega}_1 \gg 1$. There is a change in signature of the I-V curve for small ω_0 and near $\bar{\omega}_1/\bar{\omega} = 2.405 (J_0(\frac{\bar{\omega}_1}{\bar{\omega}}) = 0)$. The corrections of $O(\nu_d)$ is quantitatively important in our theory in contrast to many authors who use a model with only one collision frequency.

2. The quasistatic theory and intermediate frequency theory $\omega < O(\nu_d)$ is characterized by a decay with timescale τ (no oscillations) to the limit cycle, a linear shift of the maximum of the I-V curve $\omega_{0c} \sim \bar{\omega}_1$ and a small region of coinciding gain and PDC for $\bar{\omega}_1 > 1$.

The limit cycle can be described in a three dimensional phase space plot of $\{\omega_B(t), \mathbf{v}(t)\}$. Since we will basically be interested in conductivities, we will study the projection of the limit cycle on the Blochfrequencyvelocity plane, $\{\omega_B(t), v(t)\}$. The limit cycle will have a basic period of $T = 2\pi/\omega$, but can have a complex behavior with one or several loops at high frequencies $\bar{\omega} \gg 1$ and will due to the stiffness of the system have a tendency to align along the I-V- curve in the quasistatic limit for small $\bar{\omega}$.

A. I-V curves

The averaged velocity $v_0 = \frac{1}{T} \int_0^T v dt$ over a basic period $T\,=\,2\pi/\omega$ of the limit cycle is the dc- component of the periodic velocity. DC I-V curves (see examples in Fig. 2a) in this context is nothing else than a graph of $v_0(\omega_0; \bar{\omega}_1, \bar{\omega})$ as a function of the Blochfrequency with the amplitude and frequency of the drive as parameters. To measure this property for a nonlinearly driven superlattice numerically one has to wait until all transients has died out such that the solution sticks to the limit cycle. For the parameter regime and the collision frequencies we are interested in, it is suffient to wait 4-5 periods before one do the averaging around one period of the limit cycle. The collision frequency for a GaAs superlattice has been estimated by a fit to I-V measurements fo a specific sample given on the Quantum Institute homepage (J. Scott) to be $1/\nu_{\varepsilon} \approx 0.3 ps$ and $1/
u_p pprox 0.15 ps$. For a InAs/AlSb superlattice a reasonable guess for collision frequencies are $1/\nu_{\varepsilon} \simeq 0.6 ps$ and $1/
u_p \simeq 0.2 - 0.4 ps$. Therefore estimates of the collision frequency ratio are $\kappa_{\varepsilon p}(GaAs) \simeq 0.707$ and $\kappa_{\varepsilon p} \in [0.6, 0.8]$. The geometric mean of the collision frequencies are therefore estimated as $\nu_q(GaAs) \approx$ 4.7THz and $\nu_q(InAs/AlSb) \in [2,3]THz$. With these parameters given, the Bloch frequency can be deduced, i.e. $\omega_0, \bar{\omega}, \bar{\omega}_1 = 1$ corresponds to the physical frequencies $\omega_{B0}, \omega, \omega_1 = \nu_q$ To help the reader we give the following table which scale our nondimensional theoretical and numerical results to different type of superlattice experimental settings.

$\omega_{B0}(\omega_{B1})$	$4.7\omega_0(\text{or }\bar{\omega}_1)(\frac{\nu_g}{4.7THz})THz$
$V_0(V_1)$	$0.294(\frac{N}{100})\frac{\nu_g}{4.7THz}\omega_0(\text{or }\bar{\omega}_1)eV$
$f = \frac{\nu_g \omega}{2\pi}$	$0.748(\frac{\nu_g}{4.7THz})\bar{\omega}THz$
$v_{\varepsilon 0}$	$\frac{\Delta_1}{20meV} \frac{d}{10nm} F(\kappa) 3.79 \times 10^6 m/s$
$\kappa = \frac{\Delta_1}{2k_BT}$	$0.3868(\frac{\Delta_1}{20meV})(\frac{T}{300K})^{-1}$
σ	$(\frac{N}{100})^{-1} \frac{n_0}{10^{16} cm^{-3}} \frac{S}{20(\mu m)^2} \frac{L_{mf}}{0.1615 \mu m} \bar{\sigma}$

Tab.1 Scaling of some physical quantities from nondimensional ones. Here $\bar{\sigma} = \sigma_0 0.393 mho_{\text{and}} \sigma = \frac{e^2 n_0 L_{mf} S \sigma_0}{Nh}$. For scaling of physical σ_{1p} with nondimensional σ_1 interchange $\sigma \to \sigma_1$ and $\sigma_0 \to \sigma_{1p}$.

Here $F(\kappa) = I_1(\kappa)/I_0(\kappa)$ is plotted in Fig.1 and can also be used to infer the nonlinear temperature dependence of the dc-bias and ac-field given data for the nonlinear mean energy through our simulation(we



Figure 1 – Here we have plotted the function $F(\kappa) = I_1(\kappa)/I_0(\kappa)$ where the nondimensional parameter $\kappa = \frac{\Delta_1}{2k_BT}$. The scaling of this parameter for different superlattices is given in Tab. 1.

do not discuss the energy/temperature results here) or by experimental means. $v_{\varepsilon D}(\bar{\omega}, \bar{\omega}_1, \omega_0) = \frac{\Delta_1 d}{2h} F(\kappa) \Rightarrow$ $T(\bar{\omega}, \bar{\omega}_1, \omega_0) = \frac{2k_B}{T_0} F^{-1}(\frac{2h}{\Delta_1 d} v_{\varepsilon D}).$

This nonlinear temperature might be an important parameter to determine selfconsistent models of collision frequencies, especially for temperature regimes where kinetic energy is comparable to the phonon energy. We have also defined a characteristic collision length $L_{mf} = \nu_{c0}/\nu_g$ for superlattices. The dc current given for a nondimensional conductivity σ_0 in a superlattice with electron density n_0 , transversal crosssection of the mesa S and length L = Nd now scales as a function of dc voltage V_0 , ac electric field $E_1 = V_1/L$ and frequency f by $I_{dc} = \sigma V_0$ ([I] = Ampere if $[V_0] = Volt$). The accurrent and conductivity scale the same way given an ac nondimensional conductivity.

B. Nonlinear ac response

We will now measure the nonlinear ac response (see examples in Fig. 2b) of the superlattice velocity and energy at the first harmonic of the limit cycle. The first harmonic can be determined directly through a discrete fouriertransform of velocity and energy data from a complete period of the limit cycle. Alternatively, the real part or cosine component of the first harmonic can be determined by averaging the superlattice equations over one period assuming again that we are at the limit cycle such that periodicity can be assumed, i.e. v(t) = v(t+T). This leads to the averaged equations

$$\nu_p v_D + v_{\varepsilon D} - \frac{\omega_1}{2} v_{1c} = 1, \qquad (11)$$

$$\nu_{\varepsilon}v_{\varepsilon D} - v_D + \frac{\omega_1}{2}v_{\varepsilon 1c} = 0.$$
 (12)

The interaction terms $\mp \frac{\overline{\omega}_1}{2} v_{1c,\varepsilon 1c}$ has an interesting physical interpretation as the rescaled averaged



Figure 2 - In Fig. 2a we have plotted the normalized de I-V curve parameterized by the velocity averaged over one period of the limit cycle as a function of normalized Bloch frequency $\omega_0 \in [0, 10]$ and for a fixed nonlinear ac-drive amplitude $\bar{\omega}_1 = 5.0$. These normalized I-V curves can be scaled to I-V curves for different experimental parameters by the scaling laws given in Tab.1 and the relation $v_0 = \sigma \omega_0$. The curves are labelled as: dash-dotted curve $\rightarrow \bar{\omega} = 0.1$, curve of +'s $\rightarrow \bar{\omega} = 1.0$, curve of o's $\rightarrow \bar{\omega} = 2.079 = \bar{\omega}_1/2.405$, and solid curve $\rightarrow \bar{\omega} = 5.0$. The case $\frac{\bar{\omega}_1}{\bar{\omega}} = 2.405$ corresponds to the degenerate case of the first zero of the zeroth order Bessel function $J_0(\frac{\bar{\omega}_1}{\bar{\omega}})$.



We can deduce the ac gain through either of the two equivalent relations $\sigma_1(\omega) = -v_{1c}(\omega)/\bar{\omega}_1 =$ $-\operatorname{real}(\hat{v}_1(\omega))/(\bar{\omega}_1/2)$. Here $v_{1c}(\omega)$ and $\hat{v}_1(\omega)$ are the first harmonic cosine and real coefficient of the Fourier expansion of the limit cycle time series of the velocity. The scaling of each value of this nondimensional version nonlinear ac conductivity to a whole continuum of experimental parameters can be found through Tab. 1.

Therefore, given that there are resonances in $v_{1c}(\bar{\omega}, \bar{\omega}_1, \omega_0)$ at $n\bar{\omega} = \omega_0$ and that the peak of the I-V curve without ac-drive is at $\omega_0 = 1$ in units of the geometric mean collision frequency, we can only expect effects of the first resonance on the I-V characteristic in the form of additional bumps if $\bar{\omega} > 1$. Morover, we qualitatively deduce that if v_{1c} is slowly varying with $\bar{\omega}_1$ in the quasistatic regime $\bar{\omega} << 1$ that one can expect an approximate linear shift in v_D with increasing $\bar{\omega}_1$. E.g., a linear shift in the position of the maximum of the I-V curve can be expected.

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Figure 3 -