Phonon-limited low temperature mobility in a quasione-dimensional semiconductor quantum wire

G Y Hu and R F O'Connell

Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4001, USA

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Abstract. We derive an analytic expression for the imaginary part of the density response function for a quasi-one-dimensional semiconductor quantum wire with multi-populated subbands at finite temperature. The acoustic-phonon-limited low temperature mobility of the system is then calculated by means of the memory function formalism, neglecting electron-electron interactions. The phonon-limited relaxation rate is found to have a temperature dependence of $T^{n(T)}$ and we emphasize the temperature dependence of n. In fact the lower the temperature the larger is the n value but, in general, we find that 0 < n(T) < 2. Also, it depends on the electron density in such a way that whenever the Fermi velocity of the electrons in the top populated subband is close in magnitude to the sound velocity the phonon-limited relaxation rate reaches a peak value which also increases with increasing electron density.

In recent years, the study of semiconductor quantum wires has attracted much attention both theoretically and experimentally (for a review see [1] and references therein). Such systems can be fabricated with very high electron mobilities [2], leading to possibilities for device applications. In a semiconductor quantum wire, the Fermi wavelength is in the order of the wire width, and electrons occupy multiple subbands in quasi-one-dimensional (Q1D) states. One of the particularly interesting aspects of transport properties in these semiconductor quantum wires is the phonon-limited low temperature electron mobility [2-6]. This is because with the reduction in the impurity scattering in the high mobility samples, the phonon scattering is expected to be dominant even at low temperatures. In addition, it is well known that the Q1D electrons have a peculiar density response behaviour [7] (such as the $q = 2k_F$ divergence at T = 0 for the static density response function), which may lead to new physics in the phonon scattering problem.

The subject of the phonon-limited low temperature electron mobility was first brought to attention in the study of the two-dimensional electron gas (2DEG) [8-10], where very high mobility samples are possible. To date, there is still great interest in deducing the absolute value of the deformation coupling constant by studying the acoustic phonon scattering in a 2DEG both theoretically [9] and experimentally [10]. The study of the phonon-limited low temperature mobility in a Q1D system is unique at least from the following points of view:

(i) very high mobility samples are achievable so as to make the dominant region of the acoustic phonon scattering much wider;

(ii) it has a very distinctive $T \rightarrow 0$ behaviour (T^2 , see the discussions later) compared with T^4 for a 2DEG and T^5 for the bulk material;

(iii) the presence of electrons in multi-subbands may introduce peculiar behaviour for the acoustic phonon scattering. These are our motivations for pursuing the following study of the phonon-limited low temperature mobility in Q1D semiconductor quantum wires.

In the literature, there are already several papers which deal with Q1D electronphonon scattering [2-6]. These studies are generally explicit only for the singleoccupied subband case. Besides, a detailed analysis of the temperature and density dependence of the electron-phonon relaxation rate is still lacking. The present paper is devoted to a systematic study of the phonon-limited low temperature mobility in semiconductor quantum wires having multi-populated subbands, with the emphasis on a full analysis of the temperature and density dependence. The transport theory we will use in this paper is the generalized quantum Langevin equation (GLE) approach [11] which we developed in recent years and which has been used in studying the subband effects of the semiconductor quantum wire at T = 0. The screening effects due to the electron-electron interaction will not be discussed in this paper not only for simplicity considerations but also because some studies [9] show that a consistent description of low T mobility can be given only if the short range deformation scattering is not screened by free carriers. In addition, since our main concern here is the case where the acoustic phonon scattering is dominant, the weak localization due to the effects of disorder will be neglected. Also, we mention that there exist many studies [12] for the phonon-limited mobility in conducting polymers. The latter study is usually based on a Q1D lattice, which is different from that of the semiconductor quantum wire. Therefore, no direct comparison between the main conclusion of this paper and those of the polymer system [12] will be pursued in the present paper.

In the GLE approach [13], we visualize the centre of mass of the electrons as a quantum particle, while the relative electrons and phonons act as a heat bath, which is coupled to the quantum particle through the electron-phonon interaction. By solving the Heisenberg equation of motion for the heat bath variables, we derive the GLE for the quantum particle. According to our GLE formalism, the motion of the centre of mass of the electrons is like that of a Brownian particle subject to the frictional and fluctuation forces in a heat bath, and the mobility can be evaluated directly through the memory function formalism. The general expression for the memory function for phonon scattering in the free electron model was previously derived by us [13]. Our starting point is the phonon relaxation rate (which is the zero frequency memory function) deduced directly from (3.19) of [13]:

$$\frac{1}{\tau_{\rm ph}} = \frac{\beta}{4Nm^*\hbar} \sum_{q} q_x^2 |M(q)|^2 [-\mathrm{Im}\,\chi(q,\Omega_q)] \mathrm{cosech}^2 \frac{\beta\Omega_q}{2} \tag{1}$$

where $\beta = \hbar/k_{\rm B}T$, M(q) is the electron-phonon interaction matrix, N is the total number of electrons in the system, m^* is the effective mass of the electrons, Ω_q is the phonon energy, and $\mathrm{Im}\chi(q,\Omega_q)$ is the imaginary part of the density response function. We note that it is easy to show that, for bulk material, (1) is equivalent to the well-known Ziman formula for phonon scattering and leads to the T^5 law for phonon scattering at low temperatures. Also we note that (1) is general for all kinds of phonon scattering. In the present paper, our main concern is acoustic phonons [13], in which case one has $\Omega_q = v_s q$, with v_s the sound velocity, and also (see (4.1) of [13])

$$|M(q)|^2 = \frac{C^2 q^2}{2A\rho_{\rm m}\Omega_q} \tag{2}$$

where $\rho_{\rm m}$ is the mass density of the lattice, A is the cross-sectional area of the wire, and C is the deformation potential.

For a Q1D system in the harmonic confinement potential model, and neglecting motion in the z-direction, the density response function has the form (see appendix B of [11])

$$\chi(q,\omega) = \frac{1}{WL} \sum_{k,nn'} \frac{f_k - f_{k+q}}{\hbar\omega - (\epsilon_{k+q} - \epsilon_k) + \mathrm{i}\delta} C_n(q_l) \equiv \frac{1}{W} \sum_{nn'} \chi_{nn'}(q,w) C_n(q_l) \tag{3}$$

where W is the width, and L is the length of the Q1D sample, f_k is the Fermi distribution function, q being the wavevector along the wire (x-direction) and q_l being the quantized wavevector along the width (y-direction), so that $q = (q, q_l)$. In addition,

$$\epsilon_{k} \equiv \epsilon_{kn} = \epsilon_{n} + \frac{\hbar^{2}k^{2}}{2m^{*}}$$

where $\epsilon_n = (n + \frac{1}{2})\hbar\omega_0$ is the subband energy. In addition, the factor due to the quantum confinement [11] is

$$C_n(q_l) = \frac{n_2!}{n_1!} l^l e^{-l/2} [L_{n_1}^l(l)]^2$$
(4)

where l = |n - n'|, $n_1 = \max(n, n')$, $n_2 = \min(n, n')$, and $L_n^m(x)$ is the Laguerre polynomial.

We find that the imaginary part of (3) can be worked out analytically even at finite temperature. The result is

$$\operatorname{Im} \chi_{nn'}(q,\omega) = -\frac{m}{q\hbar^2} \frac{\sinh(\beta\omega/2)}{\cosh(\beta\omega/2) + \cosh\beta A_{nn'}}$$
(5)

where

$$\hbar A_{nn'} = \frac{m}{2} \left[\frac{\omega - (n' - n)\omega_0}{q} \right]^2 + \frac{\hbar^2 q^2}{8m} - \mu + \frac{n + n'}{2} \hbar \omega_0 \tag{6}$$

and μ is the chemical potential. The temperature dependence of (5) is easily deduced as: $\operatorname{Im} \chi_{nn'}(q,\omega) \sim m/q$ for $T \to 0$ and $\operatorname{Im} \chi_{nn'}(q,\omega) \sim \omega/T$ for $T \to \infty$, a result which will be crucial to our discussion later of the peculiar temperature dependence of the phonon-limited mobility for the QID system. Also, since we are mainly concerned with $T \to 0$, we will use the approximation $\mu \approx \epsilon_{\rm F}$, where $\epsilon_{\rm F}$ is the Fermi energy, in the following.

Substituting (2)-(5) into (1), and using the continuum approximation $\sum_q \rightarrow L/2\pi \int_0^{q_D} dq$, where q_D is the Debye wavevector, one obtains

$$\frac{1}{\tau_{\rm ph}} = \frac{1}{\tau_0} \sum_{nn'} C_n(q_l) I_{nn'}(t, \epsilon_{\rm F}) \tag{7}$$

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where $t = (2\beta k_{\rm F} v_{\rm s})^{-1}$, $\tau_0^{-1} = 2m^* C^2 / A \rho_{\rm m} v_{\rm s} \hbar$, and

$$I_{nn'}(t,\epsilon_{\rm F}) = \frac{t^2}{4s} \int_0^{x_{\rm D}} \mathrm{d}x \, x^2 \left\{ \sinh \frac{x}{2} \left[\cosh \frac{x}{2} + \cosh \beta A_{nn'} \right] \right\}^{-1}. \tag{8}$$

Here $s = v_s/v_F$, $x_D = q_D v_s/k_B T$, and

$$\beta A_{nn'} = \frac{1}{4t} \left\{ s + \frac{x^2 t^2 - k_{Fn}^2 / k_F^2}{s} + \frac{n' - n}{s b^2 k_F^2} \left(1 + \frac{n' - n}{4b^2 k_F^2 x^2 t^2} - \frac{1}{xt} \right) \right\}.$$
(9)

Equations (7)-(9) are the key results of the paper. First we analyse the temperature dependence of (7) for the momentum relaxation rate $\tau_{\rm ph}^{-1}$. When $T \to 0$, the integral in (8) becomes temperature independent. Then one obtains from (7) and (8) a $\tau_{\rm ph}^{-1} \sim T^2$ behaviour, which was previously obtained for a single subband system in [6]. What we have shown here is that the low temperature dependence of the phononlimited mobility for a multi-subband system has a low temperature behaviour similar to that of a single subband system. In our formalism, one can easily show that the corresponding two- and three-dimensional results have $\tau_{\rm ph}^{-1}$ depending on T^4 and T^5 , respectively and also that $\mathrm{Im}\chi(q,\omega)$ is independent of q (approximately in the twodimensional case) and ω as $T \to 0$. The peculiar T^2 behaviour of the Q1D momentum relaxation rate is a combined effect of the low dimensionality and the unique property of $\mathrm{Im}\chi(q,\omega) \sim m/q$ at $T \to 0$ as can be seen from (5). Apart from the fact that the impurity scattering is small in high mobility samples, the role of the phonon-limited mobility in the Q1D case is more significant compared with the twodimensional case since the respective low temperature behaviours are T^2 and T^4 .

In the $T \to \infty$ limit, it is more convenient to analyse the behaviour of $\tau_{\rm ph}^{-1}$ directly from (1). In this limit, $\beta \operatorname{cosech}^2 \beta \Omega_q/2$ has a T dependence whereas $\operatorname{Im} \chi(q, \Omega_q)$ has a T^{-1} dependence. As these two factors cancel out, the momentum relaxation rate $\tau_{\rm ph}^{-1}$ in our Q1D model is temperature independent in the very high temperature limit. It is clear that our conclusions hold regardless of the number of subbands. We also stress that the temperature independence of $\tau_{\rm ph}^{-1}$ for the Q1D system at $T \to \infty$ is different from that of the bulk system where $\tau_{\rm ph}^{-1} \sim T$. On the other hand, as our quantum description of the Q1D system clearly breaks down in the $k_{\rm B}T > \hbar\omega_0$ limit, this analysis will only serve for the purpose of understanding the behaviour of the system in the intermediate temperature region, which we discuss later.

At this stage it is perhaps useful to compare our results with those in [6]. In the latter work, only a numerical evaluation of $\tau_{\rm ph}^{-1}$ in certain temperature regions was performed (see figure 2 of [6]) and no $T \to \infty$ behaviour was extracted. We have, however, used the analysis of [6] to verify that similar results emerge for the one subband case (which is the only case treated by these investigators).

In the intermediate temperature range $\theta_D < k_BT < \hbar\omega_0$, where θ_D is the Debye temperature, one expects from these considerations that $\tau_{\rm ph}^{-1} \sim T^{n(T)}$ with 0 < n(T) < 2 and the higher T the smaller the n(T) value. This can be demonstrated by a numerical study of (7). In figure 1, we plot $\tau_{\rm ph}^{-1}$ in units of τ_0^{-1} (defined by (7)) as a function of k_BT (in units of $\hbar\omega_0$), at three different values of $\epsilon_F/\hbar\omega_0 = 2.1, 2.5, 2.9$, where we use the standard parameters (which are insensitive to the shape of the $\tau_{\rm ph}^{-1}$ curve) $q_D = k_F$, and $v_s = 5 \times 10^4$ cm s⁻¹ and we choose $\omega_0 = 2$ meV. The $\tau_{\rm ph}^{-1} \sim T^{n(T)}$ (0 < n(T) < 2) behaviour is clearly seen in that figure for all the values of ϵ_F . It is

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Figure 1. The temperature dependence (in units of the subband energy $\hbar\omega_0$) of the relaxation rate $\tau_{\rm ph}^{-1}$ (in units of $\tau_0^{-1} = 2m^*c^2/A\rho_m v_s\hbar$ defined by (7)) due to the electron-acoustic phonon scattering in a Q1D system for three different values of the Fermi energy $\epsilon_{\rm F}$. Relaxation rates with temperature dependences of $T^{1/2}$ and T are drawn in the upper right of the figure for comparison purposes.

Figure 2. The density dependence (through the variation of Fermi energy $\epsilon_{\rm F}$ in units of the subband energy $\hbar \omega_0$) of the relaxation rate $\tau_{\rm ph}^{-1}$ (in units of $\tau_0^{-1} = 2m^*c^2/A\rho_{\rm m}v_s\hbar$ defined by (7)) due to the electron-acoustic phonon scattering in a Q1D system at two different temperatures.

interesting to note that in the typical temperature ranges $0.1 < k_{\rm B}T/\hbar\omega_0 < 0.4$ and $10 \text{ K} < k_{\rm B}T < 30 \text{ K}, \tau_{\rm ph}^{-1}$ has approximately a linear dependence on T.

Next, we study the Fermi energy $\epsilon_{\rm F}$ dependence of (7) for $\tau_{\rm ph}^{-1}$. A direct analysis of (7) shows that $\tau_{\rm ph}^{-1}$ has the following properties:

(i) when $\epsilon_{\rm F}$ increases to a point where electrons start to fill another subband, there appears many new terms in the sum of (7) and the magnitude of $\tau_{\rm ph}^{-1}$ increases dramatically;

(ii) when the value of $\epsilon_{\rm F}$ changes but with a fixed number of populated subbands in the system, $\tau_{\rm ph}^{-1}$ has a maximum value at the region where the Fermi velocity of the electrons of the top populated subbands $v_{\rm Fn}$ is close to $v_{\rm s}$, where the sum appearing in (7) becomes relatively large. These features of $\tau_{\rm ph}^{-1}$ are illustrated by figure 2, where we plot $\tau_{\rm ph}^{-1}$ (in units of τ_0^{-1}) against $\epsilon_{\rm F}$ (in units of ω_0) at $k_{\rm B}T/\hbar\omega_0 = 0.1$ and 0.2. From figure 2, one concludes that for a pure electron-phonon Q1D system, $\tau_{\rm ph}^{-1}$ is an oscillating function of $\epsilon_{\rm F}/\hbar\omega_0$ with an increasing trend. It peaks when $\epsilon_{\rm F}$ is close to the bottom of the top populated subband and dips when $\epsilon_{\rm F}$ is near the lowest empty subband.

In conclusion, we have derived an analytic expression (5) for the imaginary part of the density response function for a semiconductor quantum wire with multi-populated subbands at finite temperature, and demonstrated that the GLE formalism is ideal for evaluating the phonon-limited low temperature mobility for the semiconductor quantum wires. Our results show that the acoustic phonon-limited relaxation rate

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has a temperature dependence of $T^{n(T)}$, with 0 < n(T) < 2, and the lower the temperature the larger the n(T) value. Also, in the typical experimental temperature range (1 < T < 10 K) for the semiconductor quantum wire, $n \sim 1$. In studying the density dependence, we find that whenever the Fermi velocity of the electrons in the top populated subbands is close to the sound velocity the phonon-limited relaxation rate reaches peak values which also increase with the increasing electron density.

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