Negative Transport Lifetime of Electrons in Quantum Wires

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In bulk and 2D structures, the ensemble average transport lifetime of electrons can only be a positive quantity. However, in quasi 1D structures, it can sometimes become *negative.* The negative sign is manifested whenever *forward* scattering due to acoustic phonon absorption is the dominant electron interaction. The magnitude of this negative lifetime can be increased severalfold by the application of a magnetic field which preferentially suppresses backscattering over forward scattering. Negative transport lifetimes can result in runaway electron drift (ultimately arrested by the onset of other scattering mechanisms) and possibly velocity overshoot at very low electric fields.

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In recent years, there has been a growing interest in the investigation of electron-phonon interactions in quasi-one-dimensional structures [1–31] motivated by the belief that these structures are ideal for high performance electronic devices. Most of the theoretical work in this field has concentrated on calculating the quantum lifetime or scattering rate associated with electron phonon interactions, rather than the transport lifetime or momentum relaxation rate (Ref. [30] has calculated the energy relaxation rate which is different from both the scattering and the momentum relaxation rate). The momentum relaxation rate, however, is an important quantity since it is more easily probed in transport experiments than all other relaxation rates. In this Letter, we present for the first time calculations of the ensemble average momentum relaxation rate in a quantum wire subjected to an external magnetic field. The surprising finding was that the rate can be *negative* which can then lead to a variety of profound and interesting transport effects. These effects can be observed only in quantum wires and not in quantum wells or bulk structures. Below, we present the calculations of the rates and discuss the implications.

The momentum relaxation rate associated with any type of scattering (for an electron with energy E in a subband with transverse mode indices μ and ν in a quantum wire) is calculated from the corresponding scattering rate $S(E_{\mu,\nu}, E'_{\mu',\nu'})$ as follows [32]:

$$\frac{1}{\tau_m(E_{\mu,\nu})} = \sum_{E'_{\mu',\nu'}} S\big(E_{\mu,\nu}, E'_{\mu',\nu'}\big)\big[1 - f\big(E'_{\mu',\nu'}\big)\big]\frac{k - k'}{k}, \tag{1}$$

where k is the electron wave vector in the free (current-carrying) direction and f is the occupation probability or electron distribution function. The primed and unprimed quantities relate to initial and final states of the electron. The calculations of the scattering rates $S(E_{\mu,\nu}, E'_{\mu',\nu'})$ with and without a magnetic field have been described by us previously [15–18] and will not be repeated here. The ensemble average momentum relaxation rate is calculated by averaging the energy-dependent rate $1/\tau_m(E_{\mu,\nu})$ over $E_{\mu,\nu}$ weighted appropriately by the distribution function:

$$\left\langle \frac{1}{\tau_m} \right\rangle = \frac{\sum_{E_{\mu,\nu}} f(E_{\mu,\nu}) k \tau_m^{-1}(E_{\mu,\nu})}{\sum_{E_{\mu,\nu}} f(E_{\mu,\nu}) k}. \tag{2}$$

The wave vector k in the above expression is of course related to $E_{\mu,\nu}$ by the dispersion relation in a quantum wire which is calculated rigorously (in the presence or absence of a magnetic field) according to the prescription of Ref. [33].

In bulk and two-dimensional structures, the summations over energy in Eq. (2) always result in a positive $\langle 1/\tau_m \rangle$ even if $1/\tau_m(E)$ given by Eq. (1) is negative for certain values of E [34]. This means that *ensemble averaging* in two- or three-dimensional structures always ensures a positive *average* lifetime. However, this is not true for a quasi-one-dimensional system. Here, $\langle 1/\tau_m \rangle$ can be negative if the dominant scattering processes are those for which $1/\tau_m(E_{\mu,\nu})$ given by Eq. (1) is negative, i.e., the final state wave vector k' is larger than the initial state wave vector k. This is a peculiarity of one-dimensional ensemble averaging.

To ensure a negative *average* transport lifetime, we then have to promote scattering processes for which the final state wave vector is larger than the initial state wave vector (i.e., there is a net momentum gain in the scattering process). The only scattering process that satisfies this requirement is forward scattering by phonon absorption. All other scattering processes, including phonon emission, backscattering by phonon absorption, and all elastic mechanisms (e.g., impurity scattering, boundary roughness scattering, etc.), result in positive $1/\tau_m(E_{\mu,\nu})$. This is illustrated in Fig. 1. Binary electron-electron scattering, on the other hand, does not directly contribute to the ensemble average momentum relaxation since whatever momentum one electron loses is picked up by the other owing to momentum conservation. Therefore, negative lifetimes may be observed in quantum wires only if forward scattering via phonon absorption is dominant.

The above scattering mechanism is indeed dominant in semiconductor quantum wires subjected to low driving electric fields and low temperature. Here, the only mechanisms that compete with forward scattering by phonon

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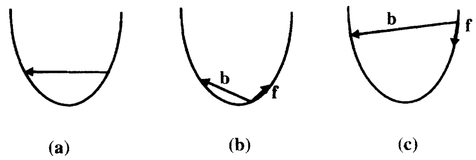

FIG. 1. Illustration of various scattering mechanisms in a quantum wire: (a) elastic scattering, (b) inelastic absorption processes, and (c) inelastic emission processes. The arrows labeled "f" and "b" indicate forward and backward scattering.

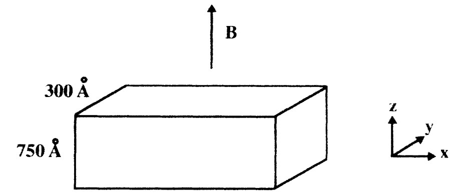

FIG. 2. Schematic of a quantum wire subjected to a magnetic field.

absorption are backscattering by phonon absorption, impurity scattering, boundary roughness scattering, and phonon emission. Impurity scattering is very infrequent in quantum wires if one or few subbands are occupied [35]. The same is true of boundary roughness [36] especially if the quantum wires are defined by split gates [37] rather than mesa etching [38]. Among the phonon emission processes, acoustic phonon emission can be inhibited by ensuring that the electron velocity along the free direction is less than the longitudinal velocity of sound, and optical phonon or surface phonon emission can be prevented by ensuring that the electron energy is less than the phonon energy. Both conditions can be met by making the Fermi velocity smaller than the longitudinal velocity of sound, i.e., by lowering the carrier concentration suitably. In this case, the only scattering mechanism that remains a contender is backscattering by phonon absorption. However, backscattering requires larger wave vector phonons than forward scattering because of momentum conservation (see Fig. 1) [39]. Such phonons have larger energy (in the case of acoustic modes) and consequently a much lower occupation probability. As a result, backscattering is relatively infrequent compared to forward scattering. Therefore, at low temperatures and low electric fields, acoustic phonon absorption will be dominant in quasidepleted semiconductor quantum wires and the ensemble average transport lifetime will be negative as we show in the following examples (optical or surface phonon absorption also yields a negative transport lifetime but is much weaker than acoustic phonon absorption in these situations).

The structure that we have chosen for illustration is a silicon quantum wire of rectangular cross section having a width of 300 Å in the y direction and a thickness of 750 Å in the z direction (see Fig. 2). The x direction is oriented along the [100] crystallographic orientation. The electron concentration is varied between 3×10^5/cm and 3.7×10^5/cm corresponding to Fermi velocities of 5.7×10^5 and 7.1×10^5 cm/sec. Only the lowest subband is occupied for such carrier concentrations and the Fermi velocity is less than the longitudinal sound velocity. Such low carrier concentrations are experimentally achievable in split gate structures fabricated with a backgate for tuning the carrier concentrations electrostatically. Mesa etched structures also result in very low carrier concentrations because of surface depletion caused by Fermi level pinning at the exposed surfaces. The lattice temperature T is 100 mK ($kT \ll E_F$). The electric field is considered weak enough that transport occurs in the linear response regime characterized by an electron distribution function that is approximately the equilibrium Fermi-Dirac distribution [40]. Under these conditions, we have verified that forward scattering by nonpolar *acoustic* phonon absorption is by far the dominant electron interaction.

In Fig. 3, we plot the ensemble average transport lifetime (inverse of the momentum relaxation rate) as a function of magnetic field for different carrier concentrations. In calculating the lifetimes, we neglected many body effects and acoustic phonon confinement effects [41], but we are sure that these will have no qualitative effect and probably only a minor quantitative effect.

It is evident that the transport lifetimes are negative and become more negative in a magnetic field. A magnetic field decreases forward scattering, but it decreases backward scattering much more [15]. Since the net momentum relaxation rate can be viewed as an *algebraic* sum of the relaxation rates associated with forward (negative lifetime) and backward (positive lifetime) scattering, the

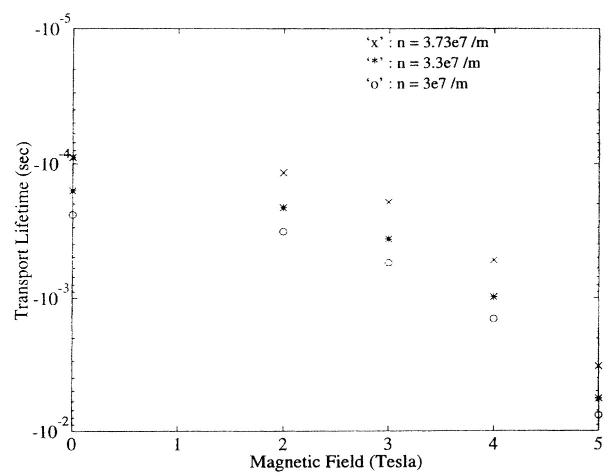

FIG. 3. Transport lifetime (inverse of momentum relaxation rate) as a function of magnetic field for a silicon quantum wire with different carrier concentrations. The wire is 40 Å thick, 750 Å wide and is oriented along the [100] crystallographic direction. The lattice temperature is 100 mK.

overall relaxation rate becomes more negative. This is clearly seen in Fig. 3.

In Fig. 4 we plot the ensemble average transport lifetimes as a function of magnetic field, just as in Fig. 3, but with the difference that the acoustic phonon scattering mechanism is treated as elastic (phonon energy $\equiv 0$). This has been a commonly used approximation [42]. In this case, we see two major *qualitative* differences: (a) the lifetime is always positive, and (b) the magnitude of the momentum relaxation rate $\langle 1/\tau_m \rangle$ *increases* with increasing magnetic field rather than decreasing as in the previous case. The reason for the first difference is that, since the interaction is elastic, the electron can only suffer backscattering (see Fig. 1) and no forward scattering. Therefore, the ensemble average transport lifetime is always positive. As for the second difference, the magnetic field has two opposing influences on the momentum relaxation rate. On the one hand, it decreases the matrix element for scattering by decreasing the overlap between initial and final state wave functions [15], while, on the other hand, it raises the subband bottom bringing it closer to the Fermi level. The former obviously decreases the momentum relaxation rate while the latter increases it. Bringing the subband bottom close to the Fermi level has two effects both of which increase the momentum relaxation rate. First, the density of final states becomes larger which enhances the scattering rate, and second, the amount of momentum transfer and hence the phonon wave vector required to effect an elastic transition is reduced. Since the phonon occupation probability increases exponentially with decreasing phonon wave vector, the relaxation rate increases. This raising of the subband has much less of an effect for inelastic absorption since the final state is always quite a bit above the subband bottom (at least by the phonon energy). In sum, the decrease in the matrix element is the dominant effect for inelastic treatment while the raising of the subband is the dominant effect for elastic treatment. The fact that the correct inelastic treatment can produce a qualitatively different result from the elastic treatment also pointed out recently by Mitin and co-workers in a different context [43].

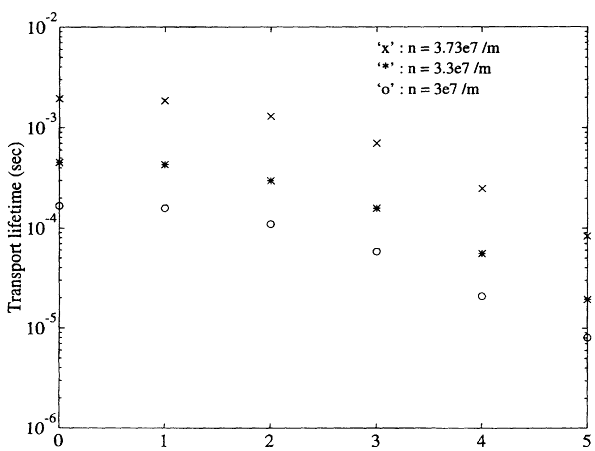

FIG. 4. Transport lifetime (inverse of momentum relaxation rate) as a function of magnetic field in the same wire as in Fig. 3 when acoustic phonon scattering is treated as elastic instead of inelastic.

Let us now conclude by examining the implications of a negative transport lifetime. It can be shown rigorously from the first moment of the Boltzmann transport equation that the current I (or equivalently the drift velocity) in response to an electric field $\mathcal{E}$ in a quantum wire obeys the relation

$$\frac{\partial I}{\partial t} + \frac{qu\nabla n}{m^*} + \frac{qn\nabla u}{m^*} + \frac{I}{\langle \tau_m \rangle} = \frac{q^2 \mathcal{E} n}{m^*}, \tag{3}$$

where n is the electron concentration (per unit length) and u is the ensemble average electron energy. With the initial condition $I = 0$ when $t = 0$, this equation has the solution

$$I = \langle \tau_m \rangle \left[\frac{q^2 \mathcal{E} n}{m^*} - \frac{qu\nabla n}{m^*} - \frac{qn\nabla u}{m^*} \right] [1 - \exp(-t/\langle \tau_m \rangle)], \tag{4}$$

if we assume that n and u are approximately time independent (the energy relaxation time, after all, is much longer than the momentum relaxation time). The above equation shows that if $\langle \tau_m \rangle$ is negative, then the current grows exponentially with time resulting in runaway. Of course, the runaway is arrested as soon as the electron energy or velocity crosses the threshold for phonon emission processes whereupon $\langle \tau_m \rangle$ changes sign to become positive. However, the short-lived runaway can still result in very low field velocity overshoot. At slightly higher fields, when the threshold for phonon emission is quickly reached, the negative lifetime may not be manifested and the velocity overshoot may be quenched. We point out that the effects of a negative lifetime are most likely to be observed in transient (rather than steady state) phenomena and that these effects can be accentuated by an external magnetic field. We are presently carrying out Monte Carlo simulations to investigate these possibilities.

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[40] The Fermi-Dirac approximation for the distribution function is not a serious assumption on this context. At low driving electric fields, the distribution function will of course not be exactly Fermi-Dirac since the system is not in equilibrium, but the deviation will be small. Since the variational principle of transport states that a first order change in the distribution function will induce only a second order change in the momentum relaxation time, the latter time is not very sensitive to the distribution function. Therefore, the assumption of a quasiequilibrium distribution will not affect the main conclusion regarding the sign of the relaxation time.

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