Anomalous conductance quantization in the inter-band gap of a one-dimensional channel

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Abstract

We report on a singular departure from the canonical step sequence of quantized conductance in a ballistic, quasi-one-dimensional metallic channel. Ideally in such a structure each sub-band population contributes its conductance quantum independently of the rest. In a picture based exclusively on coherent single-carrier transmission, unitary back-scattering may lower a conductance step below ideal but it is not possible for it to enhance it beyond the ideal conductance quantum. Precisely such an anomalous and robust voltage-dependent enhancement has already been observed over the whole density range between sub-band thresholds (de Picciotto R et al 2004 Phys. Rev. Lett. 92 036805, de Picciotto R et al 2008 J. Phys.: Condens. Matter 20 164204), a phenomenon left unexplained till now. We show theoretically that the anomalous enhancement of the ideal conductance is the hallmark of carrier transitions coupling the discrete sub-bands.

Keywords: anomalous quantized conductance, non-linear mesoscopic transport, high-field phenomena in quantum channels, interband dynamics in quantum channels

(Some figures may appear in colour only in the online journal)

1. Introduction

Understanding the conductance in quantum-confined metallic channels is a central aspect of electrical transport in meso- and nanoscopic structures and, as such, of any practical electronics built with them. Quantization of the conductance in ballistic quantum-well channels is the unique property of their one-dimensional (1D), waveguide-like nature.

The standard model of 1D quantized conductance [1–3] adopts the viewpoint of Landauer and associates [4, 5] in which a highly constricted channel is modelled as a simple barrier potential embedded in a uniform wire, modifying the free propagation of its single-electron quantum states. Strong lateral confinement of these states by the device’s quantum-well structure leads to their segregation into discrete levels (sub-bands), separated by energy gaps whose magnitude may run from tens of meV in III–V heterojunctions to several eV in carbon nanotubes.

This picture of conductance as quantum transmission accounts elegantly for the well-documented resolution of the ohmic linear response in 1D structures into a sequence of integral plateaux. As a function of increasing carrier density in the device, each successive step in the conductance extends, unaltered, throughout the energy-gap region separating the discrete sub-bands. A new plateau appears as soon as the chemical potential and thus the carrier population cross the gap to access the next higher sub-band.

That the single-particle quantum transmission picture does not address all experimental observations is known [6–9]. The reasons that it does not are also known [10]. First, quantum transmission theory is restricted to weak-field linear response; second, it does not account for the resistive dissipation that is
inevitable in every ohmic structure; third, the approach has no way to address scattering processes other than purely coherent back-scattering. These aspects of the transmission approach have been discussed in closer detail elsewhere [11–13].

One example of a crucial inelastic physical process is intra-band scattering by phonon emission, responsible for the above-mentioned dissipation. Another example is inter-band transitions, which are inherently inelastic two-body processes with substantial carrier and energy exchange between discrete bands. Owing to the necessarily finite size of actual devices, it is expected that such mechanisms should modify any entry-level description.

The physics of discrete transitions between distinct conduction sub-bands lies at the heart of this paper. The experimental findings that animate our work are those of de Picciotto, Pfeiffer, Baldwin and West [8, 9].

Let us explain the importance of the unusual non-linear, 1D conductance plateaux documented by de Picciotto and colleagues. Figure 1 reproduces the core results of their [8] and [9]. It shows a series of differential-conductance traces (normalized to the standard quantum $G_0 = 77.48 \mu S$) for a nearly ideal ballistic quantum wire, taken at fixed source–drain driving voltage and plotted as functions of gate voltage controlling the channel chemical potential and so its carrier density. The greyed region contains a complex of highly mutable shoulder structures evident at the ground-state threshold, popularly termed the ‘0.7 anomaly’, which is not of interest here.

We focus, by contrast, upon the conductance plateaux extending over the larger part of the inter-band region up to the threshold of the first excited sub-band. Unlike the ‘0.7’ features [14], they are robustly regular with a highly systematic dependence on the source–drain driving voltage.

- The anomalous steps are extremely flat and extend, with carrier density, from the early-onset ‘0.7’ feature sequence right up to the threshold of the next higher sub-band. Qualitatively and quantitatively, they are wholly distinct from the relatively ephemeral structures close to first threshold.
- The anomalous conductance steps are voltage dependent. They are beyond any linear-response description.
- These plateaux cover the entire region where the chemical potential of the carriers lies in the gap between ground- and first-excited-state bands. According to single-band quantum-transmission theory, such a structure cannot be higher than the ideal limit $G_0$.
- With increasing source–drain voltage, the enhanced steps increase in size from the expected weak-field baseline, exceeding appreciably the presumed maximum set by $G_0$. Such a scenario lies out of scope for standard models of conductance.

The devices studied in [8] and [9] are of unprecedented quality, perhaps the closest-to-perfect ballistic wires so far fabricated. We remark on the care taken by the cited authors to isolate the physics at work within their samples. It is somewhat surprising, then, that no authors since the original team [9] have commented on the violation of accepted predictions by the quantized conductance data of figure 1.

Reference [8] contains a prescient comment on the role of inter-mode coupling within the test structures; that is, that there should be some exchange of energy and possibly carriers between sub-bands, setting up a mutual dynamical feedback. To date, theoretical support for that hypothesis has not been at hand. The goal is to provide it.

In the following we present a brief description of our quantum kinetic analysis of the anomalous steps in 1D conductance. Our microscopically conserving model is based on the quantum Boltzmann formalism [10] extended to inter-band transitions. We make no appeal to customary assumptions [5]. After this short account we survey our numerical results, comparing and contrasting them with the basic data of de Picciotto and colleagues. Particular features of the results shed light on the relevant physics. The paper ends with a summary and shadows novel theoretical possibilities that could be tested in experiments in similar high-quality structures.

2. Problem and solution

The problem is to try to replicate and thus unpack the physics of anomalous non-linear enhancement of quantized conductance. Since, even in principle, the active 1D device region cannot be divorced from the large source and drain boundary leads, its operative length is no longer exclusively determined by its physical dimensions or the bulk mean free paths of its
originating substrate. Rather, its length is dictated by the longest
carrier mean free path (MFP) for the channel as embedded
in its non-ideal bounding leads. Adopting the estimate sug-
gested in [8], we take an operational channel length \( L = 2 \mu \text{m} \).
Our uniform-channel results, however, do not depend on the
absolute MFPs assumed for this ballistic scenario.

In essence we are describing carrier behaviour averaged
over an abstract ensemble of such wires, seamlessly and uni-
formly connected in series and each with maximum mean free
path \( L \). At cryogenic temperatures one expects the inelastic
mean free path to set the longer scale, fixing \( L \). On the other
hand, the observed weak-field conductance falls short of the
ideal value \( G_0 \) and we set the complementary elastic intra-
band MFP somewhat below \( L \). An elastic MFP of 0.769\( L \)
matches the mean weak-field conductance after [8].

2.1. Transport equations with inter-band coupling

Our transport equations define the behaviour of two sub-band
populations, separated by their energy gap \( E_g \). Given two
steady-state distributions \( f_{kj} \) for the lower band \( (j = 1) \) and the
next highest \( (j = 2) \) as functions of momentum \( k \), and the
expressions for modified Boltzmann–Drude form:

\[
\frac{q \mathcal{E}}{\hbar} \frac{\partial f_{k1}}{\partial k} = -R_{\text{in}}(f_{k1} - \bar{f}_{k1}) - R_{\text{el}} f_{k1}^{-}
- R_{\text{el}} \left( e^{-E_g/k_BT} f_{k1}(1 - \bar{f}_{k2}) - \bar{f}_{k2}(1 - f_{k1}) \right),
\]

\[
\frac{q \mathcal{E}}{\hbar} \frac{\partial f_{k2}}{\partial k} = -R_{\text{in}}(f_{k2} - \bar{f}_{k2}) - R_{\text{el}} f_{k2}^{-}
- R_{\text{el}} \left( f_{k2}(1 - \bar{f}_{k1}) - e^{-E_g/k_BT} \bar{f}_{k1}(1 - f_{k2}) \right).
\]

The nature of the reference distributions \( \bar{f}_{kj} \) is explained below.

Other notation is as follows. On the left-hand side of this pair
of steady-state equations, \( \mathcal{E} \) is the uniform field exerted on
the carriers by the applied source–drain voltage. On the right-
hand sides the parameters \( R_{\text{in}} \) and \( R_{\text{el}} \) are, respectively, the
intra-band inelastic and elastic scattering rates assigned to
each band while \( R_0 \) correspondingly is the inter-band trans-
port rate for the coupling between the two populations. The
elastic collision term scales with the odd part of the distribu-
tions since elastic scattering can only reverse the momentum
direction with no change in energy: \( f_{k1}^{-} = (f_{k1} - f_{k1})/2 \).

The final parameter is the Boltzmann factor \( e^{-E_g/k_BT} \) asso-
ciated with promoting a carrier from lower to upper sub-band
across their gap separation \( E_g \). In the subsequent discussion we
will express all energies in thermal units \( k_BT \), and momenta in
thermal units \( k_B T/\hbar^2 \).

We now discuss the meaning and role of the effective equi-
librium functions

\[
\bar{f}_{k1}(\mu) \equiv 1/(1 + \exp(k^2 - \mu)) \quad \text{and} \quad \bar{f}_{k2}(\mu - E_g) \equiv 1/(1 + \exp(k^2 + E_g - \mu))
\]

(2)

with momenta and energies in thermal units. Transition events
redistribute the electron population between the two sub-
bands of the channel. The change in their respective densities
is presumed to depress the effective chemical potential of the
lower band: \( \mu \) is renormalized to \( \mu - \zeta_1 \) while the augmented
population in the upper band, located above the lower by the
band gap \( E_g \), follows the rise in its effective chemical poten-
tial: \( \mu - E_g \) goes to \( \mu + \zeta_2 - E_g \). Thus both quantities \( \zeta_1 \) and
\( \zeta_2 \) should be non-negative.

For any choice of the pair of renormalized chemical poten-
tials, the coupled equation (1) are solved systematically with
the expressions for \( \bar{f}_{k1}(\mu - \zeta_1) \) and \( \bar{f}_{k2}(\mu + \zeta_2 - E_g) \), equa-
tion (2), as input. Details of the relevant Green-function algo-

2.2. Microscopic conservation

Consider the equilibrium state at zero field, for which \( \zeta_1 = 0 = \zeta_2 \).
The effective equilibria are now absolute and furthermore \( f_{kj} = \bar{f}_{kj} \). The distinct terms on either side of the
transport equation (1) all vanish individually. Detailed balance
is satisfied.

What happens at finite field? The intra- and inter-band in-
elastic collision terms on the right-hand sides of equation (1)
are not guaranteed to vanish identically when integrated sepa-
rate, although the left-hand-side expressions always do so.
As a consequence conservation must be imposed explicitly
upon the solution to the joint response: [11, 15, 16] We have a
type of generation-recombination problem; it follows that con-

The bi-linear coupling between distributions in the inter-
band transition terms means that the full problem cannot be
solved save in the trivial case of independent sub-bands (zero
transitions, \( R_{\text{in}} = R_{\text{el}} = 0 \)). Conservation then becomes a
mandatory relation linking the pair of potential shifts \( \zeta_j \) so
the system’s total density is invariant (the spin factor appears
explicitly in the integrals, which are rendered in dimension-
less units):

\[
2 \int dk \left( \bar{f}_{k1}(\mu - \zeta_1;i) + \bar{f}_{k2}(\mu - E_g;i) \right) \equiv n(\mu) \\
\equiv 2 \int dk \left( f_{k1}(\mu - \zeta_1;i) + f_{k2}(\mu + \zeta_2 - E_g;i) \right).
\]

(3)

Since there are two undetermined quantities to solve, a
second relation is needed. The new physical information to
be adduced must be independent of anything contained in the
transport equations themselves.

For the second relation we take the Helmholtz free-energy
density for the non-equilibrium carrier distribution and
remove from it the formal energy of assembly for the system,
mediated by the chemical potential. Under the action of the
external driving field, the change in this net energy should
measure the internal dynamical rearrangement of the sub-
band distributions induced by the field alone. This is mani-
fested in the renormalization of the bands’ chemical potentials
\( \mu_1 \equiv \mu - \zeta_1 \) and \( \mu_2 \equiv \mu + \zeta_2 - E_g \) as well as the form of the
distributions \( f_1(\mu_1) \) and \( f_2(\mu_2) \).

Extending the standard thermodynamic expression [17] for
the Helmholtz free energy in each band, we write its difference
with the energy of assembly as
recognizing the leading right-hand integral in equation (4) as
the total internal energy, less the assembly energy. The second
right-hand integral is the Uehling–Uhlenbeck entropy entering
into the H-theorem for fermions [18]. At global equilibrium,
minimizing $F$ (understood as a functional of the distribution
$f_j$ and subject to the latter’s variation) leads to the familiar
Fermi–Dirac form for $f_j$.
We recapitulate.

- A given gate voltage fixes the global chemical potential
  and total density within the channel.
- The source–drain field, acting independently of this,
  excites the carriers so a portion from the lower band is
  promoted to the upper band.
- The density decrease in the lower band is determined by
  the decrement $\zeta_1$ in the value of the common chemical
  potential $\mu$, while the increase in the upper band is
determined by the increment $\zeta_2$ in $\mu$.
- Any loss from the lower band must match the gain in the
  upper one. Thus the two shifts in chemical potential are
coupled by the conservation relation (3).
- To close the self-consistent solution for the $\zeta_j$, we look for
  any change in the free energy of the system as defined in
  equation (4), induced solely by application of the driving
  field.

The behaviour of $F$ above, purely as a function of chemical
potential, is quite different from its behaviour purely as a
functional of $f$. In the equilibrium state it is readily seen that
\[
\frac{dF}{d\mu}[f(\mu)] = -2 \int dk \frac{f(k^2 - \mu)}{\Delta F[\mu; \{f_j(\mu)\}] = \sum_{j=1,2} \left( F[f_j(\mu)] - F[f_j(\mu)]_{\zeta_1=0} \right). \tag{5}
\]
Wherever we find the local maximum of $\Delta F$ on the locus of
constant density $n(\mu)$ there is a unique self-consistent pair
$(\zeta_1, \zeta_2)$. This fixes the desired physical solution for the
interacting system. If no nontrivial solution exists, the maximum
defaults to the $\zeta_1$-axis (that is, $\zeta_2 = 0$) and produces the
standard quantized conductance.

2.3. Implementation

Equation (5) is taken as a measure of the non-equilibrium
excess energy built up in the system when the driving field
induces redistribution of the populations between sub-bands.
Computing the self-consistent solution requires us to connect
the intra-band MFPs, together of course with the inter-band
transition probability, to the rates $R_{inj}, R_{dis}$ and $R_{0j}$ that parametrize
the collision terms in the coupled equation (1).
It is assumed that the mean free paths are common to each
sub-band, though this need not be so more generally. Let
\( \lambda_{in} \) be the inelastic MFP and \( \lambda_{el} \) be the elastic MFP. (Recall
that, by hypothesis, the operational channel length is given by
\( L = \lambda_{in} \)) Any equilibrium distribution has its associated
characteristic velocity
\[
\tau(\mu) \equiv -\frac{\nu_0}{\bar{V}(\mu)} \int_0^\infty dk \frac{\partial f_j}{\partial k}(\mu) = \nu_0(1 + e^{-\mu}) \int_0^\infty dk \frac{f_j}{\mu}.
\]
We have scaled out the thermal velocity $\nu_0 = \hbar k_t / m^* \nu_0$ where
$m^*$ is the electron effective mass. In the low-density classical
limit, this becomes essentially $\nu_0$ while in the high-density
degenerate limit it is the Fermi velocity $\nu_0/\bar{\mu}$. The quantity $\tau$
thus sets the typical velocity scale. Accordingly we define the
rates in dimensionless units from the respective characteristic
velocities:
\[
R_{inj} \equiv \frac{L}{\nu_0} \tau(\mu_1), \quad R_{dis} \equiv \frac{L}{\nu_0} \tau(\mu_2), \quad R_{0j} \equiv \frac{L}{\nu_0} \tau(\mu_2) \tag{6}.
\]
The transition rates represent a different physical mech-
anism and are treated differently from the intra-band ones, as
a single dimensionless parameter
\[
R_{0j} \equiv \frac{L}{\nu_0} \lambda_{0}
\]
scaling inversely with a nominal ‘transition MFP’ $\lambda_0$ which,
however, is qualitatively distinct from intra-band MFPs. Its
value is an experimental unknown. Moreover $\lambda_0$ is likely to
depend strongly on device geometry and electrostatics [8].
For this work we set it an order of magnitude larger than the
operational length $L$.
To obtain the current response we sum the carrier flux over
each (parabolic) sub-band:
\[
I(\mu, V_{sd}) \equiv q \int k dk \sum_{j=1,2} f_j(\mu_1) \left( \int k dk \right) \sum_{j=1,2} f_j(\mu_1) \left( \int k dk \right) \tag{8}
\]
where the source–drain voltage is $V_{sd} = \mathcal{E} L$ and $G_0 = q^2 / \pi h$.
Note that the even parts of the distributions do not contribute to
the current. The right-hand side sum in the second line above is the equivalent of the sum of the sub-bands’ ‘transmission factors’ in the language of quantum-coherent models; it is the expectation of the flux (here normalized to appropriate units) over the non-equilibrium distributions. From equation (8) all the transport properties are derived.

The physical content of equation (8) in its low-field limit has been examined in [12] and yields the well known step sequence for 1D conductance. The chord conductance $G = I/V_{sd}$ is readily given in units of $G_0$ as

$$
\frac{G}{G_0} = \frac{2k_B T}{q^2 L} \sum_{j=1,2} \int kdk f_j^{\text{eq}}(\mu_j).
$$

(9)

3. Results

We come now to the consequences for quantized conductance away from the weak-field regime. In figure 2 below, for total channel current $I(\mu, V_{sd})$ at a series of fixed applied $V_{sd}$, we show the conductance computed from equation (9) for a device conforming to experimental specifications [8]. The dynamical scattering parameters are those of the preceding section, namely: operational length $L = \lambda_0 = 2 \mu$m; $\lambda_1 = 0.769L = 1.538 \mu$m; $\lambda_0 = 10L = 20 \mu$m.

Figure 4 of [9] gives some evidence of thermal broadening of conductance at the sub-band thresholds presumably from localized Joule heating. We compute our curves at the nominal temperature 4 K. The energy-gap value $E_g = 15$ meV and the effective mass for GaAs are used. Finally, on the horizontal axis of our figure 2 we have mapped the global chemical potential $\mu$ to values of a corresponding gate-control voltage, using the parameters provided by [8].

Our figure 2 should be compared directly with our figure 1 as taken from [9], figure 3(a). Both in the real data of figure 1 and in our calculation, the action of a substantial source–drain voltage driving the current through the channel leads to a series of elevated conductance plateaux which

(a) are inherently non-linear in origin,
(b) are extremely flat and robust,
(c) rise beyond the ideal upper bound $G_0$ on $G$ and thus
(d) exceed the normally expected limit of linear-response models.

The confluence of behaviours between experiment and theory speaks for itself.

In figure 3(a) of [9] (and figure 1 reproducing it in this paper) the plots show $\partial I/\partial V_{sd}$: the rate of change of current with driving field, plotted as the density increases. It is easily seen that when that slope is essentially flat over a broad range of gate voltage (thus density) as in figure 1, the simple conductance $I/V_{sd}$, as in figure 3, must track it closely and vice versa.

Before examining further characteristics of our theoretical conductance we discuss differences between the present implementation and the experiment. Our calculation here exhibits greater sensitivity with respect to $V_{sd}$ than the experiment so that, while in figure 2 the step increase of $G$ resulting from $V_{sd} = 1$ mV coincides with that in figure 1, its height at 3 mV is 1.43$G_0$ while its counterpart in figure 1 is 1.16$G_0$. This overestimate might be accounted for in part if the inelastic MFP $\lambda_0$ suffered shortening via optical-phonon emission at higher driving voltages (the optical-phonon energy in GaAs is 35 meV, not hugely larger than $E_g$ at 15 meV). Use of energy-dependent mean free paths within equation (1), rather than fixed ones, is an obvious aspect for exploration. Increased local Joule heating with increased driving field may also suppress the plateaux, as figure 3 below suggests.

In figure 3 we show the properties of the enhanced conductance taken at a typical mid-gap density where $G$ is steady. Device specifications are as for figure 3 with an additional choice of temperature, 8 K as well as 4 K. Our calculated $G$ exhibits an onset at finite field and asymptotic saturation at high fields. The threshold voltage value at onset depends on temperature; at low temperature the threshold value of $V_{sd}$ tends to zero and at high temperatures it rises in rough proportion to $T$.

The phenomenon above may partly explain why measurements prior to de Picciotto et al [8, 9] have not recorded the anomalous enhancement. Predominantly, experiments in quantized conductance have been carried out either at weak fields below threshold, or at higher temperatures, or on noisy
devices, or in any combination of the above. Any enhancement of \( G \) under such conditions would tend to be washed out. Saturation of \( G \) in figure 3 sets in at driving fields considerably higher than those employed in [8] and in our figure 2. The upper bound of \( G \) is close to \( 1.6G_0 \), well short of the second occupied level at \( 1.77G_0 \) in the weak-field limit. This suggests a field- and temperature-independent maximum transfer of carriers to the upper band, beyond which the feedback of transitions returning carriers to the lower band precludes any increase. While we do not at present claim quantitative accuracy in this extreme region, high-field saturation behaviour may provide a new experimental window on the dynamics of the inter-band transition.

4. Summary and implications

De Picciotto et al [8, 9] originally addressed their experiments to the topic (still unresolved) of the ‘0.7 anomaly’. Compared to earlier experiments of this genre, for their near-ideal wires they also noted substantial enhancement of the conductance steps at source–drain voltages beyond the weak-field regime. These harbour a message of potential impact on the future of textbook quantum kinetics. Beyond explaining theoretically the unusual enhancement of ballistic conductance first reported in [8] and [9], our results on temperature behaviour from figure 3 offer a basis to analyze thermal characteristics for transition-induced changes of conductance in clean quantum wires. There is a case for probing similar effects in sufficiently clean carbon nanotubes, whose energy scale and robustness at high fields far outstrip any device based on GaAs hetero-junction technology. This would call for novel experiments. Our own theoretical development will continue beyond the present effort, in the first instance with an account of calculational details too lengthy to have been covered here.

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