What is novel in quantum transport for mesoscopics? 1

Mukunda P. Das† and Frederick Green‡
†Department of Theoretical Physics, IAS, The Australian National University, Canberra, ACT 0200, Australia
‡School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia

Abstract

The understanding of mesoscopic transport has now attained an ultimate simplicity. Indeed, orthodox quantum kinetics would seem to say little about mesoscopics that has not been revealed – nearly effortlessly – by more popular means. Such is far from the case, however. The fact that kinetic theory remains very much in charge is best appreciated through the physics of a quantum point contact. While discretization of its conductance is viewed as the exclusive result of coherent, single-electron-wave transmission, this does not begin to address the paramount feature of all metallic conduction: dissipation. A perfect quantum point contact still has finite resistance, so its ballistic carriers must dissipate the energy gained from the applied field. How do they manage that? The key is in standard many-body quantum theory, and its conservation principles.

INTRODUCTION

A striking signature of mesoscopic transport, as evidenced in quantum point contacts (QPCs), is the discretization of conductance into “Landauer steps” in units of $2e^2/h$. The steps appear to be well described by the coherent transmission of independent electron waves through the contact, imagined as a perfectly lossless quantum barrier [1–3].

The techniques of single-particle scattering are universally accessible. Consequently, the pioneering insights of the Landauer school have achieved more than to open a new vista of small-scale device physics. They have also made their compact understanding available to one and all, in a toolbox of easily grasped phenomenological design aids.

Besides the great simplicity of this widely adopted approach, it is generally agreed that it cannot sustain any contradiction with the older-established principles of microscopic transport theory [4]. In this overview we clarify, in somewhat sharper detail than usual, those interrelationships that may exist between canonical kinetics on the one hand, and Landauer transport theory on the other.

Central to the Landauer description are two assumptions: (a) current flows in a QPC when a mismatch of chemical potentials is set up across the ends of the wire. In response, carriers flow more or less freely from the “high-density” lead end to the “low-density” lead end. (b) The intervening channel is a quantum tunnelling barrier that moderates the unimpeded flux of electrons. The Landauer conductance formula directly encodes this tunnelling physics.

1Invited talk presented at the 50th Golden Jubilee DAE Solid State Physics Symposium, BARC, Mumbai, 2005.
Assumptions (a) and (b) are not consistent with each other. The first asserts the validity of charge drift in the mesoscopic regime: a difference in electron density across the leads drives a current from the high to the low region. That is, the current flow is metallic because it engages carrier states that are well filled and spatially extended. In contradistinction, (b) asserts instead that the flux rate is set – quite literally – by the probability of tunnelling through some phenomenologically chosen barrier. (Surprisingly, if such a barrier had any internal physical structure it would be irrelevant to the outcome.) Here the physics is that of states separately confined to the leads on either side of the barrier. All that matters is that they have some residual overlap.

The relation between the two hypotheses itself invites two questions. To what extent do we have a picture – case (a) – of metallic conduction involving truly extended states, and to what extent is it a description – case (b) – of (self-evidently non-metallic) tunnelling involving spatially separate, autonomous in- and out-states? Should one conclude, astonishingly, that mesoscopic transport is really both at the same time?

These are intriguing, if incidental, issues. We now discuss the other thought-provoking aspects of the relation between Landauer phenomenology and conventional quantum kinetics.

THE PHYSICAL PROBLEM: DISSIPATION

The essential role (or, more accurately, the essential absence) of resistive energy dissipation has recently returned to the forefront of discussions about the microscopic basis of the Landauer approach [5–7]. In a perceptive early critique of Landauer’s picture (wherein ballistic conduction consists in perfectly coherent and, therefore, exclusively elastic transmission), Frensley [8] had already identified the singular lack of a theoretical account of dissipation (Joule heating) within the Landauer phenomenology. In admitting coherent scattering, and that only, as the origin of QPC conductance, the Landauer model leaves an enormous unhealed gap between it and the fluctuation-dissipation theorem [9], which universally quantifies the conductance in terms of the actual energy loss via the dissipative electron-hole pair processes that always accompany metallic transport [4].

In their more recent discussions, Davies [5] and Agraït et al [6] have also covered the unresolved status of ballistic dissipation. We also have summarised our own considerations from the standpoint of kinetics [7]. To date the problem seems to have had no deeper analysis on the part of any proponents of the Landauer philosophy, other than that dissipation occurs somehow, somewhere, deep in the leads and far from the active channel [2]; too far off, anyway, to spoil the undisputed simplicity of the coherent-tunnelling account of ballistic conductance.

Surveys of the dissipation issue all agree [5–8] that naïve quantum mechanical descriptions of single-carrier tunnelling are unable to settle the central problem of conduction: What causes the dissipation in a ballistic QPC? The matter goes well beyond this simple academic consideration.

Not too long from now, reliable and effective nano-electronic design will grow to demand, not models that are built for minimum effort, but ones that are microscopically grounded and therefore credible, both as basic physics and as quantitatively trustworthy engineering tools. Device designers, above all, will need every confidence to predict the dominant dissipative characteristics of their new quasi-molecular structures, operating far away from equilibrium. The Landauer approach is not made for such demands.

We now review the answer to the question posed. Its resolution has been available all the while – definitively, and free of any artificial conundrums – within many-body quantum kinetics [4, 10]. The microscopic application of many-body methods leads not only to conductance quantization by fully accounting for inelastic energy loss [11], but it also resolves a long-standing experimental enigma [12] in the noise spectrum of a quantum
point contact (QPC) [13]. Evidently, the same developments will foreshadow a systematic pathway to the truly predictive design of novel structures.

**QUANTUM KINETICS: THE SOLUTION**

The central issue in conduction is clear. Any finite conductance $G$ must dissipate electrical energy at the rate $P = IV = GV^2$, where $I = GV$ is the current and $V$ the potential difference across the terminals of the driven conductor. Physically, there must be an explicit mechanism (e.g. emission of optical phonons) through which the energy gained by carriers, when driven from source to drain, is channelled to the surroundings.

Alongside all the elastic and coherent scattering processes, inelastic processes must also act. Connected with elastic single-particle scattering, intimately and inevitably, are its dynamic and dissipative companions: the electron-hole vertex corrections [4]. This much is required by the conservation laws for the electron gas itself [14]. Over and above this (and still within the global purview of conservation), there will be additional decay modes coupling the electrons to other background excitations.

None of these dissipative effects can be described at the level of simple, one-particle coherent quantum mechanics, for they are all inherently many-body effects, requiring a genuinely microscopic description. Harnessed together, the elastic and inelastic processes fix $G$. Yet it is only the energy-dissipating mechanisms that secure the thermodynamic stability vital to steady-state conduction.

We already possess a complete quantum-kinetic understanding of the ubiquitous power-loss formula $P = GV^2$ [9, 15, 16]. It resides in the fluctuation-dissipation theorem, valid for all resistive devices at all scales, without exception. The theorem expresses the requirement for thermodynamic stability. A plain chain of reasoning follows from it: [10, 11]

(i) inelasticity is necessary and sufficient to stabilize current flow at finite conductance;
(ii) ballistic quantum point contacts have finite $G \propto \frac{2e^2}{h}$; therefore
(iii) the physics of energy loss is indispensable to a proper theory of ballistic transport.

The physics of explicit inelastic scattering is beyond the scope of transport models that rely only on coherent quantum scattering to explain the origin of $G$ in quantum point contacts. Coherence implies elasticity, and elastic scattering is always loss-free: it conserves the energy of the scattered particle. This reveals the deficiency of purely elastic models of transmission. We now review a well-defined microscopic remedy for this deficiency.

To allow for the energy dissipation vital to any microscopic description of ballistic transport, we recall that open-boundary conditions imply the intimate coupling of the QPC channel to its interfaces with the reservoirs. The interface regions must be treated as an integral part of the device model. They are the very sites for strong scattering effects: dissipative many-body events as the current enters and leaves the ballistic channel, and elastic one-body events as the carriers interact with background impurities, the potential barriers that confine and funnel the current, and so on.

The key idea in our standard treatment is to subsume the interfaces within the total kinetic description of the ballistic channel. At the same time, strict charge conservation in an open device requires the direct supply and removal of current by an external generator [15] or, equally well, a battery [16]; that is, a source for the driving field that itself is outside the system. These two criteria are equivalent. They are also prescriptive; mandated by electrodynamics whenever a metallic channel is subjected to external electromotive forces.
In truly open-system operation, therefore, the current is determined externally, independent of the local physics peculiar to the reservoirs. This canonical requirement sets the quantum kinetic approach entirely apart from the Landauer multi-reservoir scenario \[1\], which rests upon a purely intuitive phenomenology: that the current has to depend on hypothetical density gradients between the reservoirs. For an externally driven charged system, orthodox electrodynamics never entails this.

QPC CONDUCTANCE: ITS QUANTUM KINETIC EMERGENCE

It is straightforward to write the algebra for the ideal “Landauer” conductance in our model system. A uniform, one-dimensional ballistic QPC, of operational length \(L\), will be associated with two mean free paths determined by \(v_F\), the Fermi velocity of the electrons, and a pair of characteristic scattering times \(\tau_{el}, \tau_{in}\). Thus

\[
\lambda_{el} = v_F \tau_{el}; \quad \lambda_{in} = v_F \tau_{in}.
\]

Respectively, these are the scattering lengths set by the elastic and inelastic processes active at both interfaces. The device (i.e. the QPC with its interfaces) has a conductive core that is strictly collisionless. It follows from this ballistic boundary condition that \(L\) then delimits both elastic and inelastic mean free paths, leading directly to

\[
\lambda_{el} = L = \lambda_{in}.
\]

Finally, the channel’s conductance is given by the familiar formula

\[
G = \frac{ne^2}{m^*L} = \frac{2k_F}{\pi} \frac{e^2}{m^*L} \left( \frac{\tau_{in} \tau_{el}}{\tau_{el} + \tau_{in}} \right);
\]

the effective mass of the carriers is \(m^*\). In the first factor of the rightmost expression for \(G\) we rewrite the density \(n\) in terms of the Fermi momentum \(k_F\); in the final factor, we use Matthiessen’s rule \(\tau_{tot}^{-1} = \tau_{el}^{-1} + \tau_{in}^{-1}\) for the total scattering rate in the system.

Using Equations (1)–(3), the conductance reduces to

\[
G = \frac{2e^2}{\pi h} \frac{h k_F}{m^* L} \left( \frac{L/v_F}{2L/v_F} \right) = \frac{2e^2}{h} \equiv G_0.
\]

This is precisely the Landauer conductance of a single, one-dimensional, ideal channel.

None of the conjectural assumptions, otherwise invoked to explain conductance quantization \[1,3\], has been used. Rather, it is the axioms of electrodynamics and microscopic response theory, and only those, which guarantee Eq. (4). In fact, we have just seen directly how this distinctive mesoscopic result emerges from completely standard quantum kinetics.
In the left-hand panel of Figure 1 we plot the results of our model for a QPC [10] consisting of two one-dimensional conduction bands with their threshold energies separated by $12k_B T$, in thermal units at temperature $T$. We use the natural extension of Eq. (4) to cases where one or more channels may be open to conduction, depending on $T$ as well as the size of the chemical potential $\mu$. As the role of inelastic scattering is enhanced ($\tau_{\text{in}} < \tau_{\text{el}}$) the conductance deviates from the ideally ballistic “Landauer” limit.

The right-hand panel of Fig. 1 shows, as a precursor to our discussion of non-equilibrium noise (see also Fig. 3 below), the same conserving quantum-kinetic calculation of $G$ for a realistic point contact. It is noteworthy that the non-ideality of $G$ in the quasi-one-dimensional quantum channel grows progressively as the source-drain voltage that drives the mesoscopic current increases: thus the overall value of $G$ goes down as the voltage runs from low (0.5mV) to high (3mV), and the rate of optical-phonon emission increases for carriers accelerated within the channel. For a comparison with corresponding results, as extracted from raw measurements made in a QPC sample, see Fig. 2 of Ref. [12].

Most important to the microscopic derivation of the Landauer quantized conductance is the clear and central role of inelastic energy loss, one of the underpinnings of quantum transport. Charge conservation, the other underpinning, is guaranteed by our use of microscopically consistent open-boundary conditions at the interfaces. Their importance cannot be emphasised too strongly. It is fair to say that, as essential physical requirements, they are not transparent within some of the more intuitive derivations of Eq. (4).

**QPC NOISE: REVEALING MICROSCOPICS**

The noise response of a quantum point contact is a fascinating aspect of mesoscopic transport, and a more demanding one both experimentally and theoretically. In 1995, a landmark measurement of non-equilibrium noise was performed by the Weizmann group [12], which yielded a very puzzling result. Whereas conventional models [3] fail to predict any structure at all in their noise signal for a QPC driven at constant current levels, the data show an orderly series of marked and increasingly strong peaks, just where the carrier density in the
QPC starts to grow and becomes metallic.

Remarkable as they are to this day, the Weizmann results remained absolutely unexplained for a decade. We have now accounted for the Reznikov et al. measurements, within our strictly conserving kinetic description [13].

In the following Fig. 2 we display the experimental data side by side with our computation of excess QPC noise, under the same conditions [13]. In contrast to the outcome of popular mesoscopic phenomenology [3] one notes the close affinity between the measurements and the quantum kinetic calculation, as the carrier density is swept across the first conduction-band threshold, where the conductance exhibits its lowest step. At fixed values of source-drain current, the accepted noise models predict no peaks at all, but rather a featureless monotonic drop in the noise strength as the carrier density passes through threshold.

Figure 2: Non-equilibrium current noise of a QPC at constant source-drain current, as a function of gate bias. Left: data from Reznikov et al., Ref. [12]. Right: microscopically conserving kinetic calculation from Green et al., Ref. [13]. In each case the dotted line traces the currently accepted shot-noise prediction at 100nA using, as respective inputs, measured and calculated data for $G$. The prediction from Landauer theory is well wide of the mark.

To round off our survey of ballistic noise we present a final figure. It serves to show that the remarkable peaks observed in a QPC channel, at constant applied current, are by no means fortuitous artifacts. In Fig. 3 (the QPC noise measured concomitantly with $G$ in the right-hand-side panel of Fig. 1) we see an unfolding, characteristic peak sequence at constant source-drain voltage as the gate bias systematically pushes the conduction electrons upward in density: first though the lowest, and then the next higher, sub-bands in the structure. The noise maxima are very well replicated by the physics built into our conserving microscopic description. Once again they invite favourable comparison with observations. This can be checked against Fig. 2 of Ref. [12].

The constant-voltage peaks have been widely celebrated as the predictive triumph of mesoscopic transport phenomenology [3]. On that score, any alternative fluctuation theory for QPCs must do at least as well. What is unique about our quantum kinetic approach is not that it offers a microscopically founded account for effects already explained in the Landauer framework. What is really different is that it describes, faithfully, everything else that phenomenology has signally failed to predict in the noise spectrum at constant current.
Figure 3: Non-equilibrium noise in a QPC at constant levels of voltage, computed quantum kinetically as for Fig.2 [13]. Characteristic peak sequences appear at each of the two lowest sub-band energy thresholds. Note also the presence of a slower-rising signal background on which the relatively sharper maxima are superimposed. A similar background is evident in the corresponding experimental data [12]. While such maxima at constant voltage are predicted by other approaches [3], the rising background – like the unexpected structures at constant current – are not reproduced except by the fully kinetic model.

If there is a single, utterly fundamental, reason why orthodox quantum kinetics is able to open up in such a striking way the microscopics of fine-scale fluctuations, it is that – unlike other explanations of transport and noise – it starts its exploration from the universal principles of conservation, and also ends with them intact. This is exactly the reason for kinetic theory’s freedom from any and all unjustified, ad hoc assumptions. It is time to look at the mesoscopic action of conservation.

CENTRALITY OF CONSERVATION

The key to all quantum kinetic descriptions of conductance is the fluctuation-dissipation theorem, whose practical implementation is Eq. (3) (where the overall relaxation time $\tau_{\text{tot}}$ encodes all the electron-fluctuation dynamics via the Kubo formula [9]). This universal relation is one of the electron-gas sum rules [14]. In this instance, it expresses the conservation of energy, dissipatively transferred from an external source to the thermal surroundings, for any process that involves resistive transport – including that in a ballistic quantum point contact.

A second, and equally fundamental, sum rule concerns the compressibility of an electron fluid in a conductive channel. This sum rule turns out to have an intimate link with the non-equilibrium noise behavior reviewed above; here we give a brief explanation of that crucial link. For details see Refs. [13] and [17]-[19].

Recall that the carriers in a quantum point contact are stabilized by the presence of the large leads, which pin the electron density to fixed values on the outer boundaries of the interfaces (recall too that the interfaces and the channel together define the open system). No matter what the transport processes within the QPC may be, or how extreme, the system’s global neutrality is guaranteed by the stability of the large and charge-neutral reservoirs.

It follows that the total number $N$ of active electrons in the device remains independent of any current that is forced through the channel, for $N$ is always neutralized by the ionic background in its neighborhood, as well as
the stabilizing leads. The presence of the latter means that all remnant fringing fields are screened out beyond the device boundaries; hence the global neutrality.

One can then prove that the total mean-square number fluctuation $\Delta N = k_B T \partial N / \partial \mu$ is likewise independent of the external applied current [17]. The compressibility of the carriers in the QPC is given in terms of $N$ and $\Delta N$ by [14]

$$\kappa = \frac{L}{N k_B T} \frac{\Delta N}{N}, \quad (5)$$

which, in consequence, remains strictly unaffected by any transport process. This a surprising corollary of global neutrality. It asserts that, in an open conductor, the system’s equilibrium compressibility completely determines the compressibility of the electrons when driven away from equilibrium, regardless of how strong the driving field is.

The compressibility sum rule expresses the unconditional conservation of carriers in a non-equilibrium conductor. Previously unexamined in mesoscopics, this principle has an immediate importance and applicability.

How does $\kappa$ determine the noise in a QPC? The strength of the current fluctuations is, at base, the product of two contending factors:

$$S(I, t) \sim \langle I(t)I(0) \rangle \frac{\Delta N}{N}. \quad (6)$$

The first factor represents the self-correlation of the instantaneous electron current $I(t)$ evaluated as a trace over the non-equilibrium distribution of excited electrons in the device. The second factor – evidently a basic characteristic of the electron gas in the channel – is independent of $I$, meaning that the invariant compressibility (Eq. (5)) must dictate the overall scale of the noise spectrum.

Let us examine the noise spectra of Figs. 2 and 3 in light of this key result [13].

- At large negative bias $V_g$, the channel is depleted. The remnant carriers are classical, so $\Delta N/N \to 1$. The noise is then dominated by strong inelastic processes at high driving fields, as embodied in $\langle I(t)I(0) \rangle$.

- In the opposite bias limit (right-hand sector of each panel in Fig. 2), the channel is richly populated and thus highly degenerate, with a large Fermi energy $E_F$. Then $\Delta N/N \to k_B T / 2E_F \ll 1$. The noise spectrum falls off according to Eq. (6), since the current-correlation factor – now well within the regime of ballistic operation – reaches a fixed ideal value.

- In the mid-range of bias voltage, there is a point where the carriers’ chemical potential matches the energy threshold for populating the first conduction sub-band. Here there is a robust competition: on the one hand, scattering processes that reduce the correlation $\langle I(t)I(0) \rangle$ are less effective, while on the other hand the onset of degeneracy drives the compressibility down. Where this interplay is strongest, there are peaks.

Now we understand the outcome of the compressibility rule: it is, quite directly, the “inexplicable” emergence of the noise peak structures. The striking case of QPC noise gives an insight into the central importance of the conserving sum rules in the physics of transport at meso- and nanoscopic dimensions. The more imaginative treatments of noise fail to address the explicit action of microscopic conservation in ballistic phenomena, and therefore cannot offer a rational understanding of the real nature of ballistic conduction.
SUMMARY

In this paper we have recalled the most fundamental aspects of mesoscopic transport physics, and the need to make sure that descriptions of it continue to respect those aspects. They are: the primacy of microscopic conservation in charged open systems; the dominance of many-body phenomena, most of all dissipation; and the unity of conductance and fluctuations.

Quantum kinetic theory was, and remains, the sole analytical method that can guarantee all of these requirements. It provides a detailed, cohesive and inherently microscopic account of conductance and noise together. This applies to the specific case of quantum point contacts. In our own quantum-kinetic studies we have accurately reproduced – free of any and all special pleadings – the proper current response of a mesoscopic channel, including the quantized-conductance signature.

Given the keys to this standard and yet newly fruitful picture (open-system charge conservation and the efficacy of dissipative many-body scattering), our quantum kinetic analysis presents as a thoroughly orthodox development. Precisely because it is so firmly and conventionally grounded, it affords an unambiguous, natural and quantitative understanding of the non-equilibrium fluctuations of a quantum point contact, with its associated dynamics. That understanding has been successfully tested in fully explaining the long-standing puzzle posed by the noise measurements of Reznikov et al. [12].

The theoretical impact of noise and fluctuation physics is that it carries much more information on the internal dynamics of mesoscopic systems – a level of knowledge inaccessible through the I-V characteristics on their own. The capacity for a self-contained microscopic explanation of mesoscopic transport processes underwrites a matching ability to build new programs for device design that are inherently rational. The practical need for such programs can hardly be overstated in the context of nanotechnology, given the ongoing paucity of physically based techniques for it.

In the authors’ view, the time is ripe to restore the methods of microscopic quantum kinetics to a central place in mesoscopic electronics, where they seem to have been much less in evidence over recent years. The need is manifest, and is becoming more and more pressing with the advance of technology. Some of the basic tools to meet it are already at hand [9, 11, 14–17, 19].

REFERENCES

[1] Y. Imry, Introduction to Mesoscopic Physics, 2nd Edition (Oxford University Press, Oxford, 2002)
[2] Y. Imry and R. Landauer, Rev. Mod. Phys. 71, S306 (1999)
[3] Y. M. Blanter and M. Böttiker, Phys. Rep. 336, 1 (2000)
[4] G. D. Mahan, Many-Particle Physics 3rd Edition (Plenum, New York, 1990) Ch 7
[5] J. Davies, Physics of Low-Dimensional Semiconductors: An Introduction (Cambridge University Press, Cambridge, 1998) p 199 ff
[6] N. Agraït, A. Levy Yeyati, and J. M. van Ruitenbeek, Phys. Rep. 377 81 (2003); see Section IIDD5
[7] M. P. Das and F. Green, J. Phys.: Condens. Matter 17, V13 (2005)
[8] W. R. Frensley, in Heterostructures and Quantum Devices Eds. W. R. Frensley and N. G. Einspruch (Academic, San Diego, 1994) Ch 9
[9] R. Kubo, M. Toda, and M. Hashitsume, Statistical Physics II: Non-equilibrium Statistical Mechanics, 2nd Edition (Springer, Berlin, 1991)
[10] M. P. Das and F. Green, J. Phys.: Condens. Matter 15, L687 (2003)
[11] F. Green and M. P. Das, J. Phys.: Condens. Matter 12, 5233 (2000); ibid, 5251
[12] M. Reznikov, M. Heiblum, H. Shtrikman, and D. Mahalu, Phys. Rev. Lett. 75, 3340 (1995)
[13] F. Green, J. S. Thakur, and M. P. Das, Phys. Rev. Lett. 92, 156804 (2004)
[14] D. Pines and P. Nozières, The Theory of Quantum Liquids (Benjamin, New York, 1966)
[15] F. Sols, Phys. Rev. Lett. 67, 2874 (1991)
[16] W. Magnus and W. Schoenmaker, Quantum Transport in Sub-micron Devices: A Theoretical Introduction (Springer, Berlin, 2002)
[17] J. S. Thakur, F. Green, and M. P. Das, Int. J. Mod. Phys. B18, 1479 (2004)
[18] M. P. Das, J. S. Thakur, and F. Green, ArXiv preprint cond-mat/0401134 (2004)
[19] F. Green and M. P. Das in Noise and Fluctuations Control in Electronic Devices, A. A. Balandin ed (American Scientific Publishers, Stevenson Ranch, 2002), pp 31–48