We present an approach to steady-state mesoscopic transport based on the maximum entropy principle formulation of nonequilibrium statistical mechanics. This approach is valid in the nonlinear regime of high current, and yields the quantization observed in the integer quantum Hall effect at large currents. A key ingredient of this approach, and its success in explaining high-precision Hall measurements, is that the occupancy of single-electron states depends on their current as well as their energy. This suggests that the reservoir picture commonly used in mesoscopic transport is unsatisfactory outside of linear response.

We have recently developed an approach to steady-state mesoscopic transport not restricted to the linear response regime. By nonlinear here we mean that the driving force (voltage or current) is large—too large for linear response calculations, but well within the range of typical experimental values. Our approach is applicable to quasi-one-dimensional systems and to two-dimensional systems in strong magnetic fields, such as those exhibiting the integer quantum Hall effect. This work was reported in a brief form elsewhere [1]. Our study was motivated by the important but often neglected fact that the integer quantum Hall effect (IQHE) is exhibited even when the currents and voltages are very large [3]. Because the magnetic field strongly suppresses inelastic scattering, systems exhibiting the IQHE can be viewed as mesoscopic even though they are relatively large [4], and the IQHE itself can be viewed as a near-ideal manifestation of mesoscopic transport. The IQHE at low currents is well understood in terms of the Landauer-Büttiker (LB) approach to mesoscopic transport. This approach, however, appears to be fundamentally a linear response theory [5,6]. (See, however, [9,10].) When applied nonetheless at high currents, it fails to yield the observed quantization. The quantization at high currents appears to us to be an extraordinary phenomenon. It is easy to imagine many things that can end quantization (dissipation, backscattering, etc.), but it is not obvious how to restore quantization. It is perhaps possible that quantization at high current might result from conventional approaches to nonequilibrium transport (such as the Keldysh or quantum Boltzmann approaches [11]); but these are difficult even near linear response and their behaviors at large currents simply unknown. The high-current quantization is so extraordinary that it seemed likely to us that a successful theory of large-current mesoscopic transport would have to take its highly non-equilibrium nature into account from the very beginning.

We found an apparently fruitful direction in the maximum entropy approach (MEA) to nonequilibrium statistical mechanics [12], in which the density matrix is found by maximizing the information entropy of the system, subject to constraints which fix the expectation values of observables. This approach should in principle be quite generally applicable to equilibrium and nonequilibrium statistical mechanics, but in fact there have been very few examples of the latter. For reasons which we shall explain below, mesoscopic systems (including those exhibiting the IQHE) are ideally suited for the MEA, and our calculations are exact for mesoscopic systems consisting of non-interacting electrons. This gives as a first benefit an exact Hall quantization at zero temperature, for ideal systems, for almost arbitrarily large currents. A consequence of this work is that it suggests that the picture of current and voltage probes as reservoirs—which underlies nearly all approaches to transport in mesoscopic systems, and which has proven extremely successful at low currents—may not be satisfactory at high currents.

In the present and a companion paper we present our theory in detail together with discussions and applications. The present paper, part 1, develops the formal theory, and the companion, part 2, contains various applications. In the present paper, section I contains a more detailed introduction and motivation. Section II contains our maximum entropy approach together with a detailed example, and section III contains a discussion of the maximum entropy approach, the resulting electronic distributions, and the relationship between this work and more conventional approaches.

I. INTRODUCTION; LANDAUER-BÜTTIKER FORMALISM

A mesoscopic system typically consists of a ‘device’ (such as a Hall bar or quantum wire) and a number of current and voltage probes. The device itself is truly mesoscopic, by which we mean that the length of the device is smaller than the phase-breaking length. The connection between the device and the external world is provided by the probes, which are attached to the device at terminals. (In reality, the terminals consist of, for example, the $n^+$-doped regions
which connect to the inversion layer in a silicon metal-insulator field-effect transistor, or the ‘fingers’ of indium diffused through the different layers in a heterostructure. Thus, in a real device carriers pass into the device through terminals which are no larger than the device itself. The carriers in general will suffer both elastic and inelastic scattering, and so dissipate energy, in the terminals.) We presume that within the mesoscopic device itself scattering is entirely elastic and dissipationless.

It is not obvious how to handle the complicated system of device plus probes. The greatest advance in understanding mesoscopic transport came from an approach originally due to Landauer [1,6,12], in which the conduction of the entire sample is treated as a scattering problem. There are two central concepts in this model. The first is the “reservoir” — the probes are treated as macroscopically large (essentially infinite) reservoirs which inject carriers into the device through ideal leads. It is assumed that each reservoir is in local equilibrium described by a local chemical potential \( \mu_m \), and that the occupancy of electronic states entering the device from a reservoir is determined by the local chemical potential of that reservoir. We will use the term ‘reservoir’ only in this restricted sense. More generally we will refer to a source of carriers as a ‘terminal’. The second key concept is that the motion of carriers through the device itself is treated as an elastic scattering problem. Carriers entering from a reservoir into the device are scattered either back into the original reservoir or outward into the other reservoirs. The scattered electrons then equilibrate deep within the reservoir with the electrons in the reservoir. Scattering in the terminals randomizes the energy and phase of the carriers, which eliminates any quantum interference [14].

To formulate the scattering problem one needs asymptotic regions in the leads in which states carry electrons either away from or towards the device [14] (and in which evanescent modes have decayed away). Such leads are quasi-one-dimensional, and states in them can be labeled by subband index \( n \) and wavenumber \( k \). (In the presence of a magnetic field, \( n \) is a Landau level index.) Within the system consisting of the device plus the asymptotic regions scattering is elastic. This gives the conventional treatment of mesoscopic devices: conduction occurs as elastic scattering of carriers injected into the asymptotic regions from reservoirs [14]. In this paper we will adhere entirely to the scattering viewpoint. We will argue, however, that outside the linear regime one cannot treat the terminals (which inject carriers) as reservoirs in the specific sense defined above.

To be definite, we will use the following notation and conventions. For simplicity, we assume that the electrons are noninteracting and spinless. (Both restrictions can be removed—spin just adds another label, and the formulation we give later can be extended to the case of interacting many-body states.) In an \( M \)-terminal device we denote the probes by \( m = s, d, 2, \ldots, M - 2 \). Here \( s \) denotes the source of current and \( d \) the drain, since in typical experiments current flows in one lead and out one other. In general we define a complete orthogonal set of single-particle eigenstates by supposing that the leads can be treated as semi-infinite and straight [14]. In this case, a particularly useful set of eigenstates for multi-terminal \( (m > 2) \) systems is the scattering states \( | \psi^+_{mnk} \rangle \) (i.e., \( \alpha = mnk \)). The state \( | \psi^+_{mnk} \rangle \) is incoming into the device from terminal \( m; n \) and \( k \) denote the asymptotic wavenumber and subband index of the incoming wave. The state has energy \( E_{mnk} \) and carries current \( i_{mnk} \) into the device at terminal \( m \). (Landauer objects to this lead geometry as incompatible with the reservoir concept [14]. But our discussion of the LB approach needs only a subband index and wavenumber, and does not use this geometry at all. We have specified this geometry here because the scattering language it makes precise is useful for the subsequent sections.) In general, after scattering within the device, the state carries outward current through each terminal. We denote by \( t_{mnk} \) the net current of this state into the device at terminal \( m \), with the convention that current flowing into the device is positive. The state’s net current at \( m \) is related to its incoming current at \( m \) by \( i_{mnk} = i_{mnk}(\delta_{mn} - \sum_{n',k'} t_{mnk'}i_{m'n'k'}) \), where \( t_{mnk'} \) is the transition probability obtained from the scattering matrix in the \( | \psi^+_{mnk} \rangle \) representation (with a proper normalization [14]). The elastic scattering within terminals which can exist in a real system can be included as contributions to the transmission probabilities.

The reservoir and scattering concepts underlie the Landauer-Büttiker (LB) theory of mesoscopic transport [14]. A key point in this theory is that voltage as well as current contacts are treated identically and described as reservoirs [14]. The reservoirs enter this theory in several important ways: they determine the electronic distribution, they randomize the phase of occupied states (which eliminates interference), and they provide a prescription for determining voltage differences. Combined, these permit one to calculate current-voltage (\( I-V \)) curves. First consider the distribution of electrons in the device. Suppose the \( n \)th terminal is a reservoir described by a local chemical potential \( \mu_n \). Then the states in the attached lead carrying current toward the device are occupied according to the Fermi-like distribution \( f_{mnk}^{LB} = 1/[e^{(E_{mnk} - \mu_n)/k_B T} + 1] \). (Here \( \beta = 1/k_B T \), where \( T \) is the temperature and \( k_B \) is Boltzman’s constant.) The net current flowing into the system at, say, the source is \( I = \sum_{mnk} i_{mnk} f_{mnk}^{LB} \). Suppose that in a multiprobe device the current flowing in at the source and out at the drain is \( I \), with zero net current at other terminals. In the LB approach this is enough information to determine the local chemical potentials \( \mu_n \) (within an additive constant). Within the reservoir picture, it is then obvious that the measured voltage difference between
two terminals (1 and 2, say) must be \( V = (\mu_1 - \mu_2)/e \), where \( e \) is the charge of an electron.

Consider the particular case of a two-terminal device at zero temperature, with some current \( I \) flowing from source to drain. The current is in this picture caused by a voltage difference \( V = (\mu_s - \mu_d)/e = IR \) between source and drain. Following the standard LB approach, at low voltages this gives a resistance \( R = h/(je^2t) \), where \( j \) is the number of occupied subbands and \( t \) is the total transmission probability at \( \mu_s \). This resistance is quantized in the absence of backscattering (\( t = 1 \)). In real quantum Hall systems, there is a macroscopic separation between left- and right-moving states, so that in fact backscattering is highly suppressed, and indeed \( t \) is very nearly unity \( (1) \). (We have here neglected dissipation that occurs due to contact resistance at the source and drain. In a real two-terminal device this dissipation prevents perfect quantization of resistance. Resistances can be quantized only in a multi-terminal device when measured between two terminals through which no net current flows.) Here we have briefly given the two-terminal version of this explanation, but following Büttiker \( (6) \) it can be generalized to the multi-terminal case (see below), in which case the corresponding voltage is the transverse or Hall voltage. Hence the LB theory gives a very satisfying microscopic explanation of how the conductance can be so accurately quantized in the IQHE \( (4) \)—at least in the low-current regime, as we will explain below.

We have summarized the LB theory here in a way appropriate for linear response—the difference \( \mu_s - \mu_d \) is presumed to be small. This is assumed in nearly all uses of the LB approach \( (2,4,17) \). For example, we treated the transmission \( t \) as a constant, which requires in part that \( \mu_s - \mu_d \) be small. It is possible to generalize this to the case where the transmission depends significantly on energy near the Fermi level \( (5) \), as would be needed if \( \mu_s - \mu_d \) is large. In the remainder of this section, however, we will be concerned only with ideal systems (perfect transmission), so this type of generalization is not relevant here.

The LB theory of macroscopic transport has been used to interpret a wide variety of experiments (see, for example, a partial listing in Ref. \( (15) \)). In fact, the fundamental model of reservoirs at (local) equilibrium with local chemical potentials \( \mu_m \) has been used in essentially all mesoscopic calculations, including microscopic methods such as non-equilibrium Green’s functions. There is no reason to doubt the fundamental soundness of treating the terminals as reservoirs in the low-current regime.

Despite the many successes of the LB approach, there are important experiments which it seems unable to explain. Chief among these are the actual high-precision IQHE experiments. In our above application of the LB approach to the IQHE we did not mention an important point: the LB theory only predicts quantization in the IQHE when the current is small. When the current is large (as large as those typical in high-precision experiments), the same argument predicts a failure of quantization. There is at least no straightforward way to extend the LB approach to give quantization at large currents. The culprit appears to be the very reservoir concept itself.

Let us examine this in detail, first in a ideal two-terminal example. Denote the minimum energy of the \( j \)th subband by \( E_j \). Suppose to begin with that the local chemical potentials of both the source and drain exceed \( E_j \) but are less than \( E_{j+1} \). (See Fig. \( 3a \).) In an ideal system at zero temperature, the net current in each subband is, according to the LB approach, \( e(\mu_s - \mu_d)/h \). (This simple form occurs because of a cancellation between the density of states and the current carried in each single particle state. \( (1) \) With \( j \) occupied bands, this gives a current \( I = je(\mu_s - \mu_d)/h \). The two-terminal voltage in the reservoir picture is \( V = (\mu_s - \mu_d)/e \), and so the two-terminal resistance is \( R = V/I = h/(je^2) \).

Now let us suppose that the local chemical potential of the source (but not of the drain) is increased above \( E_{j+1} \), so that the source injects electrons into the \((j+1)\)st subband, while the drain does not. This is shown in Fig. \( 3b \). In an ideal system at zero temperature, the net current contributed by each of the lower \( j \) subbands is the same as above, but the net current in the \((j+1)\)st subband is \( e(\mu_s - E_{j+1})/h \). Thus the total current is \( I = je(\mu_s - \mu_d)/h + e(\mu_s - E_j)/h \). The voltage difference must still be \( V = (\mu_s - \mu_d)/e \) in the reservoir picture, so in this case the LB approach gives a two-terminal resistance \( R = V/I \) which lies between \( h/(je^2) \) and \( h/[(j+1)e^2] \). Notice that this happens whenever one or more of the subband minima lie between \( \mu_d \) and \( \mu_s \), which must occur whenever \( eV \) exceeds the subband spacing. That is, even in the case of an ideal system, with no backscattering, the LB prediction is that the two-terminal resistance should not be quantized when \( eV \) is large. And yet in the high-precision IQHE experiments quantization is found to be extremely accurate even when \( eV \) is 10 or 100 times the subband spacing \( (8) \). (The same argument has been invoked to explain the large-voltage failure of resistance quantization in quantum point contact experiments within the LB formalism \( (24) \).

The above argument also works in an ideal multi-terminal IQHE system. Suppose there are four terminals (taken to be identical for simplicity), with two current terminals \( s \) and \( d \), and two transverse voltage terminals 1 and 2 (see Fig. \( 2 \)). Then to get zero net current in terminal 1, it is necessary that \( \mu_1 = \mu_s \); similarly, \( \mu_2 = \mu_d \). A given \( \mu_s \) and \( \mu_d \) give the same total source-to-drain current as above, and the transverse (Hall) voltage is \((\mu_1 - \mu_2)/e \), also as above. Hence the ideal four-terminal LB results are identical to the ideal two-terminal measurements: the resistances are quantized at low but not at high currents.

The discussion thus far has treated the electrons as noninteracting. One might suppose that a more accurate
treatment, still within the LB picture but incorporating electron-electron interactions, might modify the large-current results. At the lowest (Hartree) level of approximation, electron-electron interactions can cause the subbands to deviate, perhaps significantly, from the wavenumber dependence which would arise in the noninteracting case [19]. This consequence of electrostatics is pictured schematically in Fig. 2(a), which shows the bending of energy levels (not too near a contact) in an IQHE sample due to the combined presence of a Hall field and an edge confinement. Of itself, this bending of bands has no effect on the argument above. If states in one level are occupied out to $\mu_s$ and $\mu_d$, then this level contributes $e(\mu_s - \mu_d)/h$ to the current, regardless of the band’s shape (because of the cancellation between density of states and current per state). So as long as all subbands shift in energy more or less together, as is the case with Hartree interactions, the picture is unchanged: a large voltage causes partial occupancy of higher subbands and hence failure of quantization.

In the above paragraph we assumed that, despite electrostatics, ideal reservoirs are able to occupy all states up to energies $\mu_s$ and $\mu_d$ (at zero temperature). Van Son and Klapwijk have recently made a serious attempt to examine more closely the consequences of electrostatics for the LB approach to the IQHE. Their starting point is that electron states (except very close to the current probes) can be described by bulk Landau levels (subbands) with a shape given by a self-consistently determined electrostatic potential (as in Fig. 2). Central to their analysis is an argument that the source injects electrons only in a range of energy $\mu_s - \Delta < \epsilon < \mu_s$. In other words, their source, because of an electrostatic barrier, does not act as a reservoir for carriers—it does not occupy all current-carrying states with energies $\epsilon < \mu_s$. Within some small length from the source, determined by inelastic scattering near the source, these electrons ‘relax’ to fill (bulk) subbands up to some energy $\mu'_s$ (with $\mu'_s < \mu_s$). Consider the case where $\sigma_H = e^2/h$. In this case, according to Van Son and Klapwijk, electrons injected at the source relax to fill only states in the lowest (bulk) subband, regardless of how large $\mu_s$ is. The result is that the lowest subband is filled from $\mu_d$ (for left-movers) to $\mu'_s < \mu_s$ (for right-movers). This is pictured in Fig. 3(b). If this relaxation occurs before the first voltage probe, they argue, a multi-terminal measurement would show the ordinary IQHE. Note that if $\mu'_s$ lies above the minimum of the next subband, this ‘relaxation’ results in some occupied states (e.g., in the lowest subband) lying at higher energies than empty states in the next subband (as in Fig. 3(b)).

We believe that Van Son and Klapwijk were correct in their conclusion that the conventional picture of terminals as reservoirs must be modified somehow at higher currents and voltages. But there appear to be some problems with the details of their arguments. Following Büttiker [6], Van Son and Klapwijk suppose that the voltage probes can be treated as reservoirs with zero net current. Let us consider what happens when $\mu'_s$ is greater than the energy minimum of the next higher subband, as pictured in Fig. 3(b). This certainly would occur if $eV_H \gg h\omega_c$. If the voltage terminals are treated as reservoirs, then the first probe ‘downstream’ from the source is at some electrochemical potential $\mu_1$ (in the geometry of Fig. 2). For simplicity let us assume that nothing complicated happens at the drain so that (in this geometry) $\mu_2 = \mu_d$. The occupied states after relaxation carry current $I = e(\mu'_s - \mu_d)/h$, and the Hall voltage is $(\mu_1 - \mu_2)/e$. This gives a quantized resistance only if $\mu_1 = \mu'_s$. But there is no reason for this to be the case. Suppose that the voltage terminal acts as an ordinary reservoir and injects carriers into all states (in all subbands) with energy $\epsilon < \mu_1$. States in the higher subband would be occupied, and so, to get zero net current at the probe, it would have to be the case that $\mu_1 < \mu'_s$. Suppose instead that the voltage terminal, like the current source, injects carriers into only a range of energies, after which the carriers relax. If the voltage and current probes are identical, then by symmetry zero net current in the former would require $\mu_1 = \mu_s > \mu'_s$. In neither of these two natural possibilities would the Hall resistance be quantized.

Second, Van Son and Klapwijk simply assume that the relaxation process is so efficient that at low temperatures states in the lowest subband end up filled continuously from $\mu_d$ to $\mu'_s$ (even though the current source and drain do not directly feed all of them), while the upper subbands all are empty. They assume this to be the case even if $\mu_s$ is high enough to inject carriers into a higher subband, as pictured in Fig. 3(b). This might work for voltages slightly above the subband spacing, but it is harder to believe that there should be no carriers in any of the higher subbands if $\mu_s - \mu_d$ is 10 or 100 times $h\omega_c$. Moreover, the relaxation into the lowest subband must be complete (to get quantization) only as long as $\mu_d$ lies below the minimum of the second band, as pictured in Fig. 3(b). Suppose that $\mu_d$ increases slightly so that it moves above the minimum of the second subband (while $\mu_s$ is held fixed). These appear to be the conditions under which one should expect a conductance of $2e^2/h$: both the source and drain attempt to occupy states in the next subband. Then according to the picture of Van Son and Klapwijk, it must be the case that states in the second subband also get filled from $\mu_d$ around to some $\mu'_s$, after relaxation, giving a conductance of $2e^2/h$. Yet why should relaxation bring all carriers to the lowest Landau level when $\mu_d$ lies slightly below the second subband’s minimum, and the same relaxation allow carriers to fill two subbands when $\mu_d$ increases to lie slightly above the minimum of the second subband? It is difficult to see how this supposition of large-scale relaxation into lower subbands can be entirely correct in detail.

Let us turn back to the usual reservoir picture, and examine whether including the interactions more accurately—by, say, including exchange—can restore the high-current quantization. The exchange interaction effectively lowers the energy of the occupied single-particle states relative to unoccupied states, and in principle this could remove
the partial occupancy of higher subbands (the cause of the failure to quantize). Suppose for example that at a low
two-terminal voltage \( V \) states in only the lowest subband are occupied. Let the voltage \( V \) increase. Suppose further
that the exchange and correlation energies effectively lower the energies of the occupied states in this subband so that
they all lie below the minima of higher subbands. Then the higher bands would remain unoccupied, and the resistance
remain quantized. The difficulty with this argument is that the quantization in high-precision IQHE measurements at
voltages 10 or 100 times the unperturbed Landau level spacing \( \hbar \omega_c \) would require the exchange and correlation energies
to exceed \( 10 \hbar \omega_c \) or even \( 100 \hbar \omega_c \). In fact the exchange and correlation energies are much smaller (of order \( 10^{-3} \hbar \omega_c \)
in the fractional quantum Hall effect), and it seems implausible that this can be used to modify the LB approach to
give the correct quantum Hall resistance at high currents and voltages.

Perhaps the electron distributions change at large current as a result of some complicated behavior (beyond elec-
trostatic considerations \( [9] \)) at the terminals where the leads and mesoscopic system are joined. There is as yet no
detailed explanation of how this could occur. Such an argument would also be outside the spirit of Landauer’s original
idea. His insight was that it should be possible to ignore the (perhaps very complicated) details of the terminals, which
are described entirely by the transmission probabilities, and concentrate on general principles (see for example the
discussion in \( [10] \)). The existence of high-current quantization in the IQHE and other mesoscopic devices argues, we
believe, that this insight is fundamentally correct. However, based on the experimental evidence of the high-precision
measurements of the quantum Hall resistance, we believe that the model of terminals as macroscopic reservoirs in local
equilibrium is unsatisfactory outside the regime of linear response. Here we will present an approach to mesoscopic
transport which can be viewed as being within the spirit of Landauer’s idea, in that we assume it is possible to neglect
the details of the terminals. Our approach leads, however, to a different occupancy of electronic states (and hence
requires modification of the reservoir concept), and appears capable of describing transport in mesoscopic devices
outside of the low-current realm.

II. MAXIMUM ENTROPY APPROACH TO MESOSCOPIC TRANSPORT

The nonlinear steady-state mesoscopic transport theory which we have developed is based on the maximum entropy
approach to nonequilibrium statistical mechanics. In this section we will develop this approach to transport and
provide a detailed example which illustrates how it can explain the IQHE even at large currents and voltages.

A. Density matrix

The central ingredient of the maximum entropy approach (MEA) is the information entropy \( S_I \) \( [12] \). If a complete
set of eigenstates of a thermodynamic system is labeled by \( \gamma \), then the information entropy is given by

\[
S_I = -c \sum_{\gamma} p_\gamma \ln p_\gamma
\]

where \( p_\gamma \) is the probability that the system is in a given microstate. Here \( c \) is an unspecified constant. (When the MEA
is applied to equilibrium thermodynamics, it can be shown that the information and thermodynamic entropies are
identical when \( c \) is chosen to be Boltzman’s constant \( k_B \). We will see that this is also true in the case of steady-state
mesoscopic transport.) As in any thermodynamic calculation, the first necessity is to define ‘the system’. We assume
that we can define the system to be the device (including the asymptotic leads), as described earlier. In general, \( \gamma \) then
simply refers to a many-body electron state. In the case of noninteracting electrons each such microstate corresponds
to a particular set of occupied single-particle scattering states. It is the fact that the device itself is mesoscopic which
allows for a straightforward description of the microstates. In the presence of dissipation, this is not so easy. In fact, in
spite of claims to its general applicability, nearly all applications of the MEA to dissipative nonequilibrium systems
have been limited to expansions about equilibrium \( [12] \).

The fundamental postulate of the MEA is that the probabilities \( p_\gamma \) are those which maximize the information
entropy—subject to constraints which describe certain given or known observables. The method itself does not give a
prescription for determining what are the constraints. These must be determined from physical considerations. (We
will discuss this point in more detail later.) In the case of equilibrium thermodynamics, it is assumed that the internal
energy \( U \) and electron number \( N \) can be taken as given, whether or not they are actually measured. In the case of
steady-state transport one knows in addition (by measurement) the net current at each terminal. We therefore include
this as an additional constraint and maximize the information entropy subject to the constraints \( \langle \hat{H} \rangle = U \),
\( \langle \hat{N} \rangle = N \), and \( \langle \hat{I}_m \rangle = I_m \). Here \( \hat{H} \) is the Hamiltonian, \( \hat{N} \) is the particle number operator, and \( \hat{I}_m \) is operator giving the net
current in lead $m$ [21]. These constraints are conveniently imposed using Lagrangian multipliers. The probability entering Eq. (1) can be written as the matrix element $p_{\gamma} = \langle \gamma | \hat{\rho} | \gamma \rangle$ of the density matrix $\hat{\rho}$. Then maximizing $S_f$ subject to the constraints gives the density matrix

$$\hat{\rho} = \exp \left[ -\beta (\hat{H} - \mu \hat{N} - \sum_m \xi_m \hat{I}_m) \right]. \quad (2)$$

As in ordinary equilibrium thermodynamics, the Lagrangian multiplier associated with the constraint on $N$ is $\mu$, the global chemical potential. The intensive variables $\xi_m$ are Lagrangian multipliers associated with the constraints on the currents. Notice that because of current conservation there are only $M - 1$ independent current constraints, and hence one $\xi_m$ can be chosen freely. It turns out to be convenient to choose $\xi_d = 0$, and we do so henceforth. Associated with the constraint on $U$ is the Lagrangian multiplier $\beta$. In equilibrium $\beta$ is the inverse temperature; we shall shortly present several arguments why this continues to be true here.

For clarity let us consider the case of non-interacting electrons. These occupy any of a complete set of single-particle eigenstates $|\psi_\alpha\rangle$ of $\hat{H}$ and $I_m$. The density matrix $\hat{\rho}$ above leads to a thermal occupancy of these single-particle states given by

$$f_\alpha = \frac{1}{\exp [\beta (\epsilon_\alpha - \mu - \sum_m \xi_m i_{m,\alpha})] + 1}. \quad (3)$$

To make this more transparent, let us look at this in the case of a two-terminal system, using scattering states $|\psi_{mnk}\rangle$ for the single-particle basis. In the two-terminal case we can drop the terminal index $m$, and understand that $k > 0$ ($k < 0$) corresponds to states injected by the source (drain). These can also be called right- and left-movers, respectively. In an ideal system with no backscattering $\{f_{nk} = \delta_{n'n} \delta_{k'k}\}$, these states carry currents $i_{nk}$ from end to end, and the distribution becomes

$$f_{nk} = \frac{1}{\exp [\beta (\epsilon_{nk} - \mu - \xi i_{nk})] + 1}, \quad (4)$$

with $\xi \equiv \xi_s$. With only one subband ($n = 0$) occupied, this is similar to the LB result; at zero temperature, states are occupied up to an energy $\mu + \xi i_{nk}$ (with $k$ here the highest occupied state on an edge). This is pictured in Fig. 4(a). Because the current has opposite signs for positive and negative $k$, right- and left-moving states are occupied up to different energies. The combination $\mu + \xi i_{nk}$ acts in this case like an effective local chemical potential. In the general case with several subbands occupied, however, states are occupied up to different energies in each subband. [See Fig. 4(b).] At zero temperature the states in subband $n$ are occupied up to $\mu + \xi i_{nk}$ which depends on the current carried by the highest occupied state in this subband. This current is in general different in different subbands, and so the distributions $f_{nk}$ cannot be described in terms of local chemical potentials. Said another way, if one insisted on defining local chemical potentials, there would need to be a different ‘local chemical potential’ for each subband.

### B. Calculating voltages

Within the reservoir model it is quite clear that ordinary voltage measurements at a contact correspond to the local chemical potential: $V_m = \mu_m / e$. (See, for example, [13].) As we have emphasized above, the distributions derived from the MEA cannot in general be described in terms of a local chemical potential, and clearly the LB prescription for finding $V_m$ cannot apply. Nor does the MEA itself give some procedure for determining voltages. The approach we take to calculate voltages comes from the following physical picture: a voltmeter determines the voltage differences between two terminals by measuring the work required to move a small amount of charge from one to the other. If moving some charge $\delta Q$ takes a work $\delta W$, then the voltage difference is the ratio $\delta W / \delta Q$. The problem is then to calculate this work.

The work required to move reversibly between equilibrium states is given by changes in thermodynamic potentials (e.g., the Helmholtz free energy, when the temperature is constant). In general potentials cannot be defined in nonequilibrium systems, which ordinarily involve dissipation. The problem of steady-state transport in mesoscopic systems, however, is a special case of nonequilibrium thermodynamics. In the device there is no inelastic scattering; this, and the steady-state condition, permit us to define thermodynamic potentials of the electron distribution [22]. For example, the information entropy is equivalent to an ordinary thermodynamic entropy, as mentioned above and explained below; and so here we can define the Helmholtz free energy as usual, $F = U - TS$. The work $\delta W$ done on the system at constant temperature is then equal to the change in free energy,
\[ \delta F = \mu \delta N + \sum_m \xi_m \delta I_m. \] (5)

That is, at constant temperature the free energy is a function of the electron number and of the net current at each terminal. However, the variables most easily varied in the theory are the intensive variables \( \mu, \xi, \xi_1, \ldots, \xi_{M-2} \). Varying any of these in general changes the occupancy \( f_{mnk} \) of incoming states at each terminal, by Eq. (5). Here for definiteness we will use the representation given by the scattering states \( |\psi_{mnk}^+\rangle \) labeled by \( \alpha = mnk \), with occupancies \( f_{mnk} \). In what follows it is useful to define a quantity \( N_m \) which is the number of occupied scattering states entering at terminal \( m \). Thus \( N_m = \sum_{nk} f_{mnk} \) and the total electron number in the device is \( N = \sum_m N_m \).

Let \( \eta \) refer to any of the independent variables \( \mu, \xi, \xi_1, \ldots, \xi_{M-2} \). Let \( \delta I_m^\eta \) denote the change in the net current entering at terminal \( m \) when variable \( \eta \) is varied while the other independent variables are held fixed. Similarly let \( \delta N_m^\eta \) be the corresponding change in \( N_m \). Then changing \( \eta \rightarrow \eta + \delta \eta \) produces a free energy change

\[ \delta F^\eta = \sum_m (\mu \delta N_m^\eta + \xi_m \delta I_m^\eta). \] (6)

We obtain the potentials \( V_m \) at the terminals by interpreting this free energy change as the work done to add \( \delta N_m^\eta \) electrons against the voltage \( V_m \) at the terminals. At each terminal the energy cost is \( e \delta N_m^\eta V_m \). Thus we can also write

\[ \delta F^\eta = \sum_m e \delta N_m^\eta V_m. \] (7)

Equating Eqs. (3) and (7) for each of the \( M \) variables \( \eta \) gives a set of \( M \) linearly independent equations,

\[ \sum_m \delta N_m^\eta (eV_m - \mu) = \sum_m \xi_m \delta I_m^\eta, \] (8)

which are to be solved for the unknown terminal voltages \( V_m \). The non-local resistance measured between two terminals \( m \) and \( m' \) is then \( R_{sd,mm'} = (V_m - V_{m'})/I \). The matrix \( \delta N_m^\eta \) on the left-hand side of Eq. (8) is invertible, and the resulting potentials are then automatically given relative to the global chemical potential \( \mu \).

C. Example

In this section we will illustrate the approach outlined above by finding the resistance of an ideal two-terminal system, and then extend the result to the ideal multi-terminal case. First consider a two-terminal device. For this we can use eigenstates which satisfy periodic boundary conditions on a length \( L \) along the device. This particular choice of boundary condition gives a simple density of states, but is of no other significance. The states are labeled by a subband index \( n \) and wavevector \( k \). Again in this case we can drop the terminal subscripts and understand that states with \( k > 0 \) are injected by the source and \( k < 0 \) by the drain. We choose \( \xi_d = 0 \) and write \( \xi \) for \( \xi_s \). The net current \( I_s \) entering at the source is just the total current \( I \) through the device. Here we consider only one simple case, for which the states have energy \( \epsilon_{nk} = \epsilon_n + \hbar^2 k^2/2m^* \) and current \( i_{nk} = e\hbar k/m^*L \). This can represent 1D transport, or a Hall bar with a parabolic transverse confinement. (In the latter case, \( \hbar^2/2m^* \rightarrow \omega_0 \ell^2/2 \), where \( \omega_0 \) is the curvature of the confining potential and \( \ell = \sqrt{\hbar eB} \) is the magnetic length.) By Eq. (3), the occupancy \( f_{nk} \) depends on energy and current in the combination \( \epsilon_{nk} - \xi i_{nk} \). This is

\[ \epsilon_n + \frac{\hbar^2 k^2}{2m^*} - \xi \frac{e\hbar k}{m^*L} = \epsilon_n + \frac{\hbar^2}{2m^*}(k - \xi n/l)^2 - \frac{e^2 \xi^2}{2m^*L^2}. \] (9)

Thus the occupancy can be written

\[ f_{nk} = f(\epsilon_{nk} - \tilde{\mu}) \equiv 1/(e^{\beta(\epsilon_{nk} - \tilde{\mu})} + 1), \] (10)

where we have defined
\[
\begin{align*}
\tilde{\epsilon}_{nk} &= \epsilon_n + \frac{\hbar^2}{2m^*}(k - \tilde{\xi})^2, \quad (11a) \\
\tilde{\xi} &= \frac{e\xi}{\hbar L}, \quad (11b) \\
\tilde{\mu} &= \mu + \frac{\hbar^2\tilde{\xi}^2}{2m^*}, \quad (11c)
\end{align*}
\]

for reasons which will shortly be apparent. The total number of electrons occupying current-carrying states in the device is

\[
N = \sum_{nk} f(\epsilon_{nk} - \tilde{\mu}) = \sum_n \int_{\epsilon_n}^{\infty} d\epsilon \rho_n(\epsilon) f(\tilde{\epsilon} - \tilde{\mu}), \quad (12)
\]

where in the limit of large \(L\) we can take the \(k\)'s and hence \(\epsilon_{nk}\) to be quasicontinuous, and define for the latter a 1D density of states,

\[
\rho_n(\tilde{\epsilon}) = \frac{(L/\pi)|2\hbar^2(\tilde{\epsilon} - \epsilon_n)/m^*|^{-1/2}}{\sqrt{2\xi}}. \quad (13)
\]

From the integral form in Eq. (12) we see that \(N\) depends on \(\mu\) and \(\xi\) only in the combination \(\tilde{\mu}\) given by Eq. (11c). Thus here \(\tilde{\mu}\) acts like a current-dependent chemical potential controlling the number of occupied current-carrying states. The total current carried by the occupied states is

\[
I = \sum_{nk} i_{nk} f(\epsilon_{nk} - \tilde{\mu}). \quad (14)
\]

Notice that \(f_{nk}\) is symmetric about \(k = \tilde{\xi}\). That is, the two states in subband \(n\) at \(k_{\pm} = \tilde{\xi} \pm |2m^*(\tilde{\epsilon} - \epsilon_n)/\hbar^2|^{1/2}\) have the same value of \(\epsilon_{nk} = \tilde{\epsilon}\) and hence, from Eq. (11), the same occupancy. The current carried by these two states is then

\[
i_n(k_+) + i_n(k_-) = e\hbar(k_+ + k_-)/m^*L = 2e\hbar\tilde{\xi}/m^*L. \quad (15)
\]

Thus the total current is

\[
I = \frac{e\hbar\tilde{\xi}}{m^*L} \sum_{nk} f(\epsilon_{nk} - \tilde{\mu}) = \frac{e\hbar}{m^*L} \tilde{\xi}N. \quad (16)
\]

With these expressions it is now straightforward to compute the current-voltage relations by inverting Eqs. (8). In this two-terminal example, it is easier to use \(\tilde{\mu}\) and \(\tilde{\xi}\) as independent variables instead of the original pair \(\mu, \xi\). Then for this example there are two Eqs. (8), labeled by \(\eta = \tilde{\mu}, \tilde{\xi}\):

\[
\begin{pmatrix}
\delta N_{s}^\mu & \delta N_{d}^\mu \\
\delta N_{s}^\xi & \delta N_{d}^\xi
\end{pmatrix}
\begin{pmatrix}
eV_s - \mu \\
eV_d - \mu
\end{pmatrix}
= \xi
\begin{pmatrix}
\delta \tilde{\mu} \\
\delta \tilde{\xi}
\end{pmatrix}. \quad (17)
\]

These equations contain \(\delta N_m^\eta\), the change in the occupation number \(N_m\) of states which carry current into terminal \(m\). We are interested in the changes in these which result when \(\eta = \tilde{\mu}, \tilde{\xi}\) are changed infinitesimally. Rather than computing these directly, consider a function

\[
Q(\tilde{\mu}, \tilde{\xi}; k_0) = \sum_{nk} f(\epsilon_{nk} - \tilde{\mu}) \text{sgn}(k - k_0). \quad (18)
\]

Notice that \(Q\) depends on \(\tilde{\xi}\) via \(\epsilon_{nk}\), which, by Eq. (11a), depends on \(\tilde{\xi}\). The quantity \(\frac{1}{2}(N \pm \pm)\) gives the number of occupied states with \(k \geq k_0\). We ultimately seek the changes in number of occupied states with \(k \geq k_0\) due to infinitesimal changes \(\delta \tilde{\mu}\) and \(\delta \tilde{\xi}\). But the changes in occupation of these states are the same as the changes in occupation numbers of states with \(k \geq k_0\), as long as \(k_0\) is not too close to the edge of occupied \(k\)'s (that is, as long as states near wavenumber \(k_0\) are either fully occupied or unoccupied). Thus we can write

\[
\delta N_{s,d}^\eta = \frac{1}{2}(\delta N^\eta \pm \delta Q^\eta), \quad (19)
\]
where the upper (lower) sign is for $m = s (d)$, and $\eta$ represents variations in either $\bar{\mu}$ or $\bar{\xi}$. Let us choose $k_0 = \bar{\xi}$. Then, more precisely, Eq. (14) is true as long as the region of $k$-space where $f(\epsilon_{nk} - \bar{\mu})$ is very close to unity (at low temperatures) brackets both $\bar{\xi}$ and $k = 0$. This will be discussed further in Part 2, since this point leads to a breakdown in quantization in point contacts.\] Clearly $Q(\bar{\mu}, \bar{\xi}; k_0 = \bar{\xi}) = 0$. We seek

$$
\delta Q \equiv Q(\bar{\mu} + \delta \bar{\mu}, \bar{\xi} + \delta \bar{\xi}; \bar{\xi}) = \sum_{nk} \frac{1}{e^{\beta(\epsilon_{nk} - \bar{\mu} - \delta \bar{\mu})} + 1} \text{sgn}(k - \bar{\xi}),
$$

(20)

where $\bar{\epsilon}_{nk} = \epsilon_n + \hbar^2 (k - \bar{\xi} - \delta \bar{\xi})^2 / 2m^*$. Since $\bar{\epsilon}_{nk}$ is symmetric about $\bar{\xi} + \delta \bar{\xi}$, the only contribution to the sum over $k$ is for $\xi \leq k \leq \xi + 2\delta \xi$, so that

$$
\delta Q = \sum_n \sum_{k=\xi}^{\xi+2\delta \xi} \left[ e^{\beta(\epsilon_{nk} - \bar{\mu} - \delta \bar{\mu})} + 1 \right]^{-1} \approx \frac{L}{\pi} \delta \xi \sum_n \left[ e^{\beta(\epsilon_n - \bar{\mu})} + 1 \right]^{-1}
$$

(21)

plus terms of second order in the quantities $\delta \bar{\xi}$, $\delta \bar{\mu}$. That is, $\delta Q \bar{\xi} = \delta Q$ and $\delta Q \bar{\mu} = 0$. From the expression for $N$ given in Eq. (12) it is evident that varying $\bar{\xi}$ and $\bar{\mu}$ changes $N$ by

$$
\delta N = -\delta \bar{\mu} \int_{\epsilon_n}^{\infty} d\bar{\epsilon} \rho_n(\bar{\epsilon}) \frac{\partial f(\bar{\epsilon} - \bar{\mu})}{\partial \bar{\epsilon}},
$$

(22)

that is, $\delta N \bar{\mu} = \delta N$ and $\delta N \bar{\xi} = 0$. Combining Eqs. (22), (21), and (19), we find

$$
\begin{align*}
\delta N_s^\mu &= \delta N_d^\mu = \frac{1}{2} \delta N, \\
\delta N_s^\xi &= -\delta N_d^\xi = \frac{1}{2} \delta Q.
\end{align*}
$$

(23)

From Eq. (14) we obtain

$$
\begin{align*}
\delta \bar{\mu} &= \frac{e\hbar}{m^* L} \bar{\xi} \delta N, \\
\delta \bar{\xi} &= \frac{e\hbar}{m^* L} N \delta \bar{\xi}.
\end{align*}
$$

(24)

It is now a simple matter to invert the matrix in Eq. (17) and solve for $V_{s,d}$. We write the final answer as the two-terminal conductance

$$
G = I/(V_s - V_d) = \frac{e^2}{\hbar} \sum_n \frac{1}{e^{\beta(\epsilon_n - \bar{\mu})} + 1}.
$$

(25)

If $\bar{\mu}$ exceeds the band minima of the first $j$ subbands (or Landau levels), then at low temperatures $G = j e^2 / h$. Finite-temperature corrections are exponentially small. This exact result is true for a system without backscattering regardless of the size of the voltage or current. This occurs because at large currents it is quite possible for states in one subband to be occupied up to energies above those of empty states in other subbands—not because relaxation has failed to occur, but because according to the MEA this is the steady-state (although highly nonequilibrium) result. Exceptions to quantization occur when either (a) the current grows so large that a subband is occupied only for carriers moving in one direction (this is connected to the saturation in quantum point contacts \[20], and will be discussed further in part 2); or (b) the current is large enough to induce breakdown in the sample as a consequence of other dissipative mechanisms \[23]. For ordinary samples exhibiting the IQHE, neither of these occurs, and the approach described above provides an explanation of the extremely accurate quantization observed outside the linear response regime. This ability to explain the high-precision IQHE experiments is non-trivial, and lends credence to the postulate of the MEA.

The above example was explained in detail to show how our approach is applied in general. In this particular case of a two-terminal system, a simplification is possible. Since $N$ depends on $\bar{\mu}$ and not $\bar{\xi}$, changing the latter while holding the former constant corresponds to moving a charge $e \delta Q / 2$ from one terminal to the other (or from edge to
edge in a quantum Hall sample. The work required to do this (at constant \(N\)) is \(\delta F \tilde{\xi} = \xi \delta \tilde{\xi}\). Hence the voltage difference is

\[
e(V_s - V_d) = \frac{\delta F \tilde{\xi}}{eBQ/2},
\]

which gives the same result.

It is easy to extend the above calculation to an ideal multi-terminal IQHE system. (The general formalism is valid regardless of the presence of a magnetic field.) Suppose there are four identical terminals, as shown in Fig. 2. Then all of the current leaving the source flows along the lower edge to terminal 1. For the net current through terminal 1 to vanish, it is necessary that \(\xi_1 = \xi_s\). Similarly \(\xi_2 = \xi_d = 0\). The work required to transfer a certain charge from terminal 1 to 2 is then precisely that required to move the same charge from \(s\) to \(d\) in the two-terminal calculation. Hence the two-terminal conductance calculated above becomes here the Hall conductance.

Finally, we mention that the parabolic example is special only in that it can be solved analytically. We have numerically studied non-parabolic energies \(\epsilon_{nk}\) and multi-terminal systems and find in these cases that the accuracy of the quantization is limited only by the numerical accuracy. This work will be reported in part 2.

III. DISCUSSION

A. Density matrix

The density matrix and distribution which result from the maximum entropy approach, and which lie at the heart of our ability to explain the high-precision IQHE experiments, are unusual, but not unheard of in the literature. The distribution \(f_\alpha\) in Eq. (4) was proposed earlier by Heinonen and Taylor [24], and more recently by Ng [25]. These authors argued argued that in a device without dissipation it should be possible to define a free energy which, presumably, would be minimized. The process of minimization, subject to the current constraint, is formally identical to the MEA’s maximization of information entropy, and leads to the same distribution. In this paper we have obtained this result on considerably more fundamental grounds—assuming only that the postulates of the maximum entropy approach to nonequilibrium statistical mechanics are, in fact, correct.

Here we will seek some understanding of the density matrix Eq. (1) and distribution Eq. (3) from other viewpoints. Note first of all that this density matrix has the general form which Hershfield recently showed should exist on quite general grounds in steady-state nonequilibrium systems [26]. In his rather more conventional approach to nonequilibrium statistical mechanics, it is quite evident that \(\beta\) in Eq. (1) is indeed \(1/k_B T\), where \(T\) is the temperature. This was not obvious in the MEA, but based on Hershfield’s work we can make the same identification, in the case of steady-state mesoscopic transport. It also then follows that the information and thermodynamic entropies are equivalent [with \(c\) in Eq. (1) set to \(k_B\)].

The distributions Eq. (3) are obviously quite different from the LB distributions. The latter follow in a very straightforward way from the model of terminals as reservoirs, and are widely considered valid by their ability to describe non-local resistances in many low-current experiments, as well as by the appealing simplicity and clarity of the reservoir model itself. How can this difference in distributions be understood physically? The LB distributions can be derived from linear response theory, with a certain assumption about how the system is driven. One can apply something very similar to the reservoir idea in a very precise calculation by modeling the leads as ideal and supposing that far from the device there is in each lead a well-defined electrochemical potential. A.D. Stone and coworkers have shown that this assumption leads in linear response to the multi-terminal LB formalism [8]. We should note, however, that this work has been criticized by Landauer, based on their use of leads of constant cross section, which do not have the geometrical spreading he believes is necessary for the reservoir picture [10]. Even so, while indeed no large reservoir is invoked in the work of Stone et al., a very similar idea—that far from the device a probe can be described as a system at constant potential—is at the heart of this calculation, entering as a boundary condition. (We should also note that since in principle linear response can be calculated using equilibrium distributions, the success of the linear theory in predicting low-current properties does not imply that the linear distributions are correct.)

We emphasize that built into Stone et al.’s and related calculations is the model of terminals as entities described by local chemical potentials. This model fits neatly into the most common way to approach nonequilibrium problems: assuming that there are two large reservoirs, each in equilibrium, and that transport (say) between them occurs when they are connected by a small channel. This is a very familiar approach to nonequilibrium statistical mechanics. And yet it amounts to an assumption as to how the system is driven. In typical transport experiments in the IQHE, say, a constant current source is connected to the sample. Using the reservoir picture amounts to a model of how a current
source (when connected to a mesoscopic device) actually drives the current. Perhaps it is valid in linear response to model the current source as two leads at different potentials. Even if valid in linear response, it is not \textit{a priori} clear that the picture should be valid at large currents. In fact, the failure of the LB approach at large currents suggests not.

Let us examine this in more detail. Suppose that the current source itself can be viewed as an object which gives rise to different potentials in the physical leads. Then the current is carried down long macroscopic lengths of lead until it is injected into the device through the terminals. Perhaps along the macroscopic wire the local potential changes gradually and smoothly (due to elastic and inelastic scattering); that is, perhaps the distribution locally can be described by a local chemical potential. Does this picture work right up to the vicinity of the mesoscopic device? In fact, there are several reasons to think not.

The simplest way to approach this is in the approximation of the Boltzmann approach to transport \cite{27}. Consider an ordinary dissipative conductor carrying a low current. Let us suppose that the current is driven by reservoirs held at two different potentials. Then at the reservoirs the Boltzmann distribution \( f(\mathbf{r}, \mathbf{k}, t) \) will have the LB form. But a perfectly standard Boltzmann calculation shows that far from the reservoirs the distribution evolves into a current-dependent form identical (in first order) to that derived from the MEA [Eq. (3)], and different from the first-order LB distributions. Suppose that the ends of an effectively one-dimensional conductor (at \( x = \pm L/2 \)) are held at different electrochemical potentials \( \mu \pm \Delta \mu/2 \). The distribution is then labeled by a wavenumber \( k \) plus a subband index \( n \): \( f = f(x, n, k, t) \). Suppose further that this gives rise to a uniform electric field \( E = \Delta \mu/eL \) through the conductor. Then in steady-state and one dimension the Boltzmann equation becomes \cite{27}

\[
\frac{v}{\partial f}{\partial x} + \frac{\partial k}{\partial t} \frac{\partial f}{\partial k} = \left( \frac{df}{dt} \right)_{\text{coll}}. \tag{27}
\]

We want the lowest-order (in \( \Delta \mu \)) solution to this, in the relaxation time approximation \cite{27}. Since the conductor’s ends are held at definite local chemical potentials, the distribution takes the LB form at the ends:

\[
f(\mp L/2, n, k, t) = 1/\left( \exp[\beta(\epsilon_{nk} - (\mu \pm \Delta \mu/2))] + 1 \right). \tag{28}
\]

The upper sign is for positive \( k \) and the lower for negative \( k \). Eq. (27) is a completely standard Boltzmann problem, with the only wrinkle provided by the boundary conditions, Eq. (28). To linear order this problem is solved by

\[
f = f_0 + \Delta \mu f_0 \frac{\partial f_0}{\partial \epsilon} \left[ \left( \frac{\hbar k \tau}{mL} + \frac{1}{2} \right) e^{-m(x \pm L/2)/\hbar k \tau} - \frac{\hbar k \tau}{mL} \right] \tag{29}
\]

where again the upper (lower) sign is for \( k > 0 \) (\( k < 0 \)). Here \( f_0(\epsilon_{nk}) = 1/\left( e^{\beta(\epsilon_{nk} - \mu)} + 1 \right) \) is the equilibrium distribution and \( \tau \) is the relaxation time (which can depend on \( k \)). Let us suppose that the relaxation time \( \tau \) is much less than the transit time across the system: \( \tau \ll L/v \), where the speed \( v = \hbar k/m \). Then at distances much farther than \( \tau v \) from the ends the distribution becomes

\[
f = f_0 - \frac{\tau \Delta \mu}{e \epsilon_{nk}} \frac{\partial f_0}{\partial \epsilon}. \tag{30}
\]

Here \( \epsilon_{nk} = ev/L \) is the current carried by the state in subband \( n \) with wavevector \( k \). Eq. (30) is the lowest-order term in an expansion in current of

\[
f_0(\epsilon_{nk} - \xi \epsilon_{nk}) = \frac{1}{\exp[\beta(\epsilon_{nk} - \mu - \xi \epsilon_{nk})] + 1}, \tag{31}
\]

where we have here identified \( \xi = \tau \Delta \mu/e \). Note that this is not equal to the corresponding first-order LB distribution \( f = f_0 \mp (\Delta \mu/2) \partial f_0/\partial \epsilon \).

That is, in a completely typical dissipative conductor, the Boltzmann distribution is precisely the lowest-order approximation to the distribution [Eq. (4)] obtained from the maximum entropy calculation. This is the case even though we chose the boundaries to model reservoirs; the distribution evolves from the LB form near the ends to the current-dependent form away from the ends. Our point with this example is the following. Even though the LB distribution has the authority of widespread usage, perhaps one should instead typically expect to find current-dependent distributions carrying steady-state currents into a mesoscopic system; for the dissipative wires carrying the current to the mesoscopic device should themselves typically have such distributions. Note that the Boltzmann equation gives current-dependent distributions also in the familiar case of a three-dimensional conductor in the relaxation-time approximation. In this case the resulting distribution is obtained by displacing the Fermi surface
in the direction of the current, and therefore here too the occupancy of single-particle states depends on their current as well as their energy.

There are special cases in which current-dependent distributions can be obtained in other ways. We have argued elsewhere that this should arise by Galilean transformation in a translationally invariant dissipationless system \cite{1}. We also have given elsewhere a detailed example in which a mechanism to switch on the current is provided, and which results in this distribution \cite{28}. These, and the general result of Hershfield mentioned earlier \cite{29}, all support our identification of $\beta$ as $1/k_BT$, as well as the notion that these distributions should be generally expected in steady-state transport.

If the reservoir picture is only adequate at low currents, how can one picture the way a current source drives a large current through a mesoscopic system? Perhaps one can think of the current source as forcing current through a region full of scatterers, like someone being forced to run a gauntlet. The current source pushes electrons in; they scatter into other states. In steady state it is reasonable that the occupancies of the various states will be influenced by their ability to carry current.

Finally, we have emphasized that the distributions resulting from the MEA (given the constraints of particle number, internal energy, and current) cannot be described in terms of a local chemical potential. Nonetheless it is evident from our calculation of the terminal voltages $V_m$ that the quantity $eV_m$ plays the role of a kind of a local chemical potential. That is, $eV_m$ is equal to the energy cost required to add an extra particle to the terminal (more precisely, to occupy an extra incoming state at terminal $m$). This is clearly not a local chemical potential in the LB sense—the MEA distributions in terminal $m$ are not of the Fermi-Dirac form with a local chemical potential $eV_m$.

B. Maximum entropy approach

Perhaps the most unorthodox part of our calculation is its use of the maximum entropy approach. The essential feature of the MEA (besides the obvious fact of the entropy maximization) is that observables enter the formalism as constraints. For example, here we have treated the current source—the object driving the system out of equilibrium—merely as something which imposes a constraint on the total current $I$. That is, the result of the driving enters the formalism. In a typical linear response calculation, the driver enters as a term in the Hamiltonian (say, a small electric field). A difficulty of the MEA is that it provides no prescription for how one should determine the constraints. It seems that one must be guided by the physical picture. This has been called “the basic problem” with the maximum entropy approach \cite{22}. In many cases it simply is not possible to know what the constraints are—for example, in the case of hot electrons in semiconductors it appears that one must somehow incorporate information about phonon interactions as a constraint \cite{22}; and nobody knows how to do this. But the fact that this approach may be difficult in some problems does not of course mean that it is always difficult. In fact, steady-state mesoscopic transport seems to be ideally suited for this approach. Guided by the physical picture, we have made the simplest possible supposition about constraints, and it appears to work. In particular, since the current source is designed to hold the current constant, we simply treat the current as a constraint.

A second difficulty with the MEA is that often it is difficult to calculate the microstates which enter the formalism. In the case of steady-state mesoscopic transport, this is not a problem. Since the thermodynamic system is the mesoscopic device plus ideal leads (in the scattering geometry), it is quite straightforward to calculate the entire set of microstates. Here we have emphasized how to do this for noninteracting electrons, but it is also possible in the interacting case. We will discuss this more in Part 2.

It is interesting to note that the LB distribution can also be obtained from the MEA by a different choice of constraint. This happens if one assumes that the current source somehow constrains the particle numbers $N_m$ entering at each terminal, rather than determining the net currents at each terminal \cite{23}. In the MEA these constraints lead to Lagrangian multipliers $\mu_m$, and the resulting occupancies are the LB distributions $f_{m,n,k}^{LB}$. Thus one might be tempted to ascribe the difference between the LB distributions and those obtained by us to the way in which the current source is modeled. At low currents the use of local chemical potentials can be justified using linear response theory, viewing the potential difference as driving the current. This cannot be extended to high currents. Since the LB distribution is associated with an ordinary electrochemical potential at each reservoir, one might suppose that it models a voltage source instead of a current source. If so, then the $I$-$V$ curve at large currents and voltages would depend on whether voltage or (as usual) current is applied \cite{23}. (In the linear regime, both approaches give the same result.) In fact, based on our arguments in section IIA this appears unlikely. Even if a voltage source is applied to the ends of the macroscopic wires leading to a device, it appears that by the time one moves far from the source (i.e., gets near the device) one should expect the distribution to have evolved to a current-dependent form.

We gratefully acknowledge discussions with C.T. Van Degrift, E. Palm, S. Girvin, S. Hershfield, M. Büttiker and A.D. Stone. This work was supported in part by the UCF Division of Sponsored Research, and by the National
Science Foundation under grant DMR-9301433.

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[3] For example, the GaAs heterojunction used to maintain the resistance standard at the U.S. National Institute of Standards and Technology shows quantization to better than one part per billion at the \( \nu = 4 \) plateau for \( eV_H > 16h\omega_c \).

[4] See, for example, J.J. Palacios and C. Tejedor, Phys. Rev. B 44, 8157 (1991).

[5] For example, the GaAs heterojunction used to maintain the resistance standard at the U.S. National Institute of Standards and Technology shows quantization to better than one part per billion at the \( \nu = 4 \) plateau for \( eV_H > 16h\omega_c \).

[6] See, for example, J.J. Palacios and C. Tejedor, Phys. Rev. B 44, 8157 (1991).

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FIG. 1. Typical energy spectrum of a one-dimensional mesoscopic device, or a laterally confined two-terminal IQHE system, and zero-temperature occupancies of the single-particle states in the Landauer-Büttiker picture. In this picture the occupancies of the states entering the device from the source and drain are described by local chemical potentials \( \mu_s \) and \( \mu_d \), respectively. Occupied states are marked by a heavy line. In (a) \( \mu_s, d \) exceed the minimum of the lowest \( j \) subbands (or Landau levels), but lie below the minimum of the \( (j+1)^{st} \) subband. In (b) \( \mu_s \) (but not \( \mu_d \)) lies above the minimum of the \( (j+1)^{st} \) subband.
FIG. 2. Schematic representation of a typical four-terminal IQHE device. Current runs along the lower edge from $s$ to terminal 1 and then to $d$. Similar currents run along the upper edge. If the device is ideal, and all terminals are identical, then in the Landauer-Büttiker picture $\mu_1 = \mu_s$ and $\mu_2 = \mu_d$ to get zero net current in terminals 1 and 2. Similarly in the maximum entropy approach $\xi_1 = \xi_s$ and $\xi_2 = \xi_d$.

FIG. 3. The typical bending of energy levels in an IQHE sample that occur due to electrostatics, here a combination of a transverse Hall electric field and confinement at the edges. (a) Occupied states are only in the first subband, and lie below the minimum of the next subband. (b) As pictured, states in only the lowest subband are occupied, even though some occupied states are higher in energy than empty states in the next subband.

FIG. 4. Current-dependent occupancies of states in an ideal two-terminal device, from the maximum entropy method. Occupied states (at zero temperature) are indicated by a heavy line. (a) When only one subband is occupied, states are occupied up to energies $\mu + \xi_{0k}$. These have different values for the outermost occupied states with for $k > 0$ and $k < 0$ (shown at $k$ and $k'$, respectively). (b) When more than one subband is occupied, states in different subbands are occupied up to different energies. Compare this with Fig. 1.