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Hydrodynamic approach to transport and turbulence in nanoscale conductors

R D'Agosta and M Di Ventra

Department of Physics, University of California—San Diego, San Diego, CA 92093, USA

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Abstract

The description of electron–electron interactions in transport problems is both analytically and numerically difficult. Here we show that a much simpler description of electron transport in the presence of interactions can be achieved in nanoscale systems. In particular, we show that the electron flow in nanoscale conductors can be described by Navier–Stokes type equations with an effective electron viscosity, i.e. on a par with the dynamics of a viscous and compressible classical fluid. By using this hydrodynamic approach we derive the conditions for the transition from laminar to turbulent flow in nanoscale systems and discuss possible experimental tests of our predictions.

1. Introduction

The electron liquid is both viscous and compressible; properties which suggest an intriguing analogy with a classical liquid [1]. This analogy is even more compelling when one recalls that the time-dependent many-body Schrödinger equation (TDSE) can be cast, quite generally, in a ‘hydrodynamic’ form in terms of the density and velocity field [2, 3]. In the classical case one can derive time-dependent equations, called Navier–Stokes equations, for the velocity field of the fluid as a function of its density, visco-elastic coefficients, pressure and the geometric confinement [1]. These equations are central to hydrodynamics and describe both laminar and turbulent regimes. If we could derive similar equations in the quantum case we would have a powerful tool to investigate a plethora of effects related to electron–electron interactions on a much simpler level than solving for the many-body Schrödinger equation. Unfortunately, the derivation of these equations in the quantum case is generally not possible.

In this paper we show that transport in nanoscale conductors satisfies the conditions for deriving quantum Navier–Stokes equations. This is simply due to the geometric constriction experienced by electrons flowing in a nanostructure which gives rise to very fast ‘collisional’ processes [4, 5]. In this regime, we show that one can truncate the infinite hierarchy of equations of motion for the electron stress tensor to second order and thus derive quantum hydrodynamic equations. With these equations we first re-derive conductance quantization in a quasi-1D non-viscous, incompressible fluid, thus making the connection between quantum transport and this hydrodynamic picture clearer. We then predict the conditions for the transition from laminar to

turbulent flow in quantum point contacts (QPCs) and suggest specific experiments to verify our predictions.

Let us start from a general many-body Hamiltonian $\hat{H} = \hat{T} + \hat{W} + \hat{V}_{\text{ext}}$, where \hat{T} is the kinetic term, \hat{V}_{ext} an external potential and

$$\hat{W} = \frac{1}{2} \int dr \int dr' \psi^\dagger(r) \psi^\dagger(r') w(|r - r'|) \psi(r') \psi(r), \quad (1)$$

where $\psi(r)$ are field operators and $w(|r - r'|)$ is the Coulomb interaction potential. It is well known that the TDSE can be equivalently written as two coupled equations of motion for the single-particle density, $n(r, t)$, and velocity field, $v(r, t)$, as obtained from the Heisenberg equation of motion for the corresponding operators [2, 3]. The single particle density is defined in terms of the field operator as $n(r, t) = \langle \psi^\dagger(r, t) \psi(r, t) \rangle$, while the velocity is given by $v(r, t) = j(r, t)/n(r, t)$ where the current density is given by $j(r, t) = e\hbar([\psi^\dagger(r, t)\nabla\psi(r, t) - \nabla\psi^\dagger(r, t)\psi(r, t)])/2mi$. For clarity we rewrite the Heisenberg equations of motion here (summation over repeated indices is understood)

$$D_t n(r, t) + n(r, t) \nabla v(r, t) = 0 \quad (2)$$

$$mn(r, t) D_t v_j(r, t) = -\nabla_i P_{i,j}(r, t) - n(r, t) \nabla_j V_{\text{ext}}(r, t) \quad (3)$$

where $D_t = \partial_t + v \cdot \nabla$ is the convective derivative, m the electron mass and $P_{i,j}$ ($i(j) \equiv r_{i(j)} = x, y, z$) is a stress tensor, exactly given by the sum of kinetic and interaction stress tensors [2, 3]. The interaction tensor is

$$W_{i,j}(r, t) = -\frac{1}{2} \int dr' \frac{r'_i r'_j}{|r'|} \frac{\partial w(|r'|)}{\partial |r'|} \int_0^1 d\lambda G_2(r + \lambda r', r - (1 - \lambda)r') \quad (4)$$

where $G_2(r, r') = \langle \psi^\dagger(r) \hat{n}(r') \psi(r) \rangle$ is the two-particle density matrix and λ is a parameter that defines the geodesic which connects two interacting particles [3]. As mentioned above, equation (3) has an appealing ‘hydrodynamic’ form where all many-body information is included in the stress tensor $P_{i,j}$. In order to solve (3) one proceeds by calculating an equation of motion for G_2 , which can be derived from the Heisenberg equation of motion of the particle creation and destruction operators. However, this equation of motion contains the three-particle density matrix. In turn, the equation of motion for the three-particle density matrix contains the four-particle density matrix and so forth, thus generating an infinite hierarchy of nested equations, making the problem practically unsolvable [2, 3].

2. Quantum Navier–Stokes equations

We show here that in the case of electrical transport in nanoscale systems we can instead close this set of equations. We proceed as follows. First, let us derive the dependence of the stress tensor $P_{i,j}$ on the rate at which the system reaches a quasi-steady state. We can obtain this dependence from the quantum kinetic equations for the non-equilibrium distribution function $f(r, p, t)$ (p is the momentum), which can be derived from the TDSE equation with standard techniques [6]¹ in a co-moving (Lagrangian) reference frame moving with velocity $v(r, t)$ [7]

$$I[f] = D_t f(r, p, t) + \frac{p}{m} \nabla f(r, p, t) + e \nabla \varphi \frac{\partial f(r, p, t)}{\partial p} - p \cdot \nabla v \frac{\partial f(r, p, t)}{\partial p} - m D_t v \frac{\partial f(r, p, t)}{\partial p} \quad (5)$$

¹ Clearly, for the definition of local equilibrium distribution to be valid any length scale entering the problem has to be larger than the system Fermi wavelength.

where I is the usual collisional integral [6] and φ is the sum of the external potential and the Hartree part of the interaction potential. The collisional integral contains two terms, one elastic and the other inelastic. In what follows, it is important to realize that both terms can drive the system toward a local equilibrium configuration.

The first two moments of the distribution give the density $n(r, t) = \sum_p f(p, r, t)$ and the condition $\sum_p p f(p, r, t) = 0$. The two-particle stress tensor is related to the distribution function as $P_{i,j} = \sum_p p_i p_j f(p, r, t)/m$. Similarly, higher order moments of the distribution function produce higher order stress tensors. Introducing these moments into (5) and comparing with (3) we can write the stress tensor in terms of the collisional integral I according to the equation of motion

$$\frac{1}{m} \int dp I[f] p_i p_j = D_t P_{i,j} + P_{i,j} \nabla \cdot v + P_{i,k} \nabla_k v_j + P_{k,j} \nabla_k v_i + \nabla_k P_{i,j,k}^{(3)}, \quad (6)$$

where $P^{(3)}$ is the three-particle stress tensor. By writing the equation of motion for $P^{(3)}$ we would again get an infinite hierarchy of equations. It is interesting to point out that the theorems of time-dependent density-functional theory establish that the stress tensor $P_{i,j}$ is a universal functional of the velocity and density only (see, for example, [8] or [9]). This implies that the hierarchy of equations for the moments of the distribution function can be formally closed to all orders in the electron–electron interaction. However, we note that $P^{(3)}$ enters into equation (6) only through its spatial derivative. If the latter is small then the hierarchy can be truncated [7]. From (6) we easily see that this derivative is small compared to the other terms whenever $\gamma = u/(L \max(\omega, v_c)) \ll 1$. Here u is the average electron velocity, L is the length of inhomogeneities of the liquid that give rise to scattering among three particles, ω is the system’s proper frequency and v_c is the collision rate. The parameter $1/L$ enters through the spatial derivative of $P^{(3)}$, ω from the frequency dependence of the interactions (in the DC limit of interest here $\omega \rightarrow 0$) and v_c through the collisional integral $I[f] \propto -v_c(f - f_0)$, where f_0 is the equilibrium Fermi distribution. This derivative is indeed small for transport in nanostructures: When electrons move into a nanojunction they adapt to the given junction geometry at a fast rate, and produce a quasi-steady state and local equilibrium distributions even in the absence of electron interactions [4, 5]. This ‘relaxation’ mechanism occurs roughly at a rate $v_c = (\Delta t)^{-1} \sim (\hbar/\Delta E)^{-1}$, where ΔE is the typical energy spacing of lateral modes in the junction. For a nanojunction of width w we have $\Delta E \sim \pi^2 \hbar^2/mw^2$ and $\Delta t \sim mw^2/\pi^2 \hbar$. If $w = 1$ nm, v_c is of the order of 10^{15} Hz, i.e. orders of magnitude faster than typical electron–electron or electron–phonon scattering rates. The condition $\gamma = u/(L \max(\omega, v_c)) \ll 1$ thus requires the length of inhomogeneities $L \gg 1$ nm, which is easily satisfied in nanostructures. Note instead that in mesoscopic structures this condition is not necessarily satisfied. In that case, the dominant relaxation rate v_c is given by inelastic effects, i.e. it is of the order of THz, so that for typical lengths of mesoscopic systems, $\gamma \approx 1$ in the DC limit. Nonetheless, the above condition could still be valid for high-frequency excitations, like plasmons, and/or very low densities, so that stress tensors of order higher than two are negligible.

Neglecting $\nabla_k P_{i,j,k}^{(3)}$ in (6) we can thus derive a form for $P_{i,j}$. Let us write quite generally the stress tensor $P_{i,j}$ as $P_{i,j} = \delta_{i,j} P - \pi_{i,j}$, where the diagonal part gives the pressure of the liquid, and $\pi_{i,j}$ is a traceless tensor that describes the shear effect on the liquid. From (6) we thus find that the tensor $\pi_{i,j}$ can be written as (in d dimensions, $d > 1$)

$$\pi_{i,j} = \eta \left(\nabla_i v_j + \nabla_j v_i - \frac{2}{d} \delta_{i,j} \nabla_k v_k \right) \quad (7)$$

where η is a real coefficient that is a functional of the density [7]. We point out that (7) is in fact a particular case of a general stress tensor with memory effects taken into account [10–12]. In our derivation this is the first non-trivial term of an expansion of the stress tensor in terms of

the density and velocity field. Consequently the Navier–Stokes stress tensor in (7) can be seen as the first-order (non-trivial) contribution to the exact stress tensor of the electron liquid (see also [3, 12, 11]).

Using this stress tensor we finally get from (3) the generalized Navier–Stokes equations for the electron liquid in nanoscale systems

$$\begin{aligned} D_t n(r, t) &= -n(r, t) \nabla \cdot v(r, t), \\ mn(r, t) D_t v_i(r, t) &= -\nabla_i P(r, t) + \nabla_j \pi_{i,j}(r, t) - n(r, t) \nabla_i V_{\text{ext}}(r, t). \end{aligned} \quad (8)$$

Equations (8) are formally equivalent to their classical counterpart [1] and thus also describe nonlinear solutions, i.e. the possibility of obtaining turbulence of the electron liquid in its normal state. In the examples that follow, we will consider only the case in which the liquid is incompressible so that the viscoelastic coefficients are spatially uniform: this approximation is practically satisfied in metallic QPCs but needs to be relaxed in the case of QPCs with organic/metallic interfaces (see e.g. [13]). In addition, for this case the Hartree potential is constant and its spatial derivative is thus zero. Therefore, equations (8) reduce to the Navier–Stokes equations for the density and velocity of a viscous but incompressible electron liquid

$$\begin{aligned} D_t n(r, t) &= 0, \\ \nabla \cdot v(r, t) &= 0, \\ mn(r, t) D_t v_i(r, t) &= -\nabla_i P(r, t) + \eta \nabla^2 v_i(r, t) - n(r, t) \nabla_i V_{\text{ext}}(r, t). \end{aligned} \quad (9)$$

3. Conductance quantization from hydrodynamics

Let us first show that we can derive from (9) the quantized conductance of an ideal ($\eta = 0$) quasi-1D liquid. We consider the electron liquid adiabatically connected to two reservoirs, and we call $v_{L(R)}$ and $\mu_{L(R)}$ the velocity and chemical potential, respectively, in the left (right) reservoir, with $\mu_L - \mu_R = eV_{\text{bias}}$. From (9) we then derive the Bernoulli equation that states the conservation of energy

$$\frac{v_L^2}{2} + h_L + \frac{\mu_L}{m} = \frac{v_R^2}{2} + h_R + \frac{\mu_R}{m} \quad (10)$$

where $h_{L(R)}$ is the enthalpy of the left (right) leads². Since we assume the fluid is incompressible $h_L = h_R$. By defining the flow velocity $v = (v_R + v_L)/2$ and the co-moving Fermi velocity³ $v_F = (v_L - v_R)/2$ we get from (10) the relation $2mvv_F = eV_{\text{bias}}$. By definition, the current is given by $I = env$ so that, by using the 1D density of states, $I = emvv_F/\pi\hbar = e^2V_{\text{bias}}/h$, which, in the linear regime, gives the quantized conductance (per spin) $G_0 = I/V_{\text{bias}} = e^2/h$. If we assume that only a fraction T of electrons is transmitted due to the presence of a barrier in the liquid, we can argue that, in linear response, the current is an equal fraction of the current in the absence of the barrier, i.e. $I = envT$. The conductance is thus $G = Te^2/h$ in accordance with the Landauer two-terminal result [14]. Corrections to this conductance in the presence of viscosity in 3D have been estimated in [13] and were found to depend non-linearly on the gradient of the electron density. Corrections to this conductance have been experimentally observed and justified with a hydrodynamical model where the conductance depends on the physical properties of the electron flow [15].

² To derive equation (10) one makes use of the relation $v\nabla \cdot v = \nabla v^2/2 - v \times (\nabla \times v)$ by projection of the equation of motion on the tangent to the current flow. The enthalpy is defined as $h = P/n$ [1]. In the 1D case $\nabla \times v = 0$ and $h(n) = (\pi\hbar n)^2/2m^2$.

³ v_F is the Fermi velocity in the reference frame moving with velocity $(v_R + v_L)/2$. Obviously the Bernoulli equation is invariant under any Galilean transformation.

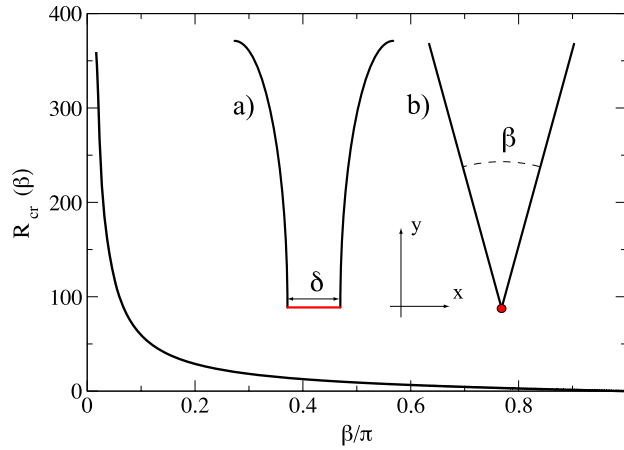


Figure 1. Critical Re number as a function of the angle β of the geometry represented in the inset (b). Inset (a) is a schematic of an adiabatic constriction.

(This figure is in colour only in the electronic version)

4. Turbulence

We know that the time-independent solutions of the Navier–Stokes equations (8) or (9) can describe many different regimes, with the non-linear (turbulent) regime generally favoured with respect to the laminar one. In fluid mechanics, in order to identify these regimes, it is customary to define a key quantity, the Reynolds number Re , as the only non-dimensional quantity that can be constructed out of the physical parameters of the system, like the density, the viscosity η , etc [1]. In the quantum case we follow a similar convention. For instance in 2D we define Re as $Re = Q/\eta = mI/e\eta$, where Q is the total mass current and I is the average total electrical current. For small Re the stable (and stationary) flow is usually laminar while for large Re the flow is turbulent [1]. In the latter case, one should then observe a local velocity field which varies in space in an irregular way, and whose pattern is very sensitive to the initial conditions.

4.1. Adiabatic QPCs

Let us apply these concepts to the transition between laminar and turbulent flow in QPCs. The microscopic geometry of these structures is quite complicated so that analytical solutions to (9) cannot generally be found. However, for an adiabatic 2D constriction, the self-consistent confining electron potential which enters (9) can be approximated with the simple form $y = k\sqrt{|x|} - \delta$ where $k > 0$ is a parameter that controls the rate at which the constriction opens up and $\delta > 0$ is the opening of the constriction (see inset (a) of figure 1). We assume electrons either originate from, or enter into, the region $\{y = 0, x = [0, \delta]\}$ of that potential to resurface on the opposite side of the structure. We know from classical hydrodynamics that, for any constriction, turbulent flow may exist only on the side where the constriction acts as a source of electrons [1]. We will therefore discuss only this side. We are interested here in the case of large k , i.e. the true adiabatic limit. Since we are dealing with a viscous liquid we assume a no-slip condition at the boundary, i.e. at the boundary the velocity component parallel to the boundary is zero. This condition can be relaxed by assuming that the velocity be finite at the boundary: the conclusions would be unchanged. We want to point out, however, that due

to the small viscosity of the electron liquid the effective boundary conditions on the electron liquid do not affect its bulk motion considerably.

The analytical stationary solution of (9) with these boundary conditions is not known. However, one can find an approximate solution by applying the transformation $x = p$, $y = \sqrt{kq}$ that maps $y = k\sqrt{|x| - \delta}$ into $q = \sqrt{k}(|p| - \delta)$, $q \geq 0$ and transforms (9) in a new set of equations where the parameter $1/k$ appears explicitly. We can then expand this equation in powers of $1/k$. The zeroth-order solution has the form $v_p(p, q) = 0$, $v_q(p, q) = \alpha q^{1/2}(p^2 - \delta^2)$ where $v_{p(q)}$ is the $p(q)$ component of the velocity in the $p - q$ plane and α is an arbitrary constant fixed by the requirement that a certain amount of charge is flowing through the system. If we transform back to the $x - y$ plane we see that the zeroth-order solution is given by $v_x(x, y) = 0$, $v_y(x, y) = \alpha(x^2 - \delta^2)$, i.e. we have obtained the classical Poiseuille flow [1]. It is well known that the Poiseuille flow is stable against small perturbation for almost all Re ; the Poiseuille flow is laminar up to $Re \simeq 2 \times 10^4$. This flow is linearly stable for any Re , but is unstable for non-linear perturbations at large Re : turbulent flow can be observed if, for example, one could force a large enough current⁴. Since for an adiabatic constriction $1/k \sim 0$ (i.e. at any given point the system is arbitrarily close to a pipe), we conclude that *in an adiabatic QPC the flow is laminar for almost any value of Re* . We note that compressibility of the liquid may instead provide a lower critical Re to observe turbulence.

4.2. Non-adiabatic QPCs

Let us now look at a case where the constriction is non-adiabatic. A simple non-adiabatic potential for which an analytical solution exists is $y = k|x|$ (see figure 1(b)). Microscopically, the point $x, y = 0$ could be, for example, a molecule sandwiched between two bulk electrodes with current flowing from one electrode to the other (see, e.g., [16]). We are interested here in the dynamics close to (but away from) this point. The present problem could also be solved by assuming a finite opening of the potential at the origin, i.e. a potential of the form $y = k(|x| - \delta)$ ($\delta > 0$). Our conclusions would be unaffected by this finite opening. In the case of the system in figure 1(b) we know there is a critical Re number, R_{cr} , determined by the angle $\tan(\beta/2) = 1/k$, above which the laminar flow is unstable. A simple calculation gives the implicit relation between the angle β and R_{cr} [1]

$$\beta(s) = \sqrt{1 - 2s^2}K(s^2) \quad (11)$$

$$\frac{R_{cr}(s)}{6} = -\frac{1 - s^2}{s^2}\beta(s) + \frac{\sqrt{1 - 2s^2}}{s^2}E(s^2) \quad (12)$$

where K and E are elliptic functions and $0 < s < 1$ is an arbitrary parameter. This critical Re is plotted in figure 1 as a function of the angle β and separates the phase space in two regions: laminar for $Re < R_{cr}$ and turbulent for $Re > R_{cr}$. Equation (12) has again been derived with the no-slip condition at the boundary. A finite velocity at the boundary (or even a larger velocity at the boundary than at the centre of the junction) would further reduce R_{cr} for any β , i.e. it would make the laminar solution even more unstable. We can thus conclude that turbulence can be observed in this case. Recently the current distribution for a two-dimensional electron gas (2DEG) QPC has been measured [17]. An irregular time-independent pattern has been observed and explained by the presence of impurities in the system. We suggest that turbulent effects could be observed in similar experiments on the 2DEG if non-adiabaticity is introduced, e.g. by

⁴ A stability analysis of the solution at large Re shows that the terms of high order appear to be important, and one cannot consider only linear perturbations (i.e. proportional to the field itself). Assuming non-linear perturbations, one can then show that the Poiseuille flow is unstable for an *arbitrary* (but small) perturbation. This is different from the usual linear perturbation case where the system is stable for *any* small linear perturbation.

asymmetric electrodes that would generate a potential of the type represented in figure 1(b). In this case we can predict the dimension λ_0 of the smallest observable eddies in the turbulent regime. A simple dimensional analysis gives [1] $\lambda_0 \sim l (R_{\text{cr}}/R)^{3/4} = l (I_{\text{cr}}/I)^{3/4}$, where I_{cr} is the critical current, i.e. the current which, from (12), gives R_{cr} , and l the linear size of the device. We easily see that λ_0 decreases rapidly with increasing β . The viscosity η can be evaluated through a perturbation theory on the 2D electron liquid [10]. For a 2DEG in a GaAs heterostructure ($m = 0.067m_e$) with a sheet density of $n \simeq 10^{15} \text{ m}^{-2}$ we have $\eta/\hbar n \simeq 0.05$ [10]⁵. For a typical current of $1 \mu\text{A}$, $Re = 145$. We then expect that a turbulent flow is developed for any angle larger than $\beta \sim \pi/10$. For instance, for $\beta = \pi/2$ ($R_{\text{cr}} \sim 10$ from figure 1), by assuming a length l of a typical device of about $1 \mu\text{m}$, we evaluate the typical dimension of the smallest eddies to be $\lambda_0 \simeq 250 \text{ nm}$. Our predictions should thus be readily verifiable experimentally.

We finally conclude by noting that the geometry of nanoscale structures, like for example a molecule between bulk electrodes, is actually closer to a conical structure for which the electron liquid is turbulent for relatively small Re [18]. The formation of eddies in proximity to an atomic or molecular junction is thus much more likely to occur than in the 2DEG case. Moreover, we expect that the finite compressibility of the electron liquid will favour the appearance of turbulent flow.

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⁵ Note that with these parameters the Fermi wavelength λ_F is about 80 nm. Assuming a lateral dimension $w = \lambda_F/2$ we get $\nu_c \simeq 10^{13} \text{ Hz}$, i.e. still orders of magnitude faster than other inelastic scattering rates in this system.