Electron transport through a nanostructure can be characterized in part using concepts from classical fluid dynamics. It is thus natural to ask how far the analogy can be taken, and whether the electron liquid can exhibit nonlinear dynamical effects such as turbulence. Here we present an ab-initio study of the electron dynamics in nanojunctions which reveals that the latter indeed exhibits behavior quite similar to that of a classical fluid. In particular, we find that a transition from laminar to turbulent flow occurs with increasing current, corresponding to increasing Reynolds numbers. These results reveal unexpected features of electron dynamics and shed new light on our understanding of transport properties of nanoscale systems.

Here, \( n \) is the electron density, \( \mathbf{u} = \mathbf{j}/n \) is the velocity field, i.e. the ratio between the current density \( \mathbf{j} \) and the density, and \( D_t = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \) is the convective derivative. \( P(\mathbf{r}, t) \) is the pressure of the liquid, \( V_{\text{ext}}(\mathbf{r}, t) \) an external potential, and \( \pi_{i,j} \) a traceless tensor that describes the shear effect on the liquid. It has the form

\[
\pi_{i,j} = \eta \left( \partial_i u_j + \partial_j u_i - \frac{2}{3} \delta_{i,j} \partial_k u_k \right),
\]

where \( \eta = \hbar n f(n) \) is the viscosity of the electron liquid and \( f(n) \) is a smooth function of the density. In analogy with the classical case we expect that the atomic structure, and in particular atomic defects in proximity to the junction, play the role of “obstacles” for the liquid and thus favor turbulence. Since we aim at showing that turbulence develops irrespective of the underlying atomic structure, we consider electrons interacting with a uniform positive background charge (i.e., the “jellium” model). The system we consider therefore consists of two large but finite jellium electrodes—subject to a bias—connected via a nanoscale jellium bridge. (The jellium edge of this system is represented with solid lines in each panel of Fig. 1.) We choose the density of the jellium at equilibrium typical of bulk gold \( (r_s \approx 3a_0) \). For computational convenience we choose a quasi-2D system, approximately 2.8 Å thick. Note that, everything else being equal, a quasi-2D geometry disfavors turbulence compared to a 3D one. We thus expect that if turbulence develops in our chosen quasi-2D geometry with given thickness, then turbulence will develop even more easily if we leave everything else unchanged (including the total current) and increase the thickness of the electrodes.

The solution of the TDSE for the many-body system is obtained within Time-Dependent Current Density Functional Theory(TDCDFT) i.e., for each single-particle state \( \phi_\alpha \), we have solved the equation of motion (in atomic units)

\[
\left\{ i \frac{\partial}{\partial t} - \frac{1}{2} \left( \frac{1}{t} \nabla - \frac{1}{c} \mathbf{a}_{\text{xc}} \right)^2 - v_{\text{jel}} - v_H - v_{\text{xc}} \right\} \phi_\alpha = 0
\]

for \( \alpha = 1,2,3,4,5,6 \).
where $c$ is the speed of light, $v_{\text{jel}}$ is the potential due to the jellium, $v_{\text{H}}$ is the Hartree potential, and $v_{\text{xc}}$ is the exchange-correlation scalar potential. The shear viscosity of the electron liquid enters the problem through the exchange-correlation vector potential $\alpha_{\text{xc}}$. If we make the approximation that, at any given time, the viscosity is a function of the density only, and does not depend on time explicitly, we find that the $i^{\text{th}}$ component of $\alpha_{\text{xc}}$ evolves according to:

$$\frac{1}{c} \frac{\partial \alpha_{\text{xc},i}}{\partial t} = \frac{1}{n} \sum_j \left\{ \frac{\partial^2 u_i}{\partial r_j^2} + \frac{\eta}{3} \frac{\partial^2 v_j}{\partial r_j^2} \right\} \frac{\partial \eta}{\partial r_j} + \frac{\partial \eta}{\partial r_j} \left( \frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} \right) - \frac{2}{3} \frac{\partial \eta}{\partial r_i} \frac{\partial u_j}{\partial r_j} \right\} \tag{4}$$

For the viscosity $\eta$ of the electron liquid we have used the one reported in Ref. [13]. We employ the approach described in Refs. [15, 16, 17, 18] to initiate electron dynamics and calculate the current. We prepare the system by placing it in its ground state; because of the applied bias, the system exhibits a separation of charge. At a time $t = 0$, we remove the bias, and let the system evolve according to eq. (4). After long time scales, the electrons encounter the far boundaries of the jellium electrodes and reflect. However, we are interested in comparing the electron dynamics calculated from eq. (4) with the one obtained by solving the Navier-Stokes equations, at times smaller than this reflection time. Equations (1) are solved by assuming the same density, initial velocity, and viscosity of the liquid employed in the TDCDFT calculation. We also solve eqs. (1) assuming the liquid to be incompressible. This simplifies the calculations enormously but leads to some minor differences with the solutions of eq. (3) (see discussion later).

Fig. 1 depicts the flow of electrons across the nanostucture, for a range of biases between 0.02V and 3.0V, after the initial transient. The panels (a)-(d) correspond to the solution of eq. (3); the panels (e)-(h) to the solution of the eqs. (1) using the same set of parameters. Panel (a) has to be compared with panel (e); panel (b) with (f), and so on. As anticipated, we observe some differences between the solutions of the eqs. (1) and the solutions of the eq. (3). These differences are due to the details of the charge configuration at the electrode-junction interface, and some degree of compressibility of the quantum liquid in the junction.

From Fig. 1 we can see the effect of surface charges, in that some electrons flow parallel to the surfaces. More importantly, at low biases, the flow is laminar and “smooth”. In addition, at these biases the current density shows an almost perfect top-bottom symmetry: the direction of the flow is symmetric with respect to the operation $z \rightarrow -z$. This symmetry is even more evident by comparing the curl of the current density in the top and bottom electrodes (see for instance Fig. 1a) and (e)).

By increasing the bias, however, a transition occurs: the symmetry $z \rightarrow -z$ of the current density breaks completely, and eddies start to appear in proximity to the junction. This is clearly evident, for instance, in Fig. 1d and (h). The outgoing current density in the bottom electrode has a more varied angular behavior, in contrast to the behavior in the top electrode, in which the electron liquid flows more uniformly toward the junction.

Since the panels (e)-(h) of Fig. 1 practically describe the dynamics of a classical fluid with the same parameters as the quantum liquid, the analogy between the electron flow and the one of a classical liquid is quite evident. We can push this analogy even further by defining a Reynolds number for the quantum system as well: $R = u_z L / \eta$, where $u_z$ is the longitudinal velocity in the junction, $L$ is the width of the junction, and $\rho$ is the density. Using the density of valence electrons in gold, and using the current density in the junction at $t = 1.4$ fs, we obtain the following Reynolds numbers: 0.216, 2.16, 10.8 and 32.5 for 0.02 V, 0.2 V, 1.0 V, and 3.0 V, respectively.

Just like in the classical case, we can then reinterpret the above results as follows. At low Reynolds numbers, the flow is highly symmetric from top to bottom. This symmetry is lost as the Reynolds number is increased. At high Reynolds numbers, the incident flow is laminar, while the outgoing flow has a jet-like character, and “turns back” on itself creating local eddies in the current density.

Having shown the similarity between the current flow obtained using the Navier-Stokes equations and the one obtained solving eq. (3) we can study the first one at times scales prohibitive for full quantum mechanical simulations. We can also study the effect of a larger thickness of the electrodes on the turbulent flow by realizing that this is equivalent to increasing the Reynolds number (which, incidentally, is also equivalent to increasing the bias). This is illustrated in Fig. 2 where the current density and the curl of the current density are plotted for the Reynolds number 32.5 of Fig. 1h (left panel of Fig. 2); same system but with a Reynolds number five times larger (middle panel of Fig. 2); and (right panel of Fig. 2) with a Reynolds number ten times larger.

From Fig. 2 it is evident that by increasing thickness the last remaining symmetry $x \rightarrow -x$ is broken at earlier times, leading to turbulent behavior closer to the junction. For instance, in the case represented in Fig. 2 (middle panel), the left-right symmetry is lost at about 14 fs, with consequent asymmetric flow within about 50 Å from the junction center. For the structure represented in Fig. 2 (right panel), the symmetry is broken at about 6 fs, and the flow asymmetry appears at about 25 Å from the junction.

We can better quantify the amount of turbulence by calculating the velocity correlation tensor:

$$B_{i,k} = \langle v_i(r) - v_i(r + \delta \mathbf{r}) \rangle \langle v_k(r) - v_k(r + \delta \mathbf{r}) \rangle \tag{5}$$

where $\delta \mathbf{r}$ is a given distance, and $i, k = x, y, z$. Here, the angle brackets denote averaging over all positions $\mathbf{r}$ within a given region. Fully developed and isotropic turbulence has a velocity correlation tensor that is a function
0.02 Volts 0.2 Volts 1.0 Volts 3.0 Volts

FIG. 1: (Color online) Panels (a)-(d): Electron current density for electrons moving from the top electrode to the bottom electrode across a nanojunction at $t = 1.4$ fs, for an initial bias of (a) 0.02 V, (b) 0.2 V, (c) 1.0 V and (d) 3.0 V. The arrows denote the current density, while the level sets denote the curl of the 2D current density. The solid lines delimit the contour of the junction. Panels (e)-(h): Velocity field solution of the equations (1), for a liquid with same velocity, density and viscosity as the quantum mechanical one.

FIG. 2: (Color online) Current density (arrows) and curl of the current density (denoted by level sets) of the electron liquid, for three different Reynolds numbers, 32.5 (left panel), 162 (middle panel), and 325 (right panel). Note that the fluid velocity has lost perfect left-right symmetry in the middle- and right-panel cases.

only of the magnitude of $\delta r$, and increases quadratically with distance. Instead, the turbulence in the examples of Fig. 2 is not fully developed. The velocity correlation tensor, $B_{ik}$, thus depends on both the magnitude of $\delta r$ as well as its direction. This is illustrated in Fig. 3 where various components of $B_{ik}$ are plotted at $t = 75.0$ fs for the system with Reynolds number 32.5 as a function of the magnitude of $\delta r$, where we have chosen $\delta r$ to point in the longitudinal ($z$) direction. The spatial averaging has been carried out over the left-hand side of the outgoing region (that is, in the region $z = [-27.3 \, \text{Å}, -72.1 \, \text{Å}], x = [-25.9 \, \text{Å}, 0.0 \, \text{Å}]$, where the origin is in the center of the junction). For comparison, the same quantity is plotted for the laminar case, i.e. for a Reynolds number of 0.216. (To compare the laminar and turbulent cases we have scaled the average turbulent velocity to the average laminar velocity.) As expected, in the laminar case the correlation tensor is essentially zero, while for the turbulent case it increases with distance.

We conclude by noting that an experiment in which the electron flow can be monitored directly may measure nonlaminar electron behavior as an asymmetry between the incoming and outgoing patterns of the current density through a nanojunction. Experiments similar to the ones reported in Ref. 20, which use scanning probe microscopy to image the flowlines, may provide such capabilities. Note, however, that since these scanning probe
FIG. 3: (Color online) Various components of the velocity correlation tensor $B_{ik}$ as a function of distance $d = |\sigma r|$, for a Reynolds number of $R = 32.5$. For the case where $R = 0.216$, the elements of $B_{ik}$ are orders of magnitude smaller, and so the corresponding curves for the laminar case coincide with the $x$ axis.

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29. Each electrode is 51.8 Å wide in the $x$ direction, and 22.4 Å long in the $z$ direction of current flow (see Fig. 3). The width of the rectangular bridge is 2.8 Å, and the gap between the electrodes is 9.8 Å.
30. We have used the adiabatic local density approximation to the scalar exchange-correlation potential $\epsilon_{xc}$ as derived by Ceperley and Alder and parametrized by Perdew and Zunger.
31. The grid spacing of the jellium system is 0.7 Å, and the timestep used to propagate the system $2.5 \times 10^{-3}$ fs. We used the Chebyshev method for constructing the time-evolution operator.
Dirchlet boundary conditions for the velocity at the inlet, and Neumann boundary conditions at the outlet.