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**Operational Estimation Method for Bare Viscosity in Fluctuating Hydrodynamics** (Role of Ultraviolet Cutoff)



# Theme of this talk : Background

### Microscopic system



microscopic particles obeying classical mechanics

### Hydrodynamic description



The motion of the system can be described by hydrodynamic theory at a macroscopic scale



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# Theme of this talk : Fluctuating hydrodynamics

- Hydrodynamics describes slow motion of conserved variables.
- We consider a situation where mass and momentum are conserved quantities.

Mass conservation

**Momentum Conservation** 

The specific properties of fluids are given by a constitutive equation.

 $\mathbf{\Pi}^{ab}(\mathbf{r},t) := p\delta_{ab} + \rho v^a v^b - \mathbf{I}_{ab} + \rho v^b - \mathbf{I}_{ab} + \mathbf{I}_$ **Fluctuating** constitutive eq. pressure advection

 $\left\langle \Pi_{R}^{ab}(\boldsymbol{r}_{1},t_{1})\Pi_{R}^{cd}(\boldsymbol{r}_{2},t_{2})\right\rangle = 2k_{B}T\delta^{2}(\boldsymbol{r}_{1}-\boldsymbol{r}_{2})\delta(t_{1}-t_{2})\left[\eta_{0}\left(\delta_{ac}\delta_{bd}+\delta_{ad}\delta_{cb}\right)+\left(\zeta_{0}-\eta_{0}\right)\delta_{ab}\delta_{cd}\right]$ 

Fluctuating hydrodynamics includes a noise term arising from thermal motion of atoms.



$$\eta_0 \left( \nabla_a v^b + \nabla_b v^a - \frac{2}{d} \delta_{ab} \nabla^c v^c \right) - \zeta_0 \delta_{ab} \nabla^c v^c + \Pi_R^a$$

viscous dissipation

b noise





## Theme of this talk : Goal

### Bare viscosity It is a parameter included in the constitutive eq. of fluctuating hydrodynamics.

Fluctuating  $\mathbf{\Pi}^{ab}(\mathbf{r},t) := p\delta_{ab} + \rho v^a v^b$ constitutive eq.

**Transport coefficient** 

 $\eta_0$ : shear

Here, bare viscosity is defined for a given UV cutoff length. (I will explain this point in detail later)

### The goal of this talk

- Demonstrating that bare viscosity  $\eta_0$  is observable.
- Specifying the value of bare viscosity  $\eta_0$  from atomic systems.

$$-\eta_0 \left( \nabla_a v^b + \nabla_b v^a - \frac{2}{d} \delta_{ab} \nabla^c v^c \right) - \zeta_0 \delta_{ab} \nabla^c v^c + \mathbf{\Pi}$$
  
viscosity,  $\zeta_0$ : bulk viscosity,





### Contents in this talk

### 1. Introduction

1.1 Why is observing bare viscosity difficult? 1.2 Why do we aim to observe bare viscosity?

### 2. Main results

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- 2.2 How robust is this result for more realistic walls
- 2.3 The determination of bare viscosity
- 2.4 Effects of varying UV cutoff length
- 2.5 Simple estimation method for bare viscosity
- 3. Summary (some remarks)





## 1.1 Why is observing bare viscosity difficult?



- We consider a practical method for measuring the shear viscosity.
- 1. We create the Couette geometry by moving two parallel walls in opposite directions. In the steady state, the simplest flow pattern, known as shear flow is realized.





Velocity field  $v^{x}(y)$ 





- We consider a practical method for measuring the shear viscosity.
- 2. We measure the noise-averaged velocity field and momentum flux in the steady state.



- Noise (or Time)-averaged  $\langle v^a(\mathbf{r}) \rangle_{\rm SS}^{\dot{\gamma}}$  velocity field
- Noise (or Time)-averaged  $\langle \Pi^{ab}(\mathbf{r}) \rangle_{\rm SS}^{\dot{\gamma}}$  momentum flux





We consider a practical method for measuring the shear viscosity.

### XY component of Fluctuating momentum flux

When velocity field is fluctuating,

 $v^{x}(t) = \dot{\gamma}y +$ the fluctuating shear flow  $v^{y}(t) = 0 +$ is given as  $\langle \delta v^{x} \rangle_{\rm ss}^{\dot{\gamma}} = \langle \delta v^{y} \rangle_{\rm ss}^{\dot{\gamma}} = \langle \Pi_{R}^{xy} (\mathbf{r}) \rangle_{\rm ss}^{\dot{\gamma}}$ 

> The noise-averaged momentum flux under shear flow is calculated as

- 3. We calculate the viscosity through the relationship between the velocity and momentum flux.

$$\mathbf{I}^{xy}(\mathbf{r},t) := \rho v^{x} v^{y} - \eta_{0} \left( \nabla_{x} v^{y} + \nabla_{y} v^{x} \right) + \mathbf{\Pi}_{R}^{xy}$$
advection shear viscosity noise
$$\delta v^{x}(t)$$

$$\delta v^{y}(t)$$

$$(t)$$

$$\langle \Pi^{xy}(\mathbf{r},t) \rangle_{\rm ss}^{\dot{\gamma}} := \langle \rho \delta v^x \delta v^y \rangle_{\rm ss}^{\dot{\gamma}} - \eta_0 \dot{\gamma}$$

advection





- We consider a practical method for measuring the shear viscosity.
- 3. We calculate the viscosity through the relationship between the velocity and momentum flux.



- The nonlinear coupling of fluctuations is NOT zero, because  $\delta v^{x}(t)$  and  $\delta v^{y}(t)$  can interact due to advection with shear flow  $\dot{\gamma}$ .
- When we try to observe the viscosity from the ratio of momentum flux to velocity gradient, the resulting viscosity always includes the correction arising from the fluctuations.

### Observing bare viscosity is difficult !!





### 1.2 How different are $\eta$ and $\eta_0$ ? Why do we aim to observe bare viscosity?

### Introduction



# How different are $\eta_0$ and $\eta$



$$\eta = \eta_0 + C_{2d} \log\left(\frac{L}{a_{uv}}\right) \quad \text{in two}$$

$$\eta = \eta_0 + C_{3d} \left(\frac{1}{L} - \frac{1}{a_{uv}}\right) \quad \text{in thr}$$

Observed viscosity  $\eta$  depends on the system size L and the ultraviolet (UV) cutoff length  $a_{\mu\nu}$ 

In the 1970s, the difference between  $\eta_0$  and  $\eta$  was calculated based on the fluctuating hydrodynamics.

$$7 \cdot \mathbf{v} = 0$$

$$(\boldsymbol{v}\cdot\nabla)\boldsymbol{v} = -\nabla p + \eta_0 \nabla^2 \boldsymbol{v} + \nabla \boldsymbol{\Pi}_{\boldsymbol{R}}$$

$$\mathbf{r}_1 - \mathbf{r}_2 \delta(t_1 - t_2) \left[ \left( \delta_{ac} \delta_{bd} + \delta_{ad} \delta_{cb} \right) - \delta_{ab} \delta_{cd} \right]$$

o dimensions

Anomalous transport in low-dimensional fluids

ree dimensions

UV cutoff dependence of fluctuating hydrodynamics



When solving continuum theory numerically or analytically, it is necessary to introduce a spatial discretization width, known as the ultraviolet (UV) cutoff length.

Simple understanding dv of UV cutoff length  $\partial x$ 

$$\eta = \eta_0 + C_{2d} \log\left(\frac{L}{a_{\rm uv}}\right) \qquad \text{in two}$$

$$\eta = \eta_0 + C_{3d} \left( \frac{1}{L} - \frac{1}{a_{\text{uv}}} \right) \quad \text{in thre}$$

depend on the UV cutoff length above two dimensions (when the UV cutoff length changes while all parameters are fixed to the same values)

## UV cutoff dependence

$$\simeq \frac{\mathbf{v}_{(i_x+1,i_y)} - \mathbf{v}_{(i_x,i_y)}}{a_{\mathrm{uv}}}$$

o dimensions



 $a_{\rm uv}$ 

### ee dimensions

### **Spatial resolution**

- Physical quantities calculated within the framework of fluctuating hydrodynamics generally









# Why do we aim to observe bare viscosity?

### Anomalous transport in low-dimensional systems



### UV cutoff dependence of fluctuating hydrodynamics





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## Anomalous transport in 2D

In low-dimensional systems, it is well known the system size.



In low-dimensional systems, it is well known that transport coefficients can diverge with

$$\eta = -\frac{\langle \rho \delta v^x \delta v^y \rangle_{ss}^{\dot{\gamma}}}{\dot{\gamma}} + \eta_0$$
$$\to \infty \ (L \to \infty)$$

The divergence of shear viscosity can be understood from the divergence of the nonlinear coupling of fluctuations.



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# Long-time tail problem

### Formula in nonequilibrium steady state

in shear viscosity in 2D.

$$\eta = \frac{1}{k_B T L^2} \int_{a_{\rm uv}/v_0}^{L/v_0} dt \left\langle \sigma^{xy}(t) \sigma^{xy}(0) \right\rangle_{\rm eq} \sim \int_{a_{\rm uv}/v_0}^{L/v_0} dt \frac{1}{t} \sim \log \frac{L}{a_{\rm uv}}$$

**Green-Kubo formula and Long-time tail** 

The existence of long-time tails in the correlation functions leads to a divergence



## Anomalous transport in 2D

the system size.



In low-dimensional systems, it is well known that transport coefficients can diverge with

$$\eta = -\frac{\langle \rho \delta v^x \delta v^y \rangle_{ss}^{\dot{\gamma}}}{\dot{\gamma}} + \eta_0$$
$$\to \infty \ (L \to \infty)$$

The nonlinear coupling of fluctuations includes the long-time tail effect, which leads to the system size dependence.

We address this problem!!

Removing the long-time tail effects completely.



By changing only the UV cutoff length  $a_{\mu\nu}$  while keeping all other parameters fixed, the predictions of fluctuating hydrodynamics change above two dimensions.

In fluctuating hydrodynamics, observed viscosity (or momentum flux) diverges as  $a_{uv} \rightarrow +0$ 



## UV cutoff dependence

$$\eta = -\frac{\langle \rho \delta v^x \delta v^y \rangle_{ss}^{\dot{\gamma}}}{\dot{\gamma}} + \eta_0$$
$$\to \infty \ (a_{uv} \to +0)$$

The UV cutoff length  $a_{\mu\nu}$  is also the parameter to determine the prediction of fluctuating hydrodynamics uniquely.





In atomic systems, the concept of UV cutoff length does not exist !! (because the classical Hamiltonian dynamics is not continuum theory.)



We also address this problem!!

**Observing bare viscosity** 



## UV cutoff dependence

$$\eta = -\frac{\langle \rho \delta v^x \delta v^y \rangle_{ss}^{\dot{\gamma}}}{\dot{\gamma}} + \eta_0$$
$$\rightarrow \infty \ (a_{uv} \rightarrow + 0)$$

The UV cutoff length  $a_{\mu\nu}$  is also the parameter to determine the prediction of fluctuating hydrodynamics uniquely.

We also address this problem!!

**Determining the value of UV cutoff length** 



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### Summary of Introduction



Including the effects of long-time tail

Observing bare viscosity is the challenging problem.



- Removing the long-time tail effects completely.
- **Determining the value of UV cutoff length**
- To address these issues, we focus on **two-dimensional dense fluids**.





## 2.1 Main idea of our study

### Main results



# Preliminary simulation

### We consider solving fluctuating hydrodynamics numerically

$$\begin{array}{l} \begin{array}{l} \displaystyle \frac{\partial\rho}{\partial t} = -\nabla\cdot(\rho\mathbf{v}) & p(\rho) = C_{\mathrm{press}}\rho & c_T := \sqrt{\left(\frac{\partial p}{\partial\rho}\right)_T} = \sqrt{C_{\mathrm{press}}} \\ \rho \left[\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v}\right] = -\nabla p + \eta_0 \nabla^2 \mathbf{v} + \zeta_0 \nabla(\nabla\cdot\mathbf{v}) + \nabla \mathbf{\Pi}_R \end{array} \end{array}$$

The sufficiently large  $C_{\text{press}}$  yields nearly incompressible fluids

We apply a common boundary condition in fluid dynamics

- The velocity field at the wall is  $(v^x, v^y) = (v_0, 0)$ 1.
- The momentum density field at the wall is  $(j^x, j^y) = (\rho v_0, 0)$ 2.

### The fluid does not fluctuate at all at the solid walls











The motivation for this simulation comes from the expectation that bare viscosity can be observed near non-fluctuating walls.

Main idea of our study : focusing on fluids near solid walls.



# Main idea of our study









Bare viscosity  $\eta_0$  is observed near solid walls. As we move away from the solid wall, it deviates from bare viscosity  $\eta_0$ 





### The idea of examining the behaviors near walls seems good!

### 2.2 Is this result robust for more realistic walls

### Main results



## Molecular dynamics (MD) simulation We perform molecular dynamics (MD) simulations. In MD simulations, molecules are represented as particles Units for the MD simulation atomic diameter $\sigma$ atomic mass $\mathcal{M}$ for $\delta < 0$ thermal velocity $v_{th} := \sqrt{k_B T/m}$ (or microscopic time $\tau = \sigma/v_{th}$ )

that follow the classical Hamiltonian dynamics.

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m} \qquad \frac{d\mathbf{p}_i}{dt} = -\frac{\partial V}{\partial \mathbf{r}_i}$$

 $\triangleright$  simple repulsive potential

 $V(r) = 10\delta^{\alpha} \quad \text{for } \delta > 0$ V(r) = 0





# Implementation of solid walls

Solid walls are implemented as a collection of particles.

1. Solid particles are trapped using an on-site potential.

$$V_{\text{onsite}}(\boldsymbol{q}) = V_0 \left[ \sin(2\pi q_x) + \sin(2\pi q_y) \right]$$

2. Solid particles are thermalized using the Langevin thermostat.

$$\frac{d\boldsymbol{q}_{j}}{dt} = \frac{\boldsymbol{p}^{w}}{m}$$
$$\frac{d\boldsymbol{p}_{j}^{w}}{dt} = -\frac{\partial V_{\text{onsite}}(\boldsymbol{q}_{j} - v_{0}t\boldsymbol{e}_{x})}{\partial \boldsymbol{q}_{j}} - \sum_{i=1}^{N} \frac{\partial V_{\text{wf}}(|\boldsymbol{r}_{i} - \boldsymbol{q}_{j}|)}{\partial \boldsymbol{q}_{j}} -$$

3. Fluid particles interact with solid particles.

4. The motion of the walls is simulated by moving the solid particles collectively at a velocity  $v_0$ .

 $V_0 = 50$ 

 $-\gamma \boldsymbol{p}_{j}^{w}+\xi_{j}(t)$ 









The local viscosity is observed in the same way as in the fluctuating hydrodynamics. fluctuating hydrodynamics.

The observed viscosity decreases near solid walls, which is consistent with the behavior in





This suggests the robustness of the results of the fluctuating hydrodynamics simulations.

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## 2.3 The determination of bare viscosity

### Main results



## Quantitative comparison



We determine the bare viscosity of the atomic system by quantitatively comparing the results of two models.

Set the same system size, density, and temperature to match the units of both models.



Use bare viscosity  $\eta_0$  and UV cutoff  $a_{uv}$ as fitting parameters.







# Quantitative agreement

We fix the UV cutoff length to  $a_{uv} = 1.0$  (i.e atomic diameter) and use only bare viscosity  $\eta_0$  as a adjustable parameter.



The fluctuating hydrodynamics with  $\eta_0 = 0.325, a_{uv} = 1.0$  reproduces the local viscosity  $\eta(x)$  of the MD simulation with high accuracy.

The agreement between the two models is observed even at the atomic diameter scale.





# Consistency check : long-time tail in EQ

▶ To validate our estimate of bare viscosity, we compare the time correlation of the momentum density field in equilibrium.

$$C_{JJ}(t) := \frac{1}{2} \langle \boldsymbol{j}(\boldsymbol{r}, t) \cdot \boldsymbol{j}(\boldsymbol{r}, 0) \rangle_{\text{eq}} \qquad \boldsymbol{j} :=$$

The fluctuating hydrodynamics with  $\eta_0 = 0.325$ reproduces the long-time tail  $C_{JJ}(t)$  of the MD simulation with high accuracy.

The agreement between the two models is observed even at the atomic time scale.









Our results suggest that fluid description is possible even at the atomic scale in such dense systems.



# Consistency check : Poiseuille flow

### As another consistency test, we perform the simulation of the Poiseuille flow.



The Poiseuille flow is realized by adding a constant force to entire fluids and imposing periodic boundary condition in the flow direction.



Even for this setup, the predictions of fluctuating hydrodynamics and MD simulations are in good agreement.





# Consistency check : Poiseuille flow



The deterministic hydrodynamics with the viscosity observed in bulk region ( $\eta = 0.464$ ) cannot reproduce the results of MD simulations. Fluctuating hydrodynamics with bare viscosity is necessary to describe fluids near walls (at least in low-dimensional systems).









## 2.4 Effects of varying UV cutoff length

### Main results



# Best value of UV cutoff length

### We investigated the best-fit bare viscosity for different UV cutoff lengths.



 $\eta_0 = 0.455$  for  $a_{uv} = 2/3$ 

**Colored: FHD** Black: MD (all the same data) (with different  $(\eta_0, a_{\mu\nu})$ ) well reproduced for any  $a_{\mu\nu}$ .

By carefully choosing  $\eta_0$ , the MD results can be











The best value of UV cutoff length is about atomic diameter!!

# Physical value of bare viscosity

We define the "bare viscosity" that reproduces the behavior in the atomic system as the physical bare viscosity  $\eta_0^P$ .



In practice, the physical bare viscosity  $\eta_0^P$  is determined to satisfy

$$\eta_{\rm MD}(x) = \eta_{\rm FH}(x:\eta_0^P,a_{\rm uv})$$

The physical bare viscosity  $\eta_0^P$  depends on the UV cutoff length.

If  $(\eta_0, a_{\mu\nu})$  lie on this relationship, any pair will reproduce the macroscopic phenomena well.





# Renormalization group

Changing the UV cutoff length is related to coarse-graining using the renormalization group.



Any parameters along the renormalization group flow can accurately reproduce the







## 2.5 Simple estimation method for bare viscosity

### Main results



# Analytical expression of local viscosity

We can calculate the theoretical expression for the noise-averaged Couette flow.



This calculation can be done using a perturbative expansion in  $\epsilon$ . (We adopted some approximations but the details are omitted here.)

$$= -\nabla p + \eta_0 \nabla^2 v + \nabla \Pi_R$$
  

$$- t_2) \Big[ (\delta_{ac} \delta_{bd} + \delta_{ad} \delta_{cb}) - \delta_{ab} \delta_{cd} \Big]$$
  

$$v^y \Big|_{y=0} = -v_0$$
  

$$v^y \Big|_{y=L} = v_0$$





# Analytical expression of local viscosity

We obtained the theoretical expression for the noise-averaged Couette flow.

$$\langle v^{y}(x) \rangle = \dot{\gamma}x - \epsilon^{2} \frac{\dot{\gamma}A}{L} \sum_{k_{x}} \frac{1}{k_{x}} \left( x - \frac{\sin(2k_{x}x)}{2k_{x}} \right) \quad k_{x} := \frac{\pi}{L}n$$

 $\dot{\gamma}$ : velocity gradient at x = 0, L

A : numerical factor depending on density, temperature...

$$\eta(x) = \eta_0 \left( 1 + \epsilon^2 \frac{A}{L} \sum_{k_x} \frac{1}{k_x} \sin^2(k_x x) \right)$$

$$\mathbf{f}$$
The information of a via incompation of a



The information of  $a_{uv}$  is included within the range of the sum.







# Validity of Analytical expression

We confirmed that this analytical expression accurately reproduces the simulation results.

$$\eta(x) = \eta_0 \left( 1 + \frac{A}{L} \sum_{k_x} \frac{1}{k_x} \sin^2(k_x x) \right)$$

We fixed  $a_{\mu\nu} = 1.0$  and compared the numerical solution (full order) of the fluctuating hydrodynamics 0.2to this analytical expression for the local viscosity.





# Simple estimation method for local viscosity

We proceed to fit the MD results to estimate the bare viscosity.







fitting the MD results using the analytical expression

We can easily estimate the bare viscosity using this analytical expression.





### Main Message

Bare viscosity is directly observed near solid walls. We believe that this result is robust even for real solid walls.

### Discussion

Fluctuating hydrodynamics and the renormalization group are strongly connected. best choice for the UV cutoff length from a microscopic perspective? (for example, mean free path?)

What happens when the mean free path is large? While this study focused on dense liquids, how might the breakdown of fluctuating hydrodynamics appear in dilute gases?

## Summary

Can we understand this connection from a microscopic perspective and is there a concept of the



