## Microscopic Dynamics

Number of particles in the system

 $D_c$  Cartesian dimension of the system – usually 3

 $D_{KY}$  Kaplan-Yorke dimension

D accessible phase space domain

 $\mathbf{q}$  ND<sub>C</sub> dimensional vector, representing the particle positions

 $\mathbf{p}$   $ND_C$  dimensional vector, representing the particle momenta

 $\Gamma$  2ND<sub>C</sub> dimensional phase space vector, representing all  $\mathbf{q}$ 's and

p's

 $\delta V_{\Gamma}(S'\Gamma)$  very small volume element of phase space centred on

 $S^{t}\Gamma \equiv \exp[iL(\Gamma)t]\Gamma$ 

 $p(\delta V_{\Gamma}(\Gamma);t)$  probability of observing sets of trajectories inside  $\delta V_{\Gamma}(\Gamma)$  at

time t

 $p_{+/-}(t)$  probability that the dissipation function is plus/minus over the

time interval (0,t)

 $M^T$  time reversal map

 $M^{K}\Gamma = M^{K}(x,y,z,p_{x},p_{y},p_{z})$  $= (x,-y,z,-p_{x},p_{y},-p_{z})$ 

Kawaski or K-map of phase space vector for

planar Couette flow,

where, 
$$\dot{\mathbf{\gamma}} = \frac{\partial \mathbf{u}}{\partial \mathbf{r}} = \begin{pmatrix} 0 & \partial u_x / \partial y & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

*L f*-Liouvillian

 $\exp[-iL(\Gamma)t]...$  *f*-propagator

L p-Liouvillean

 $\exp[iL(\Gamma)t]$  p-propagator

 $S^t$ ... p-propagator

 $K(\mathbf{p})$  peculiar kinetic energy

 $\Phi(\mathbf{q})$  interparticle potential energy

 $\phi_{i,j}(r_{ij})$  pair potential of atom i with atom j

 $\mathbf{r}_{ij} \equiv \mathbf{r}_j - \mathbf{r}_i$  position vector from atom *i* to atom *j* 

 $r_{ij} \equiv |\mathbf{r}_j - \mathbf{r}_i|$  distance between atoms i & j

 $\mathbf{F}_{ii}$  force on particle *i* due to particle *j* 

 $\nabla_{\mathbf{q}} \equiv (\partial/\partial \mathbf{q}_1, \dots, \partial/\partial \mathbf{q}_N)$ 

 $H_0(\Gamma)$  internal energy,  $H_0 = K + \Phi$ , where K is the peculiar kinetic

energy

 $H(\Gamma)$  Hamiltonian at phase vector  $\Gamma$ 

 $g(\Gamma)$  deviation function – even in the momenta

 $H_E$  extended Hamiltonian for Nosé-Hoover dynamics

 $K_{th}$  peculiar kinetic energy of thermostat

 $N_{th}$  number of thermostatted particles

 $\alpha$  Gaussian thermostat multiplier

 $\zeta$  Nosé-Hoover thermostat multiplier

 $\tau$  time constant

 $\tau_{\scriptscriptstyle M}$  Maxwell time

 $\dot{Q}$  rate of increase in heat in thermostat

 $\Lambda$  phase space expansion factor

 $S_i$  switch function

 $J(\Gamma)$  dissipative flux

 $\mathbf{F}_{e}$  external field

*m* particle mass

 $T \equiv \partial \dot{\Gamma}(\Gamma)/\partial \Gamma$  stability matrix

 $\exp_L$  latest times to left, time ordered exponential operator

tangent vector propagator

 $\lambda_i$   $i^{th}$  Lyapunov exponent

 $\lambda_{\text{max/min}}$  largest/smallest Lyapunov exponent for steady or equilibrium

state

### Statistical mechanics

 $\bar{A}_t$  time average of some phase variable, A

 $\langle A(t) \rangle$  ensemble average of A over time evolved paths

 $f(\Gamma;t)$  time dependent phases space distribution function

 $\langle . \rangle_{\mu c}$  equilibrium microcanonical ensemble average

 $\langle . \rangle_c$  equilibrium canonical enamble average

 $f_c(\Gamma)$  equilibrium canonical distribution

 $f_{\mu c}(\mathbf{\Gamma})$  equilibrium microcanical distribution

 $\Lambda$  phase space expansion factor

 $\Omega(S^t\Gamma)$  the instantaneous dissipation function, at time t on a phase space

trajectory that started at phase  $\,\Gamma\,$ 

r 3 dimensional position vector

 $\mathbf{u}(\mathbf{r},t)$  3 dimensional local fluid streaming velocity

$$S_G$$
 fine-grained Gibbs entropy - =  $k_B \int_D d\Gamma f(\Gamma) \ln(f(\Gamma)) = k_B \ln(Z_{\mu c})$ 

z partition function – normalization for the equilibrium phase space
distribution

 $Z_c$  canonical partition function

#### Mechanical variables

Q heat

V system volume

U internal energy,  $U = \langle H_0 \rangle$ 

W work performed on system of interest

Y purely dissipative generalized dimensionless work

X generalized dimensionless work

# Thermodynamic variables

T temperature

 $\beta$  Boltzmann factor (reciprocal temperature)

S entropy

A Helmholtz free energy,  $= -k_B T \ln(Z_c)$ 

 $\langle \Sigma(t) \rangle$  entropy production

 $G_0$  zero frequency elastic shear modulus

 $G_{\infty}$  infinite frequency shear modulus

Transport

 $\gamma$  strain (note:  $\gamma$  is sometimes used to fix the systems total momentum)

 $\delta \gamma$  small strain

 $\dot{\gamma}$  strain rate

 $P_{xy}$  xy-element of the pressure tensor

 $-\langle P_{xy} \rangle$  xy-element of the ensemble averaged stress tensor

 $\eta_{0^+}$  limiting zero frequency shear viscosity of a solid

 $\eta$  shear viscosity of a fluid

 $\tau_{\scriptscriptstyle M}$  Maxwell relaxation time

 $J(\Gamma)$  Dissipative flux

 $J_{\perp}(k_{y},t)$  wavector dependent transverse momentum density

 $\eta_{M}(t)$  Maxwell model memory function for shear viscosity

 $\eta_M$  zero frequency Maxwell shear viscosity

#### **Mathematics**

Θ Heaviside step function

 $\lambda$  arbitrary parameter

 $\tilde{F}(s)$  Laplace transform of F(t)

 $\hat{F}(s)$  anti-Laplace transform of F(t)

 $\oint_P$  cyclic integral of a periodic function

 $_{qs}\int_{a}^{b}$  quasi static integral from a to b

Note: Upper case sub/supers for people. Lower case for most else. Subscripts preferred to supers so as to not confuse powers with superscripts. Italics for algebraic initials. Nonitalics for word initials. (e.g. T-mixing not T-mixing because T stands for Transient, N-particle not N-particle.)