Statistical Physics and Computer Simulations
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Exercise Sheet 6

1. **Statistical Errors**
   Consider a Monte Carlo or Molecular Dynamics simulation that is strictly in equilibrium, and produces a time series of observable values $A(t)$, $t = 1, 2, \ldots, T$. The observations have been made at equidistant times. Demonstrate that the time–displaced autocorrelation function of the fluctuations of A is the central quantity that governs the statistical accuracy (i.e. the error bar) of the estimator

$$\bar{A} = T^{-1} \sum_{t=1}^{T} A(t), \tag{1}$$

   and show that the effective number of statistically independent observations is given by

$$T_{eff} = \frac{T}{1 + 2\tau}, \tag{2}$$

   where τ is a suitably (how??) defined correlation time.
   Hints: Consider the expectation value

$$\left\langle \left(\bar{A} - \langle A \rangle \right)^2 \right\rangle, \tag{3}$$

   and introduce

$$\delta A(t) = A(t) - \langle A \rangle . \tag{4}$$

   Assume that the simulation time is much longer than the correlation time.

2. **Stochastic Dynamics and Hydrodynamic Screening**
   Consider a simulation where Molecular Dynamics for N particles in a volume V is coupled to a Langevin thermostat (Stochastic Dynamics). The equations of motion are

$$\frac{d}{dt}\vec{r}_i = \frac{1}{m}\vec{p}_i, \tag{5}$$

$$\frac{d}{dt}\vec{p}_i = \vec{F}_i - \frac{\zeta}{m}\vec{p}_i + \vec{f}_i(t), \tag{6}$$

where $\vec{F}_i$ is the conservative force from the particle–particle interactions, ζ is the friction constant, $\vec{f}_i$ is a Gaussian white noise with the properties

$$\begin{aligned} \langle f_{i\alpha} \rangle &= 0, && (7) \\ \langle f_{i\alpha}(t) f_{j\beta}(t') \rangle &= 2\zeta T \delta_{ij} \delta_{\alpha\beta} \delta(t - t'). && (8) \end{aligned}$$

The Greek letters denote Cartesian indices, and we assume that the system is three–dimensional. Our aim is to study this system under the *nonequilibrium* situation of shear flow. Temperature is defined here in the pragmatic sense as the input parameter of the Langevin thermostat.

(a) Discretize the equations of motion in terms of the Euler algorithm with a time step h. Calculate the change in energy, $\mathcal{H}(t+h)-\mathcal{H}(t)$. From the limit $h \to 0$, show that

$$\left\langle \frac{d\mathcal{H}}{dt} \right\rangle = \frac{3}{m}\zeta N T - \frac{\zeta}{m^2} \sum_i \left\langle \vec{p}_i^{\,2} \right\rangle , \qquad (9)$$

where $\langle \ldots \rangle$ refers to the average over the noise (and *not* to a thermal ensemble average). Show that in thermal equilibrium the ensemble average of this expression is zero.

(b) Under nonequilibrium conditions, the average of the above expression is nonzero. Assume that for a stationary shear flow we have

$$\vec{p}_i = m\vec{u}(\vec{r}_i) + \vec{c}_i, \qquad (10)$$

where $\vec{u}$ is the macroscopic (hydrodynamic) velocity flow field (evaluated at the position of particle i), while the $\vec{c}_i$ are the so–called "peculiar momenta" that have the statistical properties (in the sense of nonequilibrium ensemble averages)

$$\begin{aligned} \langle \vec{c}_i \rangle &= 0, && (11) \\ \langle c_{i\alpha} c_{j\beta} \rangle &= \delta_{ij} \delta_{\alpha\beta} m T. && (12) \end{aligned}$$

Calculate the nonequilibrium ensemble average of $\langle d\mathcal{H}/dt \rangle$. *Hint:* $\vec{u}$ can be considered as a constant when evaluating the averages.

(c) Assume that the particle number density $n = N/V$ is constant in the sample. Re–write the sum over particles into an integral over space. Show that the thermostat induces a dissipation rate (total energy loss per unit time) of

$$\dot{E}_{thermostat} = \zeta n \int_V d^3\vec{r}\,\vec{u}^2. \tag{13}$$

(d) Even for purely Newtonian dynamics one would get dissipation due to the shear viscosity η. From hydrodynamics, we know that it is given by

$$\dot{E}_{Newton} = \eta \int_V d^3\vec{r}\,(\partial_\alpha u_\beta)\,(\partial_\alpha u_\beta)\,, \tag{14}$$

where $\partial_\alpha \equiv \partial/\partial x_\alpha$ and summation convention is implied. Assume that $\vec{u}$ is oriented in x direction and depends only on the z coordinate. Impose the boundary conditions $u(z = -L/2) = -u_0$, $u(z = +L/2) = u_0$. Find the velocity profile by minimizing the *total* dissipation rate, and interpret the result in terms of a hydrodynamic screening length λ.
Hint: Recall Lagrangian mechanics!
Remark: The assumption that the dissipation rate should be a minimum often holds in nonequilibrium thermodynamics. It is however not generally valid, in particular not in cases of nonlinear behavior (like turbulence, for instance).