Problem Set 4

Advanced Statistical Mechanics

Deadline: Friday, 24 Ordibehesht, 23:59

1 Stochastic Processes

1.1 Fokker-Planck Equation

i) Consider a system of n particles of the same species where $0 \leq n \leq N$. The state of the system is characterize by n. We shall suppose that this system evolves by transition $n \to n \pm 1$ and we denote $W_{\pm}(n)$ the probability per unit time of such a transition. The Master equation for the probability $P(n, t)$ of finding n particles at time t is

$$\frac{\partial P(n,t)}{\partial t} = (\mathcal{L}P)(n,t) \tag{1}$$

where

$$(\mathcal{L}P)(n) = W_+(n-1)P(n-1) + W_-(n+1)P(n+1) - (W_+(n) + W_-(n))P(n) \tag{2}$$

The usual approximation for large N, is the Fokker-Planck approximation. To obtain this approximation, define a concentration variable and show that

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial}{\partial x}(A(x)p(x,t)) + \frac{1}{2N}\frac{\partial^2}{\partial x^2}(D(x)p(x,t)) \equiv R_p \tag{3}$$

where

$$A(x) = w_+(x) - w_-(x), \quad D(x) = w_+(x) + w_-(x) \tag{4}$$

Hint: See problem 6 (Set 3)
ii) Now suppose the Fokker-Planck equation for a diffusing particles moving with a constant average velocity, is

$$\frac{\partial p(x,t)}{\partial t} = \frac{D}{2}\frac{\partial^2 p(x,t)}{\partial x^2} - A\frac{\partial p(x,t)}{\partial x} \tag{5}$$

Find the fundamental solution of this equation.

1.2 Random Walk and Diffusion Equation

Let $p(i, N)$ denote the probability that a random walker is at site i after N steps. Assume that walker has an equal probability to walk one step left and right.
i) Use the master equation and show that

$$p(i, N) = \frac{1}{2} p(i+1, N-1) + \frac{1}{2} p(i-1, N-1) \tag{6}$$

ii) To obtain the continuum limit of this equation, define $t = N\tau$ and $x = ia$, by assuming that $D = \frac{a^2}{2\tau}$ is finite in the limit $\tau \to 0$ and $a \to 0$, show that $p(x, t)$ satisfies the diffusion equation,

$$\frac{\partial p(x,t)}{\partial t} = D \frac{\partial^2 p(x,t)}{\partial x^2} \tag{7}$$

where D is the diffusion constant.
iii) Show that the solution of diffusion equation is given by a normal distribution.
iv) Show that the conditional probability distribution of the diffusion equation with initial condition $p(x', t|x, t) = \delta(x' - x)$ is given by:

$$p(x', t+\tau) = \frac{1}{\sqrt{4\pi D\tau}} \exp\left\{ -\frac{(x - x')^2}{4D\tau} \right\}. \tag{8}$$

v) Show that second statistical moment of x is given by

$$\left\langle x^2(t) \right\rangle = 2Dt \tag{9}$$

1.3 Kramers-Moyal Equation

From the general Kramers-Moyal equation for the probability density $p(x, t)$ derive the following differential equations for the nth-order statistical moments of x

$$\frac{\partial}{\partial t} \langle x^n \rangle = \sum_{k=1}^{n} \frac{n!}{(n-k)!} \left\langle x^{n-k} D^{(k)}(x,t) \right\rangle \tag{10}$$

1.4 Backward Kramers-Moyal Equation

Starting from the following Chapman-Kolmogorov equation

$$p(x, t|x', t') = \int p(x, t|x", t' + \tau) p(x", t' + \tau|x', t') dx" \tag{11}$$

with $t \geq t' + \tau \geq t'$ i) Show that $p(x, t|x', t')$ obey the following backward Kramers-Moyal equation

$$\frac{\partial p(x,t|x',t')}{\partial t'} = -\sum_{n=1}^{\infty} D^{(n)}(x', t') \left(\frac{\partial}{\partial x'} \right)^n p(x, t|x', t') \tag{12}$$

ii) Show that the operator

$$\mathcal{L}_{KM}^{\dagger} = \sum_{n=1}^{\infty} D^{(n)}(x', t') \left(\frac{\partial}{\partial x'} \right)^{n} \tag{13}$$

is the adjoint operator of

$$\mathcal{L}_{KM} = \sum_{n=1}^{\infty} \left(-\frac{\partial}{\partial x'} \right)^{n} D^{(n)}(x', t') \tag{14}$$

1.5 Pawula Theorem

Pawula theorem states that there are only three possible cases in the KM expansion: (i) The Kramers-Moyal expansion is truncated at $n = 1$, meaning that the process is deterministic, (ii) the KM expansion stops at $n = 2$, with the resulting equation being the Fokker-Planck equation, and describes diffusion processes and, finally, (iii) The KM expansion contains all the term up to $n = \infty$.

Show that any truncation of expansion at a finite $n > 2$ would produce non-positive probability density $p(x, t)$

Hint: See the following paper: R.F. Pawula, Phys. Rev. 162, 186 (1967)

2 Kinetic Theory

2.1 One-Dimensional Gas

A thermalized gas particle is suddenly confined to a one-dimensional trap. The corresponding mixed state is described by an initial density function $\rho(q, p, t = 0) = \delta(q) f(p)$, where $f(p) = \exp\left(-p^2/2mk_BT\right)/\sqrt{2\pi mk_BT}$

i) Starting from Liouville's equation, derive $\rho(q, p, t)$ and sketch it in the (q, p) plan.

ii) Derive the expressions for the averages $\left\langle q^2 \right\rangle$ and $\left\langle p^2 \right\rangle$ at $t > 0/$

iii) Suppose that hard walls are placed at $q = \pm Q$. Describe $\rho(q, p, t \gg \tau)$, where τ an appropriately large relaxation time.

2.2 Evolution of Entropy

The normalized ensemble density is a probability in the phase space Γ. This probability has an associated entropy $S(t) = -\int d\Gamma \rho(\Gamma, t) \ln \rho(\Gamma, t)$.

i) Show that if $\rho(\Gamma, t)$ satisfies Liouville's equation for a Hamiltonian $\mathcal{H}$, $\frac{\mathrm{d}S}{\mathrm{d}t} = 0$.

ii) Using the method of Lagrange multipliers, find the function $\rho_{max}(\Gamma)$ that maximizes the functional $S[\rho]$, subject to the constrains of fixed average energy, $\langle H \rangle = \int d\Gamma \rho \mathcal{H} = E$.

2.3 Vlasov Equation

The Vlasov equation is obtained in the limit of high particle density $n = \frac{N}{V}$, or large inter-particle interaction range λ, such that $n\lambda^3 \gg 1$. In this limit, the collision terms are dropped from the left-hand side of the equations in the BBGKY.

The BBGKY

$$\begin{aligned}\left[\frac{\partial}{\partial t} + \sum_{n=1}^{s} \frac{\mathbf{p}_n}{m} \cdot \frac{\partial U}{\partial \mathbf{q}_n} - \sum_{n=1}^{s} \left(\frac{\partial U}{\partial \mathbf{q}_n} + \sum_{l} \frac{\partial \mathcal{V}(\mathbf{q}_n - \mathbf{q}_l)}{\partial \mathbf{q}_n} \right) \cdot \frac{\partial}{\partial \mathbf{p}_n}\right] f_s \\ = \sum_{n=1}^{s} \int dV_{s+1} \frac{\partial \mathcal{V}(\mathbf{q}_n - \mathbf{q}_{s+1})}{\partial \mathbf{q}_n} \cdot \frac{\partial f_{s+1}}{\partial \mathbf{p}_n}\end{aligned} \tag{15}$$

has the characteristic time scales

$$\begin{aligned}\frac{1}{\tau_U} &\sim \frac{\partial U}{\partial \mathbf{q}} \cdot \frac{\partial}{\partial \mathbf{p}} \sim \frac{v}{L}, \\ \frac{1}{\tau_U} &\sim \frac{\partial \mathcal{V}}{\partial \mathbf{q}} \cdot \frac{\partial}{\partial \mathbf{p}} \sim \frac{v}{\lambda}, \\ \frac{1}{\tau_\times} \sum \int dx \frac{\partial \mathcal{V}}{\partial \mathbf{q}} \cdot \frac{\partial}{\partial \mathbf{p}} \frac{f_{s+1}}{f_s} &\sim \frac{1}{\tau_c} \cdot n\lambda^3\end{aligned} \tag{16}$$

where $n\lambda^3$ is the number of particles within the interaction range λ, and v is a typical velocity. The Boltzmann equation is obtained in the dilute limit, $n\lambda^3 \ll 1$, by disregarding terms of the order $\frac{1}{\tau_\times} \ll \frac{1}{\tau_c}$. The Vlasov equation is obtained in the dense limit of $n\lambda^3 \gg 1$ by ignoring terms of order $\frac{1}{\tau_c} \ll \frac{1}{\tau_\times}$.

i) Assume that the N-body density is a product of one-particle densities, that is, $\rho = \prod_{i=1}^{N} \rho_1(\mathbf{x}_i, t)$, where $\mathbf{x}_i \equiv (\mathbf{p}_i, \mathbf{q}_i)$. Calculate the densities f_s, and their normalizations.

ii) Show that once the collision terms are eliminated, all the equations in the BBGKY are equivalent to the single equation

$$\left[\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \cdot \frac{\partial}{\partial \mathbf{q}} - \frac{\partial U_{eff}}{\partial \mathbf{q}} \cdot \frac{\partial}{\partial \mathbf{p}}\right] f_1(\mathbf{p}, \mathbf{q}, t) = 0 \tag{17}$$

where

$$U_{eff}(\mathbf{q}, t) = U(\mathbf{q}) + \int d\mathbf{x}' \mathcal{V}(\mathbf{q} - \mathbf{q}') f_1(\mathbf{x}', t) \tag{18}$$

iii) Now consider N particles confined to a box of volume V, with no additional potential. Show that $f_1(\mathbf{q}, \mathbf{p}) = \frac{g(\mathbf{p})}{V}$ is a stationary solution to the Vlasov equation for any $g(\mathbf{p})$. Why is there no relaxation toward equilibrium for $g(\mathbf{p})$?

2.4 Two-Component Plasma

Consider a neutral mixture of N ions of charge $+e$ and mass m_+, and N electrons of charge $-e$ and mass m_-, in a volume $V = \frac{N}{n_0}$.

i) Show that the Vlasov equations for this two-component system are

$$
\begin{aligned}
\left[\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m_+} \cdot \frac{\partial}{\partial \mathbf{q}} + e\frac{\partial \Phi_{eff}}{\partial \mathbf{q}} \cdot \frac{\partial}{\partial \mathbf{p}}\right] f_+(\mathbf{p}, \mathbf{q}, t) = 0 \\
\left[\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m_+} \cdot \frac{\partial}{\partial \mathbf{q}} - e\frac{\partial \Phi_{eff}}{\partial \mathbf{q}} \cdot \frac{\partial}{\partial \mathbf{p}}\right] f_-(\mathbf{p}, \mathbf{q}, t) = 0
\end{aligned}
\tag{19}
$$

where the effective Coulomb potential is given by

$$
\Phi_{eff}(\mathbf{q}, t) = \Phi_{ext}(\mathbf{q}) + e \int d\mathbf{x}' C(\mathbf{q} - \mathbf{q}')[f_+(\mathbf{x}', t) - f_-(\mathbf{x}', t)] \tag{20}
$$

Here, Φ_{ext} is the potential set up by the external charges, and the Coulomb potential $C(\mathbf{q})$ satisfies the differential equation $\nabla^2 C = 4\pi\delta^3(\mathbf{q})$.
ii) Assume that the one-particle densities have the stationary forms $f_\pm = g_\pm(\mathbf{p}) n_\pm(\mathbf{q})$. Show that the effective potential satisfies the equation

$$
\nabla^2 \Phi_{eff} = 4\pi\rho_{ext} + 4\pi e(n_+(\mathbf{q}) - n_-(\mathbf{q})), \tag{21}
$$

where ρ_{ext} is the external charge density.
iii) Further assuming that the densities relax to the equilibrium Boltzmann weights $n_\pm(\mathbf{q}) = n_0 \exp[\pm\beta e \Phi_{eff}(\mathbf{q})]$ leads to the self-consistency condition

$$
\nabla^2 \Phi_{eff} = 4\pi[\rho_{ext} + n_0 e(e^{\beta e \phi_{eff}} - e^{-\beta e \phi_{eff}})], \tag{22}
$$

known as the Poisson-Boltzmann equation. Due to its non-linear form, it is generally not possible to solve the Poisson-Boltzmann equation. By linearizing the exponentials, one obtain the simpler Debye equation

$$
\nabla^2 \Phi_{eff} = 4\pi\rho_{ext} + \Phi_{eff}/\lambda^2. \tag{23}
$$

Give the expression for the Debye screening length λ.
iv) Show that the Debye equation has the general solution

$$
\Phi_{eff}(\mathbf{q}) = \int d^3\mathbf{q} G(\mathbf{q} - \mathbf{q}') \rho_{ext}(\mathbf{q}'), \tag{24}
$$

where $G(\mathbf{q}) = \exp(-|\mathbf{q}|/\lambda)/|\mathbf{q}|$ is the screened Coulomb potential.
v) Give the condition for the self-consistency of the Vlasov approximation, and interpret it in terms of the inter-particle spacing.
vi) Show that the characteristic relaxation time ($\tau \approx \lambda/$ is temperature-independent. What property of the plasma is it related to?