Aspects of kinetic theory

David Korbany
University of Heidelberg, david.korbany@gmail.com

This is a short summary of some aspects of out-of-equilibrium statistical physics and quantum field theory. Specifically, I will focus on the Langevin description.

1 Introduction

Solving the microscopic equations in many-body physics is considered practically impossible. Thus, one has to use some sort of effective description to describe macroscopic quantities of interest. Remarkably, these often obey *approximately* simple deterministic equations. The approximate nature enters in the form of *fluctuation* terms. Thus, one has *stochastic* equations, i.e. the macroscopic quantities are functions of random variables. In (out-of-equilibrium) statistical physics there are roughly speaking two approaches: The Boltzmann equation and the Langevin description, or equivalently the Fokker–Planck equation.[1] The latter is an example of a *stochastic* differential equation. These can be used to create phenomenological models for a variety of processes in physics, chemistry, biology and finance, see e.g. [1]. As an example the velocity distribution P for a Brownian particle of mass m is determined by a Fokker–Planck equation of the form

$$\frac{\partial P}{\partial t} = \frac{1}{m}\frac{\partial}{\partial \vec{v}} \cdot \left(\gamma P \vec{v} + \frac{D\gamma^2}{m}\frac{\partial P}{\partial \vec{v}} \right), \qquad (1)$$

where γ is a friction constant and D is a spatial diffusion constant. The amplitude of the random white noise is given by $2D\gamma^2$. Solving (1) we get

$$P(\vec{v},t) = \mathcal{N} \exp\left(-\frac{m\left(\vec{v} - \vec{v}_0 e^{-\gamma t/m}\right)^2}{2k_B T\left(1 - e^{-2\gamma t/m}\right)} \right), \qquad (2)$$

where $\mathcal{N} = \mathcal{N}(t)$ is determined by the normalization. For $t \to \infty$ we recover the Maxwell–Boltzmann distribution. Furthermore, (2) tells us exactly how we approach equilibrium. This is plotted in figure 1. In the following we shall discuss some ways to derive Fokker-Planck equations from fundamental microscopic dynamics on various levels of sophistication.

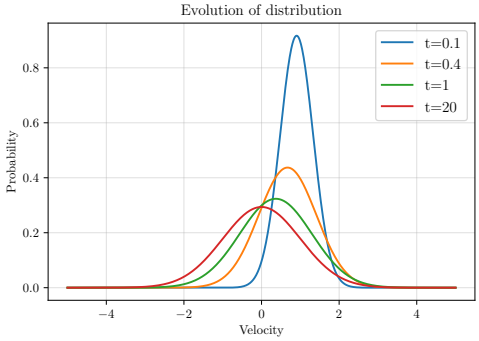

Fig. 1: *Plot of (2) for different times, with inital values $v_0 = k_B T = m = 1$. For $t = 0$ the distribution is a delta function and for large t we approach the Maxwell–Boltzmann distribution centered around $v = 0$.*

2 Relativistic phase-space distribution

The one-particle distribution of a gas of N particles is defined such that an observer at time t finds $Nf(\vec{r},\vec{p},t)\mathrm{d}^3r\mathrm{d}^3p$ particles in the volume element d^3r with momentum $\vec{p}$ within a range d^3p. It was shown by van Kampen only in 1969 that f is indeed a Lorentz scalar in the $(t,\vec{x},\vec{p})$ space [2].We can define a momentum distribution $F(\vec{p},t) = \int f(\vec{r},\vec{p},t)\mathrm{d}^3r$. For a gas of free, non-interacting particles $E_{\vec{p}}F(\vec{p},t)$ is invariant, whereas for an ideal gas in equilibrium contained in a Volume V only $\frac{F}{V}$ is invariant. Thus, the average momentum $\langle p^\alpha \rangle = \int p^\alpha F(\vec{p},t)\mathrm{d}^3p$ is a-four vector *only* in the former case. Generically,

[1] The exact equations in quantum-field theory are the Kadanoff–Baym equations.

it is a non-local quantity and thus observer dependent. Nevertheless, upon fixing a spacelike hyperplane in Minkowski space, the average momentum does transform like a four vector [3]. This has to be taken into account in simulations involving relativistic particles.

2.1 The Boltzmann equation

The dynamics of f is governed by the Boltzmann-equation

$$u^\mu \partial_\mu f + \frac{\partial}{\partial p^\mu}(K^\mu f) = C[f], \tag{3}$$

where $u^\mu = \mathrm{d}x^\mu/\mathrm{d}\tau$ is the four-velocity, $K^\mu = \mathrm{d}p^\mu/\mathrm{d}\tau$ is an external force, and $C[f]$ is the collision integral. It can be written (non-relativistically) as

$$\int \left[w(p+q,q)f(p+q) - w(p,q)f(p)\right] \mathrm{d}^3 q,$$

where $w(p,q)$ is the rate of change from $\vec{p}$ to $\vec{p}-\vec{q}$. If the collisions are dominated by low momentum (soft) scattering, we can expand

$$\begin{aligned} w(p+q,q)f(p+q) \approx & w(p,q)f(p) + q\cdot\frac{\partial}{\partial p}(wf) \\ & + \frac{1}{2}q_i q_j \frac{\partial^2}{\partial p_i \partial p_j}(wf). \end{aligned}$$

Then the collision term can be approximated as

$$C[f] = \frac{\partial}{\partial p_i}\left[A_i(p)f + \frac{\partial}{\partial p_j}\left[B_{ij}(p)f\right]\right],$$

where

$$\begin{aligned} A_i &= \int \mathrm{d}^3 k w(p,k) k_i, \\ B_{ij} &= \frac{1}{2}\int \mathrm{d}^3 k w(p,k) k_i k_j. \end{aligned}$$

Using this in (3) we have found a Fokker-Planck equation for the phase-space distribution function as an approximation to the Boltzmann equation.

3 Stochastic Dynamics

3.1 Langevin Description

The Langevin equation is a phenomenological model for stochastic processes such as Brownian motion. The equations read

$$\dot{x}^i = p^i/p^0 \tag{4a}$$

$$\dot{p}^i = -a^{ij}p^j + F^i + c^{ij}\xi^j, \tag{4b}$$

where the dot indicates proper-time derivatives and ξ^i is white noise. It is completely determined by its moments $\langle\xi^i\rangle = 0$ and $\langle\xi^i(t_1)\xi^j(t_2)\rangle = \delta^{ij}\delta(t_1-t_2)$. Due to the δ-function there is an ambiguity in the equations. To calculate expressions like

$$B = \int_t^{t+\delta t} b(x(t))\xi(t)\mathrm{d}t$$

one needs to employ some discretisation rule. The three common ones are

- Ito: $B \to b(x(t))\int_t^{t+\delta t}\xi(t)\mathrm{d}t$
- Stratonovich: $B \to (b(x(t)) + b(x(t+\delta t))/2\int_t^{t+\delta t}\xi(t)\mathrm{d}t$
- Post-Ito: $B \to b(x(t+\delta t))\int_t^{t+\delta t}\xi(t)\mathrm{d}t$

Upon expansion in δt this can be summarized as

$$B \to (b(x(t)) + \lambda\dot{b}(x(t))\delta t)\int_t^{t+\delta t}\xi(t)\mathrm{d}t,$$

for $\lambda \in \{0, 1/2, 1\}$. The right choice depends on the physical context, see [1] for a discussion. Keeping this in mind, we can determine the average displacement and correlations in phase-space. We have

$$\langle\delta x^i\rangle = \int_t^{t+\delta t}\dot{x}^i\mathrm{d}t = \frac{p^i}{p^0}\delta t,$$

assuming that the velocity is constant for small δt. Obviously then $\langle\delta x^i \delta x^j\rangle = O(\delta t^2)$. The momentum integration is slightly tricky. We have

$$\begin{aligned} \langle\delta p^i\rangle &= \int_t^{t+\delta t}\dot{p}^i\mathrm{d}t \\ &= (-a^{ij}p^j + F^i)p^i + \left\langle\int_t^{t+\delta t} c^{ij}\xi^j\mathrm{d}t\right\rangle. \end{aligned}$$

The relevant part of the last equation is upon discretesation

$$\begin{aligned} &\cdots + \lambda\left(\frac{\partial}{\partial p_l}c_{ij}\right)\dot{p}_l\delta t\int_t^{t+\delta t}\xi_j\mathrm{d}t \\ =&\cdots + \lambda\left(\frac{\partial}{\partial p_l}c_{ij}\right)c_{lk}\xi_k\delta t\int_t^{t+\delta t}\xi_j\mathrm{d}t. \end{aligned}$$

Taking the average and using $\langle\xi^i(t_1)\xi^j(t_2)\rangle = \delta^{ij}\delta(t_1-t_2)$ we find

$$\frac{1}{\delta t}\langle\delta p^i\rangle = (-a^{ij}p^j + F^i)p^i + \lambda\left(\frac{\partial}{\partial p_l}c_{ik}\right)c_{lk}.$$

Similarly we have

$$\langle \delta p^i \delta p^j \rangle = c_{ik} c_{jk} \delta t.$$

Given these results one can derive a probability distribution $P(\vec{x}, \vec{p}, t)$. The expectation value of any phase space function $g(\vec{x}, \vec{p})$ is given by $\langle g \rangle(t) = \int g(\vec{x}, \vec{p}) P(\vec{x}, \vec{p}, t) \mathrm{d}^3x \mathrm{d}^3p$. Thus, $\frac{d\langle g \rangle}{\mathrm{d}t} = \int g \frac{dP}{\mathrm{d}t}$. On the other hand

$$\frac{\mathrm{d}\langle g \rangle}{\mathrm{d}t} = \lim_{\delta t \to 0} \frac{\langle g \rangle(t + \delta t) - \langle g \rangle(t)}{\delta t} = \frac{\langle \delta g \rangle}{\delta t}.$$

To calculate $\langle \delta g \rangle$ we expand up to second order, which will be justified further below. We get

$$\begin{aligned} \delta g &= g(x + \delta x, p + \delta p) - g(x, p) \\ &= \delta x_i \frac{\partial g}{\partial x_i} + \delta p_i \frac{\partial g}{\partial p_i} + \delta p_i \delta p_j \frac{\partial^2 g}{\partial p_i \partial p_j}. \end{aligned}$$

As we have shown above, these are indeed all terms of order $O(\delta t)$. Thus,

$$\begin{aligned} \frac{\mathrm{d}\langle g \rangle}{\mathrm{d}t} &= \int g \frac{\mathrm{d}P}{\mathrm{d}t} \\ &= \lim_{\delta t \to 0} \frac{1}{\delta t} \int P \Big(\delta x_i \frac{\partial g}{\partial x_i} + \delta p_i \frac{\partial g}{\partial p_i} \\ &\quad + \delta p_i \delta p_j \frac{\partial^2 g}{\partial p_i \partial p_j} \Big) \end{aligned} \tag{5}$$

After partial integration in (5) and inserting the results for the $\langle \delta x_i \rangle$ etc., we get the Fokker–Planck equation

$$\left(\frac{\partial}{\partial t} + \frac{p^i}{p^0} \frac{\partial}{\partial x_i} \right) P = \frac{\partial}{\partial p^i} \left(A^i P + \frac{\partial}{\partial p^j} D_{ij} P \right), \tag{6}$$

where we defined

$$A^i = a^{ij} p^j - F^i - \lambda \left(\frac{\partial}{\partial p_l} c_{ik} \right) c_{lk}, \tag{7}$$

$$D_{ij} = c_{ik} c_{jk}. \tag{8}$$

The right hand side in (6) represents flow in momentum space. In equilibrium this must vanish, which, together with the known equilibrium distribution (Maxwell, Jüttner, etc.), gives rise to relations between the A^i and D^{ij}, known as fluctuation dissipation theorems (FDT). For Brownian motion (1) one obtains $D = \frac{k_B T}{\gamma}$.

3.2 Microscopic origin

Consider a density matrix $\rho[\phi_+, \phi_-]$ in a quantum field theory, i.e. instead of the position the field variables $\phi(\vec{x})$ are the degrees of freedom. The time evolution is something like

$$\begin{aligned} &\rho_{t_2}[\phi_{2+}, \phi_{2-}] \\ &= \int D\phi_{1+} D\phi_{1-} U_{t_2,t_1} \rho_{t_1}[\phi_{1+}, \phi_{1-}] U^\dagger_{t_1 t_2}, \end{aligned} \tag{9}$$

where the time evolution operator U depends on ϕ_{1+}, ϕ_{2+} and $U^\dagger$ is a functional of the other two fields. We can express the time evolution as a functional integral

$$U = \int D\phi e^{iS[\phi]}, \quad U^\dagger = \int D\phi e^{-iS^*[\phi]}. \tag{10}$$

Note that $-iS^*[\phi(t,x)] = iS^*[\phi(-t,x)]$. Thus, inserting (10) into (9) one gets a functional integral with an action with a forward and backward path in time. This is known as Schwinger–Keldysh double time path. Following [4] for the rest of this section, consider now an harmonic oscillator $H = \omega_0 a^\dagger a$. One obtains up to normalization

$$Z = \mathrm{tr} \rho_{t=\infty} = \int D\phi D\bar{\phi} e^{iS},$$

where ϕ are coherent states and the action is given by

$$S = \int_C \mathrm{d}t \bar{\phi} (i\partial_t - \omega_0) \phi. \tag{11}$$

Here C denotes the contour going from $+\infty \to -\infty \to +\infty$. Let

$$\phi(t) = \frac{1}{\sqrt{2\omega_0}} \left(P(t) - i\omega_0 X(t) \right).$$

The action (11) then reads

$$S = \int_C \mathrm{d}t \left[\frac{1}{2} \dot{X}^2 - V(X) \right], \tag{12}$$

with the potential $V(X) = \omega_0^2 X^2/2$. Let us now decompose the field into a part X^+ propagating forward in time, and X^- propagating on the backward path. Furthermore, we define classical and quantum parts via

$$X^{\mathrm{cl}} = (X^+ + X^-)/2, \quad X^{\mathrm{q}} = (X^+ - X^-)/2.$$

Then (12) becomes

$$\int_{-\infty}^{+\infty} \mathrm{d}t \left[-2X^{\mathrm{q}} \ddot{X}^{\mathrm{cl}} - V(X^{\mathrm{q}} + X^{\mathrm{cl}}) + V(X^{\mathrm{cl}} - X^{\mathrm{q}}) \right].$$

After expanding up to first order in X^q we get

$$S = \int -2X^q \left[\ddot{X}^{\mathrm{cl}} + V'(X^{\mathrm{cl}}) \right].$$

The functional integral over X^{q} gives a δ-functional, thus the only configuration contributing to Z satisfies

$$\ddot{X}^{\mathrm{cl}} = -V'(X^{\mathrm{cl}}).$$

Thus the name classical field. Now consider the particle in a bath of harmonic oscillators, where the interaction is taken as product of the coordinates. Doing the same expansion one obtains

$$\ddot{X}^{\mathrm{cl}} = -V'(X^{\mathrm{cl}}) - \gamma\dot{X}^{\mathrm{cl}}.$$

Obtaining the friction force would not be possible with one field, as it would be a boundary term. Keeping also the thermal fluctuations one gets

$$S = \int_{-\infty}^{+\infty} \mathrm{d}t \Big\{ -2X^q \Big[\ddot{X}^{\mathrm{cl}} + \gamma\dot{X}^{\mathrm{cl}} + V'\left(X^{\mathrm{cl}}\right)\Big] + 4i\gamma T \left(X^q\right)^2 \Big\}.$$

Using the identity

$$\exp\Big(-4\gamma T \int \mathrm{d}t \left(X^{\mathrm{q}}(t)\right)^2\Big) = \int D\xi \mathrm{e}^{-\int \mathrm{d}t\left[\frac{1}{4\gamma T}\xi^2(t) - 2\mathrm{i}\xi(t)X^q(t)\right]} \tag{13}$$

one finally obtains the Langevin equation

$$\ddot{X}^{\mathrm{cl}} = -\gamma\dot{X}^{\mathrm{cl}} - V'\left(X^{\mathrm{cl}}\right) + \xi(t).$$

From (13) we see that ξ is indeed white noise since

$$\langle\xi(t)\xi(t')\rangle = \int D\xi\ \xi(t)\xi(t') e^{-\int \mathrm{d}t \frac{1}{4\gamma T}\xi^2(t)} = 2\gamma T\delta(t-t').$$

This is consistent with the FDT we obtained for Brownian motion.

3.3 Langevin equation with memory

The Langevin equation (4) gives rise to Markovian processes, which is certainly only an approximation in most physical processes. The generalized Langevin equation is given by

$$\dot{x}^i = p^i/p^0 \tag{14a}$$

$$\dot{p}^i = \int_{t_0}^{t} \Gamma(t-t')p^i(t')\mathrm{d}t' + F^i + c^{ij}\xi^j, \tag{14b}$$

where Γ is a memory kernel and ξ is specified by $\langle\xi\rangle = 0$, and $\langle\xi(t_1)\xi(t_2)\rangle = K(t_1 - t_2)$, i.e. colored noise. K is the autocorrelation function and usually assumed to vanish for $|t_1 - t_2| > \tau_c$, for some $\tau_c > 0$, e.g. the scattering time. In principal, ξ may also have higher non-vanishing moments. The general fluctuation dissipation theorem [5] relates K to Γ. Note that (14) is no longer a well defined initial value problem due to the finite correlation time τ_c. Instead, one has to consider a time t_0 at which the noise is turned on. The generalized Langevin equation (14) is a nonlinear stochastic differential equation of the form

$$\dot{u}_i = F_i(u, t; \xi),$$

where u is the collection of variables. For a single realization $\bar{\xi}$ of the random functional ξ we can get a linear equation by passing to the Liouville equation

$$\partial_t\rho(u,t) = -\sum_i \partial_i \left(F_i(u,t;\bar{\xi})\rho\right). \tag{15}$$

For such a linear equation, one can then solve perturbatively in τ_c. Taking the average $\langle p(u,t)\rangle = P(u,t)$ we get a rather complicated Fokker–Planck equation for the probability distribution [1], which could be used as a starting point for numerical simulations.

Acknowledgments

I would like to thank Hendrik van Hees for many interesting discussions about physics, Jörn Knoll for the fantastic organisation and for always being helpful, and everyone else for the great time spent together.

References

[1] Van Kampen, N.G., 1992. Stochastic processes in physics and chemistry (Vol. 1). Elsevier.

[2] Van Kampen, N.G., 1969. Lorentz-invariance of the distribution in phase space. Physica, 43(2), pp.244-262.

[3] Dunkel, Jörn, and Peter Hänggi. "Relativistic brownian motion." Physics Reports 471.1 (2009): 1-73.

[4] Kamenev, A., 2011. Field theory of non-equilibrium systems. Cambridge University Press.

[5] Kubo, R., 1966. The fluctuation-dissipation theorem. Reports on progress in physics, 29(1), p.255.