This is a draft version of the lecture notes. We aim to keep improving it but at the current stage it is most likely far from perfect. Please contact us if you notice any typos, errors, subtle points, or if you have any questions or suggestions for improvements.

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January 3, 2023

8 Fokker-Planck equation

The Fokker-Planck equation is a special type of master equation, which can be used as an approximation to an actual Markov process or an elegant model for one. The trouble with the general form of the master equation is that it is an integro-differential relation and finding the probability density explicitly can be a challenging, if not impossible, task. The Fokker-Planck equation (FPE) can be derived as an approximation to the master equation in the limit of small jumps – a notion which we will formalise later. The benefit is that the FPE is a differential equation more amenable to analytical solutions. It is also called the 'Smoluchowski equation', 'generalised diffusion equation' and 'second Kolmogorov equation', depending on the context.

For a continuous random variable y and time t, the FPE has the form of a second-order partial differential equation, generally written as

$$\frac{\partial P(y,t)}{\partial t} = -\frac{\partial}{\partial y}\left[A(y)P(y,t)\right] + \frac{1}{2}\frac{\partial^2}{\partial y^2}\left[B(y)P(y,t)\right]. \tag{8.1}$$

The coefficients of the equation, $A(y)$ and $B(y) > 0$ are real differentiable functions. FPE can be written in the form of a continuity equation for the probability density

$$\frac{\partial P}{\partial t} = -\frac{\partial J}{\partial y}, \tag{8.2}$$

with the probability flux J given by a linear 'constitutive relationship'

$$J(y,t) = A(y)P - \frac{1}{2}\frac{\partial(B(y)P)}{\partial y}. \tag{8.3}$$

Note that there exists a stationary solution of Eq. (8.1), which corresponds to the vanishing flux, and is given by

$$P^s(y) = \frac{\text{const.}}{B(y)} \exp\left[2\int_0^y \frac{A(s)}{B(s)}\mathrm{d}s\right], \tag{8.4}$$

obviously only when P^s is integrable and thus can be normalised.

We can use the stationary solution to construct a Markov process. We know that a Markov process is fully specified by a pdf P_1 and a transition probability $P_{1|1}$. If now we choose a transition probability $P(y,t|y_1,t_1)$ for $t \geq t_1$ that is a solution of (8.1) which reduces to $\delta(y - y_1)$ at $t = t_1$, and take for P_1 the stationary solution P^s, the resulting Markov process is stationary.

8.1 Derivation of the Fokker-Planck equation

To arrive at the Fokker-Planck equation, we consider the Master equation (7.6) with a special form of the transition probability W. First, we rewrite $W(y|y')$ as a function of the initial point y' and jump size $r = y - y'$,

$$W(y|y') \equiv W(y', r), \tag{8.5}$$

so the master equation is recast as

$$\frac{\partial P(y,t)}{\partial t} = \int W(y-r,r)P(y-r,t)\mathrm{d}r - P(y,t)\int W(y,-r)\mathrm{d}r. \tag{8.6}$$

We now turn back to the assumption of small jumps. This means basically that there exists a length scale δ such that

$$W(y', r) \approx 0 \quad \text{for } |r| > \delta, \tag{8.7}$$

$$W(y' + \Delta y, r) \approx W(y', r) \quad \text{for } |\Delta y| < \delta. \tag{8.8}$$

In other words, W is sharply peaked around zero as a function of the jump size r but at the same time varies slowly with the first argument, the position in space. If we additionally assume that the solution also varies slowly with y, we can perform a Taylor expansion of the shift $y - r$ in the first integral of Eq. (8.6) up to second order. We have

$$\begin{aligned} W(y-r,r)P(y-r,t) \approx & W(y,r)P(y,t) - r\frac{\partial}{\partial y}\left[W(y,r)P(y,t)\right] \\ & + \frac{r^2}{2}\frac{\partial^2}{\partial y^2}\left[W(y,r)P(y,t)\right] + \text{h.o.t.} \end{aligned} \tag{8.9}$$

Note here that the dependence of W on the second argument is fully maintained – we cannot expand in this argument because of the rapid variation of W with r. Inserting this expansion into Eq. (8.6), we notice that the first and fourth terms cancel. The remaining terms can be written using the jump moments,

$$a_\nu(y) = \int r^\nu W(y,r)\mathrm{d}r \tag{8.10}$$

already defined in Eq. (7.29). We finally arrive at

$$\frac{\partial P(y,t)}{\partial t} = -\frac{\partial}{\partial y}\left[a_1(y)P(y,t)\right] + \frac{1}{2}\frac{\partial^2}{\partial y^2}\left[a_2(y)P(y,t)\right]. \tag{8.11}$$

We have thus derived Eq. (8.1) from an expansion of the master equation in the limit of small jumps by an expansion of the underlying transition rates in terms of the jump moments. Importantly, one can show that FPE preserves normalisation and positiveness of the solution.

Kramers-Moyal expansion of the master equation It would seem natural to think of a more general form of the Taylor expansion (8.9) with an arbitrary number of terms m, that would lead to

$$\frac{\partial P(y,t)}{\partial t} = \sum_{\nu=1}^{m} \frac{(-1)^\nu}{\nu!} \left(\frac{\partial}{\partial y}\right)^\nu [a_\nu(y) P(y,t)], \tag{8.12}$$

and see the effects of various types of truncations. The simplest choice is to retain just one term, to arrive at

$$\frac{\partial P(y,t)}{\partial t} = -\frac{\partial}{\partial y}[a_1(y) P(y,t)]. \tag{8.13}$$

This, however, is the deterministic Liouville equation. It cannot describe fluctuations, which was our original motivation, thus we need to include further terms; including the second-derivative term leads to FPE (8.11). However, a theorem due to Pawula [8] states that for the solution to be interpretable as a PDF (positive, with a constant integral equal to 1), the expansion must be either truncated after two terms (FPE) or contain an infinite number of terms.

Boundary conditions Two types of boundaries that are of particular interest in the context of FPE. The first is a reflecting boundary condition which contains the PDF to a bounded domain Ω. There must be no flux through the boundaries, so $J(y,t)|_{\partial\Omega} = 0$. The second is an absorbing boundary condition which reflects the fact that on the boundary $\partial\Omega$ the PDF vanishes, $P(y,t)|_{\partial\Omega} \equiv 0$. In this case, the norm of the solution of the FPE decreases and the boundary acts as a probability sink.

8.2 Fokker-Planck description of a Markov process

We have derived the Fokker-Planck equation as a model (or an approximation) for a Markov process $Y(t)$ whose individual jumps are small. There are two appealing properties of the resulting description. First, as advertised at the beginning of this Section, we arrived at a differential, rather than an integral-differential, equation. The former is much easier to handle, and therefore more practical. Second, perhaps more importantly, to construct a FPE we do not need the knowledge of the exact form of the transition kernel $W(y|y')$ but only its first and second moment. These two elements can be derived for a given process with much less effort and do not required detailed knowledge on the nature of underlying the physical process.

To illustrate this, consider a process which we choose to describe via an observable y which the physics of the process suggests to be approximately Markovian. We then choose a time interval Δt short enough for y not to change considerably but long enough for the Markov assumption to be valid. We can compute the average change $\langle \Delta y \rangle_y$ and its average square $\langle (\Delta y)^2 \rangle_y$ over this short time Δt. The subscript means that these quantities are conditional on the position y at the beginning of the time interval. Now consider the conditional probability distribution $P(y + \Delta y, t_0 + \Delta t | y_0, t_0)$ that satisfies the FPE (8.11). We can show directly by computing the moments of this distribution that for $\Delta t \to 0$ we have

$$a_1(y_0) = \frac{\langle \Delta y \rangle}{\Delta t}, \qquad a_2(y_0) = \frac{\langle (\Delta y)^2 \rangle}{\Delta t}, \qquad \frac{\langle (\Delta y)^\nu \rangle}{\Delta t} = 0 \text{ for } \nu \geq 3. \tag{8.14}$$

Thus, from the calculated averages we can compute the first and second jump moments by dividing by Δt and computing the short time limit. Note that we only need to know the short-time behaviour of the system to compute the jump moments, and the long-time behaviour can then be predicted from the FPE.

An alternative way of constructing a Fokker-Planck description relies on the phenomenological approach. From the FPE (8.11) we can show directly that

$$\frac{\partial \langle y \rangle}{\partial t} = \langle a_1(y) \rangle \tag{8.15}$$

If one now neglects fluctuations completely, we have $\langle a_1(y) \rangle = a_1(\langle y \rangle)$, and the preceding equation simplifies to

$$\frac{\partial \langle y \rangle}{\partial t} = a_1(\langle y \rangle), \tag{8.16}$$

which we identify with the macroscopic equation from Sec. 7.2. Thus the function $a_y(y)$ can be identified from the macroscopic equation. Next, the second jump moment can be found from the stationary (equilibrium) solution of the FPE. In equilibrium, the probability flux in Eq. (8.3) that corresponds to the stationary solution $P^s(y)$ must vanish, so

$$a_1 P^s - \frac{1}{2}\frac{\partial}{\partial y}(a_2(y) P^s) = 0, \tag{8.17}$$

from which we determine a_2 based on the knowledge of a_1 and the equilibrium distribution, which we typically know from statistical mechanics. Importantly, the phenomenological approach to determining a_1 and a_2, although used with great success by Einstein and others, is not generally valid and can only be used when the macroscopic equation is linear. The case of a nonlinear macroscopic equation and a consistent treatment requires a separate discussion, which we will omit for now. Instead, we will focus on the former case in the following.

Linear Fokker-Planck equation Since the FPE is always linear in P, we will reserve the name *linear Fokker-Planck equation* for the FPE in which the first jump moment is linear in y and the second jump moment is constant and equal to $B > 0$, so that

$$\frac{\partial P(y,t)}{\partial t} = -\frac{\partial}{\partial y}\left[(A_0 + A_1 y) P(y,t)\right] + \frac{B}{2}\frac{\partial^2}{\partial y^2}\left[P(y,t)\right]. \tag{8.18}$$

Then, with no approximation, we can write

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle y(t) \rangle = \langle a_1(y) \rangle = a_1(\langle y(t) \rangle) = A_0 + A_1 \langle y(t) \rangle. \tag{8.19}$$

Note that in this case A_0 can be eliminated by defining

$$P(y,t) = \tilde{P}(y - A_0 t, t). \tag{8.20}$$

We can therefore consider only the case $A_0 = 0$, which corresponds to the FPE

$$\frac{\partial P(y,t)}{\partial t} = \gamma \left[\frac{\partial}{\partial y} + \sigma^2 \frac{\partial^2}{\partial y^2} \right] P(y,t), \tag{8.21}$$

where $\gamma = -A_1 > 0$ sets the time scale and $\gamma\sigma^2 = B/2$.

We will now show a method of solving the linear FPE (8.21) that uses the method of *characteristic function*. First, we define the characteristic function $G(k,t)$ for a given probability distribution $P(y,t)$ via the Fourier transform

$$G(k) = \int \mathrm{e}^{iky} P(y) \mathrm{d}y. \tag{8.22}$$

The characteristic function has the properties that $G(0) = 1$ and $|G(k)| \leq 1$. It is also called the *moment-generating function*, because the coefficients of its Taylor expansion in k are the moments $\mu_m = \langle y^m \rangle$ of the underlying distribution, so that

$$G(k) = \sum_{m=0}^{\infty} \frac{(ik)^m}{m!} \mu_m. \tag{8.23}$$

Once $G(k)$ is known, the PDF can be found by inverse transformation

$$P(y) = \frac{1}{2\pi} \int G(k) \mathrm{e}^{-iky} \mathrm{d}k. \tag{8.24}$$

We will now solve Eq. 8.21 in an unbounded space with the initial condition $P(y, t = 0) = \delta(y - y_0)$. Taking the Fourier transform of Eq. (8.21), we arrive at a closed equation for G,

$$\frac{\partial}{\partial t} G(k,t) = -\gamma k \frac{\partial}{\partial k} G(k,t) - \gamma \sigma^2 k^2 G(k,t). \tag{8.25}$$

To solve it, we note that the general solution has the form

$$G(k,t) = e^{-\frac{1}{2}\sigma^2 k^2} \phi(k \mathrm{e}^{-\gamma t}), \tag{8.26}$$

with an unknown function ϕ which can be determined from the transformed initial condition, $G(k,0) = e^{iky_0}$, so we finally arrive at

$$G(k,t) = \exp\left(iky_0 \mathrm{e}^{-\gamma t} - \frac{1}{2}\sigma^2 k^2 (1 - \mathrm{e}^{-2\gamma t}) \right). \tag{8.27}$$

To determine the corresponding probability distribution, we should in principle apply an inverse Fourier transformation to $G(k,t)$. However, it is easier to examine the properties of the Gaussian PDF (2.52) $\mathcal{N}(y,t)$

$$\mathcal{N}(y) = \frac{1}{\sqrt{2\pi s^2}} \exp\left[-\frac{(y-\mu)^2}{2s^2} \right], \tag{8.28}$$

and note that the characteristic function reads then

$$G_{\mathcal{N}}(k,t) = \exp\left(ik\mu - \frac{1}{2}\sigma^2 k^2 \right). \tag{8.29}$$

By comparison of Eqs. (8.27) and (8.29), we see that in the linear FPE the solution is Gaussian, and reads

$$P(y,t|y_0,0) = \frac{1}{\sqrt{2\pi\sigma^2(1-\mathrm{e}^{-2\gamma t})}} \exp\left[-\frac{(y-y_0\mathrm{e}^{-\gamma t})^2}{2\sigma^2(1-\mathrm{e}^{-2\gamma t})}\right]. \tag{8.30}$$

The conditional probability $P_{1|1} \equiv P(y,t|y_0,0)$, together with the Gaussian PDF

$$P_1(y_0) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{y_0^2}{2}\right), \tag{8.31}$$

define a particularly important Markov process, called the **Ornstein-Uhlenbeck process**. By Doob's theorem, this is the only stationary and Gaussian Markov process. Its autocorrelation function reads simply

$$\kappa(\tau) = \mathrm{e}^{-\tau}. \tag{8.32}$$

8.3 Brownian motion

Brownian motion bears a long and fascinating history of its discovery, early intepretations, possible explanations, and lively discussions it has inspired in the scientific community. These endeavours are summarised in a brilliant historical account by Brush [9].

We will elaborate on the history of Brownian motion later, and now focus on the physical description of this mesoscopic phenomenon in which the key role is played by the time scales of observation which are coarse as compared to the velocity relaxation times.

We will thus focus our description on the coarse time scale, where the position of the Brownian particle $\boldsymbol{r} = (x, y, z)$ may be treated as a random variable. Since between subsequent observations of the position, the velocity of the Brownian particle has relaxed many times, we can assume the stochastic process $\boldsymbol{r}(t)$ to be Markovian. Then, a master equation can be written, from which a suitable FPE can be derived. To cut this route short, we will start with the FPE, for which we need to specify the first and second jump moments. The particle makes random jumps, which may have any length, but long jumps are highly improbable. The probability of jumping should also be isotropic and independent of the starting point. From isotropy, the first jump moment will vanish, and we assume the second jump moment to be constant

$$\boldsymbol{a}_1 = \lim_{\Delta t\to 0} \frac{\langle \Delta \boldsymbol{r}\rangle_{\boldsymbol{r}}}{\Delta t} = 0, \tag{8.33}$$

$$(a_2)_{ij} = \lim_{\Delta t\to 0} \frac{\langle \Delta r_i \Delta r_j\rangle_{\boldsymbol{r}}}{\Delta t} = 2D\delta_{ij}. \tag{8.34}$$

The FPE for the transition probability becomes then

$$\frac{\partial P(\boldsymbol{r},t)}{\partial t} = D\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) P(y,t) = D\nabla^2 P(\boldsymbol{r},t), \tag{8.35}$$

which is simply a diffusion equation for the PDF. If we assume the initial condition $P_1 \equiv P(\boldsymbol{r},0) = \delta(\boldsymbol{r}-\boldsymbol{r}_0)$, we find

$$P(\boldsymbol{r},t) = \left(\frac{1}{4\pi Dt}\right)^{3/2} \mathrm{e}^{-\frac{(\Delta \boldsymbol{r})^2}{4Dt}}, \tag{8.36}$$

which, together with P_1 defines the **Wiener process**. Note here that although we cannot measure the velocity of the particle on this coarse timescale, we can measure the mean-square displacement (MSD)

$$\left\langle (\Delta \boldsymbol{r})^2 \right\rangle = \left\langle (\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2 \right\rangle = 6Dt, \tag{8.37}$$

which grows linearly in time. Thus, the mean distance covered by the Brownian particle after time t grows as $\sqrt{t}$.

We will now follow Einstein's approach to find a microscopic expression for the diffusion coefficient. To do so, we will use the phenomenological approach presented before and apply it to a case in which there is a non-trivial macroscopic equation for a Brownian particle – consider Brownian motion in a gravitational field $\boldsymbol{g} = -g\boldsymbol{e}_z$. Then, the equilibrium distribution is known from statistical mechanics to be

$$P^{eq}(z) \sim \mathrm{e}^{-\frac{mgz}{k_B T}}. \tag{8.38}$$

Now consider the displacement of the Brownian particle over a short time Δt. The particle will exhibit random Wiener process displacements $(\Delta x_0, \Delta y_0, \Delta z_0)$ in all directions, independent of the external field. On the timescales long compared to the velocity relaxation time scale, the (Stokes) equation of motion of the particle reads $0 = mg - \zeta \langle v_z \rangle$, with ζ being the Stokes viscous friction coefficient, which for a spherical particle of radius a immersed in fluid of viscosity η reads $\zeta = 6\pi\eta a$. Hence, we find the systematic velocity $\langle v_z \rangle = \frac{mg}{\zeta}$, and we can finally write the short-time displacements of the particle in all directions

$$\Delta x = \Delta x_0, \tag{8.39}$$

$$\Delta y = \Delta y_0, \tag{8.40}$$

$$\Delta z = \Delta z_0 - \frac{mg}{\zeta}\Delta t. \tag{8.41}$$

Thus we find the components of the first jump moment to be

$$a_{1x}(\boldsymbol{r}) = 0 = a_{1y}(\boldsymbol{r}), \qquad a_{1z}(\boldsymbol{r}) = -\frac{mg}{\zeta}. \tag{8.42}$$

This systematic drift does not affect fluctuations, so the second jump moment is found as before

$$(a_2)_{ij} = \lim_{\Delta t \to 0} \frac{\langle \Delta r_i \Delta r_j \rangle_{\boldsymbol{r}}}{\Delta t} = 2D\delta_{ij}, \tag{8.43}$$

and having written these we have a complete description needed for the FPE, which now takes the form

$$\frac{\partial P(\boldsymbol{r},t)}{\partial t} = \left[\frac{mg}{\zeta}\frac{\partial}{\partial z} + D\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \right] P(y,t) = D\nabla^2 P(\boldsymbol{r},t), \tag{8.44}$$

which can be rewritten using the flux as $\partial_t P = \nabla \cdot \boldsymbol{J}$, where

$$J_x = -D\frac{\partial P}{\partial x}, \qquad J_y = -D\frac{\partial P}{\partial y}, \qquad J_z = -\left[\frac{mg}{\zeta} + D\frac{\partial}{\partial z} \right] P, \tag{8.45}$$

As before, to determine the second jump moment, we use the fact that for in equilibrium the flux vanishes, $\boldsymbol{J}^{eq} = 0$, so for P^{eq} we must have

$$\left[\frac{mg}{\zeta} + D\frac{\partial}{\partial z}\right] P^{eq} = 0. \tag{8.46}$$

Thus we find the **Stokes-Einstein formula**,

$$D = \frac{k_B T}{\zeta} = \frac{k_B T}{6\pi\eta a}, \tag{8.47}$$

which relates the macroscopic transport property (diffusion coefficient) to the microscopic parameter (radius of the particle). It is also an example of a **fluctuation-dissipation theorem**, which says that fluctuations in the medium (diffusion) are related to the dissipation (viscosity) and they cannot be independent. The fluctuation-dissipation theorem is a consequence of the second law of thermodynamics.

At the time it was derived, Eq. (8.47) was of paramount importance, because it allowed the measurement of microscopic particle sizes from macroscopic experiments. In 1908, Jean Perrin observed the positions of a Brownian particle in subsequent times to test the theoretical predictions of the theory of Brownian motion, and found excellent agreement. This has paved the way for the acceptance of "reality" of atoms amongst the scientific community of the time.

8.4 The Rayleigh particle

The Rayleigh particle is the same particle as analysed before but studied on a finer time scale. Now we will focus on time intervals Δt that are short compared to the velocity relaxation time of the particle in a gas medium, but still long compared to the time of an individual collision of the particle with a gas molecule. For simplicity, we shall now focus on the one-dimensional case, where the random variable is the velocity V of the particle.

Here, we focus on a gas rather than a liquid, because the time scales of velocity relaxation in a liquid can be as long as the Brownian time scale τ_B. If this is the case, one cannot use the Stokes law for the velocity relaxation dynamics. In other words, the Stokes equation for the particle, $m\dot{v} = \zeta v$ is not valid, because the fluid is not in a steady state. In a liquid we expect the velocity to evolve according to

$$m\frac{\mathrm{d}v}{\mathrm{d}t} = -\int_{-\infty} t\zeta(t-t')v(t')\mathrm{d}t', \tag{8.48}$$

where the friction kernel $\zeta(t)$ characterises the memory effect of the fluid. In a gas, we assume this relationship to be instantaneous and thus to depend only on the instantaneous value of the velocity. Having established that, for a gas we can write

$$\frac{\mathrm{d}v}{\mathrm{d}t} = -\gamma v, \tag{8.49}$$

with the solution $v \sim \mathrm{e}^{-\gamma t}$. Thus we see that the time intervals of interest are now such that $\Delta t \ll \gamma^{-1}$. Eq. (8.49) is thus the (linear) macroscopic equation for the velocity, from which we readily deduce the first jump moment

$$a_1(v) = \lim_{\Delta t \to 0} \frac{\langle \Delta v \rangle_v}{\Delta t} = -\gamma v. \tag{8.50}$$

For the second jump moment, we expect it to be positive even for $v = 0$, so for small v we assume that it is constant

$$a_2(v) = \alpha + \mathcal{O}(v^2) \approx \alpha. \tag{8.51}$$

Thus, the resulting FPE is the Rayleigh equation

$$\frac{\partial P(v,t)}{\partial t} = \gamma \frac{\partial}{\partial y}[vP(v,t)] + \frac{\alpha}{2}\frac{\partial^2 P(v,t)}{\partial v^2} \tag{8.52}$$

Before we solve the Rayleigh equation, note that we can find the value of α as before from the knowledge of the equilibrium distribution, which is given from statistical mechanics by the Maxwell distribution (2.41). It is straightforward to check that

$$\alpha = \frac{2\gamma k_B T}{m}. \tag{8.53}$$

Finally, we can write the Rayleigh equation as

$$\frac{\partial P(v,t)}{\partial t} = \gamma \left[\frac{\partial}{\partial y}[vP(v,t)] + \frac{k_B T}{m}\frac{\partial^2 P(v,t)}{\partial v^2} \right]. \tag{8.54}$$

This linear FPE is identical to that analysed before, hence we conclude that the solution is the transition probability of the Ornstein-Uhlenbeck process, Eq. (8.30).

It is also straightforward to compute the moments of the velocity distribution for a particle with an initial velocity v_0

$$\langle v(t) \rangle_{v_0} = v_0 \mathrm{e}^{-\gamma t}, \tag{8.55}$$

$$\left\langle v^2(t) \right\rangle_{v_0} = v_0^2 \mathrm{e}^{-2\gamma t} + \frac{k_B T}{m}(1 - \mathrm{e}^{-2\gamma t}). \tag{8.56}$$

The autocorrelation function for this stationary Gaussian function is then

$$\kappa(\tau) = \langle\langle v(t) v(t+\tau) \rangle\rangle = \langle\langle v(0) \rangle\rangle^{eq} \, \mathrm{e}^{-\gamma t} = \frac{k_B T}{m} \mathrm{e}^{-\gamma t}. \tag{8.57}$$

Note also that from the average squared velocity we can find the average kinetic energy of the Rayleigh particle

$$\frac{m \langle v \rangle^2}{2} = \frac{k_B T}{2m}, \tag{8.58}$$

which manifests the equipartition principle.