

## Chapter 2

# Brownian motion

### 2.1 Euclidean time and diffusion

When we look at Fig. 1.1 where the quantal trajectories are shown we may have an impression that we are looking at a schematic picture of the Brownian motion. As it turns out it is more than just an impression, and that there is an intimate relation between path integrals and the theory of Brownian motion. The essential difference between the two is that the mathematical basis of path integrals is very shaky [2.1], whereas the theory of Brownian motion has a solid ground and its mathematical tools were created long before the path integral approach to quantum mechanics was conceived.

Theory of Brownian motion started with the papers of Einstein [2.2] and Smoluchowski [2.3]. The mathematical basis was constructed by Wiener in a series of papers published (around the year 1922) in MIT Journal of Mathematics and Physics where the concepts of Wiener measure and Wiener integral were introduced. This work was then continued by many, notably by Kac [2.4] who also took part in development of the so called Euclidean version of Feynman's path integrals.

Let us start with the Smoluchowski equation which, in mathematical literature, is called Chapman–Kolmogoroff equation. This equation is an integral relation for the *probability density*  $\rho(x_b, x_a, t_b - t_a)$  for finding the Brown particle at  $x_b$  at the time  $t_b$ , when at the time  $t_a$  it was observed at  $x_a$ . To construct the equation we assume that the future positions are realized independently of the past positions: at the time  $t_c$ ,  $t_b > t_c > t_a$ , let the particle be at  $x_c$ , therefore in time  $t_c - t_a$  the particle moved from  $x_a$  to  $x_c$  and then, in time  $t_b - t_c$ , moved from  $x_c$  to  $x_b$ . But “the future is independent of the past”, hence the probability of transition from  $x_a$  to  $x_b$  *via*  $x_c$  is the product of probabilities  $\rho(x_b, x_c, t_b - t_c)\rho(x_c, x_a, t_c - t_a)$ . Furthermore,  $x_c$  is arbitrary. Therefore we get the following integral equation for  $\rho$

$$\rho(x_b, x_a, t_b - t_a) = \int_{-\infty}^{+\infty} dx_c \rho(x_b, x_c, t_b - t_c) \rho(x_c, x_a, t_c - t_a) \quad (2.1)$$

where  $t_b > t_c > t_a$ . Note the isomorphism of (2.1) with (1.31) for the Feynman propagators  $K(x_b, x_a, t_b - t_a)$ . Remember, however, that (2.1) is not a quantum

mechanical relation, whereas (1.31) is. As it is argued in [2.4], when we look for solutions of eq.(2.1) which depend only on distances,  $|x_b - x_a|$ , and give finite spatial dispersions:

$$\int_{-\infty}^{+\infty} dx_b (x_b - x_a)^2 \rho(|x_b - x_a|, t_b - t_a) < \infty,$$

it turns out that there exists only one solution of the Smoluchowski equation which is a gaussian density

$$\rho(x_b - x_a, t_b - t_a) = \sqrt{\frac{1}{2\pi\sigma^2(t_b - t_a)}} e^{-\frac{(x_b - x_a)^2}{2\sigma^2(t_b - t_a)}}. \quad (2.2)$$

This last expression we compare with  $K_0(b, a)$  given by (??). It turns out that, apart from different constants, we get (2.2) from (??) by replacing the time variable,  $t$ , by an imaginary variable  $-it$ . Equation (2.2) is the so called “Euclidean” version of  $K_0(b, a)$ . So, we have in this case an isomorphy of *probability densities* with *Euclidean probability amplitudes*.

The Euclidean forms of Feynman propagators are of considerable interest because, as we have already stressed above, they are well defined mathematical objects, and, as we will see below, contain all information about internal structures (such as e.g. energy levels) of quantal objects they describe. So, we will frequently work with them in these lectures. However, they are not able to describe some important quantal phenomena like e.g. diffraction, and one has to keep the “real time” version of Feynman propagators described in the Introduction in spite of their mathematical shortcomings.

In this section we will continue discussing the Euclidean propagators related to purely classical phenomenon of Brownian motions and random walks in space and time. Clearly, one can present (2.2) as a sum over paths which evolve in the Euclidean time:

$$\rho(x_b - x_a, t_b - t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} [\mathcal{D}x(t)] e^{-\frac{1}{2\sigma^2} \int_{t_a}^{t_b} dt \dot{x}^2}. \quad (2.3)$$

Also, this  $\rho$  must be a solution of the Euclidean version of the Schrödinger equation:

$$\frac{\partial \rho}{\partial t_b} = \frac{\sigma^2}{2} \frac{\partial^2 \rho}{\partial x_b^2}. \quad (2.4)$$

This is the equation of diffusion with the coefficient of diffusion  $D = \sigma^2/2$ . If we want to use it for quantal processes we have to set  $\sigma^2 = \hbar/m$ .

Let us look now at the process of diffusion as a random walk over a discretized lattice in  $(x, t)$  space. One step in space we call  $\Delta$ . We call  $\epsilon$  one step in time. Therefore the position in space and time of the particle which starts at  $(x = 0, t = 0)$  is

$$x = j\Delta, \quad t = N\epsilon, \quad j = 0, \pm 1, \pm 2, \dots, \quad N = 0, 1, 2, \dots$$

At every  $x(j)$  the particle has equal probability ( $= 1/2$ ) of moving one step to the right or to the left. Let the probability of finding the particle at  $x(j)$  in time  $t(N)$  be  $P(j, N)$ . To reach the position  $(j, N)$ , the particle executes  $\mu$  steps to the right and  $\nu$  steps to the left

$$\mu - \nu = j, \quad \mu + \nu = N, \quad N - j = 2\nu, \quad \text{hence } N - j \text{ is even.}$$

The position  $(j, N)$  can be reached through  $\binom{N}{\mu}$  different paths. Therefore  $P(j, N)$  is a sum over these paths weighted by a probability of executing  $N$  steps:

$$P(j, N) = \begin{cases} \binom{N}{\mu} \left(\frac{1}{2}\right)^N & \text{for even } N - j \\ 0 & \text{for odd } N - j. \end{cases} \quad (2.5)$$

For very large  $j$  and  $N$  we can approximate the binomial distribution by the normal distribution (for details see [2.5]) and obtain

$$P(j, N) \approx \sqrt{\frac{2}{\pi N}} e^{-\frac{j^2}{2N}}. \quad (2.6)$$

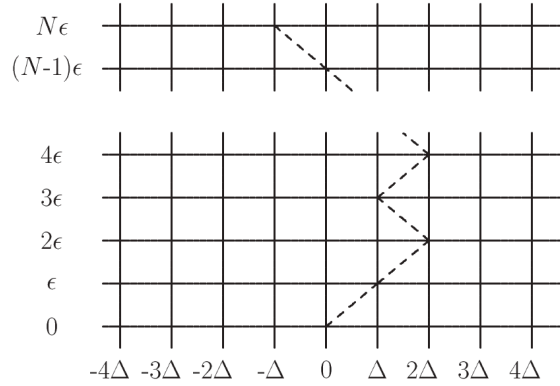


Figure 2.1: Brownian trajectory on a lattice of discretized space and time.

Now we construct the probability density per unit length:

$$\rho(x, t) = \frac{P(j, N)}{2\Delta} = \sqrt{\frac{\epsilon}{2\pi t \Delta^2}} e^{-\frac{1}{2t} \frac{\epsilon}{\Delta^2} x^2}.$$

Note that we divided  $P$  by  $2\Delta$  because the spatial resolution of particle positions is  $2\Delta$  (not  $\Delta$  since  $P(j, N) = 0$  when  $N - j$  is odd).

In order to obtain a continuous Brownian motion we let  $\Delta \rightarrow 0$  and  $\epsilon \rightarrow 0$  for fixed  $x$  and  $t$ . This can sensibly be done only if we keep

$$D = \frac{\Delta^2}{2\epsilon}$$

constant in this limiting process.  $D$  is the constant (coefficient) of diffusion. So, our probability density takes the form we already know:

$$\rho(x, t) = \sqrt{\frac{1}{4\pi Dt}} e^{-\frac{x^2}{4Dt}}. \quad (2.7)$$

## 2.2 Diffusion and the Smoluchowski equation

It is amusing and interesting to note that having (2.5) we can obtain the diffusion equation (2.4) and the Smoluchowski equation (2.1) as continuum limits of some identities of the binomial coefficients. The identity which leads to the diffusion equation is this

$$\binom{N+1}{\mu} = \binom{N}{\mu} + \binom{N}{\mu-1}. \quad (2.8)$$

Let us remind ourselves the translation of the discretized probability (2.5)

$$P(j, N) = \binom{N}{\mu} \left(\frac{1}{2}\right)^N, \quad \mu = \frac{N+j}{2},$$

into the continuum probability density  $\rho(x, t)$ :

$$P(j, N) \rightarrow \rho(x = \Delta j = \Delta(2\mu - N), t = \epsilon N). \quad (2.9)$$

Relation (2.8) comes out as

$$\rho(x, t + \epsilon) = \frac{1}{2}\rho(x + \Delta, t) + \frac{1}{2}\rho(x - \Delta, t).$$

Indeed, identification goes as follows.

In

$$\rho(x, t + \epsilon): \quad x \rightarrow j, \quad t + \epsilon \rightarrow N + 1, \quad \mu = \frac{N + j + 1}{2}$$

thus 
$$\rho(x, t + \epsilon) \rightarrow \frac{1}{2} \binom{N+1}{\mu} \left(\frac{1}{2}\right)^N.$$

In

$$\rho(x + \Delta, t): \quad x \rightarrow j + 1, \quad t \rightarrow N, \quad \mu = \frac{N + j + 1}{2}$$

thus 
$$\rho(x + \Delta, t) \rightarrow \binom{N}{\mu} \left(\frac{1}{2}\right)^N.$$

In

$$\rho(x - \Delta, t): \quad x - \Delta \rightarrow j - 1, \quad t \rightarrow N, \quad \mu' = \frac{N + j - 1}{2} = \mu - 1$$

thus 
$$\rho(x - \Delta, t) \rightarrow \binom{N}{\mu - 1} \left(\frac{1}{2}\right)^N.$$

Subtracting from both sides  $\rho(x, t)/\epsilon$  and inserting  $\Delta^2$  we get

$$\frac{\rho(x, t + \epsilon) - \rho(x, t)}{\epsilon} = \frac{\Delta^2}{2\epsilon} \frac{\rho(x + \Delta, t) - 2\rho(x, t) + \rho(x - \Delta, t)}{\Delta^2}. \quad (2.10)$$

In the continuum limit (2.10) becomes the diffusion equation

$$\frac{\partial \rho(x, t)}{\partial t} = D \frac{\partial^2 \rho(x, t)}{\partial x^2}, \quad D = \frac{\Delta^2}{2\epsilon}. \quad (2.11)$$

Now, the Smoluchowski equation follows from the identity

$$\sum_{\mu'' \leq \mu' \leq \mu} \binom{N}{\mu - \mu'} \binom{N'}{\mu' - \mu''} = \binom{N + N'}{\mu - \mu''}. \quad (2.12)$$

Indeed, we have

$$\begin{aligned} \binom{N}{\mu - \mu'} \left(\frac{1}{2}\right)^N &\rightarrow \rho(x - x', t), \\ \binom{N'}{\mu' - \mu''} \left(\frac{1}{2}\right)^{N'} &\rightarrow \rho(x' - x'', t'), \\ \binom{N + N'}{\mu - \mu''} \left(\frac{1}{2}\right)^{N + N'} &\rightarrow \rho(x - x'', t + t'). \end{aligned}$$

Finally, with the help of (2.12) we get the Smoluchowski equation

$$\int dx' \rho(x - x', t) \rho(x' - x'', t') = \rho(x - x'', t + t'). \quad (2.13)$$

We have to stress that one must not think that these two identities of the binomial coefficients contain physics of the diffusion and the Smoluchowski equations. Physics sits in the random walk process and is contained in the formula for the transition probability (2.5).

### 2.3 Euclidean form of the Schrödinger equation

As we have already seen  $\rho(x, t)$  is a solution of the diffusion equation (2.4) which, in turn, is the Euclidean form of the Schrödinger equation of a free particle. One may ask whether the Euclidean version of the Schrödinger equation for a particle moving in a potential  $V(x)$ ,

$$\frac{\partial \rho(x, t)}{\partial t} = \frac{\hbar}{2m} \frac{\partial^2 \rho(x, t)}{\partial x^2} - \frac{V(x)}{\hbar} \rho(x, t), \quad (2.14)$$

has also an interpretation in terms of the Brownian motions? The answer, in the affirmative, was given by Kac [2.4]. Indeed, let us set the particle in motion from  $x = 0$  at  $t = 0$  and assume that our particle at each  $x$  has a probability  $V(x)dt/\hbar$  (we assume  $V(x) > 0$ ) of being suppressed (annihilated). Kac calls it a random walk with holes: at  $x$  there is the probability,  $V(x)dt/\hbar$ , of falling into a hole and disappearing from existence.

The consequences of this ansatz are as follows. The particle following the path  $x(t)$  has the probability of *survival* until  $t + dt$  equal to

$$1 - \frac{V(x(t))}{\hbar} dt \approx \exp\left(-\frac{V(x(t))}{\hbar} dt\right). \quad (2.15)$$

But, in consecutive sections of time,  $dt$ , survivals are independent hence, the probability of survival in time from zero up to  $t$  is

$$\exp\left(-\frac{1}{\hbar} \int_0^t V(x(\tau)) d\tau\right). \quad (2.16)$$

Therefore, to get the complete expression for  $\rho(x, t)$ , which satisfies (2.14), in terms of the integral over paths we have to combine the above with the contribution of the free motion (2.3) and obtain

$$\rho(x, t) = \int_{x(0)=0}^{x(t)=x} [\mathcal{D}x(t)] e^{-\frac{1}{\hbar} \int_0^t [\frac{1}{2}m\dot{x}^2 + V(x)] d\tau} = \left\langle e^{-\frac{1}{\hbar} \int_0^t V(x(\tau)) d\tau} \right\rangle_{S_0}. \quad (2.17)$$

Here  $S_0$  is the free particle action. The last part of (2.17) tells us that we may interpret  $\rho(x, t)$  for a Brown particle moving under influence of the potential  $V(x) > 0$  as an averaged probability of its survival during the lapse of time  $[0, t]$ .

In fact, equation (2.17) is a special case of the following object: the paths are Brownian and we sum over them *any well defined functional of paths*, e.g.  $\exp(-\int_0^t d\tau V(x(\tau))/\hbar)$  in the above case. Sometimes one calls it a path integral over the conditional Wiener measure,  $d\mu[x(\tau)]$ , and writes

$$\langle x | e^{-\frac{t}{\hbar} H} | 0 \rangle = \int d\mu[x(\tau)] e^{-\frac{1}{\hbar} \int_0^t d\tau V(x(\tau))}. \quad (2.18)$$

Operationally this might be done through introduction of the Euclidean time,  $t \rightarrow -i\tau$  into “regular” path integrals.

Now we shall discuss some important applications of the Euclidean forms of the quantum path integral *amplitudes* (*not* the probability densities we are dealing with in the case of classical Brownian motions). Note that already the random walks with holes just discussed give not only probability *densities* but also quantal (non-conserving probability) *amplitudes*.

To avoid confusion we will change the notation, the lapse of the Euclidean time we will denote by  $\tau$ , and instead of  $\rho$  we will write  $K(x_b, x_a, -i\tau)$ . Let us employ the Euclidean analog of (??). It reads

$$\begin{aligned} K(x_b, x_a, -i\tau) &= \langle x_b | e^{-\frac{H}{\hbar} \tau} | x_a \rangle \\ &= \sum_{n, n'} \langle x_b | E_n \rangle \langle E_n | e^{-\frac{H}{\hbar} \tau} | E_{n'} \rangle \langle E_{n'} | x_a \rangle \\ &= \sum_n e^{-\frac{E_n}{\hbar} \tau} \phi_n(x_b) \phi_n^*(x_a). \end{aligned} \quad (2.19)$$

This formula implies that the lowest energy term in the sum dominates when  $\tau \rightarrow \infty$ . Therefore, having  $K(x_b, x_a, -i\tau)$  we can extract the lowest energy of the system,  $E_0$ , through the following limiting procedure:

$$E_0 = - \lim_{\tau \rightarrow \infty} \left\{ \frac{\hbar}{\tau} \ln \left( \int dx K(x, x, -i\tau) \right) \right\}. \quad (2.20)$$

This is the Feynman–Kac formula. One can write it in many other forms, e.g.

$$E_0 = - \lim_{\tau \rightarrow \infty} \left\{ \frac{\hbar}{\tau} \ln (K(x_b, x_a, -i\tau)) \right\}, \quad (2.21)$$

because the dependences on  $x_b$  and  $x_a$  are irrelevant, as long as the  $\ln$  operation does not hit one of the zeros of the eigenfunctions  $\phi_n$ .

Kac tells us in ref.[2.4] that already in 1949 he tried to estimate  $E_0$  for a few simple potentials randomly choosing a hundred of trajectories, 60 steps each (taking  $\tau$  as large as possible), and numerically performing the sum over trajectories and taking logarithm of this sum. These were, probably, the first computer simulations of this kind.

Let us sketch a more modern technique for performing the sum over paths due to Metropolis [2.6] (see also [2.7]). In order to obtain  $E_0$  and  $|\phi_0(x)|^2$  we identify  $x_b = x_a = x$  in (2.10), and for the sake of simplicity set  $\hbar = m = 1$ . Let the stretch of Euclidean time be:  $[0, \tau]$ . We discretize  $\tau$  into  $n + 1$  very small bits  $\epsilon = \tau/(n + 1)$ , and set  $x_0 = x_{n+1} = x$ . Hence our trajectory,  $\xi$ , is represented by a sequence of intermediate positions

$$\xi = (x_0 = x, x_1, x_2, \dots, x_n, x_{n+1} = x).$$

The object to simulate is

$$K_n(x, x, -i\tau) = \int dx_1 dx_2 \dots dx_n \left( \frac{1}{2\pi\epsilon} \right)^{\frac{1}{2}(n+1)} e^{-\epsilon \sum_{j=0}^n \left\{ \frac{1}{2} \left( \frac{x_{j+1} - x_j}{\epsilon} \right)^2 + V(x_j) \right\}}. \quad (2.22)$$

In what follows we shall also use the following expressions

$$E(\xi, \epsilon) = \sum_{j=0}^n \left\{ \frac{1}{2} \left( \frac{x_{j+1} - x_j}{\epsilon} \right)^2 + V(x_j) \right\}, \quad S(\xi, \epsilon) = \epsilon E(\xi, \epsilon). \quad (2.23)$$

Selection of a set of trajectories *important* in supporting (2.22) is to be decided (clearly, there must be host of them whose contribution to (2.22) is irrelevant: they contribute very little). Here is how we generate a reasonable set.

1. We choose the first trajectory  $\xi^{(0)}$ . This choice is left entirely to the industry of the person who does the simulation.
2. We choose randomly an entire number  $1 \leq j \leq n$  and a real, small, number  $0 \leq \eta \leq 1$  and we define  $\xi'$  whose only difference with  $\xi^{(0)}$  is the  $j$ -th component.

3. Let the  $j$ -th component of  $\xi'$  be

$$x'_j = x_j + (2\eta - 1)\alpha ,$$

where  $\alpha$  is of order  $\epsilon$  and is a fixed numerical parameter defining numerical integration and discretization.

4. We calculate

$$\Delta E = E(\xi', \epsilon) - E(\xi, \epsilon) .$$

- If  $\Delta E < 0$  we choose as the new trajectory

$$\xi^{(1)} = \xi' .$$

- If  $\Delta E > 0$  we choose  $\xi^{(1)} = \xi'$  with the probability

$$e^{-\epsilon\Delta E} = e^{-\Delta S} ,$$

and  $\xi^{(1)} = \xi^{(0)}$  with the probability

$$1 - e^{-\epsilon\Delta E} .$$

5. Choosing with a prescribed probability is accomplished as follows: first we randomly generate  $0 \leq \eta' \leq 1$ , and

- if  $\eta' \leq e^{-\epsilon\Delta E}$ , we choose  $\xi^{(1)} = \xi'$ ,
- if  $\eta' > e^{-\epsilon\Delta E}$ , we choose  $\xi^{(1)} = \xi^{(0)}$ .

6. We choose  $\xi^{(2)}$  from  $\xi^{(1)}$  the same way we have just chosen  $\xi^{(1)}$  from  $\xi^{(0)}$ , and continue this procedure.

7. This procedure results in a set of  $[\xi^{(k)}]$  which tends to become a set of *dominant trajectories* in a functional integral. Note: the rule which allows acceptance of  $\Delta E > 0$  prevents this procedure to get stuck in a local minimum of  $E$ .

8. Taking the sum  $\sum_k e^{-S(\xi^{(k)}, \epsilon)} [\mathcal{D}\xi^{(n)}]$  we get  $K_n(x, x, t)$ , where  $[\mathcal{D}\xi^{(n)}]$  is the coefficient in front of the exponential in (2.22). In practice (see below) we do not have to deal with  $[\mathcal{D}\xi^{(n)}]$ , as it cancels out in evaluations of e.g.  $E_0$ .

*Note:* If the classical Hamiltonian implies a minimum of energy at  $x = 0$ , the trajectories *dominating* the ground state fluctuate around  $x = 0$ . In this case it is natural to start the Monte Carlo procedure close to  $x = 0$ .

9. The process of generating trajectories gives us the square of the absolute value of the ground state wave function  $|\psi(x)|^2$ . Indeed, we divide the  $x$ -axis into bins

$$(m\Delta, (m+1)\Delta), \quad m = 0, \pm 1, \pm 2, \pm 3, \dots$$

Let us consider the  $k$ -th step in our stochastic procedure:  $x_j$  is allowed to acquire a new value  $x_j + \alpha(2\eta - 1)$ . Hence the variable  $x_j$  in the  $k+1$



step either stays the same,  $x_j$ , or becomes  $x_j + \alpha(2\eta - 1)$ . At each step the  $j$ -th component hits a bin  $(m\Delta, (m+1)\Delta)$ . Every time a bin gets hit we give it a point. While the stochastic process develops the bins collect points.  $|\psi_0(x)|^2$  is proportional to the number of points the bin containing  $x$  collects. We only have to normalize the distribution to have  $|\psi_0(x)|^2$ . (*Note:* the factor  $e^{-E_0\tau/\hbar}$  does not appear in this procedure, but  $\tau$  must be very large).

As it turns out extracting  $E_0$  directly from  $K(x, x, \tau)$  (or from  $K_n(x, x, \tau)$ ) is not effective, and it is better to work out the following expression

$$\begin{aligned} E_0 &= \lim_{\tau \rightarrow \infty} \frac{\int [\mathcal{D}x(\tau')] e^{-\frac{1}{\hbar}S[x(\tau')]} H(x, \dot{x})}{\int [\mathcal{D}x(\tau')] e^{-\frac{1}{\hbar}S[x(\tau')]} } = \frac{\langle x | e^{-\frac{1}{\hbar}H\tau} H | x \rangle}{\langle x | e^{-\frac{1}{\hbar}H\tau} | x \rangle} \\ &= \lim_{\tau \rightarrow \infty} \frac{\sum_k e^{-\frac{\tau}{\hbar}E_k} \langle k | H | k \rangle |\phi_k(x)|^2}{\sum_k e^{-\frac{\tau}{\hbar}E_k} |\phi_k(x)|^2}. \end{aligned} \quad (2.24)$$

In terms of the discretized quantities defined above we write (2.24) as follows. First, we have to generate a set of  $M$  trajectories  $[\xi_\nu]$  where  $M \gg 1$  and  $\tau$  is very large. The probability of realizing the  $\nu$ 'th trajectory is

$$P(\xi_\nu) = \frac{e^{-\frac{1}{\hbar}S[\xi_\nu, \epsilon]}}{\sum_{\nu'} e^{-\frac{1}{\hbar}S(\xi_{\nu'}, \epsilon)}}, \quad (2.25)$$

and we have

$$E_0 \approx \sum_{\nu=0}^M P(\xi_\nu) E(\xi_\nu, \epsilon). \quad (2.26)$$

We can remove (a cumbersome to deal with)  $\dot{x}$  appearing in  $E$  or  $H$  employing the virial theorem which equates these two averages

$$\langle \frac{1}{2}m\dot{x}^2 \rangle = \frac{1}{2} \langle xV'(x) \rangle, \quad (2.27)$$

hence the practical formula for evaluating  $E_0$  reads

$$E_0 = \sum_{\nu=0}^M P(\xi_\nu) \left[ \frac{1}{2}\xi_\nu V'(\xi_\nu) + V(\xi_\nu) \right]. \quad (2.28)$$

## Appendix C: Virial theorem

We prove virial theorem for a set of massive point particles having positions  $\mathbf{r}_i$  and moving under influence of forces  $\mathbf{F}_i$ . The equations of motion are

$$\dot{\mathbf{p}}_i = \mathbf{F}_i. \quad (C.1)$$

We define

$$G = \sum_i \mathbf{p}_i \cdot \mathbf{r}_i, \quad (C.2)$$

thus

$$\frac{dG}{dt} = \sum_i \dot{\mathbf{p}}_i \cdot \mathbf{r}_i + \sum_i \dot{\mathbf{r}}_i \cdot \mathbf{p}_i. \quad (\text{C.3})$$

We rewrite the second term:

$$\sum_i \dot{\mathbf{r}}_i \cdot \mathbf{p}_i = \sum_i m_i \dot{\mathbf{r}}_i \cdot \dot{\mathbf{r}}_i = 2T \quad (\text{C.4})$$

which is twice the total kinetic energy. The first term, on the other hand is

$$\sum_i \dot{\mathbf{p}}_i \cdot \mathbf{r}_i = \sum_i \mathbf{F}_i \cdot \mathbf{r}_i, \quad (\text{C.5})$$

Hence

$$\frac{dG}{dt} = 2T + \sum_i \mathbf{F}_i \cdot \mathbf{r}_i. \quad (\text{C.6})$$

Now take its average over time  $(0, \tau)$ :

$$\frac{1}{\tau} \int_0^\tau \frac{dG}{dt} dt = 2 \langle T \rangle + \left\langle \sum_i \mathbf{F}_i \cdot \mathbf{r}_i \right\rangle = \frac{1}{\tau} [G(\tau) - G(0)]. \quad (\text{C.7})$$

When the motion is bounded (e.g. periodic) the bracket [...] stays finite. Therefore, when  $\tau \rightarrow \infty$ , we obtain the virial theorem:

$$\langle T \rangle = -\frac{1}{2} \left\langle \sum_i \mathbf{F}_i \cdot \mathbf{r}_i \right\rangle. \quad (\text{C.8})$$

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