Brownian motion Masatsugu Sei Suzuki SUNY at Binghamton (Date: August 01, 2017)

The heat equation proposed by Fourier in 1822 has been applied to investigating a temperature distribution in materials. In 1827, the so-called Brownian motion was found, where the self-diffusion of water is visualized by pollen micro particles motion. Nevertheless, the Brownian motion had not been recognized as a diffusion problem until the Einstein theory of Brownian motion in 1905. Although it was a typical diffusion problem, Fick applied the heat equation to the diffusion phenomena in 1855.

https://en.wikipedia.org/wiki/Diffusion_equation

In 1905, Einstein found a general relation between a coefficient of friction on the particles and the diffusion constant related to the position of particles. On the other hand, Langevin presented an equation motion with probability, for the particles when they are influenced by irregular forces. This is called a Langevin equation. The magnitude of the fluctuating force (irregular force) which appears in the Langevin equation, is related to the diffusion co-efficient for the position of particles by the Einstein relation (fluctuation-dissipation theorem).

1. Einstein's analysis: the random walk

We now consider a simple model of Brownian movement, or the so-called random walk model, in one dimension. We consider a particle starting at x = 0 at t = 0 which suffers impacts at s steady rate v per second. Each impact causes the particle to jump a (small) distance l, of constant magnitude, either in the positive or negative direction of x. We assume that these steps of +l or -l are uncorrelated with one another. Let us denote the *n*-th step by l_n ($l_n = \pm l$) and consequently the total displacement x after N steps,

$$x = \sum_{n=1}^{N} l_n = (l_1 + l_2 + l_3 + \dots + l_N)$$

 $l_i = \pm l$

where

The average

$$\left\langle x \right\rangle = \sum_{n=1}^{N} \left\langle l_n \right\rangle = 0$$

$$\langle x^{2} \rangle = < (\sum_{n=1}^{N} l_{n})^{2} >$$

$$= < (l_{1} + l_{2} + l_{3} + \dots + l_{N})(l_{1} + l_{2} + l_{3} + \dots + l_{N}) >$$

$$= \sum_{n=1}^{N} \langle l_{n}^{2} \rangle + \sum_{n \neq m}^{N} \langle l_{n} l_{m} \rangle$$

Note that the bracket $\langle x \rangle$ signify an average taken over a large group of many similar observations of the displacement x (usually known as an ensemble average). Since

$$\left\langle l_n l_m \right\rangle = l^2, l(-l), (-l)l, l^2$$

 $\sum_{n \neq m}^N \left\langle l_n l_m \right\rangle = 0$

we have

$$\langle x^2 \rangle = N l^2$$

Suppose that we have v steps per second.

$$N = vt$$

 $\sqrt{\langle x^2 \rangle} = \sqrt{vtl^2} = \sqrt{v}l\sqrt{t}$ (complete randomness)

 \sqrt{t} is regarded as typical of any limiting random walk process.

The relative error:

$$\varepsilon = \frac{\sqrt{Nl}}{Nl} = \frac{1}{\sqrt{N}}$$

2. Brownian movement and irreversibility

If a particle subject to Newton's law of motion starts at t = 0, with velocity v_0 , then after a short time its displacement will be given by

$$x = v_0 t$$
, $x^2 = v_0^2 t^2$

or

$$\left\langle x^2\right\rangle = \left\langle v_0^2\right\rangle t^2$$

if we consider an ensemble of such particles obeying Newton's laws of motion. So we have

$$\sqrt{\langle x^2 \rangle} = \sqrt{\langle v_0^2 \rangle} t \approx t$$
. (complete regularity)

3. The Diffusion equation and viscosity

Einstein derived essentially $\sqrt{\langle x^2 \rangle} = \sqrt{\nu t l^2} = \sqrt{\nu l} \sqrt{t}$ by considering the diffusion of molecules or particles directly as a random walk problem.

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

where

 $2D = l^2 v$

D is the diffusion constant

$$D = Bk_{B}T$$

4. Diffusion equation

Einstein showed that the random walk model provided a detailed solution of the familiar diffusion equation in one dimension.

If J_n is the particle current density and *n* the particle concentration, the diffusion is described by the Fick's law

$$\boldsymbol{J}_n = -D\nabla n$$

where D is the diffusivity. The conservation equation

$$\nabla \cdot \boldsymbol{J}_n + \frac{\partial n}{\partial t} = 0$$

leads to the diffusion equation

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2} \tag{1}$$

in one dimension. Suppose at t = 0 in an infinite medium

$$n(x,t=0) = N\delta(x)$$

where $\delta(x)$ is the Dirac delta function. We have N particles concentrated at x = 0 when t = 0. Solving eq.(1), we have

$$n(x,t) = N \frac{1}{\sqrt{4\pi Dt}} \exp(-\frac{x^2}{4Dt})$$

which has the form of Gaussian,

$$\langle x^2 \rangle = 2Dt$$

Einstein demonstrated that the diffusion and Brownian movement were essentially one and the same thing, and that both were fundamentally due to molecular agitation.

5. Gaussian distribution

$$f(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp(-\frac{x^2}{4Dt})$$

which is the same as the Gaussian distribution

$$f(x,\sigma) = \frac{1}{\sqrt{2\pi\sigma}} \exp(-\frac{x^2}{2\sigma^2})$$

with

$$\sigma^2 = 2Dt$$

Note that

$$\langle x \rangle = \int_{-\infty}^{\infty} x f(x,\sigma) dx = 0$$
$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 f(x,\sigma) dx = \sigma^2 = 2Dt$$

6. Langevin's analysis: random force

Shortly after Einstein's work, Labgevin (1908) put forward an analysis of Brownian movement, which coulod also take account directly of the inertial forces acting on the system as well as viscosity.

We start with an equation of motion for a particle (mass m) with mass m with a resistive force $-\zeta v$ and a random force $\eta(t)$.

 $m\dot{v} = -\varsigma v + \eta(t)$

or

$$m\ddot{x} = -\dot{\zeta}\dot{x} + \eta(t)$$

where ζ is defined by

$$\zeta = \frac{m}{\tau}$$

and τ is a relaxation time. This leads to

$$mx\ddot{x} = -\varphi x\dot{x} + x\eta(t)$$

Noting that

$$\frac{d}{dt}(x\dot{x}) = x\ddot{x} + \dot{x}^2$$

we get

$$m\frac{d}{dt}(x\dot{x}) = m\dot{x}^2 - \varsigma x\dot{x} + x\eta(t)$$

We average this result over time. *x* and η are uncorrelated;

$$\langle x\eta \rangle = \langle x \rangle \langle \eta \rangle = 0$$

We also use the equipartition theorem for the 1 D system

$$\frac{1}{2}m\left\langle \dot{x}^{2}\right\rangle =\frac{1}{2}k_{B}T$$

Using these results, we get

$$m\frac{d}{dt}\langle x\dot{x}\rangle = m\langle \dot{x}^2 \rangle - \varsigma \langle x\dot{x}\rangle = k_B T - \varsigma \langle x\dot{x}\rangle$$

or

$$\frac{d}{dt}\langle x\dot{x}\rangle = -\frac{\varsigma}{m}[\langle x\dot{x}\rangle - \frac{k_BT}{\varsigma}]$$

The solution for $\langle x\dot{x} \rangle$ is

$$\langle x\dot{x}\rangle = C \exp(-\frac{\zeta}{m}t) + \frac{k_B T}{\zeta}$$

We use the boundary condition (x = 0 at t = 0). We find that

$$C = -\frac{k_{\scriptscriptstyle B}T}{\varsigma}$$

Using the identity

$$\left\langle x\dot{x}\right\rangle = \frac{1}{2}\frac{d}{dt}\left\langle x^{2}\right\rangle$$

we have

$$\frac{d}{dt}\left\langle x^{2}\right\rangle = \frac{2k_{B}T}{\varsigma}\left[1 - \exp\left(-\frac{\varsigma}{m}t\right)\right]$$

$$\left\langle x^{2} \right\rangle = \frac{2k_{B}T}{\varsigma} \left[t + \frac{m}{\varsigma} \exp\left(-\frac{\varsigma}{m}t\right)\right]$$
(a) For $t << \frac{m}{\varsigma}$

$$\left\langle x^{2} \right\rangle \approx \frac{k_{B}Tt^{2}}{m}$$
(b) For $t >> \frac{m}{\varsigma}$

$$\left\langle x^{2} \right\rangle = \frac{2k_{B}Tt}{\varsigma} = 2Dt.$$

where D is the diffusion constant and is defined as

$$D = \frac{k_{B}T}{\varsigma}$$

The unit of D is

$$[D] = \frac{\text{erg}}{\frac{\text{erg s}}{\text{cm}^2}} = \frac{\text{cm}^2}{\text{s}}$$

since $[\alpha] = \frac{\operatorname{erg } s}{\operatorname{cm}^2}$.

Einstein showed that the random walk model provided a detailed solution of the familiar diffusion equation in 1D system. The phenomenal solution of the familiar diffusion equation in one dimension reads

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2}$$

where f(x,t) gives the relative density of particles at x at time t. D is the diffusion constant

7. Correlation

From the definition of the derivative with respect to t,

$$\dot{v} = \frac{v(t+\tau) - v(t)}{\tau}$$
 in the limit of $\tau \to 0$

Using this relation, the equation of motion

$$\dot{v} = -\frac{\varsigma}{m}v + \frac{1}{m}\eta(t)$$

can be rewritten as

$$\frac{v(t+\tau)-v(t)}{\tau} = -\frac{\varsigma}{m}v(t) + \frac{1}{m}\eta(t)$$

Multiplying this equation by v(0) on both sides, we get

$$v(0)[\frac{v(t+\tau) - v(t)}{\tau}] = -\frac{\varsigma}{m}v(0)v(t) + \frac{1}{m}v(0)\eta(t)$$

Taking the time average,

$$\frac{\langle v(0)v(t+\tau) - v(0)v(t) \rangle}{\tau} = -\frac{\varsigma}{m} \langle v(0)v(t) \rangle + \frac{1}{m} \langle v(0)\eta(t) \rangle$$

Since v(t) and $\eta(t)$ are uncorrelated,

$$\frac{\langle v(0)v(t+\tau) - v(0)v(t) \rangle}{\tau} = -\frac{\varsigma}{m} \langle v(0)v(t) \rangle$$

In the limit of $\tau \to 0$, we have

$$\frac{d}{dt}\langle v(0)v(t)\rangle = -\frac{\varsigma}{m}\langle v(0)v(t)\rangle$$

The solution is

$$\left\langle v(0)v(t)\right\rangle = \left\langle \left[v(0)\right]^2 \right\rangle \exp\left(-\frac{\zeta t}{m}\right) = \frac{k_B T}{m} \exp\left(-\frac{\zeta t}{m}\right)$$

where

$$\frac{1}{2}m\langle \dot{x}^2 \rangle = \frac{1}{2}m\langle [v(0)]^2 \rangle = \frac{1}{2}k_BT$$

8. Langevin's equation: Einstein relation

We consider the Langevin equation with force *F*;

$$m\frac{d}{dt}v(t) = -\varsigma v(t) + \eta(t) + F$$

By taking the average,

$$m\frac{d}{dt}\langle v(t)\rangle = -\zeta \langle v(t)\rangle + \langle \eta(t)\rangle + F$$
$$= -\zeta \langle v(t)\rangle + F$$

since $\langle \eta(t) \rangle = 0$. The solution of this equation is

$$\langle v(t) \rangle = \frac{F}{\varsigma} (1 - e^{-\frac{\varsigma}{m}}) + \langle v(t=0) \rangle e^{-\frac{\varsigma}{m}}$$

When $t \to \infty$, we have the so-called terminal velocity as

$$v = \frac{F}{\varsigma} = \mu F$$

with the mobility μ as

$$\mu = \frac{1}{\varsigma}.$$

Using the relation $D = \frac{k_B T}{\varsigma}$, we obtain the Einstein relation as

$$D = \mu k_{\rm B} T$$

9. Fluctuation-Dissipation theorem))

$$\int_{0}^{\infty} \langle v(0)v(t) \rangle dt = \frac{k_{B}T}{m} \int_{0}^{\infty} \exp(-\frac{\varsigma t}{m}) dt$$
$$= \frac{k_{B}T}{\varsigma}$$

or

$$\frac{1}{\varsigma} = \frac{1}{k_B T} \int_0^\infty \langle v(0)v(t) \rangle dt$$

Since $\mu = \frac{1}{\zeta}$, we have the expression for the mobility μ as

$$\mu = \frac{1}{k_B T} \int_0^\infty \left\langle v(0) v(t) \right\rangle dt$$

10. Property of random force

$$\langle \eta(t) \rangle = 0$$
, $\langle \eta(t) \eta(t') \rangle = 2\varepsilon \delta(t-t')$

where ε is the strength of random force. Here we show that $\varepsilon = k_B T \varsigma$.

We start with

$$\dot{v}(t) = -\frac{\varsigma}{m}v(t) + \frac{1}{m}\eta(t)$$

The solution of this equation is

$$v(t) = e^{-\frac{\mathcal{A}}{m}} \left[\int_{0}^{t} e^{\frac{\mathcal{A}}{m}} \frac{\eta(s)}{m} ds + v(0) \right]$$

The fluctuation;

$$\left\langle v^{2}(t) \right\rangle = \left\langle e^{-\frac{\sigma}{m}} \left[\int_{0}^{t} e^{\frac{\sigma}{m}} \frac{\eta(s)}{m} ds + v(0) \right] e^{-\frac{\sigma}{m}} \left[\int_{0}^{t} e^{\frac{\sigma}{m}} \frac{\eta(s')}{m} ds' + v(0) \right] \right\rangle$$

$$= e^{-\frac{2\sigma}{m}} \left\langle v^{2}(0) \right\rangle + e^{-\frac{2\sigma}{m}} \frac{1}{m^{2}} \int_{0}^{t} ds \int_{0}^{t} e^{\frac{\varsigma(s+s')}{m}} \eta(s) \eta(s') ds'$$

$$= e^{-\frac{2\sigma}{m}} \left\langle v^{2}(0) \right\rangle + e^{-\frac{2\sigma}{m}} \frac{2\varepsilon}{m^{2}} \int_{0}^{t} ds \int_{0}^{t} ds' e^{\frac{\varsigma(s+s')}{m}} \delta(s-s')$$

$$= e^{-\frac{2\sigma}{m}} \left\langle v^{2}(0) \right\rangle + e^{-\frac{2\sigma}{m}} \frac{2\varepsilon}{m^{2}} \int_{0}^{t} ds e^{\frac{2\sigma}{m}}$$

$$= e^{-\frac{2\sigma}{m}} \left\langle v^{2}(0) \right\rangle + \frac{\varepsilon}{m\varsigma} (1 - e^{-\frac{2\sigma}{m}})$$

since $\langle \eta(t)v(0) \rangle = 0$. In the limit of $t \to \infty$, we have

$$\left\langle v^2(t) \right\rangle \rightarrow \frac{\varepsilon}{m\varsigma}$$

We note the energy partition relation for 1D system;

$$\frac{1}{2}m\langle v^2\rangle = \frac{1}{2}k_BT$$

Then we have

$$\frac{\varepsilon}{m\zeta} = \frac{k_B T}{m}$$

or

$$\varepsilon = k_B T \varsigma$$

From the relation $\langle \eta(t)\eta(t')\rangle = 2k_B T \varsigma \delta(t-t')$, we have

$$\varsigma = \frac{1}{k_B T} \int_{0}^{\infty} \langle \eta(t) \eta(0) \rangle dt \qquad (Fluctuation-dissipation theorem)$$

11. Power spectrum

The Fourier transform

$$x(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} x(t) dt, \qquad x(-\omega) = x^*(\omega) = \int_{-\infty}^{\infty} e^{-i\omega t} x(t) dt$$

The inverse Fourier transform:

$$x(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} x_{\omega}(\omega) d\omega$$

where

$$\int_{-\infty}^{\infty} e^{i\omega(t-t')} d\omega = 2\pi\delta(t-t')$$

((Note))

In physics, we use the Fourier transform such that

$$\chi(k,\omega) = \int dx \int dt \ e^{-i(kx-\omega t)} \chi(x,t)$$

or

$$\chi(x,t) = \frac{1}{(2\pi)^2} \int dk \int d\omega \, e^{i(kx-\omega t)} \chi(k,\omega)$$

which are different from the Fourier transform in mathematics in sign in front of ω .

12. Autocorrelation function

$$x(t)x(t+\tau) = \frac{1}{4\pi^2} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' e^{-i\omega(t+\tau)} e^{-i\omega' t} x(\omega) x(\omega')$$

The infinite time integral of this product is

$$\int_{-\infty}^{\infty} dt x(t) x(t+\tau) = \frac{1}{4\pi^2} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' e^{-i\omega(t+\tau)} e^{-i\omega't} x(\omega) x(\omega')$$
$$= \frac{1}{4\pi^2} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' e^{-i\omega\tau} x(\omega) x(\omega') \int_{-\infty}^{\infty} dt e^{-i(\omega+\omega')t}$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' e^{-i\omega\tau} x(\omega) x(\omega') \delta(\omega+\omega')$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega\tau} x(\omega) x(-\omega)$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega\tau} x(\omega) x^*(\omega)$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega\tau} |x(\omega)|^2$$

The autocorrelation function is defined by

$$\left\langle x(0)x(t)\right\rangle = \int_{-\infty}^{\infty} dt' x(t')x(t'+t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \left\langle \left| x(\omega) \right|^2 \right\rangle$$

which means that $\langle |x(\omega)|^2 \rangle$ is the Fourier transform of $\langle x(0)x(t) \rangle$,

$$\left\langle \left| x(\omega) \right|^2 \right\rangle = \int_{-\infty}^{\infty} e^{i\omega t} \left\langle x(0)x(t) \right\rangle dt$$

When t = 0, we have

$$\langle x^{2}(0) \rangle = \langle x^{2} \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \langle |x(\omega)|^{2} \rangle$$

13. Determination of e for
$$\langle \eta(t)\eta(t')\rangle = 2\varepsilon\delta(t-t')$$

We solve the equation given by

$$m\dot{v}(t) = -\varsigma v(t) + \eta(t)$$

with

$$\langle \eta(t) \rangle = 0$$
, $\langle \eta(t)\eta(t') \rangle = 2\varepsilon \delta(t-t')$

using the Fourier transform.

$$v(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} v(\omega) d\omega, \qquad \eta(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} \eta(\omega) d\omega$$
$$\dot{v}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} (-i\omega) e^{-i\omega t} v(\omega) d\omega$$

Thus we have

$$-im\omega v(\omega) = -\varsigma v(\omega) + \eta(\omega)$$

or

$$v(\omega) = \frac{\eta(\omega)}{-im\omega + \varsigma}$$

or

$$\left|v(\omega)\right|^{2} = \frac{\left|\eta(\omega)\right|^{2}}{m^{2}\omega^{2} + \zeta^{2}}$$

According to the Wiener-Khinchin theorem, we get

$$\left\langle \left| v(\omega) \right|^2 \right\rangle = \int_{-\infty}^{\infty} e^{i\omega t} \left\langle v(0)v(t) \right\rangle dt = \frac{\left| \eta(\omega) \right|^2}{m^2 \omega^2 + \varsigma^2} = \frac{2\varepsilon}{m^2 \omega^2 + \varsigma^2}$$

where

$$\left\langle \left| \eta(\omega) \right|^2 \right\rangle = \int_{-\infty}^{\infty} e^{i\omega t} \left\langle \eta(0)\eta(t) \right\rangle dt = 2\varepsilon \int_{-\infty}^{\infty} e^{i\omega t} \delta(t) dt = 2\varepsilon$$

Thus we get

$$\left\langle v^{2} \right\rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \left\langle \left| v(\omega) \right|^{2} \right\rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{2\varepsilon}{m^{2}\omega^{2} + \zeta^{2}} = \frac{\varepsilon}{\zeta m}$$

Since $m \langle v^2 \rangle = k_B T$, we obtain ε as

 $\varepsilon = k_{\rm B} T \varsigma$

14. The correlation function

The Fourier transform $x(\omega)$ of the position x(t)

$$x(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} x(\omega) d\omega, \qquad v(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} v(\omega) d\omega$$
$$v(t) = \dot{x}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} [-i\omega x(\omega)] d\omega$$

which leads to the relation

$$x(\omega) = \frac{v(\omega)}{-i\omega}$$

Then we get

$$x(\omega) = \frac{\eta(\omega)}{(-i\omega)(-im\omega + \zeta)}$$

or

$$|x(\omega)|^{2} = \frac{|\eta(\omega)|^{2}}{\omega^{2}(m^{2}\omega^{2} + \zeta^{2})}$$

According to the Wiener-Khinchin theorem, we get

$$\left\langle \left| x(\omega) \right|^2 \right\rangle = \int_{-\infty}^{\infty} e^{i\omega t} \left\langle x(0)x(t) \right\rangle dt$$
$$= \frac{\left| \eta(\omega) \right|^2}{\omega^2 (m^2 \omega^2 + \varsigma^2)}$$
$$= \frac{2\varepsilon}{m^2} \frac{1}{\omega^2 (\omega^2 + \frac{\varsigma^2}{m^2})}$$
$$= \frac{2\varepsilon}{\varsigma^2} \left(\frac{1}{\omega^2} - \frac{1}{\omega^2 + \gamma^2} \right)$$

where $\gamma = \frac{\varsigma}{m}$

From the inverse Fourier transform, we also get

$$\langle x(0)x(t)\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty}e^{-i\omega t}\frac{2\varepsilon}{\omega^2(m^2\omega^2+\varsigma^2)}$$

First we consider the integral,

$$\langle x(t)^2 \rangle = \langle x(0)^2 \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{2\varepsilon}{\omega^2 (m^2 \omega^2 + \varsigma^2)}.$$

This integral is divergent because of the extra factor of ω^2 in the denominator. So we correctly conclude that $\langle x(t)^2 \rangle$ is infinite. However, the average

$$\left\langle \left[x(t) - x(0) \right]^2 \right\rangle = \left\langle \left[\Delta x(t) \right]^2 \right\rangle$$

is finite.

$$\begin{split} \left\langle [\Delta x(t)]^2 \right\rangle &= \left\langle x(t)^2 \right\rangle + \left\langle x(0)^2 \right\rangle - 2 \left\langle x(t)x(0) \right\rangle \\ &= \frac{2}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{2\varepsilon}{\omega^2 (m^2 \omega^2 + \varsigma^2)} - \frac{2}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \frac{2\varepsilon}{\omega^2 (m^2 \omega^2 + \varsigma^2)} \\ &= \frac{2\varepsilon}{\pi} \int_{-\infty}^{\infty} d\omega \frac{1}{\omega^2 (m^2 \omega^2 + \varsigma^2)} (1 - e^{-i\omega t}) \\ &= \frac{2\varepsilon}{\pi \varsigma^2} \int_{-\infty}^{\infty} d\omega (\frac{1}{\omega^2} - \frac{1}{\omega^2 + \gamma^2}) (1 - e^{-i\omega t}) \\ &= \frac{2\varepsilon}{\varsigma^2} (|t| - \frac{1 - e^{-\gamma |t|}}{\gamma}) \end{split}$$

Since $\varepsilon = k_B T \varsigma$, we have

$$\left\langle \left[\Delta x(t)\right]^{2}\right\rangle = \frac{2k_{B}T}{\varsigma}\left(\left|t\right| - \frac{1 - e^{-\gamma|t|}}{\gamma}\right) = 2D\left(\left|t\right| - \frac{1 - e^{-\gamma|t|}}{\gamma}\right)$$

with

$$D = \frac{k_B T}{\varsigma}$$

For $t >> \frac{1}{\gamma}$,

$$\left\langle \left[\Delta x(t)\right]^2 \right\rangle = 2D(\left|t\right| - \frac{1 - e^{-\gamma |t|}}{\gamma}) = D\gamma t^2$$

$$I(t,\gamma) = \int_{-\infty}^{\infty} d\omega \frac{1}{\omega^2 + \gamma^2} (1 - e^{-i\omega t}) = \int_{-\infty}^{\infty} d\omega \frac{1}{\omega^2 + \gamma^2} - \int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega^2 + \gamma^2} = \frac{\pi}{\gamma} (1 - e^{-\gamma|t|})$$

We use the residue theorem for the second term. For t>0 we use the lower half plane of the complex plane (a single pole is at $-i\gamma$) and for t<0, we use the upper half plane (a single pole is at $i\gamma$).

$$I(t,\gamma \to 0) = \int_{-\infty}^{\infty} d\omega \frac{1}{\omega^2} (1 - e^{-i\omega t}) = \lim_{\gamma \to 0} \frac{\pi}{\gamma} (1 - e^{-\gamma |t|}) = \pi |t|$$

15. Nyquist's theorem

by K. Huang Introduction to Statistical Mechanics

((Intuitive argument))

The resistor at temperature T exchanges energy with a heat reservoir, and the average heat dissipation in the frequency range Δv is

$$\overline{I^2 R} \propto k_B T \Delta \nu$$

Using Ohm's law V = IR, we obtain

$$\overline{V^2} \propto Rk_B T \Delta v$$

((Transmission line))

We derive this law by considering a transmission line (distributed circuit) of length L and impedance R. We terminate the transmission line at both ends with resistance R, so that travelling waves along the line are totally absorbed at the ends with no reflection.



Fig. Transmission line with no reflection. The characteristic impedance (R) is equal to the loads resistance (R), where no reflection occurs. Note that the distributed circuit is very different from the lumped circuit. The distributed circuit is very significant for high frequency region.

We consider the standing wave in the transmission line with a length L. The wavelength of the standing wave is

$$\frac{\lambda_n}{2}n = L$$

or

$$\lambda_n = \frac{2L}{n}$$

where *n* is an integer (n = 1, 2, 3, ...). We assume that the dispersion relation is given by

$$\omega_n = 2\pi v_n = ck_n = c\frac{2\pi}{\lambda_n}$$

leading to the relation

$$v_n = \frac{c}{\lambda_n} = \frac{cn}{2L} = nv$$

with

$$v = \frac{c}{2L}$$

where *c* is the velocity, *k* is the wave vector, and λ is the wave length.

At a finite temperature T all higher modes are excited with frequencies nv. What is the average energy of the mode with the frequency v? To this end, we use the partition function which is defined by

$$Z_n = \sum_{k=0}^{\infty} \exp(-k\beta\hbar\omega) = \frac{1}{1 - \exp(-\beta\hbar\omega)}$$

where $\omega = 2\pi v$. The average energy of the mode with the frequency v is

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z$$

$$= -\frac{\partial}{\partial \beta} \ln \frac{1}{1 - \exp(-\beta \hbar \omega)}$$

$$= \frac{\hbar \omega}{\exp(\beta \hbar \omega) - 1}$$

For $\hbar \omega \ll k_{\scriptscriptstyle B} T$, we can use the approximation

$$\langle E \rangle = k_B T$$

The number of modes in the band width Δv is

$$\frac{\Delta v}{v} = \frac{2L}{c} \Delta v$$

The total energy is

$$E = \frac{\Delta v}{v} k_B T = \frac{2k_B T L}{c} \Delta v$$

The energy can be regarded as residing in two travelling waves in opposite directions, and the time it takes to traverse the line is

$$t = \frac{L}{c}$$

Thus the energy absorbed per second by each resistor is

$$W = \frac{E}{2t} = k_B T \Delta v$$

and the power delivered to each resistor is

$$\overline{i^2 R} = k_B T \Delta v$$

As indicated in the distributed-circuit diagram, the voltage across a resistor is

$$V = 2IR.$$

Therefore we have $I = \frac{v}{2R}$

$$=\frac{V}{2R}$$

or

$$I^2 R = \frac{V^2}{4R}$$

Hence

$$\overline{V^2} = 4k_B TR\Delta v$$

This is known as the Nyquist theorem, and predicts a universal relation between V^2 and R, true for all materials. The Nyquist relation was experimentally confirmed for the first time by Johnson (1928).



Fig. Nyquist noise: mean-square voltage fluctuation across the open ends of a resistor, as a function of resistance. The Nyquist theorem predicts the straight line with a universal

slope. K. Huang, Introduction to Statistical Physics (CRC Press, 2010). p.136. The original data is from a paper of J.B. Johnson, Phys. Rev. 32, 97 (1928). Fig.4 (p.102).

16. Noise

Here we consider a noise in the RC circuit (lumped circuit). It is well known that a fluctuation voltage across the resistance R is generated due to the thermal noise due to conduction electrons in the resistance. The thermal noise arises from thermal fluctuation in thermal equilibrium.



Fig. RC circuit. V(t) is a voltage source arising from thermal noises of conduction electrons inside the resistance R.

$$-V(t) + Ri + V_c = 0$$

with

$$i = \frac{dQ}{dt}, \qquad V_C = \frac{Q}{C}$$

We have a differential equation,

$$R\frac{dQ}{dt} + \frac{Q}{C} = V(t)$$

or

$$\frac{dQ}{dt} + \frac{Q}{CR} = \frac{1}{R}V(t)$$

Which corresponds to the equation of motion,

$$m\frac{dv}{dt} + \varsigma v = \eta(t)$$

The table of the correspondence is shown below,

$$\begin{array}{ll} Q & v \\ \dot{Q} = i & \dot{v} \\ m & R \\ \varsigma & 1/C \\ & \langle \eta(t)\eta(t') \rangle = 2\varepsilon\delta(t-t') & \langle V(t)V(t') \rangle = 2\varepsilon_R\delta(t-t') \end{array}$$

From the similarity we get

$$\langle Q^2(t) \rangle = \exp(-\frac{2t}{RC}) \langle Q^2(0) \rangle + \frac{C\varepsilon_R}{R} (1 - \exp(-\frac{2t}{RC}))$$

For $t >> \frac{RC}{2}$.

$$\left\langle Q^2(t) \right\rangle = \left\langle Q^2 \right\rangle = \frac{C\varepsilon_R}{R}$$

Using the energy partition

$$\frac{1}{2C} \left\langle Q^2 \right\rangle = \frac{1}{2} k_B T$$

we have

$$\frac{1}{2C}\frac{C\varepsilon_R}{R} = \frac{1}{2}k_BT,$$

leading to

$$\varepsilon_R = k_B T R$$

or

$$\langle V(t)V(t')\rangle = 2k_B TR\delta(t-t')$$

Then the power spectrum is given by

$$\left\langle \left| V(\omega) \right|^2 \right\rangle = \int_{-\infty}^{\infty} e^{i\omega t} \left\langle V(0)V(t) \right\rangle dt = 2\varepsilon_R \int_{-\infty}^{\infty} e^{i\omega t} \delta(t) dt = 2\varepsilon_R = 2k_B TR$$

or

$$S(\nu)\Delta\nu = 2\langle |V(\omega)|^2 \rangle\Delta\nu = 4k_B T R \Delta \nu$$

where the factor 2 is necessary when only the positive frequency ($\nu > 0$) is taken into account.

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APPENDIX

Solving the diffusion equation (Lecture Note on Mathematical Physics by M. Suzuki, 2010)

1. Thermal conductivity

Fourier's law

$$\mathbf{J}_u = -K \nabla T \,,$$

describes the energy flux density in terms of the thermal conductivity K and the temperature gradient. This forms assumes that there is a net transport of energy, but not of particles. The equation of continuity for the energy density is

$$C\frac{\partial T}{\partial t} + \nabla\cdot \mathbf{J}_u = \mathbf{0} \; , \label{eq:constraint}$$

where C is the heat capacity per unit volume. We combine these two equations to obtain the heat conduction

$$C\frac{\partial T}{\partial t}-K\nabla^2 T=0\,,$$

or

$$\frac{\partial T}{\partial t} - D\nabla^2 T = 0,$$

where D = K/C is called the thermal diffusivity. This equation describes the time-dependent diffusion for the temperature.

.2. Green's function

We want to solve the heat equation in one dimension,

$$\left(\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right)T(x,t) = Q(x,t),$$

where Q(x,t) is a heat source. First we start to find the Green's function which is defined by

$$\left(\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right)G(x,t) = -\delta(x)\delta(t),$$

Using the Fourier transform, we have

$$G(x,t) = \frac{1}{2\pi} \iint G(k,\omega) e^{i(kx-\omega t)} dkd\omega$$
$$\delta(x)\delta(t) = \frac{1}{(2\pi)^2} \iint e^{i(kx-\omega t)} dkd\omega$$

The Fourier transform of the above equation:

$$(-i\omega+Dk^2)G(k,\omega)=-\frac{1}{2\pi},$$

or

$$G(k,\omega) = -\frac{i}{2\pi} \frac{1}{\omega + iDk^2}.$$

Then the inverse Fourier transform is obtained as

$$G(x,t) = \frac{1}{2\pi} \iint G(k,\omega) e^{i(kx-\omega t)} dkd\omega$$
$$= -\frac{i}{(2\pi)^2} \iint \frac{1}{\omega + iDk^2} e^{i(kx-\omega t)} dkd\omega$$
$$= -\frac{i}{(2\pi)^2} \int_{-\infty}^{\infty} dk e^{ikx} \int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega + iDk^2}$$

We now calculate the integral



(i) *t*>0

For t>0, we use the contour C_1 in lower half plane (the complex plane). The contour integral along the path Γ_1 (radius $R = \infty$) is zero according to the Jordan's lemma. Note that the contour C_1 is the clock-wise, and that there is a simple pole at

$$z=-iDk^2,$$

inside the contour C₁. Then we have

$$\int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega + iDk^2} + \int_{\Gamma_1} dz \frac{e^{-izt}}{z + iDk^2} = \oint_{C_1} dz \frac{e^{-izt}}{z + iDk^2} = -2\pi i \operatorname{Re} s(z = -iDk^2)$$

for *t*>0. Since

$$I = \int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega + iDk^2} = \oint_{C_1} dz \frac{e^{-izt}}{z + iDk^2} = -2\pi i \exp(-Dk^2 t)$$

(ii) *t*<0

For t < 0, we use the contour C_2 in the upper half plane (the complex plane). The contour integral along the path Γ_2 (radius $R = \infty$) is zero according to the Jordan's lemma. Note that the contour C_2 is the clock-wise, and that there is no pole.

$$\int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega + \frac{i\mu k^2}{c}} + \int_{\Gamma_1} dz \frac{e^{-izt}}{z + \frac{i\mu k^2}{c}} = \oint_{\Gamma_1} dz \frac{e^{-izt}}{z + \frac{i\mu k^2}{c}} = 0,$$

or

$$I = \int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega + \frac{i\mu k^2}{c}} = 0.$$

Then we have

$$I = \int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega + iDk^2} = (-2\pi i)e^{-Dk^2 t}\Theta(t).$$

The Green's function is obtained as

$$G(x,t) = -\frac{1}{2\pi} \Theta(t) \int_{-\infty}^{\infty} dk \exp[ikx - Dk^2 t]$$
$$= -\frac{1}{\sqrt{4\pi Dt}} \exp(-\frac{x^2}{4Dt}) \Theta(t)$$

((Mathematica))

$$\int_{-\infty}^{\infty} \mathbf{Exp} \left[-\mathbf{D} \mathbf{k}^{2} \mathbf{t} + \mathbf{i} \mathbf{k} \mathbf{x} \right] d\mathbf{k} / /$$

Simplify [#, {x > 0, t > 0, D > 0}] &
$$\frac{e^{-\frac{x^{2}}{4 \text{ D} t}} \sqrt{\pi}}{\sqrt{D t}}$$

3. General solution

$$\left(\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right)T(x,t) = Q(x,t),$$

where Q(x, t) is a heat source. Green's function satisfies

$$\left(\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right)G(x - x', t - t') = -\delta(x - x')\delta(t - t'),$$

The solution of the differential equation for the heat conduction is

$$T(x,t) = -\iint dx' dt' G(x-x',t-t')Q(x',t'),$$

where

$$,G(x-x',t-t') = -\frac{1}{\sqrt{4\pi D(t-t')}} \exp[-\frac{(x-x')^2}{4D(t-t')}]\Theta(t-t')$$

or

$$T(x,t) = \int_{-\infty}^{\infty} dx' \int_{0}^{t} dt' \frac{1}{\sqrt{4\pi D(t-t')}} \exp\left[-\frac{(x-x')^{2}}{4D(t-t')}\right] Q(x',t') \,.$$

((Example)) Dirac comb

We assume that

$$Q(x,t) = \delta(x)f(t)$$

$$T(x,t) = \int_{-\infty}^{\infty} dx' \int_{0}^{t} dt' \frac{1}{\sqrt{4\pi D(t-t')}} \exp[-\frac{(x-x')^{2}}{4D(t-t')}]\delta(x')f(t')$$

$$= \int_{0}^{t} dt' \frac{1}{\sqrt{4\pi D(t-t')}} \exp[-\frac{x^{2}}{4D(t-t')}]f(t')$$

We further assume that f(t) is described by a Dirac comb given by



Fig. Dirac comb with the heat pulses at x = 0 applied periodically (T_0 is a period time).

Then we have

$$T(x,t) = \int_{0}^{t} dt' \frac{1}{\sqrt{4\pi D(t-t')}} \exp\left[-\frac{x^{2}}{4D(t-t')}\right] f(t')$$

= $\frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^{2}}{4Dt}\right) + \frac{2}{\sqrt{4\pi Dt}} \sum_{n=0}^{\infty} \frac{1}{\sqrt{t-nT_{0}}} \exp\left[-\frac{x^{2}}{4D(t-nT_{0})}\right] \Theta(t-nT_{0})$



Fig. Simulation. Plot of T(x, t) vs t with x as a parameter (x = 1 - 10). D = 1. $T_0 = 5$.

4. Initial condition

We consider the solution of the differential equation given by

,

$$\left(\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right)T(x,t) = 0$$

with the initial condition given by

$$T(x,t=0)=T_0(x),$$

which is an initial temperature distribution at t = 0. We assume that the solution is given by

$$T(x,t) = \Theta(t)u(x,t) \ .$$

Since there is no heat source, this solution satisfies

$$\left(\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right)T(x,t) = 0,$$

or

$$\Theta(t)\left[\frac{\partial}{\partial t}u(x,t) - D\frac{\partial^2}{\partial x^2}u(x,t)\right] = -\delta(t)u(x,t) = -\delta(t)T_0(x),$$

or

$$\frac{\partial}{\partial t}u(x,t) - D\frac{\partial^2}{\partial x^2}u(x,t) = -\delta(t)T_0(x).$$

where

$$\Theta'(t) = \delta(t)$$
.

The Green's function satisfies

$$\frac{\partial}{\partial t}G(x,t) - D\frac{\partial^2}{\partial x^2}G(x,t) = -\delta(x)\delta(t) \,.$$

The form of G(x, t) is given by

$$G(x,t) = -\frac{1}{\sqrt{4\pi Dt}} \exp(-\frac{x^2}{4Dt})\Theta(t).$$

The solutions of u(x, t) and T(x, t) are obtained as

$$u(x,t) = -\iint_{-\infty} d\tau d\xi G(x-\xi,t-\tau)\delta(\tau)T_0(\xi)$$
$$= -\int_{-\infty}^{\infty} d\xi G(x-\xi,t)T_0(\xi)$$

and

$$T(x,t) = -\Theta(t) \int_{-\infty}^{\infty} d\xi G(x-\xi,t) T_0(\xi)$$

((Example)) Dirac delta function

$$T_0(\xi) = \delta(\xi).$$

Then we have



Fig. *t* dependence of T(x, t) with each *x*. D = 1.



Fig. T(x,t) has a maximum $(=\frac{1}{\sqrt{2e\pi x}})$ at $t = \frac{x^2}{2D}$ as a function of t where x is fixed as a parameter. D = 1. This figure is the same as the above figure.

The derivative of T(x, t) with respect to t is obtained as

$$\frac{\partial T(x,t)}{\partial t} = \frac{D(x^2 - 2Dt)\exp(-\frac{x^2}{4Dt})}{8\sqrt{\pi}(Dt)^{5/2}}.$$

which implies that T(x, t) has a maximum $(=\frac{1}{\sqrt{2e\pi x}})$ as a function of t at

$$t = \frac{x^2}{2D}.$$

The pulse spreads out with increasing time. The mean square value of x is given by

$$\langle x^2 \rangle = \frac{\int x^2 T(x,t) dx}{\int T(x,t) dx} = 2Dt$$

The root mean square value is

$$x_{rms} = \sqrt{\langle x^2 \rangle} = \sqrt{2Dt}$$

5. Brownian motion

The width of the distribution increases as \sqrt{t} , which is a general characteristic of diffusion and random walk problem in one dimension. The connection with Brownian motion or the random walk problem follows if we let t_0 be the duration of each step of a random walk.

$$t = Nt_0$$
,

where N is the number of steps. It follows that

$$x_{rms}(t) = \sqrt{2Dt_0}\sqrt{N}$$

So that the rms displacement is proportional to the square of the number of steps. This is the result of the Brownian motion, the random motion of suspensions of small particles in liquids (Kittel and Kroemer).

6. Experiment

In the sophomore laboratory (Physics 227, Binghamton University) we have an experiment of "Thermal Wave." The purpose of this experiment is to measure the thermal diffusivity (D) of a brass rod.



Fig.1 Diagram of apparatus (from the report by Corrine Blum (Fall, 2009, Sophomore Laboratory).

Figure 1 shows a diagram of the apparatus used. There are three temperature sensors located on the brass rod. The separation distance between adjacent sensors is Δx (= 10 cm). A heat source at the one of the edge, is applied for the time *T* on and the same time *T* off, in a square wave for one hour, where $T_1 = 5$ and 10 minutes (two trials). The temperature data from each sensor are recorded as a function of time using the computer. Figures 2 and 3 show the temperature data measured by the three sensors, as a function of time t, where T = 5 minutes for the trial 1 (Fig.2) and the trial (Fig.3). As shown in Figs.2 and 3, the heat propagates from the sensor 1 to the sensor 2 and from the sensor 2 to the sensor 3 in the same finite time Δt . The diffusion diffusivity D can be estimates as

$$D = \frac{(\Delta x)^2}{2\Delta t}$$

The thermal diffusivity is found to be 3.63 x 10^{-5} m²/s for the trial 1 and 3.33 x 10^{-5} m²/s for the trial 2. Note that the theoretical value of D for the brass rod is 3.376 x 10^{-5} m²/s.



Fig.2 Temperatures measured by three sensors as a function of time (trial 1). T = 5 minutes.



Fig.3 Temperatures measured by three sensors as a function of time (trial 2). T = 10 minutes.

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