Title: Statistical Mechanics (PHYS 602) - Lecture 5

Date: Oct 08, 2010 10:30 AM

URL: http://www.pirsa.org/10100024

Abstract:

From one step to many steps

We start from the two statements that $\langle \sigma_j \rangle = 0$ and that $\langle \sigma_j \sigma_k \rangle = \delta_{j,k}$

On the average, on each step the walker goes left as much as right. Thus as a result the average displacement of the entire walk is zero

$$\langle X(t) \rangle = a \sum_{j=1}^{M} \langle \sigma_j \rangle = 0 \qquad \text{iv.1}$$

However, of course the mean squared displacement is not zero, since

$$\langle X(t)^2 \rangle = a^2 \sum_{j,k=1}^{M} \langle \sigma_j \sigma_k \rangle = a^2 \sum_{j,k=1}^{M} \delta_{j,k} = a^2 M \qquad \text{iv.2}$$

Our statement is the same that in a zero field uncoupled Ising system, the maximum magnetization is proportional to the number of spins, but the typical magnetization is only proportional to the square root of that number. Typical fluctuations are much, much smaller than maximum deviations.

We can see this fact by noting that the root mean square average of X^2 is $a \sqrt{M}$, which is the typical end-to-end distance of this random walk. This distance is is much smaller than the maximum distance which would be covered were all the steps to go in the same direction. In that case we would have had a distance aM. Thus, a random walk does not, in net, cover much ground.

Gaussian Properties of Continuous Random Walk

In the limit of large n, we can think of $X(t)$ as composed of a sum of many pieces which are uncorrelated with one another. According to the central limit theorem, such a sum is a Gaussian random variable. Hence, we know everything there is to know about it. Its average is zero and its variance is a^2t/τ where t is the number of steps. Consequently, it has a probability distribution

$$< \rho(X(t) = x) >= \left(\frac{\tau}{2\pi a^2 t}\right)^{1/2} e^{-x^2\tau/(2a^2t)} \qquad \text{iv.9}$$

Now we have said everything there is to say about the continuous random walk. As an extra we can exhibit the generating function for this walk:

$$< \exp[iqX(t)] >= e^{-q^2a^2t/(2\tau)}$$

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An example:

The difference between maximum length and RMS length (root mean square length) needs to be emphasized by an example. Consider a random walk that consists of M= one million steps steps. If each step is one centimeter long the maximum distance traveled is M centimeters, or 10 thousand meters or 10 kilometers. On the other hand the typical end to end distance of such a walk is $M^{1/2}$ centimeters or ten meters. That is quite a difference!

Higher Dimensions

Reason for putting many different calculations on a lattice is that the lattice provides a simplicity and control not available in a continuum system.   There is no ambiguity about how things very close to one another behave, because things cannot get very close. They are either at the same point or different points.
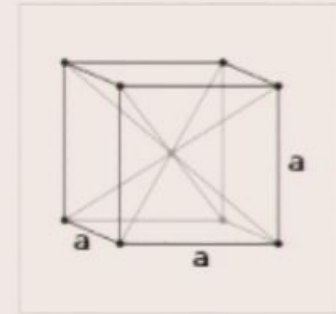

Body-centered cubic

So now I would like to talk about a random walk in a d-dimensional system by considerin a system on a simple lattice constructed as in the picture. The lattice sites are given by $\mathbf{x} = a(n_1, n_2, n_3, ...)/2$. The n's are integers. There are two possible kinds of assignments for the n's: Either they are all even e.g. $\mathbf{x} = a(0, 2, -4, ...)/2$ or they are all odd, for example $\mathbf{x} = a(1, 3, -1, ...)/2$.   If all hopping occurs from one site to a nearest neighbor site, the hops are through one of 2^d vectors of the form $\xi_\alpha = a(m_1, m_2, m_3, ...)/2$, where each of the m's have magnitude one, but different signs for example $a(1, -1, -1, ...)$. We use a lattice constant, a, which is twice as big as the one shown in the picture.

We then choose to describe the system by saying that in each step, the coordinate hops through one of the nearest neighbor vectors, ξ_α , which one being choosen at random. This particular choice makes the entire coordinate, $\mathbf{x}$, have components which behave entirely independently of one another, and exactly the same as the one-dimensional coordinate we have treated up to now.

RANDOM WALKS

http://particlezoo.files.wordpress.com/2008/09/randomwalk.png
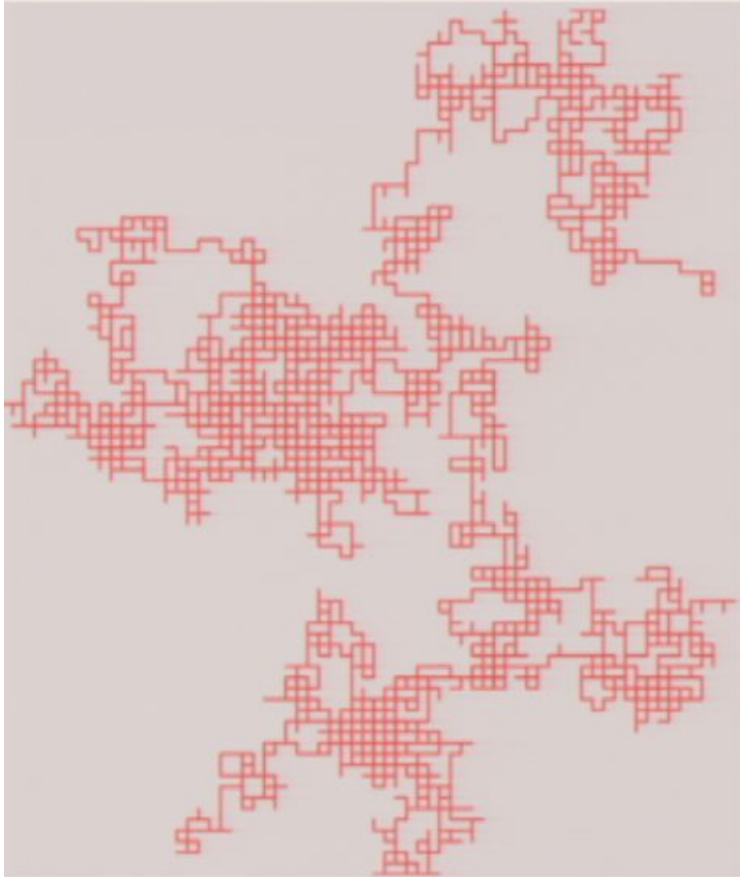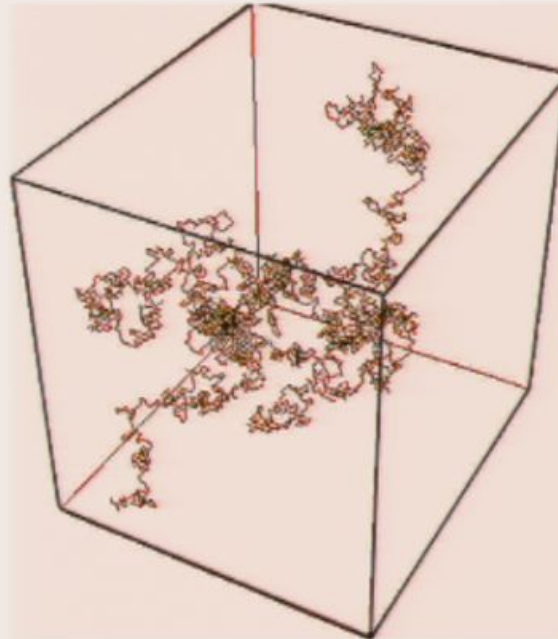
dspace.mit.edu/.../CourseHome/index.htm

Higher Dimensions.....continued

We denote the probability density of this d-dimensional case by a superscript d and the one for the previous one-dimensional case of by a superscript 1. As an additional difference, the d-dimensional object will be a function of space and time rather than n and M. After a while, we shall focus entirely upon the higher dimensional case and therefore drop the superscripts. We have

$$\rho^d_{an,M\tau} = \prod_{\alpha=1}^{d} \rho^1_{n_\alpha,M}$$

However, we can jump directly to the answer for the continuum case, If the probability distribution for the discrete case is simply the product of the one-dimensional distributions so must be the continuum distribution. The one-dimensiona equation answer in eq iv.9 was

$$< \rho(X(t) = x) >= \left(\frac{\tau}{2\pi a^2 t}\right)^{1/2} e^{-x^2\tau/(2a^2 t)} \qquad \text{iv.9}$$

so that the answer in d dimensions must be

$$< \rho(R(t) = r) >= \left(\frac{\tau}{2\pi a^2 t}\right)^{d/2} e^{-r^2\tau/(2a^2 t)}$$

Here the bold faced quantities are vectors, viz $r^2 = x^2 + y^2 + ...$

Higher dimensional probability density: again

one dimension

d dimensions is a product of ones

$$< \rho(X(t) = x) >= \left(\frac{\tau}{2\pi a^2 t} \right)^{1/2} e^{-x^2 \tau / (2a^2 t)}$$

$$< \rho(R(t) = r) >= \left(\frac{\tau}{2\pi a^2 t} \right)^{d/2} e^{-r^2 \tau / (2a^2 t)}$$

Notice that the result is a rotationally invariant quantity, coming from adding the x^2 and y^2 and....
in separate exponents to get $r^2 = x^2 + y^2 + ...$. This is an elegant result coming from the fact that
the hopping has produced a result which is independent of the lattice sitting under it. We would
get a very similar result independent of the type of lattice underneath. In fact, the result come
from what is called a diffusion process and is typical of long-wavelenth phenomena in a wide
variety of systems.

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Diffusion Process

Diffusion here is a result of a **conservation law:** a global statement that the total amount of something is unchanged by the time development of the system. $dQ/dt=0$. In our case the Q in question is the total probability of finding the diffusing particle someplace. Diffusion has a second element: **locality.** The local amount of Q, called ρ, changes because things flow into and out of a region of space. The flow is called a current, j, and the conservation law is written as

$$\frac{\partial \rho(r,t)}{\partial t} + \nabla \cdot j(r,t) = 0 \qquad \text{conservation law}$$

The time derivative of the density is produced by a divergence of the curent flowing into a point. On a one dimension lattice, the rule takes the simpler form:

$$\rho_{n,M+1} - \rho_{n,M} = l_{n-1/2,M} - l_{n+1/2,M} \qquad \text{conservation law}$$

This equation says that the change of probability over one time step is produced by the flow of probability in from the left minus the flow out to the right.

Here, I'm going to visualize a situation once more in which we have a discrete time coordinate M and a discrete space coordinate, n. I shall assume that the initial probabilities is sufficiently smooth so that even and odd n-values have rather similar occupation probabilities so that we can get away with statement like

$$\rho_{n,M+1} - \rho_{n,M} \approx \partial \rho_{n,M} / \partial M \qquad \text{The conservation law then takes the form}$$

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$$X(t) = \sum_{j=1}^{M} a\sigma_j \qquad \sigma_j = \pm 1$$

$$\rho(r,t)$$

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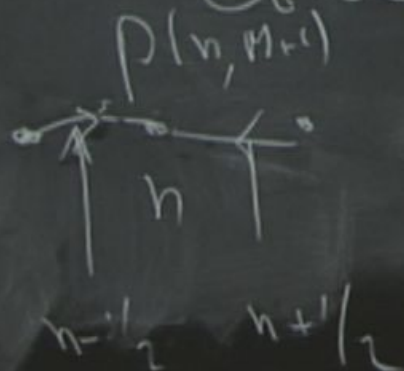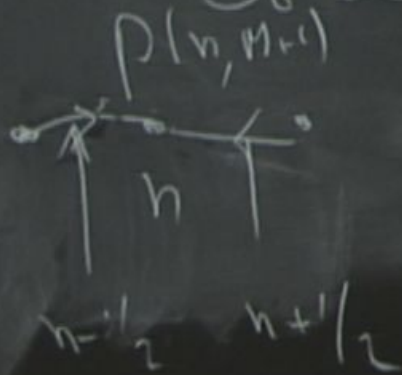
for Atoms   Molecules

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$\rho(n, M+1)$

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The Current

We do not have a full statement of the of what is happening until we can specify the current. An approximate definition of a current in a conservation law is called a constitutive equation. We now write this down.

Our hopping model says that a $I_{n+1/2,M}$ is given a contribution +1 when the site at n is occupied at time M, and σ_n is equal to +1. On the other hand it is given a contribution -1 when the site at n +1 is occupied at time M, and σ_{n+1} is equal to -1. Since there is a probability 1/2 for each of the σ−events the value of I is

$$I_{n+1/2,m} = (\rho_{n,m} - \rho_{n+1,m}) / 2 \qquad \text{constitutive equation}$$

Once again, we write the difference in terms of a derivative, getting

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which can be written in dimensional form as

$$\frac{\partial \rho}{\partial t} = \lambda \frac{\partial^2 \rho}{\partial x^2} \qquad \text{diffusion equation}$$

with the diffusion coefficient being given by $\lambda = a^2/(2\,\tau)$. It has dimensions L^2/t.

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Higher Dimension

In higher dimensions, the current is proportional to the gradient of the current

$$j(r,t) = -\lambda \nabla \rho(r,t)$$

so that the diffusion equation becomes, as before,

$$\partial_t \rho(r,t) = \lambda \nabla^2 \rho(r,t)$$

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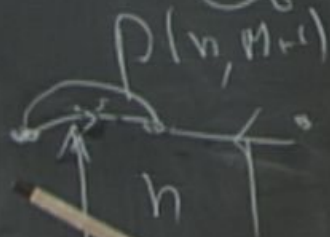with the diffusion coefficient being given by $\lambda = a^2/(2\tau)$. It has dimensions L^2/t.

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Conservation

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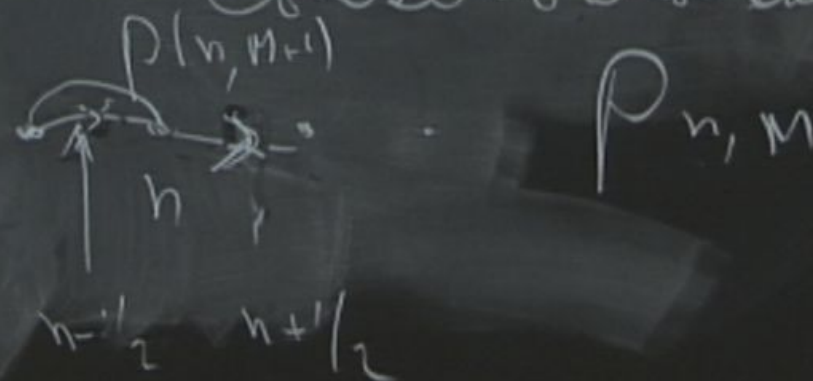
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$$\left.\begin{array}{l} \rho(r,t) \\ \rho = \sigma \cdot \vec{E}(v,t) \end{array}\right|$$

$$X(t) = \sum_{j=1}^{M} a\sigma_j \qquad \sigma_j = \pm$$

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Conservation law

$\rho(n, M+1)$

$\rho_{n, M}$

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Here, I'm going to visualize a situation once more in which we have a discrete time coordinate M and a discrete space coordinate, n. I shall assume that the initial probabilities is sufficiently smooth so that even and odd n-values have rather similar occupation probabilities so that we can get away with statement like

$$\rho_{n,M+1} - \rho_{n,M} \approx \partial \rho_{n,M} / \partial M \qquad \text{The conservation law then takes the form}$$

$$\partial \rho_{n,M} / \partial M + \partial I_{n,M} / \partial n = 0 \qquad \text{conservation law}$$

Higher dimensional probability density: again

one dimension

$$< \rho(X(t) = x) > = \left(\frac{\tau}{2\pi a^2 t}\right)^{1/2} e^{-x^2\tau/(2a^2 t)}$$

d dimensions is a product of ones

$$< \rho(R(t) = r) > = \left(\frac{\tau}{2\pi a^2 t}\right)^{d/2} e^{-r^2\tau/(2a^2 t)}$$

Notice that the result is a rotationally invariant quantity, coming from adding the x^2 and y^2 and.... in separate exponents to get $r^2 = x^2 + y^2 + ...$. This is an elegant result coming from the fact that the hopping has produced a result which is independent of the lattice sitting under it. We would get a very similar result independent of the type of lattice underneath. In fact, the result come from what is called a diffusion process and is typical of long-wavelenth phenomena in a wide variety of systems.

Diffusion Process

Diffusion here is a result of a conservation law: a global statement that the total amount of something is unchanged by the time development of the system. dQ/dt=0. In our case the Q in question is the total probability of finding the diffusing particle someplace. Diffusion has a second element: locality. The local amount of Q, called ρ, changes because things flow into and out of a region of space. The flow is called a current, j, and the conservation law is written as

$$\frac{\partial \rho(r,t)}{\partial t} + \nabla \cdot j(r,t) = 0 \qquad \text{conservation law}$$

The time derivative of the density is produced by a divergence of the curent flowing into a point. On a one dimension lattice, the rule takes the simpler form:

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The Current

We do not have a full statement of the of what is happening until we can specify the current. An approximate definition of a current in a conservation law is called a constitutive equation. We now write this down.

Our hopping model says that a $I_{n+1/2,M}$ is given a contribution +1 when the site at n is occupied at time M, and σ_n is equal to +1. On the other hand it is given a contribution -1 when the site at n +1 is occupied at time M, and σ_{n+1} is equal to -1. Since there is a probability 1/2 for each of the σ−events the value of I is

$$I_{n+1/2,m} = (\rho_{n,m} - \rho_{n+1,m}) / 2 \qquad \text{constitutive equation}$$

Once again, we write the difference in terms of a derivative, getting

$$I_{n,m} = -(\partial \rho_{n,m} / \partial n) / 2 \qquad \text{constitutive equation}$$

This can then be combined with the conservation law to give the diffusion equation

$$\partial \rho_{n,M} / \partial M = \partial^2 \rho_{n,M} / \partial n^2 / 2$$

which can be written in dimensional form as

$$\frac{\partial \rho}{\partial t} = \lambda \frac{\partial^2 \rho}{\partial x^2} \qquad \text{diffusion equation}$$

with the diffusion coefficient being given by $\lambda = a^2/(2\tau)$. It has dimensions L^2/t.

Higher Dimension

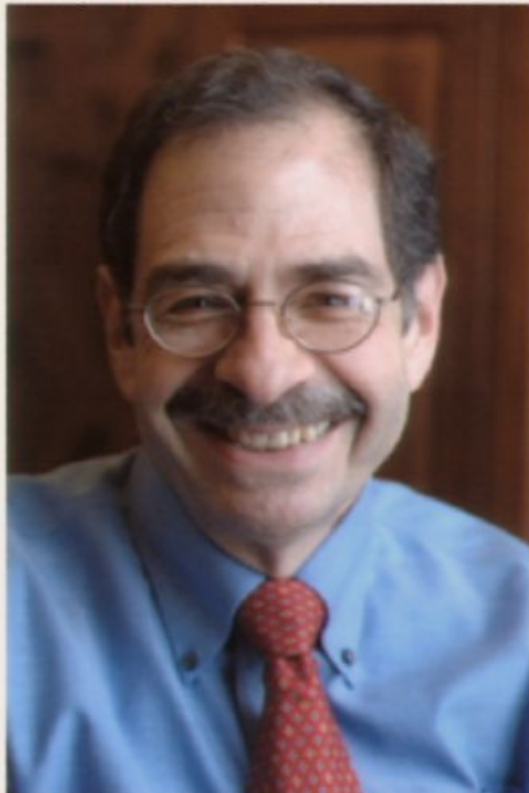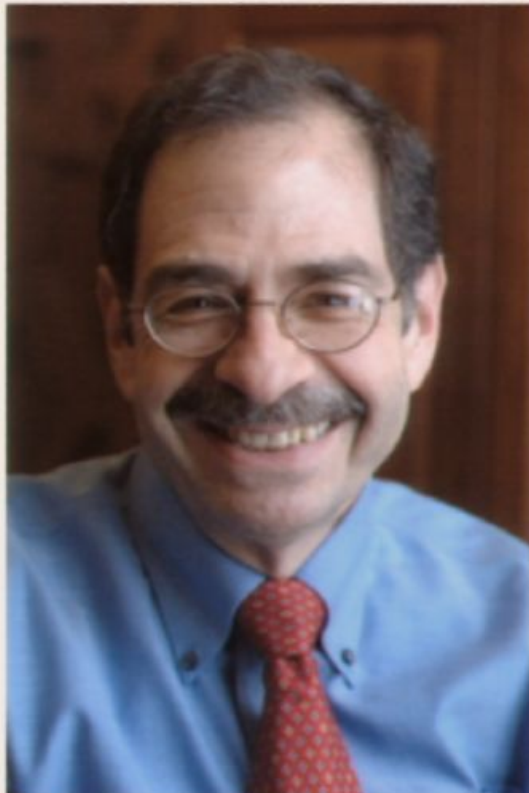In higher dimensions, the current is proportional to the gradient of the current

$$j(r,t) = -\lambda \nabla \rho(r,t)$$

so that the diffusion equation becomes, as before,

$$\partial_t \rho(\mathbf{r},t) = \lambda \nabla^2 \rho(\mathbf{r},t)$$

Diffusion Equation

This equation is one of several equations describing the slow transport of physical quantities from one part of the system to another. When there is slow variation is space, the conservation law guarantees that the rate of change in time will also be slow. In fact this is part of a general principle which permits only slow changes as a result of a conservation law. This general principle is much used in the context of quantum field theory and condensed matter physics. The idea is connected with the construction of the kind of particle known as a Nambu-Goldstone boson, named for two contemporary physicists, my Chicago colleague Yoichiro Nambu and the MIT theorist Jeffrey Goldstone.

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Solution to Diffusion Equation Cannot be Carried Backward in Time

The wave equation is $(\partial_t^2 - c^2\partial_x^2)F = 0$

Its general solution is $F(x,t) = G(x-ct) + H(x+ct)$

This is a global solution. It enables you to look forward or back infinitely far in the future or the past without losing accuracy. Find solution from $F(x,0) = \partial_x F(x,0) = 1$ for $0 < x < 1$ and $F(x,0) = \partial_x F(x,0) = 0$ otherwise. Use $c=2$

A global solution to the diffusion equation is $\rho(x,t) = \int dk \ \exp[ikx - \lambda k^2 t] \ g(k)$

with $g(k) = \int dx \ \exp[-ikx] \ \rho(x,0)/(2\pi)$ as initial data.

Small rapidly varying errors at $t=0$ will produce small errors for positive t and huge errors for negative t. You cannot extrapolate backward in time. Information gets lost as time goes forward.

Solve for $\rho(x,0)=1$ for $0 < x < 1$ and $\rho(x,0) = 0$ otherwise. Use $\lambda=2$. Plot solution for $t=0,2,4$. What happens for $t=-2$?

Boltzmann noted that equations of classical mechanics make sense if t is replaced by $-t$. (In fact, it just replaces momenta, p, by $-p$.) But diffusion equation has a solution which does not make sense. Where did we go from sense to nonsense?

$$\partial_t \rho = \lambda \partial_x^2 \rho$$

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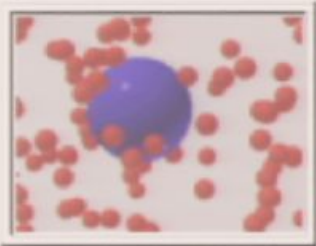$\partial_x F(x, t=0)$

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$$dp/dt = \ldots\ldots + \eta(t) - p/\tau$$

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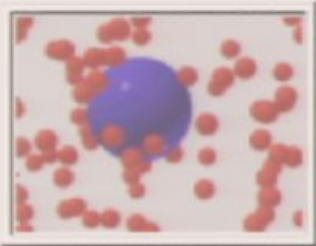$$\langle \eta_j(t) \, \eta_k(s) \rangle = \Gamma \delta(t-s) \delta_{j,k} \qquad \qquad v.2$$

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$$\langle \eta(A) \rangle = 0$$

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Solution:
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<div align="right">v.4</div>

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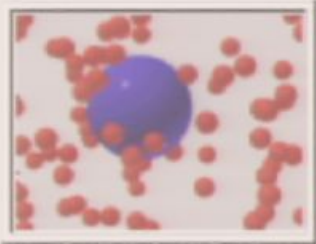
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The relaxation time, τ, describes friction slowing down as the particles moves through the medium. In contrast Γ describes the extra momentum picked up via the collisions. Both represent the same physical effect, little particles hitting our big one. However, they operate in a somewhat different fashion. The individual kicks point in every which direction and only in the long run produce any concerted change in momentum. On the other hand the term in τ is a friction tending to continually push our particle toward smaller speeds relative to the

Calculate momentum from $d\mathbf{p}/dt = \ldots + \eta(t) - p/\tau$

In physics, an equation with a random term is called a Langevin equation

Solution:
$$P(t) = \int_{-\infty}^{t} dt' \; \eta(t') \exp\left(-\frac{t - t'}{\tau}\right) \qquad \text{v.3}$$

Because *P(t)* is a sum of many random variables according to the central limit theorem, it must be a Gaussian random variable.   Therefore it has a Gaussian probability distribution. In equilibrium, *P(t)* should have the variance, M kT, with M now being the mass of the Brownian particle. In equilibrium it will have the Maxwell-Boltzmann probability distribution

$$\rho(\mathbf{p}) = \left(\frac{\beta}{2\pi M}\right)^{3/2} \exp[-\beta p^2/(2M)]$$

Notice that if this works out for us, it will be our first "proof" that the ideas of Gibbs, Boltzmann, and Maxwell about the canonical distribution was correct. So we would have a proof that this "law" works, at least in this situation.   In physics, we often use laws long before there is any substantial proof that they are correct. We use little bits of evidence, intuition, and guesswork and gradually convince ourselves that idea X "must be" right. If X is attractive, we hold on to that view until there is overwhelming evidence to the contrary.

Calculate Average

$$< p_j(t)p_k(s) > = \int_{-\infty}^{t} du \int_{-\infty}^{s} dv < \eta_j(u)\eta_k(v) > \exp[-(t-u+s-v)/\tau]$$

$$< p_j(t)p_k(s) > = \int_{-\infty}^{t} du \int_{-\infty}^{s} dv \, \Gamma \delta_{j,k} \delta(u-v) \exp[-(t-u)/\tau - (s-v)/\tau]$$

.... if $t > s$ the integral over v always gets a contribution from the delta-function integral in u so that this expression then becomes

$$< p_j(t)p_k(s) > = \int_{-\infty}^{s} dv \, \Gamma \delta_{j,k} \exp[-(t+s-2v)/\tau]$$

$$= \frac{\delta_{j,k}}{2} \Gamma \tau \exp[-|t-s|/\tau]$$

so we see that $p_j^2/(2M)$, where M is the mass of the Brownian particle is on one hand given by

$$< \frac{p_j^2}{2M} > = \Gamma \tau / (4M)$$ note: no Einstein summation convention

On the other hand, we know that in classical physics this quantity is $kT/2$. Thus we obtain th relation between the two parameters in the Einstein model.

Probability distribution

$\Gamma\tau = 2MkT$

Whenever this relation is satisfied, p has the right variance, MkT, and the right Maxwell-Boltzmann probability distribution for the Brownian particle!

$$\rho(\mathbf{p}) = (\frac{\beta}{2\pi M})^{3/2} \exp[-\beta p^2/(2M)]$$

More generally, if we have a Hamiltonian, $H(\mathbf{p},\mathbf{r})$, for the one-particle system, the Maxwell-Boltzmann distribution takes the form

$\rho(\mathbf{p},\mathbf{r})=exp[-\beta H(\mathbf{p},\mathbf{r})]/Z,$ v.7

where, the the simplest case the Hamiltonian is

$H(\mathbf{p},\mathbf{r}) = p^2/(2M) +U(\mathbf{r})$

Maxwell and Boltzmann expected that, in appropriate circumstances, if they waited long enough, a Hamiltonian system would get to equilibrium and they would end up with a Maxwell-Boltzmann probability distribution. But we have not yet derived this for the molecules in the fluid! We want to do this derivation.

Question: Should we not be able to derive this distribution from classical mechanics alone? Maybe we should have to assume also that we must long enough to reach equilibrium? What to do?

Something of the form v.7 is called by mathematicians a Gibbs measure and by physicists a Boltzmann distribution or often a Maxwell-Boltzmann distribution.

Statistical and Hamiltonian Dynamics

We have that the equilibrium $\rho = \exp(-\beta H)/Z$. How can this arise from time dependence o
system? One very important possible time-dependence is given by Hamiltonian mechanics

$$\frac{dq_\alpha}{dt} = \frac{\partial H}{\partial p_\alpha}$$

$$\frac{dp_\alpha}{dt} = -\frac{\partial H}{\partial q_\alpha}$$

The simplest case is a particle moving in a potential field with a Hamiltonian

$$H = \mathbf{p}^2/(2M) + U(\mathbf{r})$$ and consequently equations of motion

$$\frac{d\mathbf{p}}{dt} = -\nabla U$$

$$\frac{d\mathbf{r}}{dt} = \mathbf{p}/M$$

The statistical mechanics of such situations is given by a probability density function $\rho(\mathbf{p},\mathbf{r},t)$ such that the probability of finding the particle in a volume element **dp dr** about **p,r** at time t is $\rho(\mathbf{p},\mathbf{r},t)$ **dp dr**. The next question is, what is the time-dependence of this probability density? Or maybe, how do we get equilibrium

Time Dependence of Dynamical systems: A much more general problem

Instead of carrying around the variables **p** and **r**, let me do something with much simpler formulas. I'm going to imagine solving the dynamical systems problem in which there is a differential equation $dX/dt=V(X(t),t)$ to get a solution $X(t)$. I will have a probability function $\rho(x,t)\,dx$ which is the probability that the solution will be in the interval dx about x. This is a probability because, when we start out the initial data is not just one value of x but a probability distribution, given by $\rho(x,0)$. So the situation at a later time must be described by a probability distribution then as well. So what is the time dependence of the probability distribution? One way to approach this problem is to ask what does the distribution mean. Specifically, if we have some function $g(X)$ of the particle coordinates at time t, that function has an average at time t given by

$\int dx\, g(x)\, \rho(x,t)$. Naturally the average at time $t + dt$ is $\int dx\, g(x)\, \rho(x,t+dt)$. That same average is obtained by taking the solution at time $t+dt$, which is

$$X(t+dt) \approx X(t)+V(X(t),t))dt \qquad\qquad \text{v.7}$$

and calculate its average using the probability distribution which is appropriate at the earlier time, i.e. the average is $\int dx\, g(x+dt\,V(x,t))\, \rho(x,t)$. Equate those two expressions for the average

$$\int dx\, g(x)\, \rho(x,t+dt) \;=\; \int dx\, g(x+dt\,V(x,t))\, \rho(x,t) \qquad\qquad \text{v.8}$$

Calculation Continued .....

$$\int dx \; g(x) \; \rho(x,t+dt) \;\; = \;\; \int dx \; g(x+dt \, V(x,t)) \; \rho(x,t)$$

expand to first order in dt

$$\int dx \; g(x) \; \rho(x,t) + dt \int dx \; g(x) \partial_t \rho(x,t) \;\; = \;\; \int dx \; g(x) \; \rho(x,t) + \int dx \; dt \, V(x,t)[d_x g(x)] \; \rho(x,t)$$

throw away the things that cancel against each other to get

$$\int dx \; g(x) \partial_t \rho(x,t) \; - \; \int dx \, V(x,t)[\partial_x g(x)] \; \rho(x,t) = 0$$

integrate by parts on the right hand side, using the fact that $\rho(x,t)$ vanishes at x=± infinity

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$$\partial_t \rho(x,t) + \rho(x,t) \sum_j (\partial_{x_j} V_j) + \sum_j V_j \partial_{x_j} \rho(x,t) = 0 \qquad \text{v.9}$$

We call the second term on the left the divergence term. It describes the dilation of the volume element by the changes in the x's caused by the time development. The last term is the direct result of the time-change in each coordinate X(t) Now we have the general result for the time development of the probability density. We go look at the Hamiltonian

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for Atoms

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$$\frac{d \vec{X}(t)}{dt} = V(X(t), t)$$

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$$dt \rightarrow 0$$

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$$\frac{d \vec{X}(t)}{dt} = V(X(t), t)$$

$$X(t + dt) = X(t)$$

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$$dt \to 0$$

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$$\frac{d \vec{X}(A)}{dA} = V(X(A), t)$$

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$$P(\vec{X}(A)) = \vec{X}$$

$$\frac{d \vec{X}(t)}{dt} = V(X(t), t)$$

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$$+ dt \, V(x(t), t)$$

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$$\partial_t \, \rho(\vec{x}(t) = \vec{x}, t)$$

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$\langle g(x) \rangle$

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$= \int dx$

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$$\langle g(x) \rangle_{t}$$

$$= \int dx \, g(x) \, p(x,t)$$

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general

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c.m.

$$\partial_t \rho = - \frac{\partial}{\partial q} \frac{\partial H}{\partial q} (pq)$$

$$\partial_t g = \frac{\partial}{\partial p} \frac{\partial H}{\partial q} (pq)$$

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