August 21, 1980

Wick ordering (Simon's book). One suppose given a random variable x on a probability space. Then the Wick-ordered powers $:x^n:$ are defined so that

$$\langle :x^n: \rangle = 0 \qquad n \geq 1$$

$$\frac{d}{dx} :x^n: = n :x^{n-1}: \qquad ?$$

This second condition might be explained as follows — that if y is another random variable, then

$$:(x+y)^n: = :x^n: + n(:x^{n-1}:)y + O(y^2)$$

The ultimate formula is that if

$$:e^{tx}: = \sum \frac{t^n}{n!} :x^n:$$

then

$$\boxed{:e^{tx}: = \frac{e^{tx}}{\langle e^{tx} \rangle}}$$

as power series in t. If x is a Gaussian r.v. then

$$\langle e^{tx} \rangle = \frac{1}{\sqrt{2\pi\sigma}} \int e^{tx} e^{-\frac{x^2}{2\sigma}} dx = e^{+\sigma\frac{t^2}{2}}$$

where $\sigma = \langle x^2 \rangle$

hence

$$:e^{tx}: = e^{tx - \sigma\frac{t^2}{2}}$$

and this means for $\sigma = 1$, that the Wick powers $:x^n:$ are essentially Hermite polynomials

August 22, 1980

Back to the harmonic oscillator:

$$H_0 = \omega a^* a \qquad\qquad \omega > 0$$

Let's consider a time-dependent perturbation

$$H_J = H_0 + \tilde{J} a^* + J a$$

where $J, \tilde{J}$ are compact support fns. of t. Then we have the S-matrix

$$S_J = T\left\{ e^{-i\int (\tilde{J}\tilde{a}^*(t) + J\tilde{a}(t))\,dt} \right\}$$

where

$$\tilde{a}^*(t) = e^{iH_0 t} a^* e^{-iH_0 t} = e^{i\omega t} a^*$$
$$\tilde{a}(t) = \quad " \quad a \quad " \quad = e^{-i\omega t} a$$

Computation of the S-matrix may be done by using

$$e^A e^B = e^B e^A e^{[A,B]} \qquad \text{if } [A,B] \text{ commutes with } A, B$$

and breaking time into intervals dt. We have

$$\prod_{t \le T} e^{-(i\tilde{J}(t)e^{+i\omega t}dt)a^*} e^{-(iJ(t)e^{-i\omega t}dt)a}$$

$$= \text{const}\; e^{-i\int^T \tilde{J}(t)e^{i\omega t}dt\; a^*} \; e^{-i\int^T J(t)e^{-i\omega t}dt\; a}$$

and multiplying this by $e^{-i\tilde{J}(T)e^{i\omega T}dt\; a^*} e^{-iJ(T)e^{-i\omega T}dt\; a}$ we have to move the a past the a^* factor so we pick up

$$e^{[-iJ(T)e^{-i\omega T}dt\, a,\; -i\int^T \tilde{J}(t)e^{i\omega t}dt\; a^*]}$$

Doing this for each T gives the formula

$$S_J = e^{-\int_{t_1>t_2} J(t_1)\, e^{-i\omega(t_1-t_2)}\tilde{J}(t_2)} \; e^{\left(-i\int \tilde{J}(t) e^{i\omega t} dt\right) a^*}$$

$$\times e^{\left(-i\int J(t)\, e^{-i\omega t} dt\right) a}$$

The constant in front is

$$\langle 0 | S_J | 0 \rangle = \exp\left(-\int_{t_1>t_2} J(t_1)\, e^{-i\omega(t_1-t_2)} \tilde{J}(t_2)\right)$$

so

$$S_J = \langle 0 | S_J | 0 \rangle \, e^{-i\tilde{\gamma} a^*} \, e^{-i\gamma a}$$

where
$$\gamma = \int J(t)\, e^{-i\omega t} dt$$
$$\tilde{\gamma} = \int \tilde{J}(t)\, e^{i\omega t} dt$$

so that $\tilde{\gamma} = \bar{\gamma}$ when $\tilde{J} = \bar{J}$. An easy computation shows in this case that

$$2\,\mathrm{Re} \int_{t_1>t_2} J(t_1)\, e^{-i\omega(t_1-t_2)} \bar{J}(t_2) = \gamma\bar{\gamma}$$

so that
$$|\langle 0 | S_J | 0 \rangle| = e^{-|\gamma|^2}.$$

Finally notice that

$$S_J |0\rangle = \langle 0 | S_J | 0 \rangle \sum \frac{(-i\gamma)^n}{n!} (a^*)^n |0\rangle$$

so that the probability of the n-particle state after the scattering is

$$P_n = |\langle 0 | S_J | 0\rangle|^2 \, \frac{|\gamma|^{2n}}{(n!)^2}\, n! = e^{-|\gamma|^2} \frac{(|\gamma|^2)^n}{n!}$$

which is a Poisson distribution with mean $|\gamma|^2$. (see Feb. 3, 1980).

Suppose a constant perturbation $c(a+a^*)$ acts for $0 \leq t \leq T$. Then

$$-i\gamma = \int_0^T c(-i)e^{-i\omega t}\,dt = c\,\frac{e^{-i\omega T}-1}{\omega}$$

so

$$|\gamma|^2 = c^2\,\frac{1}{\omega^2}\sin^2\!\left(\frac{\omega T}{2}\right)$$

This is not linear in T. However the philosophy of Fermi's Golden Rule is as a function of ω, this for large T is essentially $T\cdot\delta(\omega)$. Note:

$$\int_{-\infty}^{\infty}\frac{\sin^2\left(\frac{\omega T}{2}\right)}{\omega^2}\,d\omega = \frac{T}{2}\underbrace{\int_{-\infty}^{\infty}\frac{\sin^2\omega}{\omega^2}\,d\omega}_{\pi}$$

Parseval: $$\int_{-1}^{1} e^{i\omega t}\,dt = \frac{e^{i\omega}-e^{-i\omega}}{i\omega} = 2\,\frac{\sin\omega}{\omega}$$

$$\therefore \int\frac{d\omega}{2\pi}\left(2\,\frac{\sin\omega}{\omega}\right)^2 = \int_{-1}^{1} dt = 2$$

or $$\int d\omega\,\frac{\sin^2\omega}{\omega^2} = \pi$$

What I would like to do is to cook up a good example of a system of harmonic oscillators with different frequencies (e.g. a scalar Bose field), so that I could actually see the meaning of probability per unit time.

Recall some path integral formulas. Let's begin with the fermion case. Let $\psi_j, \tilde{\psi}_j$ be generators for an exterior algebra Λ. Then this exterior algebra has a top-dimensional element

$$\Lambda \psi_j \cdot \Lambda \tilde{\psi}_j$$

well-defined up to sign. Hence we can define

$$\int : \Lambda \longrightarrow \mathbb{C}$$

unique up to a scalar. Then

$$\int e^{-\Sigma \tilde{\psi}_j A_{jk} \psi_k} = \int \frac{(-1)^n}{n!} \left(\Sigma \tilde{\psi}_j A_{jk} \psi_k \right)^n$$

$$= c \det(A_{jk}) \qquad c \text{ const.}$$

Now diff. wrt A_{kj} to get

$$\frac{\int e^{-\Sigma \tilde{\psi}_j A_{jk} \psi_k} \psi_j \tilde{\psi}_k}{\int e^{-\Sigma \tilde{\psi}_j A_{jk} \psi_k}} = \frac{\partial}{\partial A_{kj}} \log \det(A)$$

$$= \frac{1}{\det(A)} \; kj\text{-th minor}$$

By Cramer's Rule: $\quad = (A^{-1})_{jk}$

Thus without indices we have

$$\frac{\int e^{-\tilde{\psi} A \psi} \psi \tilde{\psi}}{\int e^{-\tilde{\psi} A \psi}} = A^{-1}$$

think of ψ as a column vector and $\tilde{\psi}$ as a row vector

In the boson case we take complex variables z_j and a matrix $A = (A_{jk})$ with pos-def hermitian part. Then one has

$$\int e^{-\sum \bar{z}_j A_{jk} z_k} \text{ Lebesgue measure} = \frac{c}{\det A}$$

so

$$\frac{\int e^{-\sum \bar{z}_j A_{jk} z_k} z_j \bar{z}_k}{\int e^{-\sum \bar{z}_j A_{jk} z_k}} = -\frac{\partial}{\partial a_{kj}} \log\left(\frac{c}{\det A}\right) = (A^{-1})_{jk}$$

Next suppose we want to evaluate

$$\int e^{-z^* A z + z^* \tilde{J} + J z} \Big/ \int e^{-z^* A z}$$

$$-z^* A z + z^* A A^{-1} \tilde{J} + J A^{-1} A z$$

$$= -(z^* - J A^{-1}) A (z - A^{-1} \tilde{J}) + J A^{-1} \tilde{J}$$

Thus using translation invariance of Lebesgue measure we get

$$\boxed{\frac{\int e^{-z^* A z + z^* \tilde{J} + J z}}{\int e^{-z^* A z}} = e^{J A^{-1} \tilde{J}}}$$

Master equation: Let a system have [redacted] states $|n\rangle$, and let [redacted] P_n be the probability of finding it in the state $|n\rangle$. Under suitable "Golden Rule" assumptions a perturbation $\mathcal{H}'$ induces transitions, [redacted] and the probability per unit time of the transition $m \longrightarrow n$ is

$$V_{nm} = \left|\langle n|\mathcal{H}'|m\rangle\right|^2 ,$$

Thus

$$\frac{dP_n}{dt} = \underbrace{\sum_m{}' V_{nm} P_m}_{\substack{\text{transitions} \\ \text{into } |n\rangle}} - \underbrace{\sum_m V_{mn} P_n}_{\substack{\text{transitions} \\ \text{out of } |n\rangle}}$$

Since $V_{nm} = V_{mn}$ we get

$$\frac{dP_n}{dt} = \sum_m V_{nm}(P_m - P_n)$$

(Note that this implies $\sum{}' P_n$ is constant in time)

Next

$$\frac{d}{dt}\left(-\sum{}' P_n \log P_n\right) = -\sum_n\left(+\frac{dP_n}{dt}\log P_n + \cancel{P_n}\frac{1}{\cancel{P_n}}\underset{\overset{\shortparallel}{0}}{\frac{dP_n}{dt}}\right)$$

since $\sum P_n = 1$.

$$= -\sum_n \sum_m V_{nm}(P_m - P_n)\log P_n$$

$$= \frac{1}{2}\sum_n \sum_m{}' V_{nm} \underbrace{(P_m - P_n)(\log P_m - \log P_n)}$$

$\geqslant 0$ because $P_m > P_n \Rightarrow \log P_m > \log P_n$

In fact this is > 0 unless $V_{nm} \neq 0$ [redacted] $\Rightarrow P_m = P_n$. So that if the states are connected by transitions we conclude that the entropy is strictly increasing unless all P_n are equal.

Prop. [redacted] Form a graph whose vertices are the states $|n\rangle$ and in which there is an edge [redacted] between $|n\rangle$ and $|m\rangle$ when $V_{mn} > 0$. If this graph is connected, then the entropy $-\sum P_n \log P_n$ is strictly increasing unless all the P_n are equal.

Look more closely at the DE

$$\frac{dP_n}{dt} = \sum_{m[redacted]}' V_{nm}(P_m - P_n) \qquad \text{can forget } m=n$$

$$= \sum_{m\neq n}' V_{nm} P_m + \Big(-\sum_{m\neq n}' V_{nm}\Big) P_n$$

In other words one has taken the V-matrix and adjusted the diagonal elements [redacted] so that $(1,\dots,1)$ is an eigenvector. Thus we have a symmetric matrix with positive off-diagonal entries such that the row sums are zero. Moreover the graph is connected.

Hence I should review the Mumford theorem. It tells me that this matrix is ≤ 0 with exactly one null eigenvector. (Recall the proof: Given any vector v orthogonal to $(1,1,\dots,1)$ we split its into its positive + negative component $v = v^+ - v^-$ [redacted]. Because off-diag entries >0, the form $v\cdot Av = v^+Av^+ + v^-Av^- - 2\underbrace{v^+Av^-}_{>0}$ $\leq v^+Av^+ + v^-Av^-$ and then one uses induction)

[redacted]

[redacted]

[redacted]

Time-dependent perturbation theory: Suppose we have a small interaction Hamiltonian V depending on t, and $H = H_0 + V$. Then to first order in V

$$\psi(t) = \psi_0(t) - \frac{i}{\hbar}\int^t dt_1 \, e^{-\frac{i}{\hbar}H_0(t-t_1)} V(t_1)\, \psi_0(t)$$

Suppose H_0 has eigenstates $|n\rangle$ of energy $E_n = \hbar\omega_n$, and

$$\psi_0(t) = e^{-i\omega_m t}|m\rangle$$

Then

$$\langle n|\psi(t)\rangle = e^{-i\omega_m t}\langle n|m\rangle - \frac{i}{\hbar}\int^t dt_1\, e^{-i\omega_n(t-t_1)} \langle n|V(t_1) e^{-i\omega_m t_1}|m\rangle$$

or

$$\langle n|e^{i\omega_n t}|\psi(t)\rangle = \delta_{nm} - \frac{i}{\hbar}\int^t dt_1\, e^{+i\omega_{nm}t_1}\langle n|V(t_1)|m\rangle$$

where

$$\omega_{nm} = \omega_n - \omega_m = \frac{1}{\hbar}(E_n - E_m).$$

Suppose $n \neq m$ and that V is constant for $[0,t]$. Then the amplitude for the transition $m \mapsto n$ is

$$\underset{\substack{\uparrow \\ \text{call this} \\ a_{nm}(t)}}{e^{i\omega_n t}\langle n|\psi(t)\rangle} = -\frac{i}{\hbar}\underbrace{\int_0^t dt_1\, e^{+i\omega_{nm}t_1}}_{\frac{e^{+i\omega_{nm}t}-1}{+i\omega_{nm}}}\langle n|V|m\rangle$$

or

$$a_{nm}(t) = \frac{1}{\hbar}\langle n|V|m\rangle \frac{1-e^{i\omega_{nm}t}}{\omega_{nm}}$$

Thus

$$|a_{nm}(t)|^2 = \frac{1}{\hbar^2}|\langle n|V|m\rangle|^2 \frac{4\sin^2(\omega_{nm}\frac{t}{2})}{\omega_{nm}^2}$$

is the probability of the transition with the interaction switched on [redacted] for the time [redacted] t.

Now suppose the states $|n\rangle$ to which the transition takes place form a continuous family (as in scattering). Then one wants to interpret $|a_{nm}(t)|^2$ as a probability density in n. The point is somehow to use that

$$\int \underbrace{\frac{\sin^2(\omega t/2)}{\omega^2}}_{\text{peaks around } \omega = 0.} d\omega = \frac{t}{2}\pi$$

Thus

$$\frac{\sin^2(\omega t/2)}{t\omega^2} \longrightarrow \frac{\pi}{2}\delta(\omega)$$

and so

$$|a_{nm}(t)|^2 \sim \frac{2\pi}{\hbar^2}|\langle n|V|m\rangle|^2 \, \delta(\omega_n - \omega_m) \cdot t$$

$$= \frac{2\pi}{\hbar}|\langle n|\mathbf{V}|m\rangle|^2 \, \delta(E_n - E_m) \cdot t$$

Addition to master equation: If A is a matrix with off-diagonal entries ≥ 0, then for $t \geq 0$

$$e^{tA} = \lim_{n\to\infty}\left(1 + \frac{t}{n}A\right)^n$$

has entries ≥ 0, since for large n this is true for $1 + \frac{t}{n}A$.

August 24, 1980

Master equation: Have states $|n\rangle$ and P_n is the probability of finding the system in the state $|n\rangle$, W_{nm} is the transition rate for $m \mapsto n$. Then

$$\frac{dP_n}{dt} = \sum_{m \neq n} W_{nm}(P_m - P_n)$$

i.e.

$$\frac{dP_1}{dt} = W_{12}(P_2 - P_1) + W_{13}(P_3 - P_1) + \cdots\cdots$$

It seems that only transitions between states of the same energy give rise to a transition rate. The limiting distribution is when all P_n are equal (assuming all states are mutually accessible).

Now we want to consider a system with different energy levels: ε_n in the n-th state, and we suppose it is connected to a thermal reservoir so that the total system has energy E. We've seen how the equilibrium is described by the Boltzmann distribution. Recall: Let $\sigma(E)$ be the number of states in the reservoir of energy E. The number of states of the combined system such that the small system has energy ε_n is $\sigma(E - \varepsilon_n)$. Since at equilibrium all states of the combined system of the same energy are equally probable we get

$$P_n = C\sigma(E - \varepsilon_n).$$

with C independent of n. As $\log \sigma(E - \varepsilon) = \log \sigma(E) - \frac{\sigma'(E)}{\sigma(E)}\varepsilon \cdots$ we get

$$P_n \text{ prop. to } e^{-\beta \varepsilon_n} \qquad \text{with } \beta = \frac{\sigma'(E)}{\sigma(E)}$$

Next I'd like to get a master equation to show [redacted] how a given distribution $\{P_n\}$ evolves into the Boltzmann distribution. Let's consider the simplest case where the small system has 2 states, which means that the states of the combined system of the fixed energy E are partitioned into 2 gps. So our DE looks as follows.

$$\frac{dP}{dt} = \left(\begin{array}{c|c} \quad & \quad \\ \hline \quad & \quad \end{array}\right) P$$

Take the simplest case of 3 states partitioned as follows:

$$\underbrace{1, 2}, \underbrace{3}$$

Now we are not interested in the states of the reservoir, so we would like a DE for $P_1 + P_2$, P_3

$$\frac{dP_1}{dt} = W_{12}(P_2 - P_1) + W_{13}(P_3 - P_1)$$

$$\frac{dP_2}{dt} = W_{21}(P_1 - P_2) + W_{23}(P_3 - P_2)$$

$$\frac{d}{dt}(P_1 + P_2) \text{ [redacted] } = (W_{13} + W_{23})P_3 - W_{13}P_1 - W_{23}P_2$$

$$= (W_{13} + W_{23})\left(P_3 - \frac{(P_1 + P_2)}{2}\right) \text{ [redacted]}$$

if either $W_{13} = W_{23}$ or $P_1 = P_2$

similarly under these conditions

$$\frac{dP_3}{dt} = W_{31}(P_1 - P_3) + W_{32}(P_2 - P_3) = (W_{31} + W_{32})\left(\frac{P_1 + P_2}{2} - P_3\right)$$

So the equations become

$$\frac{d}{dt}\begin{pmatrix} P_1+P_2 \\ P_3 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2}(W_{13}+W_{23}) & W_{13}+W_{23} \\ \frac{1}{2}(W_{13}+W_{23}) & -(W_{13}+W_{23}) \end{pmatrix}\begin{pmatrix} P_1+P_2 \\ P_3 \end{pmatrix}$$

Let's generalize. Suppose we have N states partitioned into blocks α of size N_α. Let P_j, $j\in N$ satisfy

$$\frac{dP_j}{dt} = \sum_{k} W_{jk}(P_k - P_j) .$$

Then

$$\frac{d}{dt}\underbrace{\left(\sum_{j\in\alpha} P_j\right)}_{\rho_\alpha} = \sum_\beta \sum_{k\in\beta}\sum_{j\in\alpha} W_{jk}(P_k - P_j)$$

$$= \sum_\beta \left(\sum_{\substack{j\in\alpha \\ k\in\beta}} W_{jk}\right)\left(\frac{\rho_\beta}{N_\beta} - \frac{\rho_\alpha}{N_\alpha}\right)$$

assuming P_j is constant over each block. Another possible notation is

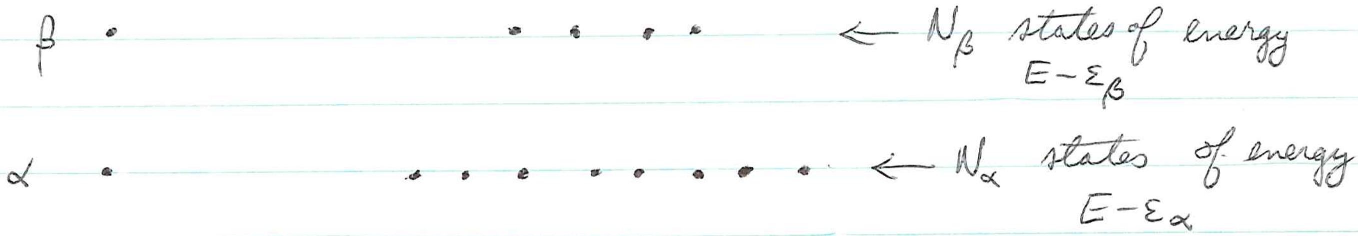
$$\tilde{\rho}_\alpha = \frac{1}{N_\alpha}\sum_{j\in\alpha} P_j$$

and the equation becomes

$$\frac{d\tilde{\rho}_\alpha}{dt} = \frac{1}{N_\alpha}\sum_\beta \underbrace{\left(\sum_{\substack{j\in\alpha \\ k\in\beta}} W_{jk}\right)}_{\text{denote this } W_{\alpha\beta}}\left(\tilde{\rho}_\beta - \tilde{\rho}_\alpha\right)$$

Anyway the first notation seems better because the blocks correspond to states of the small system, and ρ_α is the probability of the state α.

<u>Summary</u>: Suppose the small system has states α and that α can be combined with N_α states of the reservoir to get a state of the combined system of the right energy.



We assume transition rates $n \to m$, $m \to n$ for the combined system are the same. We also assume that the reservoir has a short relaxation time, so any uneven distribution of probabilities at a given energy $E-\varepsilon_\alpha$ evens out very fast. Then if we have a distribution of probabilities $\{\rho_\alpha\}$, the distribution for the combined system will have $\frac{\rho_\alpha}{N_\alpha}$ in the N_α states of energy $E-\varepsilon_\alpha$. These will transition to different states and even out, so that the <u>modified master equation</u> is

$$\boxed{\frac{d\rho_\alpha}{dt} = \sum_\beta{}' \, W_{\alpha\beta}\left(\frac{\rho_\beta}{N_\beta} - \frac{\rho_\alpha}{N_\alpha}\right)}$$

where $W_{\alpha\beta} = W_{\beta\alpha} \geq 0$. The limiting distribution is when

$$\rho_\alpha = C N_\alpha \qquad C \text{ const.}$$

August 25, 1980

Langevin approach to Brownian motion. Let $u(t)$ be the velocity of a Brownian particle. We suppose the force on the particle is the sum of a frictional force proportional to $-u$ and a random force. Thus

$$(1) \qquad \frac{du}{dt} = -\gamma u + A(t) \qquad \gamma \text{ constant} > 0$$

where A is a random fn. of t. How do we make sense out of random fn? We imagine an ensemble of similar particles. If ξ labels the member of the ensemble then the set of ξ's forms a probability space $\mathcal{E}$, and $\xi \mapsto A(t,\xi)$ is a random variable for each t.

The solution of the Langevin equation (1) is

$$u(t) = e^{-\gamma t} u_0 + e^{-\gamma t} \int_0^t e^{\gamma t_1} A(t_1)\, dt_1$$

where u_0 is the velocity at $t=0$. u_0 can in general depend on ξ. Thus $u(t)$ is a random variable for each t.

We suppose that the random force is zero on the average, i.e. $\langle A(t) \rangle = 0$. Then

$$\langle u(t) \rangle = e^{-\gamma t} \langle u_0 \rangle = e^{-\gamma t} u_0$$

assuming u_0 the same for all ξ. This shows that the mean velocity decays exponentially as expected.

Next we suppose that $A(t)$ is a stationary random process, which implies that

$$\langle A(t_1) A(t_2) \rangle$$

depends only on $t_1 - t_2$. In general it means that all the moments $\langle A(t_1)\cdots A(t_n)\rangle$ are unchanged by time translation. (One can suppose I think that there is a 1-parameter group $\xi \mapsto \xi(t)$ of autos. of the prob. space $\mathcal{E}$ such that

$$A(t,\xi) = A(t+\tau, \xi(\tau)))$$

Let's compute the variance of $u(t)$.

$$\langle (u(t) - e^{-\gamma t}u_0)^2 \rangle = e^{-2\gamma t}\int_0^t dt_1 \int_0^t dt_2\, e^{\gamma(t_1+t_2)}\langle A(t_1)A(t_2)\rangle$$

$$= e^{-2\gamma t}\, 2\int_{t\ge t_1\ge t_2\ge 0} dt_1\,dt_2 \quad e^{\gamma(t_1+t_2)}\langle A(t_1)A(t_2)\rangle$$

put $t_1 = t_2 + u$

$$= e^{-2\gamma t}\, 2\int_0^t dt_2 \int_0^{t-t_2} du \quad e^{\gamma(2t_2+u)} \underbrace{\langle A(t_2+u)A(t_2)\rangle}_{\langle A(u)A(0)\rangle}$$

$$= 2\int_0^t dt_2\, e^{-2\gamma(t-t_2)}\int_0^{t-t_2} du\, e^{\gamma u}\langle A(u)A(0)\rangle$$

$$= 2\int_0^t dv\; e^{-2\gamma v}\int_0^v du\; e^{\gamma u}\langle A(u)A(0)\rangle$$

$$= 2\int_0^t du\; e^{\gamma u}\langle A(u)A(0)\rangle \underbrace{\int_u^t e^{-2\gamma v}\,dv}_{\frac{e^{-2\gamma u} - e^{-2\gamma t}}{2\gamma}}$$

$$= \frac{1}{\gamma}\int_0^t du\,\langle A(u)A(0)\rangle\left(e^{-\gamma u} - e^{\gamma u - 2\gamma t}\right)$$

Thus $$\boxed{\lim_{t\to\infty}\left\langle \left(u(t) - e^{-\gamma t}u_0\right)^2\right\rangle = \frac{1}{\gamma}\int_0^\infty du\,\langle A(u)A(0)\rangle e^{-\gamma u}}$$

August 26, 1980

$$\frac{du}{dt} = -\gamma u + A(t)$$

$$u(t) = e^{-\gamma t} u_0 + e^{-\gamma t} \int_0^t e^{+\gamma t_1} A(t_1)\, dt_1$$

$$\langle u(t) \rangle = e^{-\gamma t} u_0$$

$$\langle (u(t) - e^{-\gamma t} u_0)^2 \rangle = e^{-2\gamma t} \int_0^t dt_1 \int_0^t dt_2 \; e^{\gamma(t_1+t_2)} \langle A(t_1) A(t_2) \rangle$$

In the stationary case Bochner's thm. yields

$$\langle A(t_1) A(t_2) \rangle = \int e^{-i\omega(t_1-t_2)}\, d\mu(\omega)$$

for some measure $d\mu$ with $\int d\mu < \infty$. Thus the variance becomes

$$e^{-2\gamma t} \int d\mu(\omega) \int_0^t dt_1\, e^{(\gamma - i\omega)t_1} \int_0^t dt_2\, e^{(\gamma+i\omega)t_2}$$

$$= e^{-2\gamma t} \int d\mu(\omega) \frac{|e^{(\gamma+i\omega)t} - 1|^2}{\gamma^2 + \omega^2}$$

As $t \to \infty$ this approaches

$$\longrightarrow \int d\mu(\omega) \frac{1}{\gamma^2+\omega^2}$$

But

$$\int \frac{e^{+i\omega t}}{\gamma^2+\omega^2} \frac{d\omega}{2\pi} = \frac{e^{-\gamma|t|}}{2\gamma}$$

so

$$\int \frac{d\mu(\omega)}{\gamma^2+\omega^2} = \int d\mu(\omega) \int dt \; e^{-i\omega t} \frac{e^{-\gamma|t|}}{2\gamma} = \frac{1}{\gamma} \int_0^\infty e^{-\gamma t} \langle A(t) A(0) \rangle\, dt$$

which is the expression obtained before.

Next suppose that $A(t)$ is a Gaussian process. This means

$$\left\langle e^{i\int J(t)A(t)\,dt}\right\rangle = e^{-\frac{1}{2}\int dt\,dt'\, J(t)\langle A(t)A(t')\rangle J(t')}$$

i.e. the moments $\langle A(t_1)\cdots A(t_n)\rangle$ are computed via Wick's thm.

(Question: The elements $A(t)$ generate a subspace $\mathcal{H}$ of $L^2(\mathcal{E})$, $\mathcal{E}$ = the ensemble behind $A(t)$. When $A(t)$ is a Gaussian process, does it follow that the symmetric algebra of $\mathcal{H}$ embeds in $L^2(\mathcal{E})$? ~~It~~ seems reasonable that $L^2(\mathcal{E})$ can be assumed to be $\mathrm{Sym}(\mathcal{H})$.)

When working with mutually Gaussian random variables, one can combine them linearly and compute the variance as if one were in a (real) Hilbert space. Thus from

$$u(t) - e^{-\gamma t}u_0 = e^{-\gamma t}\int_0^t e^{\gamma t_1} A(t_1)\,dt_1$$

we see that $u(t) - e^{-\gamma t}u_0$ is a Gaussian random variable for each t, hence is completely determined by its variance.

Therefore we see that no matter what initial velocity u_0 our Brownian particle has the velocity of $u(t)$ for large t has a Gaussian distribution with variance computed above from the auto-correlation function of A. But equi-partition says the equilibrium velocity distribution is Maxwell's: Hence [redacted] it is a Gaussian distribution with mean kinetic energy $\frac{1}{2}kT$:

$$\frac{1}{2} m \langle u^2 \rangle = \frac{1}{2} kT$$

This gives the formula

$$\boxed{\frac{k}{m} T = \frac{1}{\gamma} \int_0^\infty e^{-\gamma t} \langle A(t) A(0) \rangle \, dt}$$

(If we [redacted] write the Langevin DE in the form

$$m \frac{du}{dt} = -m\gamma u + mA$$

the above becomes

$$kT = \frac{1}{m\gamma} \int_0^\infty e^{-\gamma t} \langle mA(t)\, mA(0) \rangle \, dt$$

which isn't much help.)

Next consider the position $r(t)$ of the Brownian particle:

$$\frac{dr}{dt} = u(t) = e^{-\gamma t} u_0 + \int_0^t dt_2 \, e^{-\gamma t + \gamma t_2} A(t_2)$$

$$r(t) = r_0 + \int_0^t u(t_1) dt_1 = \underbrace{r_0 + \frac{1 - e^{-\gamma t}}{\gamma} u_0}_{\text{constant over the ensemble}} + \int_0^t dt_1 \int_0^{t_1} dt_2 \, e^{-\gamma t_1 + \gamma t_2} A(t_2)$$

$$\int_0^t dt_1 \int_0^{t_1} dt_2 \, e^{-\gamma t_1 + \gamma t_2} A(t_2) = \int_0^t dt_2 \underbrace{\int_{t_2}^t dt_1 \, e^{-\gamma t_1}}_{\frac{e^{-\gamma t_2} - e^{-\gamma t}}{\gamma}} \left(e^{+\gamma t_2} A(t_2) \right)$$

$$= \int_0^t dt_2 \, \frac{1-e^{-\gamma(t-t_2)}}{\gamma} A(t_2)$$

Another way to see this is to use the Green's function for

$$\underbrace{\left(\frac{d^2}{dt^2} + \gamma \frac{d}{dt}\right)}_{} r = A$$

has
$$G(t,t') = \begin{cases} \dfrac{1-e^{-\gamma(t-t')}}{\gamma} & t > t' \\ 0 & t < t' \end{cases}$$

So we see that except for the constant part $r_0 + \frac{1-e^{-\gamma t}}{\gamma} u_0$, the position is a suitable average of $A(t)$. Suppose $r_0 = u_0 = 0$ to simplify. Then $\langle r(t) \rangle = 0$ and

$$\langle r(t)^2 \rangle = \int_0^t dt_1 \int_0^t dt_2 \, \frac{\left[1-e^{-\gamma(t-t_1)}\right]\left[1-e^{-\gamma(t-t_2)}\right]}{\gamma^2} \langle A(t_1) A(t_2) \rangle$$

$$= \int_0^t dt_1 \int_0^t dt_2 \, \frac{(1-e^{-\gamma t_1})(1-e^{-\gamma t_2})}{\gamma^2} \underbrace{\langle A(t-t_1)\, A(t-t_2) \rangle}_{\langle A(t_2 - t_1)\, A(0) \rangle}$$

By assumption the self-correlation $\langle A(t) A(0) \rangle$ decays as $t \to \pm\infty$. (Note that $\langle A(t) A(0) \rangle = \langle A(0) A(-t) \rangle$ by stationarity $= \langle A(-t) A(0) \rangle$ since $A(0), A(-t)$ commute

$$\cancel{\langle r(t)^2 \rangle = 2\int_0^t dt_1 \int_{t_1}^t dt_2 \cdots \neq 2\int_0^t dt \int_0^t dt}$$

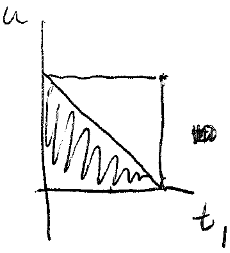
$$r(t) = \int_0^t \frac{1-e^{-\gamma(t-t_1)}}{\gamma} A(t_1)\,dt_1$$

$$\langle r(t)^2 \rangle = \iint_0^t dt_1 dt_2 \; \frac{1-e^{-\gamma(t-t_1)}}{\gamma} \; \frac{1-e^{-\gamma(t-t_2)}}{\gamma} \langle A(t_1) A(t_2) \rangle$$

$$= \int_0^t dt_1 \int_0^t dt_2 \; \frac{1-e^{-\gamma t_1}}{\gamma} \; \frac{1-e^{-\gamma t_2}}{\gamma} \; \underbrace{\langle A(t-t_1)\, A(t-t_2) \rangle}_{\langle A(t_2-t_1)\, A(0) \rangle}$$

$$= 2 \int_{0 \le \underbrace{t_1 \le t_2}_{u} \le t} dt_1 dt_2 \quad \cdots\cdots$$

$$= 2 \int_0^t dt_1 \int_0^{t-t_1} du \; \frac{(1-e^{-\gamma t_1})(1-e^{-\gamma t_1 - \gamma u})}{\gamma^2} \; \langle A(u) A(0) \rangle$$



$$= 2 \int_0^t du \underbrace{\int_0^{t-u} dt_1 \left(1 - e^{-\gamma t_1} - e^{-\gamma t_1 - \gamma u} + e^{-2\gamma t_1 - \gamma u}\right)}_{t-u - \frac{e^{-\gamma(t-u)}-1}{-\gamma}(1+e^{-\gamma u}) + \frac{e^{-2\gamma(t-u)}-1}{-2\gamma} e^{-\gamma u}} \frac{\langle A(u) A(0) \rangle}{\gamma^2}$$

$$= 2 \int_0^t t \frac{\langle A(u) A(0) \rangle}{\gamma^2} du \; + \frac{2}{\gamma^2} \int_0^t du \langle A(u) A(0) \rangle \left\{ -u \quad \cdots\cdots \right\}$$

as $t \to \infty$ we get

$$\langle r(t)^2 \rangle = t \frac{2}{\gamma^2} \int_0^\infty \langle A(u) A(0) \rangle du \; + \; \frac{2}{\gamma^2} \int_0^\infty du \, \langle A(u) A(0) \rangle \left\{ -u - \frac{1}{\gamma}(1+e^{-\gamma u}) + \frac{1}{2\gamma} e^{-2\gamma u} \right\}$$

Thus we see that

$$\langle r(t)^2 \rangle \sim t\left(\frac{1}{\gamma}\int_{-\infty}^{\infty} \langle A(t)A(0)\rangle dt\right) + \text{messy constant depending on } \langle A(t)A(0)\rangle.$$

Thus our Brownian particle for large times has position described by a Gaussian with variance proportional to t like ordinary diffusion.

$$\boxed{\text{Einstein assumption:} \quad \langle A(t)A(0)\rangle = \tau\delta(t).}$$

Using this we can work out the formulas in detail.

$$\langle r(t)^2 \rangle = \int_0^t dt_1 \int_0^t dt_2 \, \frac{1-e^{-\gamma t_1}}{\gamma} \, \frac{1-e^{-\gamma t_2}}{\gamma} \langle A(t_2-t_1)A(0)\rangle$$

assuming $r_0 = v_0 = 0$

$$= \frac{\tau}{\gamma^2}\int_0^t dt_1 \, \underbrace{(1-e^{-\gamma t_1})^2}_{1-2e^{-\gamma t_1}+e^{-2\gamma t_1}}$$

$$= \frac{\tau}{\gamma^2}\left[t + 2\,\frac{e^{-\gamma t}-1}{+\gamma} + \frac{e^{-2\gamma t}-1}{-2\gamma}\right]$$

$$= \frac{\tau}{2\gamma^3}\left[2\gamma t + 4e^{-\gamma t} - 4 - e^{-2\gamma t} + 1\right]$$

$$\boxed{\begin{aligned} \langle r(t)^2 \rangle &= \frac{\tau}{2\gamma^3}\left[2\gamma t - 3 + 4e^{-\gamma t} - e^{-2\gamma t}\right] \\ &\sim \frac{\tau}{2\gamma^3}(2\gamma t - 3) \qquad \text{as } t \to \infty \end{aligned}}$$

$$\langle u(t)^2 \rangle = \frac{1}{2\gamma}\int_{-\infty} \langle A(t)A(0)\rangle e^{-\gamma t} dt = \frac{\tau}{2\gamma}$$

Recall $\quad \frac{m}{2}\langle u^2(t)\rangle = \frac{1}{2}kT \quad \therefore \quad \frac{kT}{m} = \frac{\tau}{2\gamma}$

Now the diffusion coefficient D is defined so the fundamental solution is

$$\frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{x^2}{4Dt}}$$

Therefore $\boxed{\langle x^2 \rangle = 2Dt \quad \text{for diffusion in one dimension}}$

So

$$\langle r(t)^2 \rangle \sim \frac{\tau}{\gamma^2} t \quad \Rightarrow \quad 2D = \frac{\tau}{\gamma^2}$$

$$\tau = \frac{2\gamma k T}{m}$$

$\therefore$ $\boxed{\text{Einstein relation} \qquad D = \frac{kT}{\gamma m}}$

Under the Einstein assumption we should compute $\langle u(t)^2 \rangle$ exactly

$$\langle u(t)^2 \rangle = \int_0^t dt_1 \int_0^t dt_2\, e^{-\gamma(t-t_1)} e^{-\gamma(t-t_2)} \langle A(t_1) A(t_2) \rangle$$

$$= \tau \int_0^t dt_1\, e^{-2\gamma(t-t_1)}$$

$$= \tau \frac{1 - e^{-2\gamma t}}{+2\gamma} = \frac{\tau}{2\gamma}\left(1 - e^{-2\gamma t}\right)$$

$$\boxed{\langle u(t)^2 \rangle = \frac{\tau}{2\gamma}\left(1 - e^{-2\gamma t}\right)}$$

Let us compare the above with the Einstein derivation, which is based upon direct fiddling with the DE. Work with x instead of r. Then

$$\ddot{x} + \gamma \dot{x} = A$$

As in the virial thm. multiply by x and average:

$$\underbrace{\langle x\ddot{x}\rangle} + \gamma\langle x\dot{x}\rangle = \langle xA\rangle$$

$$\frac{d}{dt}\langle x\dot{x}\rangle - \langle \dot{x}^2\rangle$$

yields ($\Longrightarrow$)

$$\left(\frac{d}{dt}+\gamma\right)\langle x\dot{x}\rangle = \langle \dot{x}^2\rangle + \langle xA\rangle$$

Then one argues that

$$\langle xA\rangle = 0 \qquad \text{because } A(t) \text{ is indep. of } A(t') \text{ for } t'<t$$

$$\langle \dot{x}^2\rangle = \frac{kT}{m} \qquad \text{by equi-partition}$$

The first formula is correct because of

$$x(t) = \int_0^t \frac{1-e^{-\gamma(t-t_1)}}{\gamma} A(t_1)\,dt_1$$

and the fact the kernel vanishes at $t_1 = t$. The second formula is correct for equilibrium conditions, i.e. large times. The exact formula is on the preceding page.

Note the analogous argument that $\langle \dot{x}A\rangle = 0$ is false

So we have from ($\Longrightarrow$) (for large times)

$$\left(\frac{d}{dt}+\gamma\right)\langle x\dot{x}\rangle = \frac{kT}{m}$$

The steady-state solution is

$$\langle x\dot{x}\rangle = \frac{kT}{\gamma m}$$

or

$$\frac{d}{dt}\langle x^2\rangle = 2\frac{kT}{\gamma m}$$

which show that $\langle x^2\rangle$ increases as a constant rate.

Notice that if we took

$$\langle \dot{x}\ddot{x} \rangle + \gamma \langle \dot{x}^2 \rangle = \langle \dot{x} A \rangle$$

and tried to argue that $\langle \dot{x} A \rangle = 0$ because $\dot{x}(t)$ depends on $A(t')$ for $t < t'$ and $A(t)$ is independent of these, then we would get

$$\left(\frac{1}{2} \frac{d}{dt} + \gamma \right) \langle \dot{x}^2 \rangle = 0$$

which $\Longrightarrow$ $\langle \dot{x}^2 \rangle \to 0$ for large time. Hence $\langle xA \rangle = 0$ but $\langle \dot{x} A \rangle$ is a constant.

So we see Einstein's argument is brilliant but maybe unreliable, and that Langevin's equation allows a precise understanding.

Fokker-Planck equation. Integrating the Langevin equation

$$\frac{du}{dt} = -\gamma u + A$$

leads to a flow on the set of probability distributions on u-space in the following manner. Think of A as being given by an ensemble of functions $A(t, \xi)$ $\xi \in \mathcal{E}$. Then given a distribution u_0 for initial velocity we imagine it given by a separate ensemble $\mathcal{E}_0$. Then we take the ensemble $\mathcal{E}_0 \times \mathcal{E}$. What this means is that we make u_0 and A independent of each other. Assuming A has independent increments, i.e. $\langle A(t_1) A(t_2) \rangle = c\delta(t_1 - t_2)$, $u(t)$ should remain independent of A.

?

August 27, 1980

Fokker-Planck equation: The idea is that integrating the Langevin equation

(1) $$\frac{du}{dt} = -\gamma u + A(t)$$

yields a flow on the space of probability distributions on u-space. How? Given a distribution u_0 we make it independent of the process $A(t)$. This means that if u_0 is realized as a function on $\mathcal{E}_0$ and if the process is realized on $\mathcal{E}$, then we work on $\mathcal{E}_0 \times \mathcal{E}$. The solution of the Langevin equation is

(2) $$u(t) = e^{-\gamma t} u_0 + \int_0^t dt_1\, e^{-\gamma(t-t_1)} A(t_1)$$

These two summands are independent. We are assuming that

(3) $$\langle A(t_1) A(t_2) \rangle = \tau\, \delta(t_1 - t_2),$$

and strictly speaking, probably $A(t)$ doesn't make sense, rather it is a distribution with values being random variables. For example, if $E(t)$ is a increasing family of projections in a Hilbert space, then the path $E(t)v$ has orthogonal increments, so

$$A(t) = \frac{d}{dt} E(t) v \qquad \text{(formally)}.$$

In any case when we use (3) we always use integrals of $A(t)$, and then integrals with disjoint supports are orthogonal. Hence the process $e^{\gamma t} u(t)$ defined by (2) has independent increments.

So now it's more or less clear to me that

I have some sort of flow on the measures on u-space. This is a *Markov* process, because ~~[illegible] $u(t')$ depends only upon $u(t_0)$ and not~~ given $t' < t$, one can compute $u(t)$ from $u(t')$ without knowing $u(t'')$ for $t'' < t'$. There's the Chapman-Kolmogorov equation

$$(*) \qquad W(x, t+\Delta t) = \int K(x, t+\Delta t; x', t)\, W(x', t)\, dx'$$

where $W(x,t)\,dx$ denotes the probability distribution of $u(t)$.

So let's now recall how to derive a diffusion-style equation from $(*)$. Take a test function $\phi(x)$ and integrate

(assume process stationary)

$$\int dx\, \phi(x)\, W(x, t+\Delta t) = \int dx' \underbrace{\int dx\, \phi(x)\, K(x, x'; \Delta t)}\; W(x', t)$$

$$= \int dx \left[\phi(x') + \phi'(x')(x-x') + \frac{\phi''(x')}{2}(x-x')^2 + \cdots \right] K(x, x'; \Delta t)$$

At this point we need to know the moments of the distribution $dx\, K(x, x', \Delta t)$ which represents what happens when we start with δ fn. at x' and let it evolve a time Δt. In previous notation

$$u_0 = \text{const } x'$$

$$dx\, K(x, x', \Delta t) = \text{distribution of } u(\Delta t).$$

Thus

$$\text{mean} = \langle u(\Delta t) \rangle = e^{-\gamma \Delta t} x'$$

$$\text{variance} = \langle (u(\Delta t) - e^{-\gamma \Delta t} x')^2 \rangle = \frac{I}{2\gamma}\left(1 - e^{-2\gamma \Delta t}\right)$$

$$\therefore \int dx\, (x-x')\, K(x,x';\Delta t) = e^{-\gamma\Delta t}x' - x' \approx -\gamma(\Delta t)x'$$

$$\int dx\, (x-x')^2\, K(x,x';\Delta t) = \langle x^2\rangle - 2\langle x\rangle x' + x'^2$$

$$= \langle (x-\langle x\rangle)^2\rangle + \langle x\rangle^2 - 2\langle x\rangle x' + x'^2$$

$$= \frac{\tau}{2\gamma}\left(1-e^{-2\gamma\Delta t}\right) + \underbrace{e^{-2\gamma\Delta t}(x')^2 - 2e^{-\gamma\Delta t}x'^2 + x'^2}_{x'^2\left(1-e^{-\gamma\Delta t}\right)^2}$$

$$= (\tau)\Delta t + O\left((\Delta t)^2\right)$$

Thus we get

$$\int dx\, \phi(x)\, \frac{W(x,t+\Delta t)-W(x,t)}{\Delta t} = \int dx' \left[-\phi'(x')\gamma x' + \tfrac{1}{2}\phi''(x')\tau\right] \times W(x',t)$$

so integrating by parts yields

$$\boxed{\frac{\partial W}{\partial t} = \gamma \frac{\partial}{\partial x}(xW) + \frac{1}{2}\tau \frac{\partial^2 W}{\partial x^2}}$$

which is the Fokker-Planck eqn. Here x denotes velocity, so should be replaced by v or u.

Similarly if we consider the Langevin equation as defining a flow of distributions on phase space (position + velocity) one gets a PDE called the Chandrasekhar equation:

$$\frac{\partial W}{\partial t} + v\frac{\partial W}{\partial v} = \gamma \frac{\partial}{\partial v}(vW) + \frac{1}{2}\tau \frac{\partial^2 W}{\partial v^2}$$

Wiener – Khinchin theorem. Suppose that $A(t)$ is a random periodic function with period L. Random here is interpreted to mean there is an ensemble around so that averages can be computed via time averages. Thus we have

$$\langle A(t+s)A(t)\rangle = \frac{1}{L}\int_0^L A(t+s)A(t)\,dt$$

Call the quantity $K(s)$. Take Fourier series

$$A(t) = \sum_{\omega\in\frac{2\pi}{L}\mathbb{Z}} e^{-i\omega t}\hat{A}(\omega) \qquad \hat{A}(\omega) = \frac{1}{L}\int_0^L e^{i\omega t}A(t)\,dt$$

Then

$$K(s) = \frac{1}{L}\int_0^L A(t+s)A(t)\,dt = \sum_{\omega} e^{-i\omega s}\left|\hat{A}(\omega)\right|^2$$

where we have used that $A(t)$ is real. This is one form of Wiener – Khinchin: The self-correlation fn. $\frac{1}{L}\int_0^L A(t+s)A(t)\,dt$ is the Fourier transform of the power function $|\hat{A}(\omega)|^2$. The point is that $\hat{A}(\omega)$ is the amplitude of $A(t)$ of frequency ω, and $|\hat{A}(\omega)|^2$ is the intensity.

Actually we didn't use an ensemble at all.

$$A(t) = \sum_{\omega\in\frac{2\pi}{L}\mathbb{Z}} e^{-i\omega t}\hat{A}(\omega) \qquad \hat{A}(\omega) = \frac{1}{L}\int_0^L e^{i\omega t}A(t)\,dt$$

$$\Longrightarrow \quad \frac{1}{L}\int_0^L A(t+s)\overline{A(t)}\,dt = \sum_{\omega\in\frac{2\pi}{L}\mathbb{Z}} e^{-i\omega s}\left|\hat{A}(\omega)\right|^2$$

But now let us bring in the ensemble idea. Then $A(t)$ is a family of functions and so is $\hat{A}(\omega)$. We have

$$(*) \qquad \langle A(t+s)\,\overline{A(t)}\rangle = \sum_{\omega_1,\omega_2} e^{-i\omega s}\, e^{-i\omega_1 t\,\text{[redacted]} + i\omega_2 t\,\text{[redacted]}} \langle \hat{A}(\omega_1)\,\overline{\hat{A}(\omega_2)}\rangle$$

and the fact that this is independent of t tells me[redacted] that

$$\langle \hat{A}(\omega_1)\,\overline{\hat{A}(\omega_2)}\rangle = 0 \qquad \omega_1 \neq \omega_2$$

Therefore the fact that $A(t)$ is a stationary process should mean that the different Fourier components are [redacted] independent random variables. [redacted] This [redacted] is true for Gaussian random variables [redacted] at least, where independence is the same as orthogonal.

The above equation $(*)$ yeilds

$$\langle A(t+s)\,\overline{A(t)}\rangle = \sum_{\omega} e^{-i\omega s} \langle |\hat{A}(\omega)|^2\rangle$$

which is another version of Wiener-Khinchin.