refs: ① N.G. Van Kampen, "Stochastic Processes in Physics and Astronomy"
② Zwanzig, "Nonequilibrium Statistical Mechanics"

II. Master Equation

→ Master equation, dating from Nordsieck, Lamb, Uhlenbeck, 1940, is a general form/structure for evolution of pdf due transitions between states.

→ Master equation structure applicable to both classical and quantum problems.

To derive:

Recall Chapman-Kolmogorov equation:

Generic to Markov Process

$$\boxed{\underbrace{T_{\tau+\tau'}(y_3|y_1)}_{\substack{\text{transition from } y_3 \text{ to } y_1\\ \text{in interval } \tau+\tau'}} = \underbrace{\int dy_2}_{\text{sum over intermediates}} \underbrace{T_{\tau'}(y_3|y_2)}_{\substack{\text{transition from } 2\to 3\\ \text{in } \tau' \text{ probability}}} \underbrace{T_{\tau}(y_2|y_1)}_{\substack{\text{transition from}\\ 1\to 2 \text{ in } \tau\\ \text{probability}}}}$$

→ general statement of evolution for Markov process.

Now, for small/short (relative to what?) transition time, can write:

$$T_{\tau'}(y_2|y_1) = (1-\alpha_0\tau')\,\delta(y_2-y_1) + \tau' W(y_2|y_1) + \text{h.o.t.}$$

- $W(y_2|y_1) \equiv$ transition probability per unit time for $y_1 \to y_2$

$W(y_2|y_1) > 0$

- $(1-\alpha_0\tau')\,\delta(y_2-y_1) \equiv$ probability that no transition takes place during τ'

and $P_{\text{trans}} + P_{\text{no trans}} = 1 \Rightarrow$

$$\alpha_0 = \int dy_2\, W(y_2|y_1) \quad \to \text{loss rate}$$

Now, insert $T_{\tau'}$ in C-K equation:

$$T_{\tau+\tau'}(y_3|y_1) = \int dy_2\, T_\tau(y_2|y_1)\left\{(1-\alpha_0\tau')\,\delta(y_3-y_2) + \tau' W(y_3|y_2)\right\}$$

$$= T_\tau(y_3|y_1)(1-\alpha_0\tau') + \tau'\int dy_2\, W(y_3|y_2)\,T_\tau(y_2|y_1)$$

$$= T_\tau(y_3|y_1) - \tau'\left\{\int dy_2\, W(y_2|y_3)\, T_\tau(y_3|y_1) - \int dy_2\, W(y_3|y_2)\, T_\tau(y_2|y_1)\right\}$$

so, re-grouping:

$$T_{\tau+\tau'}(y_3|y_1) - T_\tau(y_3|y_1) = \tau'\left\{\int dy_2\, W(y_3|y_2)\, T_\tau(y_2|y_1) - \int dy_2\, W(y_3|y_2)\, T_\tau(y_3|y_1)\right\}$$

and expanding (short τ):

$$\cancel{T_\tau(y_3|y_1)} - \cancel{T_\tau(y_3|y_1)} + \cancel{\tau'}\,\frac{\partial T}{\partial t}(y_3|y_1)$$

$$= \cancel{\tau'}\left\{\int dy_2 \left[W(y_3|y_2)\, T_\tau(y_2|y_1) - W(y_3|y_2)\, T_\tau(y_3|y_1)\right]\right.$$

Now, $T_\tau(y_2|y_1) = P(y_2,t)$

transition probability of $1 \to 2$ in τ

↳ pdf of y_2, at t

so

$$\frac{\partial T}{\partial t}(y_3|y_1) = \int dy' \left[W(y|y')\, T(y',t) - W(y'|y)\, T(y,t) \right]$$

or, more transparently:

(avoid need of interchange ?!)

$$\boxed{\frac{\partial P(y,t)}{\partial t} = \int dy' \left\{ W(y|y')\, P(y',t) - W(y'|y)\, P(y,t) \right\}}$$

– the Master Equation.

in discrete form (i.e. quantized states):

$$\boxed{\frac{d}{dt} P_n(t) = \sum_{n'} \left\{ W_{n,n'}\, P_{n'}(t) - W_{n',n}\, P_n(t) \right\}}$$

here, in QM, transition probabilities determined by Fermi Golden Rule, i.e.:

$$W_{n,n'} = \frac{2\pi}{\hbar} \underbrace{|H'_{n,n'}|^2}_{\text{matrix element of pert. Hamiltonian}} \underbrace{\rho(E_{n'})}_{\text{density of states}}$$

$$|H'_{n,n'}|^2 = |\langle n|H'|n'\rangle|^2 = \left|\int d^3x\, \varphi_n(\underline{x})\, H' \varphi_{n'}(\underline{x})\right|^2$$

→ What does the Master Equation mean?

→ simply : birth vs death

i.e. $\frac{\partial P_n(t)}{\partial t} = \sum_{n'} \Big\{ \underbrace{W_{n,n'} P_{n'}(t)}_{\text{birth}} - \underbrace{W_{n',n} P_n(t)}_{\text{death}} \Big\}$

birth
i.e. transition into state n from states n'

death
i.e. transition out of state n into states n'

→

Contrast : Master Equation vs. Fokker-Planck Eqn.

a la' Pblm #3 of Set #1, can derive F-P equation from Master equation, with additional assumption of small deflection/increment, i.e.

$$\frac{\partial}{\partial t} f(V,t) = \text{in} - \text{out}$$

$$= \int d\Delta V \Big\{ \overset{\text{in}}{T(V-\Delta V, \Delta V, T)\, f(V-\Delta V, t)} - \overset{\text{out}}{T(V, \Delta V, T)\, f(V,t)} \Big\} \to \text{Master Equation}$$

at this point, nothing said about ΔV being "small"

Now, expand for small ΔV,

$$\cong \cancel{f(V,t)} - \frac{\partial}{\partial V}\int d\Delta V\, \Delta V\, T f + \frac{1}{2}\frac{\partial^2}{\partial V^2}\int d\Delta V (\Delta V)^2 T f$$

$$- \cancel{f(V,t)}$$

$$\frac{\partial f(v,t)}{\partial t} = -\frac{\partial}{\partial v}\left\{ \langle \Delta v \rangle f - \frac{\partial}{\partial v} \frac{\langle \Delta v \Delta v \rangle}{2} f \right\}$$

here $\langle \;\rangle = \int d\Delta v \, T$

transition-per-time, so $1/\Delta t$ understood.

$\Rightarrow$ F.-P. E.

Morals: - Master equation is more general than Fokker-Planck equation.

- Fokker-Planck equation is small deflection/increment limit of Master equation.

Another Contrast: Master Equation vs. Chapman-Kolmogorov Equation

- C-K. equation is nonlinear and expresses Markov character, but contains no process-specific info.

- Master equation is process specific, via transition probability, and is linear given transition probability.

Moral: Master equation only as useful as transition probabilities input to it!

→ Simple Examples of Master Equation

① Radioactive Decay

- Consider a group of n radioactive nuclei which survive at some time t, from some initial batch

- each nuclei has decay probability-per-time of γ

Find $P(n,t)$
↳ probability of n at time t.

Now, decay only, so:

$$
\begin{aligned}
T_{\Delta t}(n|n') &= 0 \,, & n > n' \\
&= n'\gamma\Delta t \,, & n = n'-1 \\
&= \text{h.o.} \,, & n = n'-2
\end{aligned}
$$

$$
\begin{aligned}
T_{2\Delta t}(n'-2|n') &= (n'\gamma\Delta t)((n'-1)\gamma\Delta t) \\
&= n'(n'-1)\gamma^2(\Delta t)^2
\end{aligned}
$$

i.e. - higher # jumps higher order in Δt, which is small

- 1 step cascade process.

so $\quad W_{nn'} = \gamma n' \delta_{n,n'-1}$

$$\frac{\partial P_n}{\partial t} = \sum_{n'} \left(W_{nn'} P_{n'}(t) - W_{n'n} P_n(t) \right)$$

$$= \sum_{n'} \left(\gamma n' \delta_{n,n'-1} P_{n'}(t) - \gamma n \delta_{n',n} P_n(t) \right)$$

$$= \gamma(n+1) P_{n+1}(t) - \gamma n P_n(t)$$

∴ have Master Equation:

$$\frac{\partial P_n}{\partial t} = \underbrace{\gamma(n+1) P_{n+1}(t)}_{\substack{\text{birth of } n\text{-population} \\ \text{from } (n+1) \text{ population}}} - \underbrace{\gamma n P_n(t)}_{\substack{\text{death of } n \text{ population} \\ \text{into } n-1 \text{ population}}}$$

and need i.c. $\quad P_n(0) = \delta_{n,n_0}$.

For this type (linear!) Master equation, convenient to write:

$$\langle N \rangle = \sum_n n P_n \qquad \rightarrow \text{ i.e. defines avg.}$$

then $$\frac{d\langle N\rangle}{dt} = \sum_{n=0}^{\infty} n\dot{P}_n$$

$$= \gamma\left\{\sum_{n=0}^{\infty} n(n+1)P_{n+1} - \sum_{n=0}^{\infty} n^2 P_n\right\}$$

shifting sum

$$= \gamma \sum_{n=0}^{\infty}\left\{(n-1)nP_n - \sum_{n=0}^{\infty} n^2 P_n\right\}$$

$$= \gamma\left(-\sum_{n=0}^{\infty} nP_n\right) = -\gamma\langle N\rangle$$

$\therefore$ $\langle N\rangle = \langle N\rangle_0 e^{-\gamma t}$, as expected.

Exercise: $\left\{\begin{array}{l}\text{Compute } \langle N(t)^2\rangle \text{ and } \langle N(t)^2\rangle - \langle N(t)\rangle^2 \\ = \Delta(N^2) \text{ for decay.}\end{array}\right.$

② Chemical Kinetics

Consider bimolecular reaction:

$$A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A + A$$

k_1 – forward rate constant

k_2 – backward rate constant

Now, # A molecules $- m$

B molecules $- n$

as reaction converts B to A,

$$N = m + n = \text{const, throughout}$$

Thus, have two possible (microscopic) transitions

forward rate const   #A   #B — for reaction

$$W(m+1, n-1 \,|\, m, n) = k_1 \frac{m \; n}{V}$$

forward transition   ↳ volume norm factor

→ makes AA from AB

and

backward rate const   #A   #A

$$W(m-1, n+1 \,|\, m, n) = k_2 \frac{m \; m}{V}$$

back transition

→ makes AB from AA

so can write Master equation:

Finally, as $m+n=N$

can put $n = N-m$

so

$$W(m+1|m) = k_1 \frac{m(N-m)}{V} \quad \rightarrow \text{forward}$$

$$W(m-1|m) = k_2 \frac{m^2}{V} \quad \rightarrow \text{backward.}$$

Now, $\frac{dP_m}{dt}$ = (gains) − (losses)

= (① forward transitions $m-1 \rightarrow m$; ② back transitions $m+1 \rightarrow m$) − (③ forward transitions $m \rightarrow m+1$; ④ back transitions $m \rightarrow m-1$)

∴

$$\frac{dP_m(t)}{dt} = \overset{①}{\frac{k_1}{V}(m-1)(N-m+1)\,P_{m-1}(t)} + \overset{②}{k_2\frac{(m+1)^2}{V}\,P_{m+1}(t)}$$

$$- \overset{③}{\frac{k_1}{V}m(N-m)\,P_m(t)} - \overset{④}{k_2\frac{m^2}{V}\,P_m(t)}$$

is Master eqn. for reaction.

Furthur, can take V big, so

$c = m/V$ → concentration of m

$c_0 = N/V$ → concentration of total

$\rho(c,t)$ – pdf of concentration

so

$$\frac{dP_m}{dt} = V\Big\{ k_1 (c - 1/V)(c_0 + 1/V - c) P_{m-1} + k_2 (c + 1/V)^2 P_{m+1} - k_1 c (c_0 - c) P_m - k_2 c^2 P_m \Big\}$$

and can furthur take:

$$P_{m+1} - P_m \cong \frac{1}{V}\frac{\partial \rho}{\partial c} \qquad \text{i.e. } m \gg 1$$

All said, for large V, can convert to F.-P. equation, i.e.

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial c}\Big\{ (k_1 c (c_0 - c) - k_2 c^2)\rho - \frac{1}{2V}\frac{\partial}{\partial c}\Big[(k_1 c (c_0 - c) + k_2 c^2)\rho \Big] \Big\}$$

→ General Properties of the Master Equation

$$\frac{\partial P_n}{\partial t} = \sum_{n'} \left\{ W_{n,n'} P_{n'}(t) - W_{n',n} P_n(t) \right\}$$

so entire content is $W_{n,n'}$ ⇒ useful to consider general structure of W.

Useful to define $\mathcal{W}$-matrix:

i.e.

$$\mathcal{W}_{n,n'} = W_{n,n'} \,, \quad n \neq n'$$

$$\mathcal{W}_{nn} = -\sum_{n' \neq n} W_{n',n}$$

so

$$\mathcal{W}_{n,n'} = \underset{n\neq n'}{W_{n,n'}} - \delta_{n,n'} \left(\sum_{n''} W_{n'',n} \right)$$

advantage of this is that can write:

$$\dot{P}_n(t) = \sum_{n'} \mathcal{W}_{n,n'} P_{n'}(t)$$

i.e.

$$\dot{\underline{P}}(t) = \underline{\underline{\mathcal{W}}} \cdot \underline{P}(t) \Rightarrow \underline{P}(t) = e^{t\mathcal{W}} \underline{P}(0)$$

$$\dot{P}_n(t) = \sum_{n'} \left(\underset{n\neq n'}{W_{n,n'}} - \delta_{n,n'} \left(\sum_{n''} W_{n'',n} \right) \right) P_{n'}(t)$$

$$\Rightarrow \dot{\rho}_n(t) = \sum_{n'} \left(W_{n,n'} \rho_{n'}(t) - W_{n',n} \rho_n(t) \right)$$
$n \neq n'$

upon re-label.

Now, as $W_{n,n'}$ is transition probability;

① $\Rightarrow$ $W_{n,n'} \geq 0$ for $n \neq n'$

② $\Rightarrow$ $\sum_n W_{n,n'} = 0$ (Exercise : Show this!).

defines W - matrix.

What of structure of W matrix ??

$\Rightarrow$ structure ~~determines~~ determined by class of transitions....

i.e. (i) W completely reducible or decomposable if can be put (via permutation / relabeling of rows columns) in form:

$$\underline{\underline{W}} = \begin{pmatrix} A, & 0 \\ 0, & B \end{pmatrix}$$

where A, B square matrices.

— Decomposable $\mathcal{W}$ matrix $\leftrightarrow$ A, B break whole system into non-interacting subsystems

— no transitions between A, B subsystems

(ii) $\mathcal{W}$ incompletely reducible if can be cast in form:

$$\mathcal{W} = \begin{pmatrix} A, & D \\ 0, & B \end{pmatrix}$$

A, B square, but D, in general, is not.

Meaning of incomplete reducibility: $\leftrightarrow$ type of subsystem coupling

$$\dot{P}_a = \sum_{a'} A_{a,a'} P_{a'} + \sum_{b} D_{a,b} P_{b'}$$

$$\dot{P}_b = \sum_{b'} B_{b,b'} P_{b'}$$

subsystems couple.

i.e. - can determine probability of B (i.e. P_b's) without knowing a's.

- but a, b couple via D

i.e. $$\frac{d}{dt}\sum_b P_b = \sum_b \sum_{b'} B_{b,b'} P_{b'}$$

$$= \sum_{b'} \left(\sum_b B_{b,b'}\right) P_{b'}$$

but $$\sum_n W_{nn'} = 0$$

$$\Rightarrow \quad \frac{d}{dt}\sum_b P_b = -\sum_{b'}\left(\sum_a D_{a,b'}\right) P_{b'}$$

so $\Rightarrow$ b states depleted by coupling via D.

b states $\rightarrow$ transient i.e. ultimately must $\rightarrow 0$ for stationary solution

a states $\rightarrow$ absorbing, i.e. gain probability from b's as $t \to \infty$.

(iii) W is called splitting, if can be written in form:

$$W = \begin{bmatrix} A, & 0, & D \\ 0, & B, & E \\ 0, & 0, & C \end{bmatrix}$$

where $\begin{cases} A, B \text{ are } W\text{-matrixes.} \\ C \text{ is square} \\ \text{some elements } D, E \neq 0 \end{cases}$

For splitting W matrix:

- c-states transient
- these deplete into A, B, time asymptotically.

General Properties of Master Equation, cont'd.

Recall Master Equation: for Markovian stochastic process

$$\frac{\partial}{\partial t} P_n = \sum_{n'} \{ \underbrace{W_{n,n'}}_{\text{transition probability per time}} \underbrace{P_{n'}(t)}_{\text{in}} - \underbrace{W_{n',n} P_n(t)}_{\text{out}} \}$$

where: Chapman-Kolmogorov $\supset$ Master $\supset$ Fokker-Planck

and can conveniently re-write as:

$$\dot{\underline{P}}_n = \underline{\underline{\mathcal{W}}} \cdot \underline{P}_n(t)$$

$$\mathcal{W}_{n,n'} = \underset{n' \neq n}{W_{n,n'}} - \delta_{n,n'} \left(\sum_{n''} W_{n'',n} \right)$$

structure of $\mathcal{W}$-matrix allows classification of systems and processes, i.e.

$$\mathcal{W} = \begin{pmatrix} A, & 0 \\ 0, & B \end{pmatrix} \quad ; \quad \mathcal{W} = \begin{pmatrix} A, & D \\ 0, & B \end{pmatrix}$$

"decomposable"
→ non-interacting subsystems (i.e. decoupled)

"incompletely reducible/decomposable"

D not, in general, square.

→ subsystems coupled

i.e. b-states: transient, must → 0 at stationarity

a-states: ~~absorbing~~ - pumped by b's.

and can go furthur to define "splitting"

$$\mathcal{W} = \begin{pmatrix} A, & 0, & D \\ 0, & B, & E \\ 0 & 0 & C \end{pmatrix}$$

→ where C-states transient and a, b absorbing ...

Moral of the story: Structure of $\mathcal{W}$ matrix determines classes of dynamics in Master Eqn.

Now consider:

a.) closed isolated physical systems

b.) entropy and detailed balance

c) eigenfunctions of $\mathcal{W}$-matrix

d.) macroscopics.

a.) Closed, Isolated, Physical Systems

– meaning?

"physical" ↔ there exists underlying microscopic description (i.e. Hamiltonian equations)

"isolated" ↔ no external forces act, E is C.O.M., dynamics constrained to energy shell

"closed" ↔ microscopic variables fixed – no exchange of matter with outside.

- What happens, how describe?

→ microcanonical ensemble sets equilibrium distribution for given value of energy.

i.e. $\underbrace{\Omega(E)}_{\text{microcanonical partition function}} = \underbrace{\int dx_i \int dp_i}_{\text{phase space volume}} \underbrace{\delta(H-E)}_{\text{energy shell}}$

→ if additional COMs, energy shell decomposes into uncoupled sub-shells, etc.

∴ for Master equation for such a system:

→ $\underline{\underline{W}}$ decomposes into separate blocks for separate subshells

→ subshell is indecomposable (i.e. ergodicity)

∴ $\underline{\underline{W}}$ matrix for subshell is square.

and

→ Master equation has single, stationary solution ρ_n^s (ergodicity!)

and $\rho_n^s = \rho_n^e$ ⇒ solution must be identical to equilibrium distribution

so, stationarity ⇒

$$\boxed{\sum_{n'} W_{n,n'} \rho_{n'}^e = \left(\sum_{n'} W_{n',n} \right) \rho_n^e}$$

- relates W's, as ρ_n^e known from eqbrm. stat mech.

- no p_n^e vanishes, no transient states.

Note, however, that stationarity condition $\not\Rightarrow$ detailed balance, i.e.

$$\sum_{n'} W_{n,n'}\, p_{n'}^e = \Big(\sum_{n'} W_{n',n}\Big)\, p_n^e \quad \rightarrow \text{ state integrated } \Big(\sum_{n'}\Big) \text{ condition}$$

vs detailed balance:

$$W_{n,n'}\, p_{n'}^e = W_{n',n}\, p_n^e \quad \rightarrow \text{ state-by-state criterion}$$

N.B.: ① Detailed balance $\Leftrightarrow$ microscopic time reversed symmetry (with $B \Rightarrow -B$)

② For system in contact with heat bath at temperature T

$$p_n^e = \underbrace{g_n}_{\text{phase volume factor}}\, e^{-\overbrace{\epsilon_n}^{\text{energy}}/T}$$

Exercise: show this!

b) Entropy

- How does system approach stationary state of Master equation?

N.B. - strictly speaking, discussion limited to closed, isolate physical systems

$\rightarrow$ positive p_n^e known

— but, discussion generalizable provided no transient states [N.B.: Is this all?]

? How would transient state violate H-thm?

Now, consider Master equation

$$\frac{\partial P_n}{\partial t} = \sum_{n'} \left\{ W_{n,n'} P_{n'} - W_{n',n} P_n \right\}$$

with stationary solution P_n^e existing, with $P_n^e > 0$.

take $f(x)$ to be arbitrary, non-negative, convex function $f(x)$ s/t

$$0 \leq x < \infty, \quad f(x) \geq 0, \quad f''(x) > 0$$

and, (surprise!) define H via: H-function

$$\boxed{H(t) = \sum_n P_n^e f\left(P_n(t)/P_n^e \right) \equiv \sum_n P_n^e f(x_n)}$$

$H(t) \geq 0$, by construction, and; $\boxed{x_n = P_n / P_n^e}$

$$\frac{dH(t)}{dt} = \sum_n \left\{ \cancel{\dot{P}_n^e f(x_n)} + \dot{x}_n f'(x_n) P_n^e \right\}$$

eqbm

$$= \sum_{n,n'} \frac{f'(x_n)}{\cancel{P_n^e}} \left(W_{n,n'} P_{n'} - W_{n',n} P_n \right) \cancel{P_n^e}$$

so

$$\frac{dH(t)}{dt} = \sum_{n,n'} W_{n,n'} \rho_n^e \left\{ x_{n'} f'(x_n) - x_{n'} f'(x_{n'}) \right\}$$

i.e. $n \Leftrightarrow n'$ interchange in second term.

Now, have for arbitrary $\psi_n, \psi_{n'}$:

$$\sum_{n,n'} W_{n,n'} \rho_{n'}^e (\psi_n - \psi_{n'}) = 0$$

if detailed balance applies

i.e. $n \Leftrightarrow n'$

$$\sum_{n,n'} W_{n,n'} \rho_{n'}^e (\psi_n - \psi_{n'}) = \sum_{n,n'} W_{n',n} \rho_n^e (\psi_{n'} - \psi_n)$$

$$= \sum_{n,n'} W_{n',n} \rho_{n'}^e (\psi_{n'} - \psi_n)$$

so $X = -X \Rightarrow X = 0$.

Now, choosing $\psi_n = f(x_n) - x_n f'(x_n)$

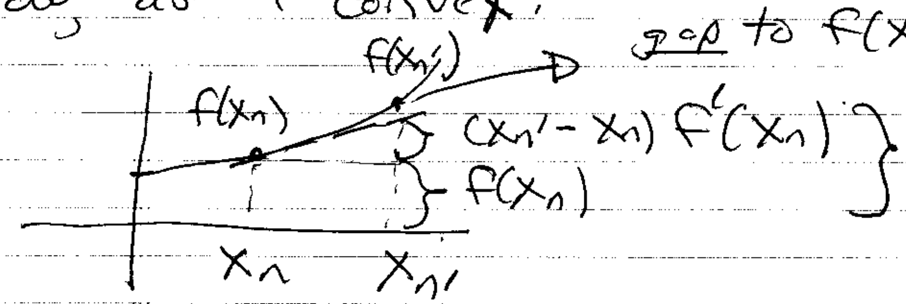
and using above to write zero creatively,

$$\frac{dH(t)}{dt} = \sum_{n,n'} W_{n,n'} \rho_{n'}^e \Big\{ x_n' f'(x_n) - x_{n'} f'(x_{n'}) + f(x_n) - x_n f'(x_n) - f(x_{n'}) + x_{n'} f'(x_{n'}) \Big\}$$

so

$$\frac{dH}{dt}(t) = \sum_{n,n'} w_{n,n'}\, p^{e}_{n'} \Big\{ (x_{n'} - x_n)\, f'(x_n) + f(x_n) - f(x_{n'}) \Big\}$$

Now, as f convex:



$\rightarrow f(x_n) + (x_{n'} - x_n) f'(x_n)$

so

$$\boxed{\frac{dH}{dt}(t) = \sum_{n,n'} w_{n,n'}\, p^{e}_{n'} \Big\{ f(x_n) + (x_{n'} - x_n)\, f'(x_n) - f(x_{n'}) \Big\}} \quad *$$

≤ 0

(i.e. "=" if $x_n = x_{n'}$)

so

$\Rightarrow dH/dt < 0$

but

$\Rightarrow H > 0$

so H tends to limit, for which $*$ vanishes

i.e. $dH/dt = 0$.

Now $dH/dt = 0$ possible only if
$x_n = x_{n'}$ for all n, n' s/t $w_{n,n'} \neq 0$.

So

① → either n covers all states [i.e. each $x_{n'}$ equals all x_n which can be reached by a string of transitions with non-zero probability]

or

② → n covers a 'disconnected' subset of all states

if ①, $\rho_n(\infty) = \rho_n^e$ (i.e. $x \to$ const $= 1$)

if ②, W decomposable, and $\rho_n(\infty) \to \rho_n^e$ (up to factor) within disjoint subsets

either way, $\frac{dH}{dt} = 0 \Rightarrow \rho_n \to \rho_n^e$.

Note: the usual choice of f is
$f = x \ln x$, $H = \sum_n \rho_n \ln(\rho_n/\rho_n^e)$

→ makes contact with Boltzmann H-thm from kinetic theory

→ H additive, etc.

Consider 2 independent subsystem

states	probability
n	p_n
m	q_m

and can combine:

(n, m)	$p_n q_m$
combined state	combined probability

$$H = \sum_{n,m} p_n q_m \ln\left\{\frac{p_n q_m}{p_n^e \, q_m^e}\right\} = \sum_n p_n \ln \frac{p_n}{p_n^e} + \sum_m q_m \ln \frac{q_m}{q_m^e}$$

Ex: Show This!

c.) Eigenfunctions of W Matrix

→ Useful to consider dynamics, relaxation, etc. in terms of "modes" of system of transition events. (i.e. a/a' linear chain ...)

Point: Master Equation is linear...

→ Obviously here:

1 mode with zero frequency
all other modes damped } why?

Now, assume
→ detailed balance (↔ symmetry)
→ $\mathcal{W}$ indecomposable

for eigenvalues/functions:

$$\mathcal{W}\Phi_\lambda = -\lambda\Phi_\lambda$$

as eigenvalues non-positive definite (from stability).

Have:

→ one $\lambda = 0$, with $\Phi_{\lambda=0} = \Phi_0 = \rho^e$ (equilibrium). Here $\Phi_0 > 0$.

so

→ $\rho(t) = \sum_\lambda c_\lambda \Phi_\lambda e^{-\lambda t}$ (damped modes as relaxation to equilibrium...)

→ general representation of ρ.

→ assumed detailed balance ⇒

$$w(y|y')\rho^e(y') = w(y'|y)\rho^e(y)$$

$$\rho^e(y) = \Phi_0$$

so, if define scalar product

$$(\Phi, \Psi) = \int dy \frac{\Phi(y)\Psi(y)}{\Phi_0(y)} = (\Psi, \Phi)$$

with $\|\Phi\| = |(\Phi, \Phi)|^{1/2}$

Detailed balance $\Leftrightarrow$ symmetry of $\mathcal{W}$ $\Leftrightarrow$

$$(\Phi, \mathcal{W}\Psi) = (\Psi, \mathcal{W}\Phi) = (\mathcal{W}\Phi, \Psi)$$

Moral: Detailed balance $\Leftrightarrow$ symmetry, self-adjointness of $\mathcal{W}$

$\Rightarrow$ eigenfunctions form complete set:

$$\sum_{\lambda} \frac{\Phi_{\lambda}(y)\, \Phi_{\lambda}(y')}{\Phi_0(y')} = \delta(y-y')$$

so, can write general solution of M.E. in terms of eigenmodes and projections of initial value data, i.e.

$$\boxed{P(y,t) = \sum_{\lambda} \Phi_{\lambda}(y) e^{-\lambda t} \int dy' \frac{\Phi_{\lambda}(y')}{\Phi_0(y)} P(y', 0)\, dy'}$$

Now, can express several useful quantities in terms of modes...

(i) Transition Probability $T(y, y')$

Now, $T(y,y') = P(y,t \mid y', t=0)$

i.e. $P(y', 0) = \delta(y''-y')$

$$P(y,t) = \sum_\lambda \Phi_\lambda(y)\, e^{-\lambda t} \int dy'' \frac{\Phi_\lambda(y'')}{\Phi_0(y'')}\, \delta(y'-y'')\, dy''$$

$$\boxed{P(y,t) = \sum_\lambda \Phi_\lambda(y) \frac{\Phi_\lambda(y')}{\Phi_0(y')} e^{-\lambda t}}$$

(ii) autocorrelation function, at equilibrium:

$$K(\tau) = \int dy'\, P_{eq}(y', 0) \int dy\, P(y,t)\, y' y \qquad \text{(phase space)}$$

$$= \langle Y(0)\, Y(\tau) \rangle \qquad \text{('Lagrangian')}$$

$P_{eq}(y') = \Phi_0(y')$

$$P(y,t) = \sum_\lambda \Phi_\lambda(y) \frac{\Phi_\lambda(y')}{\Phi_0(y')} e^{-\lambda t}$$

$$K(\tau) = \int dy' \cancel{\Phi_0(y')} \int dy \sum_\lambda \frac{\Phi_\lambda(y)\, \Phi_\lambda(y')}{\cancel{\Phi_0(y')}}\, y y' e^{-\lambda\tau}$$

$$= \sum_\lambda e^{-\lambda\tau} \left(\int dy\, y\, \Phi_\lambda(y) \right)^2$$

label irrelevant

and understood $\sum_\lambda$ excludes $\lambda = 0$, as equilibrium state does <u>not</u> contribute to decay of correlation (i.e. analogous to translation mode in coupled oscillators ...)

so

$$\boxed{K(\tau) = \langle Y(0) Y(\tau) \rangle = \sum_{\lambda \neq 0} e^{-\lambda\tau} \left(\int dy\, y\, \Phi_\lambda(y) \right)^2}$$

Note that for comparable projections, most weakly damped mode controls relaxation.

iii.) <u>Fluctuation spectrum</u>

$$S(\omega) = \int_0^\infty e^{i\omega t} K(t)\, dt = \int_0^\infty \langle Y(0) Y(t) \rangle dt\, e^{i\omega t}$$

Spectrum as Fourier transform of correlation function.

$$A_\lambda \equiv \left(\int dy\, y\, \Phi_\lambda(y)\right)^2$$

$$K(t) = \sum_{\lambda \neq 0} e^{-\lambda t} A_\lambda$$

$$S(\omega) = \sum_{\lambda \neq 0} A_\lambda \int_0^\infty e^{i\omega t} e^{-\lambda t}\, dt$$

$$= \sum_{\lambda \neq 0} A_\lambda \frac{(i)}{\omega + i\lambda}$$

$$= \sum_{\lambda \neq 0} A_\lambda \frac{\lambda}{\omega^2 + \lambda^2}$$

$\Rightarrow$

$$S(\omega) = \sum_\lambda \frac{\lambda}{\lambda^2 + \omega^2} \left(\int dy\, \Phi_\lambda(y)\, y\right)^2$$

$\Rightarrow$

$$S(\omega) < S(0)$$

i.e. $S(\omega)$ decreases monotonically with frequency.

iv.) Behavior of $S(\omega)$, the Fluctuation Spectrum

Now,

$$S(\omega) = \sum_\lambda \frac{\lambda}{\lambda^2 + \omega^2} \left(\int dy\, \Phi_\lambda(y)\, y\right)^2$$

expand in $(\omega^2/\lambda^2)^{-1}$ ...

so expanding ...

$$S(\omega) = \sum_{r=0}^{\infty} \frac{(-1)^r}{\omega^{2r+2}} \sum_\lambda \lambda^{2r+1} \left(\int y \Phi_\lambda(y)\, dy \right)^2$$

$$= \sum_{r=0}^{\infty} \frac{(-1)^r}{\omega^{2r+2}} \sum_\lambda \int dy' \Phi_\lambda(y')\, dy' \int y (-W)^{2r+1} \Phi_\lambda(y)\, dy$$

since: $W \Phi_\lambda(y) = -\lambda \Phi_\lambda(y)$

$$W^n \Phi_\lambda(y) = (-\lambda)^n \Phi_\lambda(y)$$

Now, since detailed balance renders W-matrix symmetric:

$$W^\dagger(y|y') = W(y'|y)$$

$\Rightarrow$ can pull transpose thru:

$$S(\omega) = \sum_{r=0}^{\infty} \frac{(-1)^{r+1}}{\omega^{2r+2}} \sum_\lambda \int dy' \Phi_\lambda(y')\, dy' \int \Phi_\lambda(y)\, W^{\dagger\,2r+1}_{y}\, dy$$

but $\sum \Phi_\lambda(y) \Phi_\lambda(y') = \Phi_0(y') \delta(y-y')$

(from before)

so

$$S(\omega) = \sum_{r=0}^{\infty} \left(\frac{-1}{\omega^2} \right)^{r+1} \iint dy'\, y' \Phi_0(y') \delta(y-y')\, W^{\dagger\,2r+1}_{y}\, dy$$

finally:

$$\boxed{\begin{aligned} S(\omega) &= \sum_{\nu=0}^{\infty}\left(\frac{-1}{\omega^2}\right)^{\nu+1}\int dy\, \Phi_0(y)\, y\, \mathbb{W}^{2\nu+1} y \\ &= \sum_{\nu=0}^{\infty}\left(\frac{-1}{\omega^2}\right)^{\nu+1}\langle y\, \mathbb{W}^{2\nu+1} y\rangle^e \end{aligned}}$$

So why care ?? → can obtain asymptotic expansion of fluctuation spectrum WITHOUT solving Master eqn.

→ need only operate with $\mathbb{W}$!
and only need eigen vectors/values ...?

Now, Applying the Master Equation

→ One-Step Processes ... — Cascades

Of particular interest are $\left\{\begin{array}{l}\text{one-step} \\ \text{birth and death} \\ \text{generation-recombination}\end{array}\right\}$

processes where $\mathbb{W}$ permits jumps only between adjacent sites

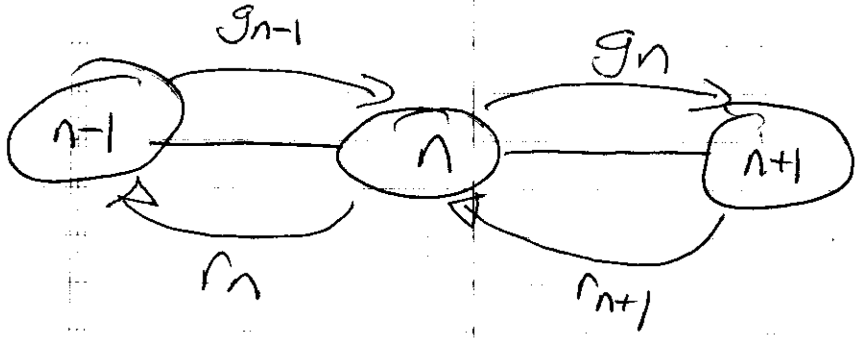
i.e. $\mathbb{W}_{n,n'} = r_{n'}\,\delta_{n,n'-1} + g_{n'}\,\delta_{n,n'+1}$, $n \neq n'$

Now, to write Master Equation:

$\mathbb{W}_{n,n} = -(r_n + g_n)$

so

$$\dot{P}_n = r_{n+1} P_{n+1} + g_{n-1} P_{n-1} - (r_n + g_n) P_n$$



g's → forward flow

r's → back flow.

system is local cascade process.

Now, can classify cases:

i) coefficients r, g constant, independent of n, except at boundaries

⇒ random walks

ii) r, g ~ linear functions of n ⇒ "linear one-step processes"

Can formulate a general solution ...

iii) Other form r, g ⇒ "nonlinear one-step processes".

Here focus on i), ii)

Can write some examples;

1.) symmetric random walk

$r = g = \text{const.}$ Const absorb into time

$$\dot{P}_n = P_{n+1} + P_{n-1} - 2P_n$$

$\Rightarrow$ Diffusion (see HW)

2.) asymmetric random walk

$$\dot{P}_n = \alpha P_{n+1} + \beta P_{n-1} - (\alpha+\beta) P_n$$

$\rightarrow$ diffusion with external force.

3.) Poisson Process

$r_n = 0$, $g_n = \text{const} = \Sigma$

$$\boxed{\dot{P}_n = \Sigma (P_{n-1} - P_n)}$$

$\rightarrow$ corresponds to random walk over integers, with steps to right (increasing n), only

$\rightarrow$ can view as steps at random times.

$\rightarrow$ corresponds to probability for step to occur between t and $t+dt$ in process $y(t)$ = # steps between $t=0$, T.

N.B: Note Σ is probability of step to occur at time t.

Looking at Poisson Process:

$$\rightarrow \quad \left. p_n(t) = (qt)^n e^{-qt}/n! \right] \quad \rightarrow$$ pdf for Poisson process

check:

$$\dot{p}_n = q\left(\frac{(qt)^{n-1}e^{-qt}}{(n-1)!} - \frac{(qt)^n e^{-qt}}{n!}\right)$$

$$= q\left(\frac{(qt)^{n-1}e^{-qt}}{(n-1)!} - \frac{(qt)^n e^{qt}}{n!}\right) = 0 \quad \checkmark$$

→ Note $p_n(t)$ is <u>not</u> stationary for Poisson process, as

$y(t)$ = total # events from initial time

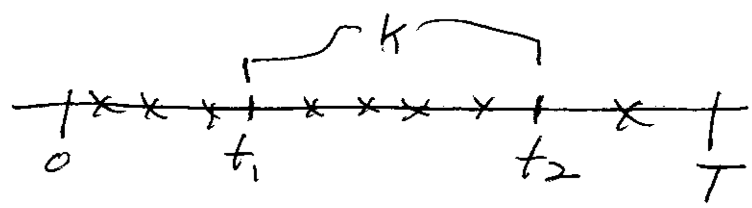
i.e. unlike diffusion, Poisson process accumulates.

→ Alternate Approach:

– 'randomly' place n points in interval $(0, T)$.

What is probability that k of these points lie in (t_1, t_2) interval?

i.e.



Now, from simple binomial distribution:

$$P(k \text{ points in } (t_1, t_2)) = \underbrace{\binom{n}{k}}_{\substack{\#\text{ ways}\\ \text{to pick } k\\ \text{of } n}} p^k q^{n-k}$$

q → prob. not $= 1-p$

p → (probability of event in interval) $= \left(\frac{t_2 - t_1}{T}\right)$, as independent

Now, what happens if n gets big?

→ if n large enough such that

$n \gg 1, \quad p \ll 1$

but $np \sim npq \gg 1$

then $\quad P_n(k) \simeq \dfrac{1}{\sqrt{2\pi npq}} e^{-(k-np)^2/2npq}$ (De Moivre–LaPlace Theorem)

→ Gaussian, diffn, etc.

now, if $np \sim 1$, ⇒ Poisson theorem

$$\frac{n!}{k!\,(n-k)!} p^k q^{n-k} \cong e^{-np} \frac{(np)^k}{k!}$$

→ Poisson distribution!

i.e.

re-considering:

$$P\{k \text{ in } (t_1, t_2)\} = \binom{n}{k} p^k q^{n-k}$$

$$p = \Delta t / T = (t_2 - t_1)/T$$

$$n \gg 1$$

$$\Delta t / T \ll 1 \quad \rightarrow \quad q = 1 - p \sim 1$$

So for $n \dfrac{\Delta t}{T} \sim k \Rightarrow$

$$P\{k \text{ in } \Delta t\} \cong e^{-n \Delta t / T} \left(n \frac{\Delta t}{T} \right)^k / k!$$

using Poisson distribution formula.

If now $\dfrac{n}{T} = \lambda$ $\quad$ ($\lambda \equiv$ uniform event rate)

$\Rightarrow$

$$P\{\underline{k} \text{ in } \Delta t\} = e^{-\lambda \Delta t} (\lambda \Delta t)^k / k!$$

prob. k events in interval Δt, where n events and n/T = <u>event rate</u>

n.B.: Poisson Processes are quite common in queueing theory and detection theory i.e. if designing business service, useful to know distribution of customer load, i.e.

If system to service customers and expect base rate of λ customers per hour, what is probability of k customers arriving in a 10-minute interval?

$$\Rightarrow \quad P = P\{k \text{ in } 1/6 \text{ hour}\} = e^{-\lambda/6}(\lambda/6)^k/k!$$

then use to determine statistics of queue, etc.!

→ Theory of 1-Step Processes ('Cascades'), cont'd

To develop the theory:

1.) general considerations of structure of solution for 1-step process

2.) some 'linear' 1-step processes

3.) boundary effects

4.) generating function solutions - a general approach.

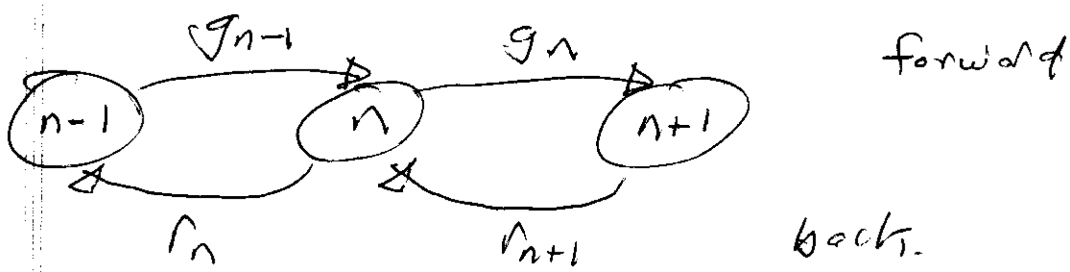
combine

→

i.) General Considerations

Recall concerned with Master Equation for local cascades, i.e.

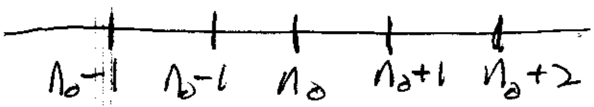
$$\dot{P}_n = r_{n+1} P_{n+1} + g_{n-1} P_{n-1} - (r_n + g_n) P_n$$



a particularly simple case is $\quad (r = g = \text{const})$

$$\frac{\partial p_n}{\partial t} = p_{n+1} + p_{n-1} - 2p_n$$

contrast: ① 'simple random walk' i.e. walker starts from $n = n_0$ and takes 1 step every Δt to right or left, depending on coin-toss



time and space jumps quantized

here can calculate pdf via binomial distribution

② above $\rightarrow$ differential-difference equation
i.e. n discrete, t continuous
$\Rightarrow$ generic structure of Master equation

Now,

- observed often useful to shift indexes in sums, i.e. $n \rightarrow n \pm 1$, so ....

→ if $-\infty < n < +\infty$, can define <u>shift operator</u> <u>in function space</u>

$$\mathcal{E} f(n) = f(n+1) \, , \qquad \mathcal{E}^{-1} f(n) = f(n-1)$$

if n bounded, view $\mathcal{E}$ as shorthand.

→ Properties of Shift Operator

$$\sum_{n=0}^{N-1} g(n)\, \mathcal{E} f(n) = \sum_{n=0}^{N-1} g(n) f(n+1)$$

$$= \sum_{n=1}^{N} f(n)\, \mathcal{E}^{-1} g(n)$$

$$= \sum_{n=1}^{N} f(n)\, g(n-1) = \sum_{n=0}^{N-1} f(n+1)\, g(n)$$

<u>so</u> $\boxed{\sum_{n=0}^{N-1} g(n)\, \mathcal{E} f(n) = \sum_{n=1}^{N} f(n)\, \mathcal{E}^{-1} g(n)}$ for any pair f, g.

<u>so</u>

→ can economically write Master Equation as

$$\dot{p}_n = (\mathcal{E} - 1)\, r_n p_n + (\mathcal{E}^{-1} - 1)\, g_n p_n$$

this is especially convenient for moments, i.e.

$$\frac{d}{dt}\langle n(t)\rangle = \frac{d}{dt}\sum_n n\,P_n = \sum_n \left(n(\mathcal{E}-1)\, r_n P_n + n(\mathcal{E}^{-1}-1)\, g_n P_n \right)$$

using shift identity $\Rightarrow$

$$= \sum_n \left\{ r_n P_n (\mathcal{E}^{-1}-1)\, n + g_n P_n (\mathcal{E}^{+1}-1)\, n \right\}$$

but $(\mathcal{E}^{-1}-1)\, n$

$$= n-1-n = -1$$

$$(\mathcal{E}-1)\, n = n+1-n = +1$$

so

$$\frac{d\langle n(t)\rangle}{dt} = \sum_n -r_n P_n + g_n P_n$$

$$\boxed{\frac{d\langle n(t)\rangle}{dt} = -\langle r_n\rangle + \langle g_n\rangle}$$

Similarly, have:

$$\boxed{\frac{d}{dt}\langle n^2\rangle = 2\langle n(g_n - r_n)\rangle + \langle g_n + r_n\rangle}$$

Exercise: Show this!

→ Now, can use shift operator to elucidate general solution $r_n = r_n(n)$, $g_n = g_n(n)$

$$\frac{\partial P_n}{\partial t} = (\mathcal{E}-1)\, r_n P_n + (\mathcal{E}^{-1}-1)\, g_n P_n$$

stationarity ⇒ stationary solution

$$0 = (\mathcal{E}-1)\, r_n P_n^s + (\mathcal{E}^{-1}-1)\, g_n P_n^s$$

$$= (\mathcal{E}-1)\left\{ r_n P_n^s - \mathcal{E}^{-1} g_n P_n^s \right\}$$

⇒ stationary solution of { } independent of n

$$\Rightarrow \boxed{\left(r_n P_n^s - \mathcal{E}^{-1} g_n P_n^s \right) = -J}$$

the stationarity condition.

{ what is J?

note:

- here J corresponds to flow in n or "current" of probability
- $J < 0$ convention, as flow $n \to n-1$
- need consider different cases for different ranges of n.

i.e. 3 cases:

a) $-\infty < n < \infty$

b) $n = 0, 1, 2 \ldots$

c) $n = 0, 1, \ldots N$

For c), $\dot{P}_0 = r_1 P_1 - g_0 P_0$ $\Rightarrow J = 0$ from $\dot{P}_0 = 0$

$r_0 = g_{-1} = 0$ (boundary contribution! sets $J = 0$)

so

$$r_n P_n^s = g_{n-1} P_{n-1}^s$$

and $$r_{n-1} P_{n-1}^s = g_{n-2} P_{n-2}^s$$

etc

so

$$\boxed{P_n^s = \frac{g_{n-1} g_{n-2} \cdots g_1 g_0}{r_n r_{n-1} \cdots r_2 r_1} P_0^s}$$

$$= \left(\prod_{i=0}^{n-1} g_i \Big/ \prod_{i=1}^{n} r_i \right) P_0^s$$

Now, have

$$\sum_{n=1}^{N} P_n^s + P_0^s = 1$$

$\Rightarrow$

$$\boxed{1/P_0^s = 1 + \sum_{n=1}^{N} \frac{g_0 g_1 \cdots g_{n-1}}{r_1 r_2 \cdots r_n}}$$

general solution (finite range)

$\left\{ J = 0 \text{ cascade process} \right.$

→ for half-infinite range, can construct similar
→ for two-sided, can have constant flow from $-\infty \to +\infty$ ⇒ must deduce J from problem.

Note Important Contrast:

– $J = 0$ stationarity condition

$$r_n P_n^s = g_{n-1} P_{n-1}^s \quad ;$$

$\left\{ \begin{array}{l} \text{a definition for } J=0 \\ \Rightarrow \text{determines } P_n^s \end{array} \right.$

no physics

– statement of detailed balance:

$$r_n P_n^e = g_{n-1} P_{n-1}^e \quad ;$$

$\left\{ \begin{array}{l} \text{a consequence of} \\ \text{time-reversal symmetry} \\ \text{of micro-dynamics} \end{array} \right.$

here P_n^e given a-priori by equilibrium stat. mech.

has physical content

2) → Some Examples of 'Linear' (i.e. $r_n \sim n$, $g_n \sim n$) 1-step Processes

a) Planck Distribution from Kinetics

b.) Population Growth

c.) Cosmic Ray Cascades

a.) Planck Law – Black Body Radiation

recall Planck distribution for radiation from black body:

$$dE_\omega = \frac{V\hbar}{\pi^2 c^3} \frac{\omega^3 d\omega}{(e^{\hbar\omega/T}-1)}$$

'Usual' derivation from equilibrium stat mech :

– N photons variable, but for minimum of free energy F

$$\partial F/\partial N = 0$$

but $\partial F/\partial N\big|_{T,V} = \mu$ $\Rightarrow$ $\mu = 0$ (Photon chemical potential vanishes) so Gibbs thermodynamic potential Ω:

$$\Omega = -T \ln Z$$

$$= -T \ln \sum_{n_k} \left(e^{-\epsilon_k/T}\right)^n$$

$$\Rightarrow \quad \left.\bar{n}_k = 1 \Big/ e^{\epsilon_k/T} + 1 \right\} \Rightarrow \left\{ \begin{array}{l} \text{\# photons in} \\ n^{th} \text{ quantum} \\ \text{state} \end{array} \right.$$

For total # photons $\Rightarrow$ $\mapsto V\, 4\pi k^2 dk/(2\pi)^3$

$$d N_\omega = (\text{density of states})\, \bar{n}_k$$

$$= \frac{V}{\pi^2 c^3} \frac{\omega^2 \, d\omega}{e^{\hbar\omega/T} - 1}$$

and $dE_\omega = \hbar\omega \, dN_\omega$.

From kinetics: (ala' Einstein)

"Black body" $\leftrightarrow$ QM harmonic oscillator
$\rightarrow$ photons emitted in quanta of allowed transitions

states of oscillator: $E_n = (n + 1/2)\hbar\omega$

Dipole emission $\Rightarrow$ $T_{n,n'} = T(n)\,\delta_{n-1,n} + T'(n)\,\delta_{n+1,n}$

(i.e. $\langle n|x|n'\rangle = \delta_{n,n\pm1}$)

and harmonic oscillator Q.M. $\Rightarrow T, T' \sim n$

so forward jump $n-1 \to n$ $\rightarrow$ $g_{n-1} = \beta n$ $\mapsto$ coeffs

backward jump $n \to n-1$ $\rightarrow$ $r_n = \alpha n$

here $\alpha, \beta = \alpha(\rho(\omega)), \beta(\rho(\omega))$, but independent of n.

$\rho \equiv$ radiation density

so, can write Master equation as:

$$\dot{p}_n = \alpha(\mathcal{E}-1)\,n p_n + \beta(\mathcal{E}^{-1}-1)(n+1)p_{n+1}$$

$\Rightarrow$ for stationarity: $r_n p_n^s = g_{n-1} p_{n-1}^s$

$$\alpha p_n^s = \beta p_{n-1}^s$$

$$p_n^s = (\beta/\alpha)\, p_{n-1}^s$$

$$\Rightarrow \boxed{p_n^s = C\,(\beta/\alpha)^n}$$

norm constant

stationary solution
$\rightarrow$ Poscal distribution

but also know:

- at stationarity, oscillator ⊕ radiation field come to equilibrium, so p_n given by equilibrium statistical mechanics

- blackbody equilibrium with radiation field is one of detailed balance of radiator (black body) and radiation field

so

$$p_n^e = \underset{\text{norm const.}}{c} \; e^{-n\hbar\omega/T}$$

$$(\beta/\alpha)^n = e^{-n\hbar\omega/T} \Rightarrow \boxed{\beta/\alpha = e^{-\hbar\omega/T}}$$

Can further say:

- $\beta = A\rho$ as transition probability can depend on radiation intensity

and

- $\alpha = \underset{\text{const.}}{B} + C\rho$ similarly

$$\Rightarrow \frac{A\rho}{B + C\rho} = e^{-\hbar\omega/T} \Rightarrow \boxed{\rho = \frac{B}{A e^{\hbar\omega/T} - C}}$$

and can determine constants from large T asymptotics.

b.) Population Growth (again ....)

Consider population of n beasties. Each beastie has:

- probability rate α to die
- probability rate β to produce another beastie

$\Rightarrow$ back flow: $\quad r_n = \alpha n$
forward flow: $\quad g_n = \beta n$

so

$$\frac{dp_n}{dt} = \sum_n \left\{ n(E-1)\,\alpha\, p_n + n(E^{-1}-1)\,\beta\, p_n \right\}$$

For mean, mean-square population (i.e. average, fluctuation levels)

have:
$$\frac{d}{dt}\langle n\rangle = -\langle r_n\rangle + \langle g_n\rangle$$
$$= -\alpha\langle n\rangle + \beta\langle n\rangle$$
$$= (\beta-\alpha)\langle n\rangle$$

agrees with intuition from macroscopics (Malthusian growth)

Also have:

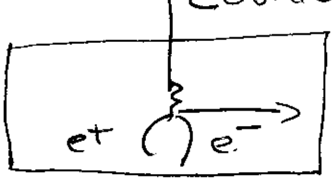
$$\frac{d}{dt}\langle n^2\rangle = 2\langle n(g_n - r_n)\rangle + \langle g_n + r_n\rangle$$

$$\frac{d}{dt}\langle n^2\rangle = 2\langle n^2\rangle(\beta-\alpha) + (\beta+\alpha)\langle n\rangle$$

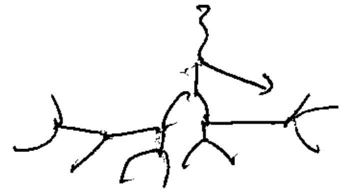
$\Rightarrow \langle n^2\rangle$ grows exponentially for $(\beta-\alpha)>0$.

c.) Cosmic Ray 'Cascade'

"cosmic ray" electron (i.e. energetic electron)



⤳ absorber



dendritic growth.

i.e. – creates additional electrons via Bremsstrahlung
– pair creation (electron, positron pair)

so → electrons accumulate, only
→ no back flow.

n = # electrons
β = creation rate / distance, in absorber (density of scatterers)
T = thickness of absorber traversed

$\therefore$ $r_n = 0$ (no back flow)
$g_n = \beta$
$\Rightarrow$ i.e. electrons accumulate! $\Rightarrow$ Poisson Process

so $$\frac{dP_n}{dT} = \beta \left(P_{n-1} - P_n \right)$$

$$\Rightarrow \quad P_n(T) = \frac{(\beta T)^n}{n!} e^{-\beta T}$$

→ Poisson distribution

but $P_n(0) = \delta_{n,1}$ (start from 1 electron)

$$\boxed{P_n(T) = \frac{(\beta T)^{n-1}}{(n-1)!} e^{-\beta T}} \quad (n = 1, 2, \ldots)$$

↓

probability of n electrons at thickness T.

3.4) Generating Function Solution, with Boundary Condition

- seek general approach to solution of Master equation
- first consider constant coefficients...

exploiting constant coefficients approach via use of

$$\boxed{\text{generating function} \quad F(z,t) = \sum_n z^n P_n(t)}$$

strategy: convert differential-difference equation to differential equation for F, solve and then use:

$$P_n(t) = \frac{1}{n!}\left[\left(\frac{\partial}{\partial z}\right)^n F(z,t)\right]_{z \to 0}$$

or:

$$P_n(t) = \frac{1}{2\pi i}\oint z^{-n-1} F(z,t)\,dz \quad , \quad \text{integral on unit circle}$$

Exercise - Show this!

Now observe since $\left\{\begin{array}{l} \sum_n P_n = 1 \\ P_n \geq 0 \end{array}\right. \Rightarrow F(z,t)$ exists.

and:

$$F(1,t) = 1 \qquad \text{(normalization)}$$

$$F'(1,t) = \sum_n n z^{n-1} P_n \Big|_{z \to 1} = \langle n(t) \rangle$$

$$F''(1,t) = \langle n(t)^2 \rangle - \langle n(t) \rangle \qquad \Rightarrow \text{all moments...}$$

etc.

or alternatively:

$$\left.\frac{\partial \ln F}{\partial z}\right|_{z=1} = \langle n(t)\rangle$$

$$\left.\frac{\partial^2 \ln F}{\partial z^2}\right|_{z=1} = \langle n(t)^2\rangle - \langle n(t)\rangle^2 - \langle n(t)\rangle$$

i.e. $F \leftrightarrow$ effective partition function.

Now, to implement in solution:

$$\dot{p}_n = p_{n+1} + p_{n-1} - 2p_n \qquad (-\infty < n < \infty)$$

$$\sum_n z^n \dot{p}_n = \underbrace{\sum_n z^n p_{n+1}}_{F/z} + \underbrace{\sum_n z^n p_{n-1}}_{z\,F} - 2\sum_n z^n p_n$$

$$\Rightarrow \frac{\partial F}{\partial t} = \sum_n \left(\frac{z^{n+1}}{z} p_{n+1}\right) + \sum_n \left(z\, z^{n-1} p_{n-1}\right) - 2F$$

$$= z\,F + \frac{F}{z} - 2F$$

can re-label sums

$$\Rightarrow \boxed{\frac{\partial F(z,t)}{\partial t} = \left(z + \frac{1}{z} - 2\right) F(z,t)}$$

simple differential equation!

i.e. match Ω

and $F(z,t) = \Omega(z) \exp\left[\left(z + \frac{1}{z} - 2\right) t\right]$

$p_n(0) = \delta_{n,0} \Rightarrow F(z,0)\Big|_{z\to 0} = 1$

$\Rightarrow \Omega(z) = 1$

$\Rightarrow F(z,t) = \exp\left[t\left(z + \frac{1}{z} - 2\right)\right]$

and expanding in z $\Rightarrow$

$$F(z,t) = e^{-2t} \sum_{k,\ell=0}^{\infty} \frac{t^{k+\ell}}{k!\,\ell!} z^{k-\ell}$$

and

$$\boxed{p_n(t) = e^{-2t} \sum_{\ell} t^{2\ell+n} / (\ell+n)!\,\ell!}$$

$\ell, n+\ell \neq 0$

$\rightarrow$ solution!

N. B. Compare with Problem 5 of Set III
(i.e. series representation of $e^{-\omega t} I_j(\omega t)$)

Exercise: Consider asymmetric random walk with:

$$\dot{p}_n = \alpha p_{n+1} + \beta p_{n-1} - (\alpha+\beta) p_n$$

Solve via generating function approach.

→ Now, let's try a non-trivial case: a <u>Linear</u> <u>1-Step</u> <u>Process</u>!

¿ Why the distinction between 'Linear' and 'Nonlinear' i.e. $\underset{g}{r} \sim n$, vs $\underset{g}{\hat{r}} \sim n^2$, etc. ?

For <u>general</u> <u>linear</u> <u>case</u>:

$$\rightarrow \dot{P}_n = a\,(\mathcal{E}-1)\,(r+n)P_n + b\,(\mathcal{E}^{-1}-1)\,(g+n)\,P_n$$

a, b, r, g constants. $\quad (a \neq b \neq 0)$

→ neglect b.c.'s at first, and solve on $-\infty < n < \infty$

<u>so</u>

$$\frac{d}{dt}\sum_n z^n P_n = a\sum_n (z^{n-1}-z^n)(r+n)\,P_n$$

$$+\; b\sum_n\,(z^{n+1}-z^n)\,(g+n)\,P_n$$

and re-grouping as before:

$$\frac{\partial F(z,t)}{\partial t} = ar\left(\frac{1}{z}-1\right)F + a(1-z)\frac{\partial F}{\partial z}$$

$$+ bg(z-1)F + b(z^2-z)\frac{\partial F}{\partial z}$$

N.B. : Now Generating function equation is PDE !

so

$$\boxed{\frac{\partial F(z,t)}{dt} = (1-z)(a-bz)\frac{\partial F}{\partial z} + (1-z)\left(\frac{ar}{z}-bg\right)F}$$

is generating function equation.

$\Rightarrow$ now, solve via characteristics ! (general for first order in space-time pde)

$$\frac{\partial F}{\partial t} - (1-z)(a-bz)\frac{\partial F}{\partial z} = (1-z)\left(\frac{ar}{z}-bg\right)F$$

$$\frac{dF}{dt} = (1-z)\left(\frac{ar}{z}-bg\right)F$$

$$dF/dt = \partial F/\partial t + u(z)\frac{\partial}{\partial z}F$$

$$u(z) = \frac{dz}{dt} = -(1-z)(a-bz)$$

$\rightsquigarrow$ characteristic equation on z, t plane.

so $\quad -dt = dz \big/ (1-z)(a-bz)$

$$\Rightarrow \quad \frac{(1-z)}{(a-bz)} e^{(b-a)t} = \underset{\substack{\text{integration} \\ \text{constant}}}{C} \rightarrow \text{labels characteristics}$$

$\rightarrow$ parametrizes characteristics

then $$\frac{dF}{dt} = (1-z)\left(\frac{ar}{z} - bg\right) F$$

$$\Rightarrow \frac{dF}{F} = \cancel{(1-z)}\left(\frac{ar}{z} - bg\right)\left(\underbrace{\frac{-dz}{\cancel{(1-z)}(a-bz)}}_{\text{from characteristic equations}}\right)$$

$$\therefore \quad \boxed{F(z,t) = \text{const } z^{r} (a-bz)^{r-g}}$$

Now, constant chosen for each characteristic curve

$$\text{const} = \Omega(C) = \Omega\left(\frac{1-z}{a-bz} e^{(b-a)t}\right)$$

$$\Rightarrow \boxed{F(z,t) = z^{-r}(a-bz)^{r-g}\,\Omega\left(\frac{1-z}{a-bz}\,e^{(b-a)t}\right)}$$

For Ω: $\quad p_n(0) = \delta_{n,m}$

$$\Rightarrow \quad F(z,0) = z^m$$

so

$$\Omega\left(\frac{1-z}{a-bz}\right) = z^{m+r}(a-bz)^{g-r}$$

define $\varphi = \dfrac{1-z}{a-bz}$, $\quad z = \dfrac{a\varphi-1}{b\varphi-1}$

so

$$\Omega(\varphi) = \left(\frac{a\varphi-1}{b\varphi-1}\right)^{m+r}\left(\frac{b-a}{b\varphi-1}\right)^{g-r}$$

so --- plugging it all in --- $\Rightarrow$ THE ANSWER:

$$\boxed{F(z,t) = z^m\left[\frac{a\varepsilon-b+a(1-\varepsilon)z^{-1}}{a-b}\right]^{m+r}\left[\frac{a-b\varepsilon-b(1-\varepsilon)z}{a-b}\right]^{-m-g} \qquad \varepsilon = e^{(b-a)t}}$$

i.e. General solution for Linear One-Step Process Possible ..... !

but ... the boundary conditions ... ??

recall had:

$$\dot{p}_n = [r(n+1)]p_{n+1} + [g(n-1)]p_{n-1} - \{r(n)+g(n)\}p_n$$

for $n = 1, 2 \ldots N-1$

and need

$$\dot{p}_0 = r(1) - g(0)\,p_0$$

$$\dot{p}_N = g(N-1)\,p_{N-1} - r(N)\,p_N$$

Call $n=0$ boundary "natural" (i.e. tractable) if:

i.) Master eqn. valid to $n=1$
ii.) $r(0) = 0$

if so, $\left\{\begin{array}{l}\text{can extend to } -\infty < n < +\infty \\ \text{with } p_n(0) = 0, \quad n < 0.\end{array}\right.$

$\Rightarrow$ Convert b.c. to i.c.

For further discussion of b.c.'s, see Van Kampen.