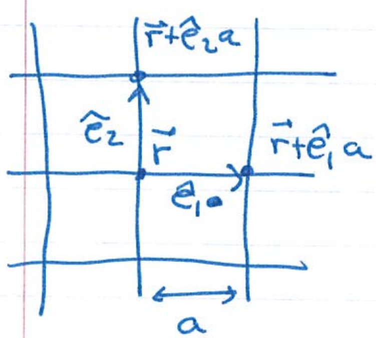
Random Walks

Consider a~~n~~ regular array of points in space, a lattice.

Consider now a "particle" that moves on this lattice (for simplicity we will assume that it is a cubic lattice) but that ~~the~~ its motion is completely random: at a given time the walker is at site $\vec{r}$ and it randomly chooses ~~to go~~ to hop to



one of its nearest-neighboring sites $\{\vec{r} \pm \hat{e}_\mu a\}$ $(\mu = 1, 2, 3)$. Since the probability that it will hop somewhere is 1 and there are $z = 2d$ neighbors in a cubic lattice ($d = 3$) (z: coordination number) $\Rightarrow$ the probability of any one of these hops is $\frac{1}{z} = \frac{1}{2d}$

Suppose the random walker begins its journey at $\vec{R} = 0$, what is the probability that it will arrive at a given site $\vec{R}$ in N hops? If a hop takes a time $\tau \Rightarrow$ after N hops it takes $t = N\tau$

Total displacement : $\vec{R} = \sum_{i=1}^{N} \vec{d}_i$

where $\vec{d}_i$ are the displacements at every intermediate time. These displacements are taken randomly from the set $\{\pm \hat{e}_\mu a\}$ with equal probability $\frac{1}{2\cancel{d}}$.

$$\Rightarrow \langle \vec{R} \rangle = \sum_{i=1}^{N} \langle \vec{d}_i \rangle = 0$$

But

$$\langle \vec{R}^2 \rangle = \langle \left(\sum_{i=1}^{N} \vec{d}_i \right)^2 \rangle =$$

$$= \sum_{i,j=1}^{N} \langle \vec{d}_i \cdot \vec{d}_j \rangle$$

$$= \sum_{i,j=1}^{N} \delta_{ij}\, a^2 = N a^2$$

since $\cancel{\langle \vec{d}^2 \rangle}$ $\langle \vec{d}_i \cdot \vec{d}_j \rangle = \langle \vec{d}_i \rangle \cdot \langle \vec{d}_j \rangle = 0$

$i \neq j$
(uncorrelated and zero average)

and $$\langle \vec{d}_i^{\,2} \rangle = \frac{\sum \vec{d}_i^{\,2} P[\vec{d}_i]}{\sum P[\vec{d}_i]} = \frac{3\cancel{d}\, a^2 \frac{1}{3\cancel{d}}}{3\cancel{d} \cdot \frac{1}{2\cancel{d}}} = a^2$$

$$\Rightarrow \langle \vec{R}^2 \rangle = N a^2$$

or $\sqrt{\langle \vec{R}^2 \rangle} = a\sqrt{N}$ which is very slow.

Let $\rho(\frac{\vec{r}}{a}, \frac{t}{\tau})$ be the probability to find the walker at $\underline{\underline{\vec{r}}}$ after a step which was completed at time $\underline{\underline{t}}$.

$$\rho_L(\frac{\vec{r}}{a}, \frac{t}{\tau}) = \langle \delta_{\vec{R}(t),\vec{r}} \rangle$$

"Lattice"

Consider now a region Ω centered at $\vec{r}_0$ but same point containing many sites (still small compared to the size of the system).

$$\Rightarrow \int_{\vec{r}\in\Omega} d\vec{r}\ \rho(\vec{r},t) = \sum_{\vec{r}\in\Omega} \rho_L(\frac{\vec{r}}{a}, \frac{t}{\tau})$$

Since a site (or unit cell) has volume a^D (D: dimension) $\Rightarrow$ $\rho(\vec{r},t) = \frac{1}{a^D}\rho_L(\frac{\vec{r}}{a}, \frac{t}{\tau})$

This equation will help us take a continuum ~~limit~~ limit

If the walk begins at $\vec{r}=0$ at $t=0$

$\Rightarrow \quad \rho_L\left(\frac{\vec{r}}{a}, 0\right) = \delta_{\vec{r},0}$ ← (Kronecker delta)

$$\rho_L\left(\frac{\vec{r}}{a}, \frac{t}{\tau}\right) = \left\langle \delta_{\vec{R}(t),\vec{r}} \right\rangle =$$

$$= \int \frac{d\vec{q}^{\,D}}{(2\pi)^D} \left\langle e^{i\vec{q}\cdot(\vec{R}(t)-\vec{r})/a} \right\rangle$$

Brillouin zone

$$= \int_{BZ} \frac{d\vec{q}^{\,d}}{(2\pi)^d} \, e^{-i\vec{q}\cdot\vec{r}/a} \left\langle \prod_{i=1}^{N} e^{i\vec{q}\cdot\vec{d}_i/a} \right\rangle$$

$$\vec{R}(t) = \sum_{i=1}^{N} \vec{d}_i$$

$t = N\tau$

Since the $\vec{d}_i$'s are uncorrelated

$$\left\langle \prod_{i=1}^{N} e^{i\vec{q}\cdot\vec{d}_i/a} \right\rangle = \prod_{i=1}^{N} \left\langle e^{i\vec{q}\cdot\frac{\vec{d}_i}{a}} \right\rangle$$

$$= \left\langle e^{i\vec{q}\cdot\vec{d}/a} \right\rangle^N =$$

any allowed displacement

$$\left\langle e^{i\vec{q}\cdot\frac{\vec{d}}{a}} \right\rangle = \sum_{\mu=1}^{d} \frac{1}{2d} \left(e^{iq_\mu} + e^{-iq_\mu}\right) = \frac{1}{d}\sum_{\mu=1}^{d} \cos q_\mu$$

$$\Rightarrow \left\langle \prod_{i=1}^{N} e^{i\vec{q}\cdot\frac{\vec{d}_i}{a}} \right\rangle = \left(\frac{1}{d} \sum_{\mu=1}^{d} \cos q_\mu \right)^N$$

$$\Rightarrow \rho_L\left(\frac{\vec{r}}{a}, \frac{t}{\tau}\right) = \int_{BZ} \frac{d^d q}{(2\pi)^d} \, e^{-i\vec{q}\cdot\frac{\vec{r}}{a}} \left(\frac{1}{d} \sum_{\mu=1}^{d} \cos q_\mu \right)^N$$

For N large enough this integral can be estimated by the method of steepest-descents. Which effectively amounts to the approximation.

$$\left(\frac{1}{d} \sum_{\mu=1}^{d} \cos q_\mu \right)^N \approx e^{-\frac{\vec{q}^{\,2} N}{2d}}$$

$$\text{and } \frac{1}{a^d} \rho_L\left(\frac{\vec{r}}{a}, \frac{t}{\tau}\right) = \frac{1}{a^d} \underbrace{\int}_{\text{all space}} \frac{d^d q}{(2\pi)^d} \, e^{-i\vec{q}\cdot\frac{\vec{r}}{a} - \frac{N\vec{q}^{\,2}}{2d}}$$

$$\frac{t}{\tau} = N$$

$$\rho(\vec{r}, t) = \left(\frac{\tau d}{2\pi t a^2} \right)^{\frac{d}{2}} e^{-\frac{\vec{r}^{\,2}}{4Dt}} = \frac{e^{-\vec{r}^{\,2}/4Dt}}{(4\pi D t)^{d/2}}$$

$$D = \frac{a^2}{2\tau d} = \text{Diffussion constant}$$

Hence for long times $t = N\tau$ ($N \gg 1$)

$$\rho(\vec{r},t) = \frac{e^{-\vec{r}^{\,2}/4Dt}}{(4\pi D t)^{d/2}}$$

is the probability we were looking for.

Note: $\langle \vec{r}^{\,2} \rangle = 2Dtd$

or $\left\langle \frac{\vec{r}^{\,2}}{a^2} \right\rangle = \frac{2Dtd}{a^2} = \cancel{\frac{2}{a^2}}\ \cancel{\frac{a^2}{2\tau d}}\ N\cancel{\tau}\cancel{d}$

$= \frac{N}{\cancel{d}}\cancel{d}$

$\Rightarrow \langle \vec{r}^{\,2} \rangle = N a^2$ ✓

Equation of Motion for $\rho_L\left(\frac{\vec{r}}{a}, \frac{t}{\tau}\right)$:

What is the probability to find the walker at $\vec{r}$ after N steps? = equal to the probab to find the walker in any of its neighbors in $(N-1)$ steps $\times$ probability of the last step.

$$\Rightarrow \rho_L\left(\frac{\vec{r}}{a}, \frac{t}{\tau}\right) = \frac{1}{2d} \sum_{\pm \hat{e}_\mu a} \rho_L\left(\frac{\vec{r}}{a} \mp \hat{e}_\mu, \frac{t}{\tau} - 1\right)$$

$$\Rightarrow \rho(\vec{r}, t+\tau) - \rho(\vec{r}, t) = \sum_{\vec{\xi} \in \text{neighbors}} \frac{\rho(\vec{r}-\vec{\xi}, t) - \rho(\vec{r}, t)}{2d}$$

$$\Rightarrow \rho(\vec{r}, t+\tau) - \rho(\vec{r}, t) \approx \tau \frac{\partial \rho}{\partial t}(\vec{r}, t)$$

$$\rho(\vec{r}-\vec{\xi}, t) - \rho(\vec{r}, t) = -\vec{\xi} \cdot \vec{\nabla}\rho + \frac{1}{2}\left(\vec{\xi} \cdot \vec{\nabla}\right)^2 \rho$$

$$\sum_{\vec{\xi}} \vec{\xi} = 0 \quad \text{and} \quad \sum_{\vec{\xi}} \xi_i \xi_j = \delta_{ij} a^2$$

$$\Rightarrow \quad \tau \frac{\partial \rho}{\partial t} = \frac{a^2}{2d} \nabla^2 \rho$$

or $$\frac{\partial \rho}{\partial t} = \frac{a^2}{2\tau d} \nabla^2 \rho \Leftrightarrow \boxed{\frac{\partial \rho}{\partial t} = D \nabla^2 \rho}$$

Diffussion Equation.

$$D = \frac{a^2}{2\tau d}$$

Browmian Motion and Random Walks

Consider a particle of mass M moving in a gas. We will assume that the gas is in equilibrium at some temperature T. The interactions between the particle and the atoms are random: random forces, $\vec{\eta}(t)$.

Hamilton's Equations:

$$\frac{d\vec{R}}{dt} = \frac{\vec{P}}{M} = \frac{\partial H}{\partial \vec{P}}$$

$$\frac{d\vec{P}}{dt} = \underbrace{-\frac{\partial H}{\partial \vec{R}}}_{\text{conservative force.}} + \underbrace{\vec{\eta}(t)}_{\text{random force}} \underbrace{- \frac{\vec{P}}{\tau}}_{\text{friction}}$$

τ ← "relaxation time"

The random forces $\vec{\eta}(t)$ will be assume to be uncorrelated (i.e. a Markov process)

$$\mu=1,\dots,d \quad \langle \eta_\mu(t)\ \eta_\nu(t') \rangle = \Gamma\ \delta_{\mu\nu}\ \delta(t-t')$$

i.e. very short kicks

Impulse: $\vec{I} = \int_t^{t+\delta t} dt' \; \vec{\eta}(t')$

$$\Rightarrow \langle I_\mu I_\nu \rangle = \int_t^{t+\delta t} dt' \int_{t}^{t+\delta t} dt'' \langle \eta_\mu(t') \eta_\nu(t'') \rangle$$

$$= \Gamma \int_t^{t+\delta t} dt' \int_t^{t+\delta t} dt'' \; \delta_{\mu\nu} \, \delta(t'-t'')$$

$$\langle I_\mu I_\nu \rangle = \Gamma (\delta t) \, \delta_{\mu\nu}$$

and $\langle I_\mu \rangle = 0$

$\Rightarrow$ random walk in momentum space

$\Rightarrow$ I_μ are gaussian variables

$$\Rightarrow \langle e^{i \vec{q} \cdot \vec{I}} \rangle = e^{-\frac{1}{2} \Gamma \, \delta t \, \vec{q}^{\,2}}$$

An equation s.t.

$\dfrac{d\vec{P}}{dt} = - \dfrac{\vec{P}}{\tau} + \eta(t)$ is a <u>Langevin Equation</u>

Consider the case $H = 0$ (no conservative forces)

$$\Rightarrow \vec{P}(t) = \vec{P}(t_0) \, e^{-\frac{t-t_0}{\tau}} + \int_{\tau_0}^{t} dt' \, \vec{\eta}(t') \, e^{-\frac{t-t'}{\tau}}$$

$$\Rightarrow \quad \langle \vec{P}(t) \rangle = \vec{P}(0)\, e^{-t/\tau}$$

and $$\langle e^{i \vec{q} \cdot \vec{P}(t)} \rangle = \, ?$$

$$\left(t_0 \to -\infty \Rightarrow \vec{P}(t) = \int_{-\infty}^{t} dt'\, \eta(t')\, e^{-\frac{t-t'}{\tau}} \right)$$

$$\left\langle e^{i q_\mu \int_{-\infty}^{t} dt'\, \eta_\mu(t')\, e^{-\left(\frac{t-t'}{\tau}\right)}} \right\rangle =$$

$$= e^{-\frac{1}{2} q_\mu q_\nu \int_{-\infty}^{t} dt' \int_{-\infty}^{t} dt'' \langle \eta_\mu(t')\, \eta_\nu(t'') \rangle}$$

$$e^{-\left(\frac{t-t'}{\tau}\right)} e^{-\left(\frac{t-t''}{\tau}\right)}$$

$$= e^{-\frac{1}{2} q_\mu q_\nu \int_{-\infty}^{t} dt' \int_{-\infty}^{t} dt''\, \Gamma\, \delta_{\mu\nu}\, \delta(t'-t'')}$$

$$= e^{-\frac{\Gamma}{2} \vec{q}^{\,2} \int_{-\infty}^{t} dt'\, e^{-\frac{2}{\tau}(t-t')}}$$

$$= e^{-\frac{\Gamma}{4} \tau \vec{q}^{\,2}}$$ which is also Gaussian.

If $\vec{P}$ where to satisfy a Maxwell-Boltzmann distribution at Temperature $T \Rightarrow$

$$\rho(\vec{P}) = \frac{1}{(2\pi MkT)^{d/2}} e^{-\frac{\vec{P}^2}{2MkT}}$$

$$\Rightarrow \langle e^{i\vec{q}\cdot\vec{P}} \rangle = e^{-\frac{\vec{q}^2}{2}MkT}$$

$\Rightarrow$ both gaussians agree if

$$MkT = \frac{\Gamma\tau}{2} \quad \text{or} \quad \underbrace{\Gamma\tau}_{\text{dissipation}} = \underbrace{2MkT}_{\text{fluctuation}}$$

$\Rightarrow$ the rate at which momentum is added to the particle (Γ) is determined by kT and by τ.

(Fluctuation-Dissipation Thm.).

Let $$f(\vec{r},\vec{p},t) = \left\langle \sum_{j=1}^{N} \delta(\vec{P}_j(t)-\vec{p})\,\delta(\vec{R}_j(t)-\vec{r}) \right\rangle$$

$$\equiv N(2\pi\hbar)^3 \rho(\vec{r},\vec{p},t)$$

$(2\pi\hbar)^3$ (norm.)

one-particle distribution function. (one particle)

$$\frac{d\vec{R}}{dt} = \frac{\vec{P}}{m} \doteq \frac{\partial H}{\partial \vec{P}}$$

$$\frac{d\vec{P}}{dt} = -\frac{\partial H}{\partial \vec{R}} + \vec{\eta}(t) - \frac{\vec{P}}{\tau}$$

$$H = \frac{\vec{P}^2}{2m} + U(\vec{R})$$

Let $\mathcal{O}(\vec{p},\vec{r})$ be any observable

$$\Rightarrow \langle \mathcal{O}(\vec{p},\vec{r}) \rangle (t) = \int d\vec{r}\wedge d\vec{p}\; \mathcal{O}(\vec{p},\vec{r})\, \rho(\vec{r},\vec{p},t)$$

We know that

$$\frac{\partial f}{\partial t} + \{H, f\} = \left(\frac{\partial f}{\partial t}\right)_{\text{collisions}}$$

what expression do we get for $\left(\frac{\partial f}{\partial t}\right)_{\text{coll}}$?

Over some interval δt

$$(\delta\vec{p})_{\text{collision}} = -\vec{p}\,\frac{\delta t}{\tau} + \vec{I}$$

$$\vec{I} = \int_t^{t+\delta t} dt'\,\vec{\eta}(t')$$

$$\delta\langle O(t)\rangle = \int dr\wedge dp\; O(\vec{r},\vec{p})\;\delta t\;\frac{df(r,p,t)}{dt}\Big|_{coll}$$

$$\delta\langle O\rangle(t) = \Big\langle \int dr\wedge dp\;\big[O(\vec{r},\vec{p}+\delta\vec{p}) - O(\vec{r},\vec{p})\big]\Big\rangle$$

$$= \int dr\wedge dp\; f(\vec{r},\vec{p},t)\Big[\big\langle O(\vec{p}-\vec{p}\tfrac{\delta t}{\tau}+\vec{I},\vec{r})\big\rangle - O(\vec{r},\vec{p})\Big]$$

$$O(\vec{p},\vec{r}) = \int d\vec{q}\; e^{i\vec{p}\cdot\vec{q}}\;\tilde{O}(\vec{q},\vec{r})$$

$$\big\langle O(\vec{p}-\vec{p}\tfrac{\delta t}{\tau}+\vec{I},\vec{r})\big\rangle =$$

$$= \int d\vec{q}\;\tilde{O}(\vec{q},\vec{r})\;\Big\langle e^{i\vec{p}\cdot\vec{q} - i\vec{p}\cdot\vec{q}\frac{\delta t}{\tau} + i\vec{I}\cdot\vec{q}}\Big\rangle$$

$$= e^{i\vec{p}\cdot\vec{q}}\;e^{-i\vec{p}\cdot\vec{q}\frac{\delta t}{\tau}}\;e^{-\frac{1}{2}\Gamma\delta t\,\vec{q}^{\,2}}$$

$$\langle O(\vec{p} - \vec{p}\frac{\delta t}{\tau} + \vec{\xi}, \vec{r})\rangle - O(\vec{p}, \vec{r}) =$$

$$= \int d\vec{q}\, \left(e^{i\vec{p}\cdot\vec{q}}\, e^{-i\vec{p}\cdot\vec{q}\frac{\delta t}{\tau}}\, e^{-\frac{\Gamma\delta t}{2}\vec{q}^2} - e^{i\vec{p}\cdot\vec{q}}\right) \tilde{O}(\vec{q}, \vec{r})$$

$$= \int d\vec{q}\, e^{i\vec{p}\cdot\vec{q}} \left(e^{-i\vec{p}\cdot\vec{q}\frac{\delta t}{\tau}}\, e^{-\frac{\Gamma\delta t}{2}\vec{q}^2} - 1\right) \tilde{O}(\vec{q}, \vec{r})$$

$$\approx \int d\vec{q}\, e^{i\vec{p}\cdot\vec{q}} \left[-i\vec{p}\cdot\vec{q}\frac{\delta t}{\tau} - \frac{\Gamma\delta t}{2}\vec{q}^2 + \cdots\right] \tilde{O}(\vec{q}, \vec{r})$$

$$\vec{p}\cdot\vec{\nabla}_p O(\vec{p}, \vec{r}) = \vec{p}\cdot\vec{\nabla}_p \int d\vec{q}\, e^{i\vec{q}\cdot\vec{p}}\, \tilde{O}(\vec{q}, \vec{r})$$

$$= \int d\vec{q}\; i\,\vec{p}\cdot\vec{q}\, e^{i\vec{q}\cdot\vec{p}}\, \tilde{O}(\vec{q}, \vec{r})$$

$$\nabla^2_{\vec{p}} O(\vec{p}, \vec{r}) = \int d\vec{q}\, (-\vec{q}^2)\, e^{i\vec{q}\cdot\vec{p}}\, \tilde{O}(\vec{q}, \vec{r})$$

$\Rightarrow$ we get $\; -\frac{\delta t}{\tau}\vec{p}\cdot\vec{\nabla}_p O(\vec{p}, \vec{r}) + \frac{\Gamma\delta t}{2}\nabla^2_{\vec{p}} O(\vec{p}, \vec{r})$

$$\Rightarrow \delta\langle O\rangle = \int dr\wedge dp\left[-\frac{\delta t}{\tau}\,\vec{p}\cdot\vec{\nabla}_p O + \frac{\Gamma\delta t}{2}\,\nabla^2_{\vec{p}} O\right] f(r,p,t)$$

$$= \int dr\wedge dp\ O(r,p)\,\delta t\ \vec{\nabla}_{\vec{p}}\cdot\left\{\left[\frac{\vec{p}}{\tau} + \frac{\Gamma}{2}\vec{\nabla}_p\right] f(\vec{r},\vec{p},t)\right\}$$

$$\Rightarrow \left(\frac{\partial f}{\partial t}\right)_{\text{collisions}} = \vec{\nabla}_p\cdot\left\{\left(\frac{\vec{p}}{\tau} + \frac{\Gamma}{2}\vec{\nabla}_{\vec{p}}\right) f(\vec{r},\vec{p},t)\right\}$$

$\Rightarrow$ Fokker-Planck Equation:

$$\boxed{\frac{\partial f}{\partial t} + \{H, f\} = \vec{\nabla}_p\cdot\left\{\left(\frac{\vec{p}}{\tau} + \frac{\Gamma}{2}\vec{\nabla}_p\right) f(r,p,t)\right\}}$$

Equilibrium solutions: $\frac{\partial f}{\partial t} = 0$ and $f = \Phi(H)$

$\Rightarrow \{H, f\} = 0$ but

r.h.s $\neq 0$ unless

$$\vec{\nabla}_{\vec{p}}\cdot\left[\left(\frac{\vec{p}}{\tau} + \frac{\Gamma}{2}\vec{\nabla}_p\right)\Phi[H]\right] = 0$$

since $\frac{\vec{p}}{M} = \frac{\partial H}{\partial \vec{p}}$ $\Rightarrow$

$$\nabla_{\vec{p}} \cdot \left\{ \left[\frac{M}{\tau} (\vec{\nabla}_{\vec{p}} H) + \frac{\Gamma}{2} \vec{\nabla}_{\vec{p}} \right] f \right\} = 0$$

if $\quad \frac{M}{\tau} (\vec{\nabla}_p H) f + \frac{\Gamma}{2} \vec{\nabla}_p f = 0$

$$\Rightarrow \frac{M}{\tau} \vec{\nabla}_p H = - \frac{\Gamma}{2} \vec{\nabla}_{\vec{p}} \log f$$

$$\vec{\nabla}_p \left[\frac{M}{\tau} H + \frac{\Gamma}{2} \log f \right] = 0$$

$$\Rightarrow \frac{M}{\tau} H + \frac{\Gamma}{2} \log f = \text{const.}$$

$$\log f = \text{const} - \frac{2M}{\Gamma \tau} H$$

$$f = \text{const} \times e^{-\frac{2M}{\Gamma\tau} H}$$

$\Rightarrow$ Gibbs $\quad \frac{\Gamma \tau}{2M} = kT \quad \checkmark$

Fokker-Planck: $\boxed{\frac{\partial f}{\partial t} + \{H, f\} = \vec{\nabla}_p \cdot \left\{ \left[\frac{MkT}{\tau} \vec{\nabla}_p + \frac{\vec{p}}{\tau} \right] f \right\}}$

General Langevin Processes

Consider a system described by some coordinates $q_i(t)$ subject to the action of dissipative forces and random external forces. We will assume that the system is <u>overdamped</u> and write

$$\frac{d q_i(t)}{dt} = + \frac{1}{\gamma} f_i[\vec{q}(t)] + \eta_i(t)$$

Note: $[\eta] = \frac{L}{T}$ not F!

where f_i are external forces and $\eta_i(t)$ are random forces. The random forces obey
(γ : friction constant)

$$\langle \eta_i(t) \rangle = 0$$

Note : $[\Gamma] = \frac{L^2}{T}$ = Diffusion constant

$$\langle \eta_i(t)\, \eta_j(t') \rangle = \Gamma\, \delta(t-t')\, \delta_{ij}$$

i.e. are Markov processes ("no memory")

Hence the probability density of a particular random process $\eta_i(t)$ is

$$d\mathcal{P}[\eta] = \underset{\substack{\uparrow \\ \text{"measure"}}}{\mathcal{D}\eta}\; e^{-\frac{1}{2\Gamma}\int_{-\infty}^{+\infty} dt\, \vec{\eta}^{\,2}(t)}$$

What is the Fokker-Planck Equation associated with this problem?

$$P[\vec{q},t] = \left\langle \prod_{i=1}^{d} \delta(q_i(t) - q_i) \right\rangle$$

The same line of reasoning as used before leads to the equation

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial q_i}\left[\frac{\Gamma}{2}\frac{\partial P}{\partial q_i} + \frac{1}{2\gamma} f_i(q)\, P\right] \qquad (FP)$$

There is an interesting analogy with Quantum Mechanics. Let H be a Q.M. hamiltonian, ~~and~~ $|\vec{q}\rangle$ be a final state and $|\vec{q}\,'\rangle$ be an initial state $\Rightarrow$

$$\langle \vec{q} |\, e^{-tH} \,| \vec{q}\,' \rangle \equiv \tilde{F}(\vec{q}, \vec{q}\,'; t)$$

In quantum mechanics the quantity that is ~~usually~~ computed is

$$\langle \vec{q} |\, e^{-\frac{i}{\hbar} t H} \,| \vec{q}\,' \rangle \equiv F(\vec{q}, \vec{q}\,'; t)$$

and it is known as the evolution operator $\hat{U}$

F and $\tilde{F}$ are related through the analytic continuation ($\hbar = 1$) $t \to it$ (i.e. "imaginary time")

It is easy to show that, if we define $\vec{\hat{p}} = -i\frac{\partial}{\partial \vec{q}}$, the "Hamiltonian" is

$$H = \frac{\Gamma}{2}\hat{\vec{p}}^{\,2} + \frac{i}{\gamma}\hat{\vec{p}}\cdot\vec{f}[\vec{q}]$$

which is in general clearly not hermitean.

How do observables ~~evolve~~ evolve in time?

Let $A[\vec{q}(t)]$ be an observable $\Rightarrow$

$$\langle A[\vec{q}(t)]\rangle = \int d\vec{q}\; A[\vec{q}]\,\langle \vec{q}|\, e^{-tH}\,|\vec{q}\,'\rangle$$

where $\vec{q}\,' = \vec{q}(0)$

Let us define the "Heisenberg representation"

$$A[\vec{q},t] = \int d\vec{q}\,'\; A[\vec{q}\,']\,\langle \vec{q}\,'|\, e^{-tH}\,|\vec{q}\rangle$$

$$\Rightarrow \quad \frac{\partial A}{\partial t} = \left(\frac{\Gamma}{2}\frac{\partial}{\partial q_i} - \frac{1}{2\gamma}f_i[\vec{q}]\right)\frac{\partial}{\partial q_i}A$$

is the Eqn of motion.

<u>Equilibrium:</u> $\quad P_0[\vec{q}] = \lim_{t\to\infty} P[\vec{q},t]$

Since $\quad \partial_t P = \vec{\partial}_q\cdot\left[\frac{\Gamma}{2}\partial_{\vec{q}}P + \frac{1}{2\gamma}\vec{f}\,P\right]$

$$\Rightarrow \int_\Omega d\vec{r}\,\partial_t P = \partial_t\int_\Omega d\vec{r}\;P = \int_\Omega d\vec{r}\;\partial_{\vec{r}}\cdot\left[\frac{\Gamma}{2}\partial_{\vec{q}}P + \frac{1}{2\gamma}\vec{f}\,P\right]$$

$$= \int_{\partial\Omega} d\vec{S}\cdot\left(\frac{\Gamma}{2}\partial_{\vec{q}}P + \frac{1}{2\gamma}\vec{f}\,P\right) = 0$$

$\Rightarrow \int_\Omega d\vec{r}\;P \equiv 1$ is <u>conserved</u>.

$\Rightarrow$ P_0 must be a right eigenvector of H (recall that H is not Hermitean $\Rightarrow$ right and left eigenvectors are $\neq$). In general, the right eigenvectors have a positive real part which guarantees the existence of a "ground state", i.e. an equilibrium distribution.

Furthermore, if the forces $f_i(q)$ are conservative, i.e. $f_i = -\partial_i E(q)$ for some "potential" $E(q)$ $\Rightarrow$

$$\frac{\partial \vec{q}}{\partial t} = -\frac{1}{2\gamma}\, \partial_{\vec{q}}\, E(\vec{q}) + \vec{\eta}(t)$$

Let us write $P(\vec{q},t)$ in the form:

$$P(t,\vec{q}) = e^{-\frac{1}{2\gamma\Gamma}E(\vec{q})} \langle \vec{q} \,|\, U(t,0) \,|\, \vec{q}\,' \rangle\, e^{\frac{E(\vec{q}\,')}{2\gamma\Gamma}}$$

where $\vec{q}\,' = \vec{q}(0)$ $\quad$ [i.e. $P(\vec{q},0) = \delta(\vec{q}-\vec{q}\,')$]

$\Rightarrow$

$$\frac{\partial}{\partial t} \langle \vec{q} \,|\, U(t,0) \,|\, \vec{q}\,' \rangle = -\frac{\Gamma}{2}\left(-\frac{\partial}{\partial \vec{q}} + \frac{1}{2\gamma\Gamma}\frac{\partial}{\partial \vec{q}}E(\vec{q}) \right) \cdot$$

$$\cdot \left(\frac{\partial}{\partial \vec{q}} + \frac{1}{2\gamma\Gamma}\frac{\partial E(\vec{q})}{\partial \vec{q}} \right) \langle \vec{q} \,|\, U(t,0) \,|\, \vec{q}\,' \rangle$$

where the new "Hamiltonian" $\tilde{H}$ is

$$\tilde{H} = \frac{\Gamma}{2}\hat{P}^2 + \frac{\Gamma}{8}\left(\partial_{\tilde{q}}\tilde{E}(q)\right)^2 - \frac{\Gamma}{4}\partial_q^2\tilde{E}(q)$$

with $\tilde{E}(\vec{q}) = \frac{1}{\gamma\Gamma}E(\vec{q})$ and $\vec{p} = i\frac{\partial}{\partial\vec{q}}$

$\tilde{H}$ is clearly Hermitean.

Note: $[\Gamma] = \frac{L^2}{T}$ and $[\gamma] = E/(L^2/T) \Rightarrow [\Gamma\gamma] = E$

The (normalizable) ground state wave function of $\tilde{H}$ is $\psi_0(\vec{q}) = \# e^{-\frac{1}{2}\tilde{E}(\vec{q})}$

Its eigenvalue is zero

$$\tilde{H}\psi_0 = 0$$

and in general

$$P(\vec{q},t) = e^{-\frac{1}{2}\tilde{E}(\vec{q})}\langle\vec{q}|e^{-t\tilde{H}}|\vec{q}'\rangle e^{\frac{1}{2}\tilde{E}(}$$

Let $|n\rangle$ the n-th eigenstate of $\tilde{H}$ with eigenvalue λ_n,

$$\tilde{H}|n\rangle = \lambda_n|n\rangle$$

Clearly $\langle\vec{q}|0\rangle = \psi_0(\vec{q})$ and $\underline{\underline{\lambda_0 = 0}}$

Let $\psi_n(\vec{q}) = \langle\vec{q}|n\rangle$

since $\{|n\rangle\}$ are complete (and discrete)

$\hat{I} = \sum_n |n\rangle\langle n|$ is the identity operator.

$\Rightarrow$

$$\langle \vec{q} |\, e^{-t\tilde{H}} \,| \vec{q}\,' \rangle =$$

$$= \sum_{n=0}^{\infty} \langle \vec{q} | n \rangle \, e^{-t\lambda_n} \, \langle n | \vec{q}\,' \rangle$$

$$= \sum_{n=0}^{\infty} \psi_n(q)\, \psi_n^{*}(q')\, e^{-\lambda_n t}$$

Since $\tilde{H}$ is not only hermitian but also <u>real</u> $\Rightarrow$ λ_n are real (and positive), and ψ_n are also real.

$$\Rightarrow P(\vec{q},t) = e^{-\frac{1}{2}\tilde{E}(\vec{q})} \sum_{n=0}^{\infty} \psi_n(q)\, \psi_n^{*}(q')\, e^{-\lambda_n t}$$

$$e^{\frac{1}{2}\tilde{E}(\vec{q}\,')}$$

$$\Rightarrow P(\vec{q},t) = e^{-\frac{1}{2}\tilde{E}(q)} \Big[\psi_0(\vec{q})\, \psi_0^{*}(\vec{q}\,')\, 1 + \psi_1(\vec{q})\, \psi_1^{*}(\vec{q}\,') \times e^{-\lambda_1 t} + \dots \Big] e^{\frac{1}{2}\tilde{E}(q')}$$

but $\psi_0(\vec{q}) = e^{-\frac{1}{2}\tilde{E}(\vec{q})}$ (up to a normalization)

$$\Rightarrow P(\vec{q},t) = e^{-\tilde{E}(\vec{q})} + \psi_1(\vec{q})\, e^{-\frac{\tilde{E}(q)}{2}}\, \psi_1^{*}(\vec{q}\,')\, e^{\frac{\tilde{E}(\vec{q}\,')}{2}} \, e^{-\lambda_1 t} + \dots$$

$$\Rightarrow \lim_{t\to\infty} P(\vec{q},t) \equiv P_0(\vec{q}) = e^{-E(\vec{q})/\gamma\Gamma}$$

(This makes sense if ψ_0 is normalizable.) (caveat)

Hence, asymptotically, $P(\vec{q},t)$ converges to a Gibbs distribution with $kT = \gamma\Gamma$

Notice that in general there is a <u>spectrum of relaxation times</u> $\tau_n = \frac{1}{\lambda_n}$, where $\{\lambda_n\}$ are the eigenvalues of $\tilde{H}$. Thus, at long times, the correction to $P_0(\vec{q})$ is exponentially small <u>if</u> there is a gap in the spectrum of $\tilde{H}$, i.e. if $\lambda_1 > 0$. If the spectrum is continuous, there is no normalizable solution and the time dependence changes. For instance for a random walker, $\vec{f}=0$ and the asymptotic solution is $P_0=0$. In this case the time dependence was much more singular $\sim \frac{1}{t^{\#}} e^{-\frac{\#}{t}}$

<u>Note</u>: For $\vec{f}=0$ (i.e. free particle) the Fokker-Planck equation becomes: $\frac{\partial P}{\partial t} = \frac{\Gamma}{2} \partial_{\vec{q}}^2 P \Rightarrow$ diffusion equation with $D = \frac{\Gamma}{2}$

$$\Rightarrow P(\vec{q},t) = (2\pi\Gamma t)^{-d/2} \exp(-\vec{q}^{\,2}/2\Gamma t) \xrightarrow[t\to 0]{} \delta^d(\vec{q})$$