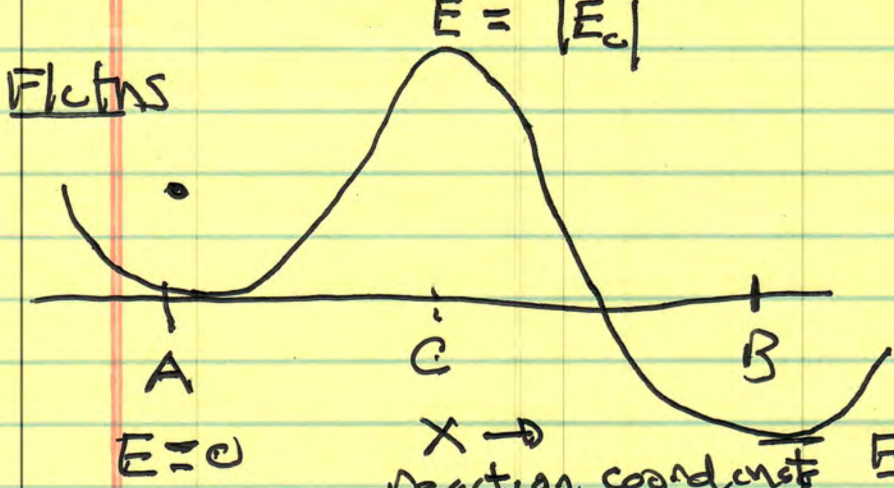
Physics 210B

Kramers Problem - Part II

→ weak friction ⟺ Energy Diffusion

(c.f. Zwanzig)

Recall the Kramers Problem:



$\boxed{T}$

drag ~ β

~ $6\pi\eta a$

- Seek probability of passage $A \rightarrow B$.

- noise / drag essential → many kicks

- in general, have

$$\frac{dv}{dt} = -\frac{\beta}{m} v + \underbrace{q_{ext}(x)}_{-\nabla U(x)/m} + \underbrace{\tilde{q}}_{\tilde{f}/m} \quad , \quad \frac{dx}{dt} = v$$

before:

- strong friction / high viscosity

$$v = -\frac{\nabla U(x)}{\beta} + \frac{\tilde{f}}{\beta} = \frac{dx}{dt}$$

$\Rightarrow$ Schmoluchowski

$$\frac{\partial n}{\partial t} = -\frac{\partial}{\partial x}\left[-\frac{\nabla U(x)}{\beta} n - \frac{\partial}{\partial x} D n\right]$$

$$D = T/\beta$$

$$\frac{\partial n}{\partial t} + \partial_x J = 0$$

Re-write:

$$J = -\frac{D_v}{\beta^2} \exp\left[-\frac{\beta U}{D_v}\right] \partial_x \left(n \exp\left(\frac{\beta U}{D_v}\right)\right)$$

etc. $\quad D_v = \beta^2 D = \beta T.$

look for $J = \text{const.}$, with i.c near A

- now, weak friction / low viscosity
  - no longer make terminal velocity approximation
  - need $f(v,x,t)$, with random scattering in v due thermal noise, and drag.

So use Full Fokker-Planck Eqn for f:

$$\partial_t f + v\partial_x f = -\partial_v \left\{ q_{ext} f - \frac{\beta}{m} v f - \partial_v (D_v f) \right\}$$

$\Rightarrow$

$$\partial_t f + v\,\partial_x f + q_{ext}\,\partial_v f = \partial_v \left\{ \frac{\beta}{m} v f + \partial_v (D_v f) \right\}$$

LHS: $\frac{df}{dt}$, along Hamiltonian orbits

$D_v \sim \beta T$

RHS $\sim \beta$

$\rightarrow$ small

$$\frac{df}{dt} = \partial_v \left\{ \frac{\beta}{m} v f + \partial_v (D_v f) \right\}$$

$$= \beta \cdot \partial_v \left\{ \frac{v f}{m} + \partial_v (T f) \right\}$$

can re-write as:

$$\frac{\partial f}{\partial t} + L_0 f = \beta T \frac{\partial}{\partial p} f_{eq} \frac{\partial}{\partial p}\left(\frac{f}{f_{eq}}\right)$$

particle Liouville Operator

check:

$$RHS = \beta T \frac{\partial}{\partial p}\left[f_{eq} \frac{1}{f_{eq}} \partial_p f - \frac{f_{eq}}{f_{eq}^2} \frac{\partial f_{eq}}{\partial p} f \right]$$

$$= \beta T \frac{\partial}{\partial p}\left[\frac{\partial}{\partial p} f\right] + \beta \cancel{T} \frac{\partial}{\partial p}\left[\frac{p}{M \cancel{T}} f\right]$$

$$= \beta T \frac{\partial}{\partial p}\left[\partial_p f\right] + \frac{\beta}{M} \frac{\partial}{\partial p}\left[p f\right]$$

$$\rightarrow \partial_v \left\{ \left(\frac{\beta}{M} v f\right) + \partial_v (D_v f) \right\} \checkmark$$

so

$$\boxed{\frac{\partial f}{\partial t} + L_0 f = \beta T \frac{\partial}{\partial p} f_{eq} \frac{\partial}{\partial p} \frac{f}{f_{eq}}}$$

is general FPE for Kramers Problem.

LHS akin Vlasov eq. (no Poisson)

Low β $\rightarrow$ $\frac{\partial f}{\partial t} + L_0 f = C(f) \rightarrow$ akin weakly collisional Boltzmann.

$$L_0 = \frac{p}{m}\partial_x + (-\nabla U)\frac{\partial}{\partial p}$$

$$\boxed{\begin{aligned} f_{eq} &= f_{eq}(H) \\ H &= \frac{p^2}{2m} + U(x) \end{aligned}}$$

expect diffusion in energy

For distribution of energy;

$$g(E,t) = \int dx \int dp\, \delta(H(x,p) - E)\, f(x,p,t)$$

- delta selects pts on $E = \text{const}$ surface

- so $L_0 H = 0$ after $\int dx \int dp\, \delta(H-E)$ on F-P Eqn.

$$\boxed{\partial_t g(E,t) = \beta T \int dx \int dp\, \delta(H-E) \frac{\partial}{\partial p} f_{eq} \frac{\partial}{\partial p} \frac{f}{f_{eq}}}$$

- reduced Fokker Planck eqn.
- only most scott evolves $g(E,t)$ b.

Now seek equation for $g(E,t)$:

① replace $f(x,p,t) \Rightarrow \phi(H,t)$

require:

$$\int dx \int dp\, \delta(H-E)\, \phi(H,t) = \int dx \int dp\, \delta(H-E)\, f(x,p,t)$$

$$= g(E,t)$$

$$= \phi(E,t) \int dx \int dp\, \delta(H-E)$$

② $\Omega(E) = \int dx \int dp\, \delta(H-E)$ is microcanonical partition function

so

③ $\phi(E,t)\,\Omega(E) = g(E,t)$

④ $\dfrac{f}{f_{eq}} \cong \dfrac{g(H,t)}{g_{eq}(H)}$

so

(5) $-\frac{\partial}{\partial p}\frac{f}{f_{eq}} = \frac{p}{M}\frac{\partial}{\partial H}\frac{g(H,t)}{g_{eq}(H)}$

so

$$\frac{\partial g(E,t)}{\partial t} = \beta T \int dx \int dp\, \delta(H-E)\, \frac{\partial}{\partial p} f_{eq}\, \frac{\partial}{\partial p}\frac{f}{f_{eq}}$$

$$= \beta T \int dx \int dp\, \delta(H-E)\, \frac{\partial}{\partial p} f_{eq}\, \frac{p}{M}\frac{\partial}{\partial H}\frac{g(H,t)}{g_{eq}(H)}$$

Now, integrate by parts:

$$\int dp\, \delta(H-E)\frac{\partial}{\partial p} = -\int dp\, \frac{\partial}{\partial p}\delta(H-E)$$

$$= \frac{\partial}{\partial E}\int dp\, \frac{p}{M}\,\delta(H-E)$$

so, have:

$$\boxed{\frac{\partial g(E,t)}{\partial t} = \beta T \frac{\partial}{\partial E}\int dx \int dp \left(\frac{p}{M}\right)^2 \delta(H-E)\, f_{eq}(E)\, \frac{\partial}{\partial E}\frac{g(E,t)}{g_{eq}(E)}} \; *$$

Can re-write as: Diffusion / Schmoluchowski

$$\boxed{\frac{\partial g(E,t)}{\partial t} = \frac{\partial}{\partial E} D(E) g_{eq}(E) \frac{\partial}{\partial E} \frac{g(E,t)}{g_{eq}}}$$

where: (reminiscent QL → here th noise)

$$\boxed{D(E) = \beta T \frac{\int\int dx\,dp\,(p/m)^2 \delta(H-E)}{\int dx \int dp\, \delta(H-E)}}$$

energy diffusion 'coefficient' $\sim \Omega$

→ N.B. – replacing spatial diffusion with energy diffusion
– x, p dependence is thru of Hamiltonian → weak friction & RHS small, zeroth order is Vlasov.

cranking further.

$$\int dp\, \underbrace{f(p)}_{\text{some fctn}}\, \delta(p^2 - a^2) = \frac{f(a)}{2a}$$

so $$D(E) = 2\underbrace{\frac{\beta T}{m}}\frac{\int dx\sqrt{E-U(x)}}{\int dx\ 1/\sqrt{E-U(x)}}$$

Now,

- integration over x s/t $E > U(x)$

- $\int dx\sqrt{E-U} = \oint dx\, p(x) = I(E)$

  numerator — action

  $$p(x) = [2m(E-U(x))]^{1/2}$$

- $$\int dx \frac{1}{\sqrt{E-U(x)}} = 1/\partial I/\partial E$$

  $$= \frac{\omega(E)}{2\pi} \to \frac{\omega(E)}{2\pi}$$

so, have energy diffusion

$$\frac{\partial g(E,t)}{\partial t} = \frac{\partial}{\partial E}\frac{\beta}{m} I(E)\left[\left[1 + T\frac{\partial}{\partial E}\right]\left(\frac{\omega(E)\, g(E,t)}{2\pi}\right)\right]$$

$$\Leftrightarrow \quad \frac{\partial g}{\partial t} = \beta T D(E)\, g_{eq}(E) \frac{\partial}{\partial E} \frac{g(E,t)}{g_{eq}(E)}$$

$$\boxed{\frac{\partial g(E,t)}{\partial t} = \frac{\partial}{\partial E}\left[\frac{\beta}{m} I(E) \left[1 + T\frac{\partial}{\partial E} \right] \frac{\omega(E)}{2\pi} g(E,t) \right]}$$

Recall for large friction, spatial Schmoluchowski Eqn:

$$\boxed{\frac{\partial f}{\partial t} = D \frac{\partial}{\partial x} e^{-U/T} \frac{\partial}{\partial x}\left(e^{U/T} f\right)}$$

so have analogy

Large Friction	Small friction
x	E
$e^{-U/T}$	$\Omega(E)\, e^{-U/T}$
$D(x)$	$D(E)$
use terminal vel.	use unperturbed orbits

Recall, for first passage time:

$$D^{+}\tau = -1$$

adjoint of F-P operator

so

$$\frac{\partial f}{\partial t} = D\frac{\partial}{\partial x} e^{-U/T}\frac{\partial}{\partial x}\left(e^{U/T} f\right)$$

then

$$D e^{U/T}\frac{\partial}{\partial x} e^{-U/T}\frac{\partial}{\partial x}\tau = -1$$

Can argue analogously:

$$\tau(E) = \int_{E}^{E_b} dE' \frac{1}{D(E')\, g_{eL}(E')} \int_{0}^{E'} dE'' g_{eL}(E'')$$

plugging in $D(E')$, $g_{eL}(E')$

$$\boxed{T(E) = \frac{2m}{\beta T}\int_E^{E_b} dE'\, \frac{e^{E'/T}}{I(E')}\int_0^E dE''\,\Omega(E'')\, e^{-E''/T}}$$

$I(E) \simeq \frac{2m}{\omega_0} E$, $\Omega(E) = \frac{\pi}{\omega_0}$ near min.

$$\Rightarrow \quad \boxed{\tau = \frac{2\pi m T}{\beta}\,\frac{1}{\omega_0 I(E_b)}\, e^{E_b/T}}$$

- Mean First passage time $\underline{(\text{Rate})}^{-1}$ $\sim 1/\beta$ small β
- Recall $\frac{1}{\tau} \sim 1/\beta$ large β

So