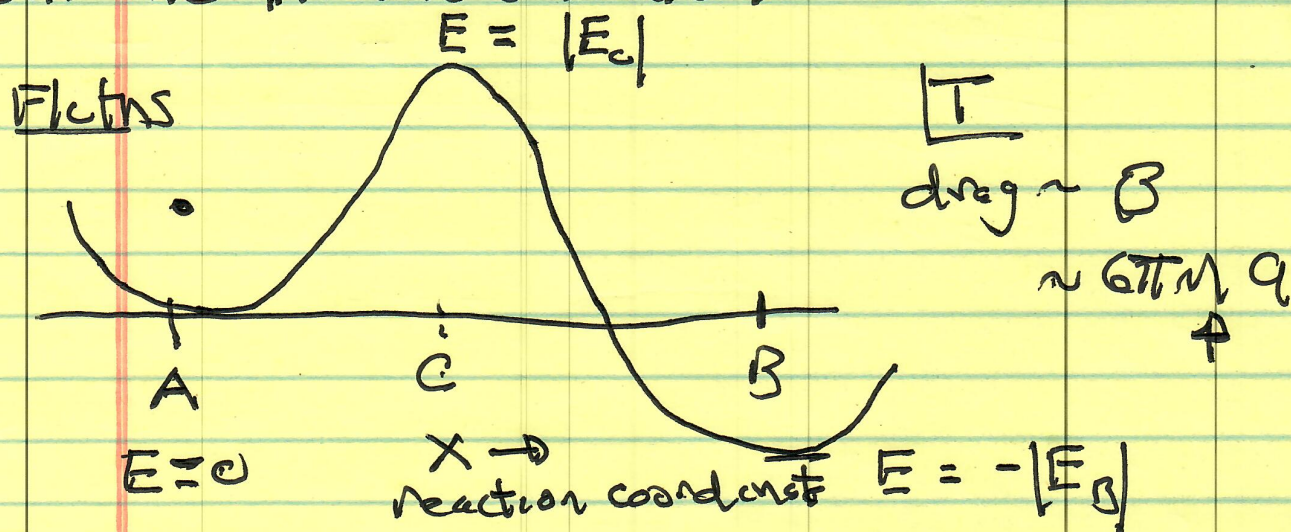


Physics 210B

Kramers Problem - Part II

→ weak friction ↔ Energy Diffusion
(c.f. Zwanzig)

Recall the Kramers Problem:



- Seek probability of passage $A \rightarrow B$.
- noise / drag essential $\rightarrow$ many kicks
- in general, have

$$\frac{dv}{dt} = -\frac{\beta}{m} v + \frac{q_{ext}(x)}{m} + \frac{\tilde{q}}{m}, \quad \frac{dx}{dt} = v$$

$-\frac{DU(x)}{m}$
 $\frac{\tilde{p}}{m}$

before:

- strong friction / high viscosity

$$v = - \frac{\partial U(x)}{\beta} + \frac{p^2}{\beta} = \frac{dx}{dt}$$

⇒ Schmuckowski

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

$$D = T/\beta$$

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

Re-write:

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

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

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 Egn
for F ;

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

$\Rightarrow$

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

LHS: $\frac{df}{dt}$, along Hamiltonian orbits $D_v \sim \beta T$

$$\begin{aligned} \frac{df}{dt} &= \partial_v \left\{ \frac{\beta}{m} v f + \partial_v (D_v f) \right\} & \text{RHS} \sim \beta \\ &= \beta \cdot \partial_v \left\{ \frac{v}{m} f + \partial_v (T f) \right\} & \rightarrow \text{small} \end{aligned}$$

Can re-write as:

$$\frac{\partial F}{\partial t} + L_0 F = \beta T \frac{\partial}{\partial p} f_{e2} \frac{\partial}{\partial p} \left(\frac{F}{f_{e2}} \right)$$

↓
1 particle's Liouville Operator

check:

$$\begin{aligned} \text{RHS} &= \beta T \frac{\partial}{\partial p} \left[f_{e2} \frac{1}{f_{e2}} \frac{\partial p F}{\partial p} - \frac{f_{e2}}{f_{e2}^2} \frac{\partial f_{e2}}{\partial p} F \right] \\ &= \beta T \frac{\partial}{\partial p} \left[\frac{\partial F}{\partial p} \right] + \beta T \frac{\partial}{\partial p} \left[\frac{1}{m} F \right] \end{aligned}$$

$$= \beta T \frac{\partial}{\partial p} \left[\frac{\partial F}{\partial p} \right] + \frac{\beta}{m} \frac{\partial}{\partial p} [p F]$$

$$\rightarrow \frac{\partial}{\partial p} \left\{ \left(\frac{\beta}{m} v F \right) + \frac{\partial}{\partial p} (Q F) \right\} \quad \checkmark$$

$$\boxed{\frac{\partial F}{\partial t} + L_0 F = \beta T \frac{\partial}{\partial p} f_{e2} \frac{\partial}{\partial p} \frac{F}{f_{e2}}}$$

LHS akin $V/\epsilon_0 v$ d. (no Poisson) $\rightarrow$ general FPE for Bremers Problem.

Low $\beta \rightarrow \frac{\partial f}{\partial t} + L_0 f = C(f) \rightarrow$ akin weakly collisional Boltzmann. $\frac{S_0}{\beta}$

$$L_0 = \frac{1}{m} \frac{\partial}{\partial x} + (-\partial u) \frac{\partial}{\partial p}$$

$$\begin{cases} f_{e2} = f_{e2}(H) \\ H = \frac{p^2}{2m} + u(x) \end{cases}$$

expect difference in energy

For distribution of energy,

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

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

$\xrightarrow{-\infty} L_0 H = 0$ after $\int dx \int dp \delta(H - E)$ on $F \rightarrow E$ surface.

$$\partial_t g(E, t) = \beta T \int dx \int dp \delta(H - E) \frac{\partial}{\partial p} f_{e2} \frac{\partial}{\partial p} \frac{p}{f_{e2}}$$

— reduced Fokker-Planck eqn.

— only non-steady evolves $g(E, t)$ $\downarrow$

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

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

require:

$$\begin{aligned} \int dx \int dp \delta(H-E) \phi(H, t) &= \int dx \int dp \delta(H-E) P(x, p, t) \\ &= g(E, t) \\ &= \phi(E, t) \int dx \int dp \delta(H-E) \end{aligned}$$

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 $\frac{f}{f_{\text{eq}}} \approx \frac{g(H, t)}{g_{\text{eq}}(H)}$

so

①

$$\frac{\partial}{\partial p} \frac{F}{g_{eq}} = \frac{A}{M} \frac{\partial}{\partial H} \frac{g(CH, t)}{g_{eq}(CH)}$$

②

$$\begin{aligned} \frac{\partial g(E, t)}{\partial t} &= (\beta T \int dx \int dp \delta(H-E)) \frac{\partial}{\partial p} F_{eq} \frac{\partial}{\partial p} \frac{F}{F_{eq}} \\ &= \beta T \int dx \int dp \delta(H-E) \frac{\partial}{\partial p} F_{eq} \frac{A}{M} \frac{\partial}{\partial H} \frac{g(CH, t)}{g_{eq}(CH)} \end{aligned}$$

Now, integrate by parts:

$$\begin{aligned} \int dp \delta(H-E) \frac{\partial}{\partial p} &= - \int dp \frac{\partial}{\partial p} \delta(H-E) \\ &= \frac{\partial}{\partial E} \int dp \frac{p}{M} \delta(H-E) \end{aligned}$$

so, we've:

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

Can re-write as:

Diffusion/Schrodinger

$$\frac{\partial g(E,t)}{\partial t} = \frac{\partial}{\partial E} D(E) g_E(E) \frac{\partial}{\partial E} g(E,t)$$

where:

(remember cent $\Omega \rightarrow$ here the noise)

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

energy diffusion coefficient

Ω

- $\rightarrow$ N.B. - replacing spatial diffusion with energy diffusion
 - x, p dependence is that of Hamiltonian $\rightarrow$ weak friction $\downarrow$
 RHS small, zeroth order is v_{esc} .

cranking further.

$$\int_{\text{some } p \text{ etc.}} dp F(p) \delta(p^2 - a^2) = \frac{F(a)}{2a}$$

so

$$D(E) = \frac{2}{\hbar} \frac{BT \int dx \sqrt{E - U(x)}}{\int dx \sqrt{E - U(x)}}$$

Now,

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

- $\int dx \sqrt{E - U} = \oint dx p(x) = I(E)$
 numerator: action
 $p(x) = [2m(E - U(x))]^{1/2}$

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

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

so, have energy difference

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

$$\Leftrightarrow \frac{\partial g}{\partial t} = \partial T D(E) \rho_0(E) \frac{\partial}{\partial E} \frac{g(E,t)}{\rho_0(E)} \quad 10.$$

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

Recall, for large friction, spatial

Schmoluchowski $E \propto \lambda$

$$\frac{\partial F}{\partial t} = D \frac{\partial}{\partial x} e^{-u/T} \frac{\partial}{\partial x} (e^{u/T} F)$$

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:

$$D^T \tau = -1$$

So

adjoint of F-N operator.

so

$$\frac{\partial F}{\partial t} = D \frac{\partial}{\partial x} e^{-u/t} \frac{\partial}{\partial x} (e^{u/t} f)$$

then

$$D e^{u/t} \frac{\partial}{\partial x} e^{-u/t} \frac{\partial}{\partial x} \tau = -1$$

Can argue analogously:

$$\tau(E) = \int_E^{E_b} dE' \frac{1}{D(E') g_L(E')} \int_0^{E'} dE'' J_{e_L}(E'')$$

plugging in $D(E')$, $J_{e_L}(E')$

$$\Gamma(E) = \frac{2m}{\beta T} \int_E^{E_0} dE' \frac{e^{-E'/T}}{I(E')} \int_0^E dE'' \Omega(E'') e^{-E''/T}$$

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

$$\Rightarrow \Gamma = \frac{2\pi m T}{\beta} \frac{1}{\omega_0 I(E_0)} e^{E_0/T}$$

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

