Fission75-Summer School-VECC-Kolkata-May2014

## Stochastic dynamical model of fission

Santanu Pal
Formerly with VECC, Kolkata

Fission75-Summer School-VECC-Kolkata-May2014

## Stochastic dynamical model of fission

We discuss only stochastic model, not the "Dynamical cluster decay model" of Greiner,Gupta (Int.J.Mod.Phys.E3,supp01(1994)3350)

How does a nucleus undergo fission, EX> fission barrier

For EX< fission barrier, q.m. tunneling, not discussed here

Statistical model of Bohr and Wheeler
(N. Bohr and J.A. Wheeler, 1939) Phys.Rev.56(1939)426

Statistical $\rightarrow$ Full phase space equally accessible for an equilibrated system

Fission probability will depend upon the phase space available at the saddle point ( the transition point)


Deformation $\longrightarrow$
$\rho\left(\mathrm{E}^{*}\right)=$ density of states at ground state
No. of states between $E^{*}$ and $E^{*}+\delta E^{*}=\rho\left(E^{*}\right) \delta E^{*}$
Choose an ensemble such that there is only one nucleus in each state

No. of nucleus in ground state $=\rho\left(\mathrm{E}^{*}\right) \delta \mathrm{E}^{*}$
Collective kinetic energy= $\varepsilon$; collective speed=v; $\mathrm{d} \varepsilon=\mathrm{vdp}$
No. of collective states with momentum between $p$ and $\mathrm{p}+\mathrm{dp}$ and over one unit of length along fission direction $=1 \times \mathrm{dp} / \mathrm{h}=\mathrm{dp} / \mathrm{h}$

Excitation energy at saddle $=\mathrm{E}^{*}-\mathrm{V}_{\mathrm{B}}-\varepsilon$
No. of nuclei at saddle over a distance $v$
$=v \times \operatorname{dp} \times \rho^{*}\left(\mathrm{E}^{*}-\mathrm{V}_{\mathrm{B}}-\varepsilon\right) \delta \mathrm{E}^{*} / h$

Number of nuclei at saddle over a distance $v$
$=v d p \rho^{*}\left(E^{*}-V_{B}-\varepsilon\right) \delta E^{*} / h$
Total number crossing the saddle per unit time
$=\delta \mathrm{E}^{*} \int_{\mathrm{vdp}} \rho^{*}\left(\mathrm{E}^{*}-\mathrm{V}_{\mathrm{B}}-\varepsilon\right) / h$
$=\delta \mathrm{E}^{*} \int \mathrm{~d} \varepsilon \rho^{*}\left(\mathrm{E}^{*}-\mathrm{V}_{\mathrm{B}}-\varepsilon\right) / h$
Fission probability/time=r

$$
\begin{aligned}
& =\left[\delta \mathrm{E}^{*} \int \mathrm{~d} \varepsilon \rho^{*}\left(\mathrm{E}^{*}-\mathrm{V}_{\mathrm{B}}-\varepsilon\right) / h\right] / \rho\left(\mathrm{E}^{*}\right) \delta \mathrm{E}^{*} \\
& =\left[\int \mathrm{d} \varepsilon \rho^{*}\left(\mathrm{E}^{*}-\mathrm{V}_{\mathrm{B}}-\varepsilon\right)\right] / h \rho\left(\mathrm{E}^{*}\right)
\end{aligned}
$$

From radioactive decay law, fission life-time $\tau=1 / r$

Fission width $\quad \Gamma_{\mathrm{Bw}}=\hbar / \tau=\hbar \mathrm{r}$

$$
=\left(1 / 2 \pi \rho\left(\mathrm{E}^{*}\right)\right) \int \mathrm{d} \varepsilon \rho^{*}\left(\mathrm{E}^{*}-\mathrm{V}_{\mathrm{B}}-\varepsilon\right)
$$

$$
\Gamma_{B W}=\frac{1}{2 \pi \rho\left(E^{*}\right)} \int_{0}^{E^{*}-V_{B}} \rho^{*}\left(E^{*}-V_{B}-\varepsilon\right) d \varepsilon
$$

Approximate form: (Assume little "a" and "l" shape independent)

Level density (Fermi gas): combinatorial, BohrMottelson, Nuclear Structure, Vol.I

$$
\begin{aligned}
& \rho\left(E^{*}, l\right)=\frac{2 l+1}{24}\left(\frac{\hbar^{2}}{2 I}\right)^{\frac{3}{2}} \frac{\sqrt{a}}{E^{* 2}} e^{2 \sqrt{a E^{*}}} \approx \frac{e^{2 \sqrt{a E^{*}}}}{E^{*^{2}}} \\
& \Gamma_{B W}=\frac{1}{2 \pi} \int_{0}^{E^{*}-V_{B}} \frac{E^{*^{2}}}{\left(E^{*}-V_{B}-\varepsilon\right)^{2}} e^{2 \sqrt{a\left(E^{*}-V_{B}-\varepsilon\right)-2 \sqrt{a E^{*}}} d \varepsilon}
\end{aligned}
$$

For $\mathrm{E}^{*} \gg \mathrm{~V}_{\mathrm{B}}$
$\frac{E^{*}}{E^{*}-V_{B}-\varepsilon} \approx 1$ Note: when $\varepsilon=\mathrm{E}^{*}-\mathrm{V}_{\mathrm{B}}$, integrand very small
$\Gamma_{B W} \approx \frac{1}{2 \pi} \int_{0}^{E^{*}-V_{B}} e^{2 \sqrt{a\left(E^{*}-V_{B}-\varepsilon\right)}-2 \sqrt{E^{*}}} d \varepsilon$
$\sqrt{a\left(E^{*}-V_{B}-\varepsilon\right)}=\sqrt{a E^{*}}-\frac{V_{B}+\varepsilon}{2} \sqrt{\frac{a}{E^{*}}}=\sqrt{a E^{*}}-\frac{V_{B}+\varepsilon}{2 T}$
$\Gamma_{B W}=\frac{T}{2 \pi} e^{-\frac{V_{B}}{T}}$


Sadhukhan,Pal:PRC79,064606(2009)

## Strutinsky's correction (Phys.Lett.47B(1973)121)

We have missed out something

We have included collective phase space at saddle But we have not accounted for the collective phase space at ground state

Assume an oscillator potential near ground state $=m \omega^{2} x^{2} / 2$
Distribution function (Boltzman) $=\exp \left[-\left(p^{2} / 2 m+m \omega^{2} x^{2} / 2\right) / T\right]$

$$
\begin{aligned}
& \Delta x=\sqrt{ }\left(2 \pi T / m \omega^{2}\right) \\
& \Delta p=\sqrt{ }(2 \pi m T)
\end{aligned}
$$

Collective phase space factor at g.s. $=\Delta \mathrm{x} \Delta \mathrm{p} / \mathrm{h}=\mathrm{T} / \hbar \omega$ (to be multiplied with $\rho\left(\mathrm{E}^{*}\right)$ in denominator)

Aproximate Gaussian by rectangle in obtaining $\Delta x, \Delta p$
$=\frac{\hbar_{\omega}}{2 \pi} e^{-V_{E} / T}$
Strutinsky corrected

Crucial assumption in BW $\rightarrow$ equilibrium everywhere True if flux across fission barrier is very small

Fission width is very small $\rightarrow \mathrm{V}_{\mathrm{B}} \gg \mathrm{T}$


If not (e.g. heavy ion reactions), not enough nuclei near barrier after initial crossing

To maintain steady flux at saddle, fission dynamics to be considered

## Dynamical model



Expt. $\rightarrow$ V. Singh et al. Phys. Rev.C86(2012)014609 Line $\rightarrow$ Stat. model with Bohr-Wheeler width

Bohr-Wheeler over predicts fission rate
Fission is slower than predicted by Bohr-Wheeler theory

Collective dynamics of interacting particles-> dissipative

When fission is slower, more time for particle evaporation

Fission $\Rightarrow$ shape evolution $\Rightarrow$ shape variables $\Rightarrow$ dynamical coordinates

Elongation (c)
Neck (h)
Asymmetry ( $\alpha$ )
Brack (funny hill)


Nucleus $\Rightarrow$ 3A coordinates
->a few shape (collective) variables(x)

+ many intrinsic (almost 3 A ) coordinates ( $\xi$ )
Consider effect of $\mathrm{V}_{\text {int }}$ on $\mathrm{H}_{\text {intr }}$ as a first-order perturbation and take average over all intrinsic states (Linear Response Theory)
$\mathrm{d}\left\langle\mathrm{H}_{\text {intr }}\right\rangle / \mathrm{dt} \propto(\mathrm{dX} / \mathrm{dt})^{2} \Rightarrow$ energy is pumped into intrinsic system (heating)
energy is lost from collective motion $\mathrm{H}_{\text {coll }}$ (dissipative energy loss)

Eqn. of motion of collective coordinates averaged over intrinsic states
$d\langle P\rangle / d t=-(d U / d X)-\eta(d\langle X\rangle / d t)$
Gives average trajectory in deformation (collective coordinate) space

- H.Hofmann \& P.J.Siemens, Nucl. Phys. A 257 (1976)165
- S.E. Koonin \& J.Randrup, Nucl. Phys. A 289 (1977) 475

Stochastic dynamics:
$>$ Consider an ensemble of fissioning compound nuclei.
$>$ Shape evolution not same for all CN (Had it been same, all CN would have reached the saddle point simultaneously and we would not have the law of radioactive decay, but same life-time for all CN).
$>$ Some reach saddle point earlier, some later.
$>$ For a given time interval, average trajectory may or may not cross saddle. In reality, some trajectories cross saddle, some do not, the ratio gives the fission probability
$>$ Average trajectory not of much use in fission dynamics. We need to trace individual trajectories.

We need observables averaged over many trajectories and not observables for the average trajectory
$>$ We need eqn. of motion of individual trajectories

$$
H_{\text {tot }}=H_{\text {coll }}(x)+H_{\text {intr }}(\xi)+V_{\text {int }}(x, \xi)
$$

The force on the collective dynamics due to $\mathrm{V}_{\text {int }}(\mathrm{X}, \xi)$ is random in nature essentially due to the large number of intrinsic degrees of freedom ( $\xi$ )

Force $=\langle$ Force $\rangle+$ fluctuation (R)

$$
d P / d t=-(d U / d X)-\eta(d X / d t)+R(t)
$$

## Langevin equation of motion

Fission->Brownian motion of a heavy particle in a viscous heat bath

Collective dynamics (large inertia) ->Brownian particle
$\langle R(t)\rangle=0$
$\left\langle R(t) R\left(t^{\prime}\right)\right\rangle=2 D \delta\left(t-t^{\prime}\right)$
$R(t)$ is assumed to follow a Gaussian distribution
Fluctuation-dissipation theorem: $D=\eta T$
Markovian Process (zero memory time) assumed

## How to solve a stochastic eqn. of motion?

Start with uniform random no. generator $(0,1)$
$p(x) d x=d x$ for $0<x<1,=0$ otherwise
$y(x)$-> prescribed function of $x$
$f(y)=$ ? (prob. of $y$ )
$f(y) d y=p(x) d x->$ area under the curve for each transformed element must remain same (illustrate)

$$
\begin{aligned}
& f(y)=p(x) \frac{d x}{d y} ; p(x)=1: f(y)=\frac{d x}{d y} ; d x=f(y) d y \\
& x=\int_{-\infty}^{y} f(y) d y=F(y)
\end{aligned}
$$

Make a table of $(y, F(y)) ; F(y)$ numerically obtained

Take a uniform random number $x$, read from the table the corresponding $y$ through interpolation
$\{x 1, x 2, x 3, \ldots . . .\}-.>\{y 1, y 2, y 3, \ldots . . .$.$\} , the y$-sequence wil follow $f(y)$ (Illustrate with Gaussian)

Now back to Langevin equation:

$$
d P / d t=-(d U / d X)-\eta(d X / d t)+R(t)
$$

and $\quad d X / d t=P / m$
$\Rightarrow \quad d P / d t=-(d U / d X)-\beta P+g G(t)$ where $\beta=\eta / m$ and $g G(t)=R(t)$
or $\quad d P / d t=H(P(t), X(t))+g G(t)$ and $\langle G(t) G(t)\rangle=2 \delta\left(t-t^{\prime}\right)$ and $g=\sqrt{ }(\eta T)$

## Discretizing

$$
P(t+\tau)-P(t)=\int_{t}^{t+\tau} d t^{\prime} H(t)+g \int_{t}^{t+\tau} d t^{\prime} G(t) \cong
$$

$\tau H(t)+g G_{1}(t)$

$$
X(t+\tau)-X(t) \cong \tau P(t) / m
$$

Here $G_{1}(t)=\int_{t}^{t+\tau} d t^{\prime} G\left(t^{\prime}\right)$ is also a Gaussiandistributed random number

How? $\left\langle G_{1}(t)\right\rangle=\int_{t}^{t+\tau} d t^{\prime}\langle G(t)\rangle=0$ and

$$
\left\langle G^{2}{ }_{1}(t)\right\rangle=\int_{t}^{1+\tau} d t_{1} \int_{t}^{t+\tau} d t_{2}\left\langle G\left(t_{1}\right) G\left(t_{2}\right)\right\rangle=2 \tau
$$

generate Gaussian numbers $\omega$ with $\left\langle\omega^{2}\right\rangle=2$ and use $G_{1}(t)=\sqrt{ } \tau \omega(t)$.

Perform integration choosing the random force at each step from sampling a Gaussian distribution.

Since random numbers are used at each time step, each Langevin trajectory will be different though started with same initial condition $\left(X_{0}, P_{0}\right)$.

After each time step, check if $X>X_{\text {sci }}$ (scission point) or not.

## If YES,

count the event as a fission event, record the instant, $n_{C N}=n_{C N}-1$.

## If NO,

continue the process ( till some very large time $t_{\max }$ ).
Repeat the procedure for a large number of events
Show typical plot along with potential profile


## At the end of a run

we have a distribution of life-time of fission events
$n_{C N}(t-\Delta t / 2)=$ No. of $C N$ at time $(t-\Delta t / 2)$
$n_{C N}(t+\Delta t / 2)=$ No. of CN at time $(t+\Delta t / 2)$
Assuming law of radioactive decay, decay rate at time ' $t$ ',

$$
\lambda(t)=\frac{\ln \left\{n_{C N}(t-\Delta t / 2) / n_{C N}(t+\Delta t / 2)\right\}}{\Delta t}
$$


1.Y. Abe et al., Phys. Rep. 275 (1996) 49
2. P. Frobrich \& I.I.Gontchar, Phys. Rep. 292 (1998)131 Input for solving Langevin equation:

- Collective potential U $\Rightarrow$ LDM
- Collective inertia $m \Rightarrow$ hydro-dynamical model assuming no vortex
- Dissipation coefficient $\eta \Rightarrow$ nuclear bulk property, one-body dissipation (sometimes treated as a parameter)


## Potential (Finite Range Liquid Drop Model

 potential)AJ Sierk, PRC33(1986)2039double folding of Yukawa+exponential
$U\left(X(\right.$ shape - parameter $)=\iint d^{3} r_{1} d^{3} r_{2} \rho\left(r_{1}\right) \rho\left(r_{2}\right) v_{\text {eff }}\left(r_{1}-r_{2}\right)$
Illustrate with figure
Parameters of $\mathrm{v}_{\text {eff }}$ fixed by fitting fission barriers of heavy nuclei

Add Coulomb + rotational


Discuss only the lower plot

## Collective inertia

Nucleus $\rightarrow$ incompressible and irrotational (no vortex) fluid (Davies , Sierk \& Nix, PRC13(1976)2385)

$$
\begin{aligned}
& T=\frac{1}{2} \sigma_{m} \int \nu^{2} d^{3}{ }_{m} \\
& \vec{\partial}=\sum\left(\theta \overrightarrow{\omega^{2}} / \theta q_{\theta}\right) q_{x}
\end{aligned}
$$

$q_{i}$ collective (shape) coordinate

$$
T=\frac{1}{2} \sum \pi_{0}\left(\frac{1}{q}\right) \dot{q}_{2}
$$

$\mathrm{m}_{\mathrm{ij}}$-> analytically obtained

## One-body dissipation

## Wall formula

Particle hits moving wall (Brownian particle)
Receives kick from wall
Wall motion slows down
Dissipation in wall motion results

$$
\begin{aligned}
& -\dot{E}^{w a d l}=\rho_{m} \bar{v} \oint \dot{n}^{2} d s, \\
& -\dot{E}_{d i s}=\sum_{i, j} \eta_{i j}(\vec{q}) \dot{q}_{i} \dot{q}_{j},
\end{aligned}
$$

Analytical form of $\eta$ obtained
J. Blocki et al., Ann. Phys. 113 (1978) 330
J.Randrup \& W.J. Swiatecki, Ann. Phys. 125 (1980)193

Window dissipation
Transfer of particles $\rightarrow$ transfer of momentum Irreversible

Net effect $\rightarrow$ dissipation
Effective only when a window is open (neck is formed)


Classical expression $\rightarrow$

$$
-\dot{E}^{w \dot{n} d o w}=\frac{1}{2} \rho_{m} \bar{v} \Delta \omega v^{2}
$$

$U \rightarrow$ relative speed between left and right pieces

$$
\begin{aligned}
& u=\dot{R}=\sum\left(\partial R / \partial q_{i}\right) \dot{q}_{i} \\
& \eta_{\Rightarrow}^{w n d o w}(\vec{q})=\frac{1}{2} \rho_{m} \bar{v} \Delta \sigma \frac{\partial R}{\partial q_{i}} \frac{\partial R}{\partial q_{i}}
\end{aligned}
$$

Blocki et al. Ann.of Phys.113,330(1978)
Inertia, dissipation co-efficient depend on nuclear shape


Sadhukhan \& Pal:Phys.Rev.C82, 021601(R)(2010)
How to couple particle emission in a Langevin dynamical calculation?

During each time-step of Langevin integration, consider emission of particles also

Algorithm for compound nuclear (CN) decay
Fission-> Langevin dynamics; evaporation->statistical


## Start with a $\mathrm{CN}\left(\mathrm{E}_{\mathrm{x}}, \mathrm{I}\right)$

Solve Langevin eqn. for time step $\Delta \mathrm{t}$ If fission occurs, stop (count as a fission event)

If not, do a Monte-Carlo sampling to decide if the CN has decayed in $\Delta t$

If YES, decide decay type ( $n, p, \alpha, \gamma$ ) by another MonteCarlo

Re-adjust ( $A, E_{X}, I$ ) of residual nucleus and continue Otherwise $\rightarrow$ go to the next time step and continue How to Monte-Carlo a decay probability?

We shall assume the radioactive law of CN decay
i.e. Probability of a CN to decay in $\Delta \mathrm{t} \propto \Delta \mathrm{t}$

$$
=r \Delta t=(\Gamma / \hbar) \Delta t
$$

Here, $\Gamma$ is the total width of a CN decay given as

$$
\Gamma=\Gamma_{\mathrm{n}}+\Gamma_{\mathrm{p}}+\Gamma_{\alpha}+\Gamma_{\gamma} \text { etc. }
$$

Underlying assumption: all the processes are independent

Particle/gamma decay widths (Feshbach formula)
(Puhlhofer;NPA280,278(1977))
All the decay widths depend upon excitation energy and spin of the CN

$$
\Gamma_{i}=\Gamma_{i}\left(E_{x}, I\right)
$$

Probability of a CN to decay in $\Delta \mathrm{t}=\mathrm{p}=(\Gamma / \hbar) \Delta \mathrm{t}<1$ and constant

So we do a uniform sampling
We call a subroutine which generates uniformly distributed random numbers in the range 0 to 1 , output $\rightarrow$ r

If $r \leq p \rightarrow C N$ has decayed in $\Delta t$
If $r>p \rightarrow C N$ has survived $\Delta t$
If it decays, the type of decay (i.e. $f$ or $n$ or $p$ or $\alpha$ or $\gamma$ ) can also be decided by uniform sampling of partial widths $\left(\Gamma_{i} / \Gamma\right)$


initial total excitation energy ( MeV )
Frobrich,Gontchar;NPA563(1993)326


Karpov et al.,J.Phys.G.Nucl.Phys.29,2365(2003)
$\square \longrightarrow$ experimental data
Other symbols $\rightarrow$ different ' $a$ '

## 3-D results

Karpov et al. PRC63,054610(2001)


FIG. 8. The theoretical (a) and experimental (b) mass distributions of fission fragments of ${ }^{260} \mathrm{Rf}, E^{*}=74.2 \mathrm{MeV}$. The theoretical histogram was calculated with the reduction coefficient $k_{s}=0.1$. The experimental distribution was taken from Ref. [57].


FIG. 6. The theoretical (a) and experimental (b) MED of fission fragments of ${ }^{260} \mathrm{Rf}$ at the total excitation energy $E^{*}=74.2 \mathrm{MeV}$. The numbers at the contour lines in percents indicate the yield, which is normalized to $200 \%$. The theoretical diagram was calculated with the reduction coefficient $k_{s}=0.1$. The experimental diagram was taken from Ref. [57].


Frobrich et al.(1993)


Karpov et al.(2001)
Wall formula too strong to reproduce experimental
data:
A reduction factor seems necessary
Why a reduction factor?
$\eta_{C W W F}=\mu \eta_{W F}$
Magnitude of $\eta$ is an open problem
Often used as a fit parameter

Alternative approach to stochastic dynamics $\Rightarrow$
Fokker-Planck equation
$\square$ Consider the total ensemble of Langevin trajectories

The evolution of the ensemble with time can be viewed as a diffusion process

In stead of individual trajectories, we can discuss in terms of a probability distribution function $\rho(X, P, t)$
$\rho(\mathrm{X}, \mathrm{P}, \mathrm{t}) \mathrm{dXdP} \Rightarrow$ probability of finding a CN with collective coordinate and momentum in the range $X \rightarrow X+d X$ and $P \rightarrow P+d P$ at time ' $t$ '.

Fokker-Planck equation from Langevin equation
Liouville's theorem:
$\frac{d \rho}{d t}=\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial X} \dot{X} \rho+\frac{\partial}{\partial P} \dot{P} \rho=0$
density conservation
$\frac{d P}{d t}=-\frac{d U}{d X}-\eta \frac{d X}{d t}+R(t)$
$\frac{d X}{d t}=\frac{P}{m} \quad$ Langevin eq.

$$
\begin{gathered}
\frac{\partial \rho}{\partial t}=-\left(\frac{\partial}{\partial X} \dot{X}+\frac{\partial}{\partial P} \dot{P}\right) \rho(X, P, t) \\
=\Omega(X, P, t) \rho(X, P, t) \\
\Omega(X, P, t)=\frac{\partial}{\partial P}\left(\frac{d U}{d X}+\frac{\eta}{m} P-R(t)\right)-\frac{\partial}{\partial X}\left(\frac{P}{m}\right) \\
\rho(X, P, t+\Delta t)=\rho(X, P, t)+\int_{t}^{t+\Delta t} \Omega\left(X, P, t_{1}\right) \rho\left(X, P, t_{1}\right) d t_{1} \\
=\rho(X, P, t)+\int_{t}^{t+\Delta t} d t_{1} \Omega\left(X, P, t_{1}\right)\left[\rho(X, P, t)+\int_{t}^{t_{1}} \Omega\left(X, P, t_{2}\right) \rho\left(X, P, t_{2}\right) d t_{2}\right] \\
=\left[1+\int_{t}^{t+\Delta t} d t_{1} \Omega\left(X, P, t_{1}\right)+\int_{t}^{t+\Delta t} d t_{1} \Omega\left(X, P, t_{1}\right) \int_{t}^{t_{1}} d t_{2} \Omega\left(X, P, t_{2}\right)+\ldots .\right] \rho(X, P, t)
\end{gathered}
$$

## $\Delta t \gg$ time-scale of $R(t)$

$$
\begin{aligned}
& \langle R(t)\rangle=0 \\
& \left\langle R(t) R\left(t^{\prime}\right)\right\rangle=I_{R} \delta\left(t-t^{\prime}\right) \\
& I_{R}=2 \eta T
\end{aligned}
$$

$$
\begin{aligned}
& \int_{t}^{t+\Delta t} d t_{1} \Omega\left(X, P, t_{1}\right)=\Delta t\langle\Omega(X, P, t)\rangle=\Delta t\left(\frac{\partial}{\partial P}\left(\frac{d U}{d X}+\frac{\eta}{m} P-R(t)\right)-\frac{\partial}{\partial X}\left(\frac{P}{m}\right)\right\rangle \\
& \left.\int^{\partial P}\left(\frac{d U}{d X}+\frac{\eta}{m} P\right)-\frac{\partial}{\partial X}\left(\frac{P}{m}\right)\right]
\end{aligned}
$$

## Remembering time-average->ensemble average

$$
\int_{t}^{t+\Lambda t} \int_{t}^{t_{1}} d t_{1} d t_{2} \Omega\left(t_{1}\right) \Omega\left(t_{2}\right)=\frac{1}{2} \int_{t}^{t+\Delta t} \int_{t}^{t+\Delta t} d t_{1} d t_{2} \Omega\left(t_{1}\right) \Omega\left(t_{2}\right)
$$


Let

$$
F=\frac{\partial}{\partial P}\left(\frac{d U}{d X}+\frac{\eta}{m} P\right)-\frac{\partial}{\partial X}\left(\frac{P}{m}\right)
$$

int egral $=\iint\left\{F-R\left(t_{1}\right) \frac{\partial}{\partial P}\right\}\left\{F-R\left(t_{2}\right) \frac{\partial}{\partial P}\right\} d t_{1} d t_{2}$
$=F^{2}(\Delta t)^{2}+\frac{\partial^{2}}{\partial P^{2}} \iint R\left(t_{1}\right) R\left(t_{2}\right) d t_{1} d t_{2}$
$=F^{2}(\Delta t)^{2}+I_{R} \Delta t \frac{\partial^{2}}{\partial P^{2}}$
Substituting,

$$
\begin{aligned}
& \rho(t+\Delta t)=\left[1+F \Delta t+\frac{1}{2} F^{2}(\Delta t)^{2}+\frac{1}{2} I_{R} \Delta t \frac{\partial^{2}}{\partial P^{2}}+\ldots .\right] \rho(t) \\
& \frac{\rho(t+\Delta t)-\rho(t)}{\Delta t}=F \rho(t)+\frac{1}{2} I_{R} \frac{\partial^{2}}{\partial P^{2}} \rho(t)+\frac{1}{2} \Delta t F^{2} \rho(t)+\ldots . . \\
& \Delta t \rightarrow 0 \\
& \frac{\partial}{\partial t} \rho(X, P, t)=\left\{-\frac{\partial}{\partial X} \frac{P}{m}+\frac{\partial}{\partial P} \frac{d U}{d X}+\frac{\partial}{\partial P}\left(\beta P+m \beta T \frac{\partial}{\partial P}\right)\right\} \rho(X, P, t) \\
& \beta=\frac{\eta}{m}
\end{aligned}
$$

Fokker-Planck eqn.,
Kramers,Physica(Amsterdam)7,284(1940)
Generalized Liouville's eqn. to include dissipation
Diffusion eqn. in phase space
Kramers' analytical solution of Fokker-Planck equation:
Fokker-Planck equation in one-dimension
$\frac{\partial \rho}{\partial t}+\frac{P}{m} \frac{\partial \rho}{\partial X}-\frac{d U}{d X} \frac{\partial \rho}{\partial P}=\beta \frac{\partial(P \rho)}{\partial P}+m \beta T \frac{\partial^{2} \rho}{\partial P^{2}}$
$U=\frac{1}{2} m \omega_{g}^{2}\left(X-X_{g}\right)^{2}$
$=V_{B}-\frac{1}{2} m \omega_{s}^{2}\left(X-X_{s}\right)^{2}$


- Ensemble of large number of CN at A
- Weak diffusion current at $\mathrm{C}\left(\mathrm{V}_{\mathrm{B}}>\mathrm{T}\right) \rightarrow$ density at A does not change
- Steady state $\rightarrow \partial \rho / \partial t=0$

Steady state F-P eqn.
$\frac{P}{m} \frac{\partial \rho}{\partial X}-\frac{d U}{d X} \frac{\partial \rho}{\partial P}=\beta \frac{\partial(P \rho)}{\partial P}+m \beta T \frac{\partial^{2} \rho}{\partial P^{2}}$
Desired solution $\rightarrow$
At $\mathrm{A} \rightarrow$ Boltzmann
$\rho=K \exp \left[-\frac{\frac{P^{2}}{2 m}+U}{T}\right]$
$\rho=K \exp \left[-\frac{\frac{P^{2}}{2 m}+\frac{1}{2} m \omega_{g}^{2}\left(X-X_{g}\right)^{2}}{T}\right]$
At $\mathrm{C} \rightarrow$ With modification
At B $\rightarrow$ Zero

## General solution

$\rho=K F(X, P) \exp \left[-\frac{\frac{P^{2}}{2 m}+U}{T}\right]$
$\rho=K F(X, P) e^{-V_{s} / T} \exp \left[-\frac{\frac{P^{2}}{2 m}-\frac{1}{2} m \omega_{s}^{2}\left(X-X_{s}\right)^{2}}{T}\right]$
$F(X, P) \approx 1$ at $X=X g$
$\approx 0$ at $X \gg X_{s}$
Aim is to find $F$
Re-define $X=X-X_{s}$
$m \beta T \frac{\partial^{2} F}{\partial P^{2}}=\frac{P}{m} \frac{\partial F}{\partial X}+\frac{\partial F}{\partial P}\left(m \omega_{s}^{2} X+\beta P\right)$

Solution exists if we assume $\varsigma=P-a X$ (Zeta)
$F(X, P)=F(\varsigma)$
$m \beta T \frac{d^{2} F}{d \varsigma^{2}}=-\left(\frac{a}{m}-\beta\right)\left(P-\frac{m \omega_{s}^{2}}{\frac{a}{m}-\beta} X\right) \frac{d F}{d \varsigma}$
We must have $a=\frac{m \omega_{s}^{2}}{\frac{a}{m}-\beta}$
$m \beta T \frac{d^{2} F}{d \varsigma^{2}}=-\left(\frac{a}{m}-\beta\right) \varsigma \frac{d F}{d \varsigma}$

Solution:
$F(\zeta)=0$ for $\zeta \rightarrow-\infty$ implying a=+ve when $X \rightarrow \infty$ at far right of saddle
$F(\zeta)=1$ for $\zeta \rightarrow+\infty$ implying a=+ve when $X \rightarrow-\infty$ at far left of saddle (May not hold at large spin)
' $a$ ' should be positive

$$
\text { Defining eqn. } \rightarrow a=\frac{m \omega_{s}^{2}}{\frac{a}{m}-\beta}
$$

Taking +root
$a=\frac{m \beta}{2}+\sqrt{\omega_{s}^{2} m^{2}+\frac{m^{2} \beta^{2}}{4}}$
Full solution: $\rho=K F(X, P) e^{-V_{s} / T} \exp \left[-\frac{\frac{P^{2}}{2 m}-\frac{1}{2} m \omega_{s}^{2}\left(X-X_{s}\right)^{2}}{T}\right]$

With $F(\varsigma)=\sqrt{\frac{1}{2 \pi m \beta T}\left(\frac{a}{m}-\beta\right)} \int_{-\infty}^{\varsigma} e^{-\frac{1}{2 m \beta T}\left(\frac{a}{m}-\beta\right) \varsigma^{2}} d \varsigma$
Our task is to calculate the fission rate
Current across C

$$
j=\int_{-\infty}^{+\infty} \rho\left(X=X_{s}, P\right) \frac{P}{m} d P
$$

$$
=K T e^{-\frac{V_{B}}{T}} \sqrt{\frac{a / m-\beta}{a / m}}
$$

$$
=K T e^{-\frac{V_{B}}{T}}\left\{\sqrt{1+\left(\frac{\beta}{2 \omega_{s}}\right)^{2}}-\frac{\beta}{2 \omega_{s}}\right\}
$$

## integrating by parts

No. of particles in pocket at ' $A$ ' =

$$
\begin{aligned}
& n_{g}=\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \rho(\text { near }-A) d P d X=\frac{2 \pi K T}{\omega_{g}} \\
& \Gamma_{K}=\hbar \frac{j}{n_{g}}=\frac{\hbar \omega_{g}}{2 \pi} e^{-\frac{V_{B}}{T}}\left\{\sqrt{1+\left(\frac{\beta}{2 \omega_{s}}\right)^{2}}-\frac{\beta}{2 \omega_{s}}\right\}
\end{aligned}
$$

