Methods of statistical physics in description of nuclear reactions at low energies

1. Langevin equations
2. Fokker-Planck equations
3. Master-equations

Characteristics of binary reactions under consideration

- total dissipation of kinetic energy in the entrance channel

- wide mass (charge) distributions of the reaction products in the exit channel

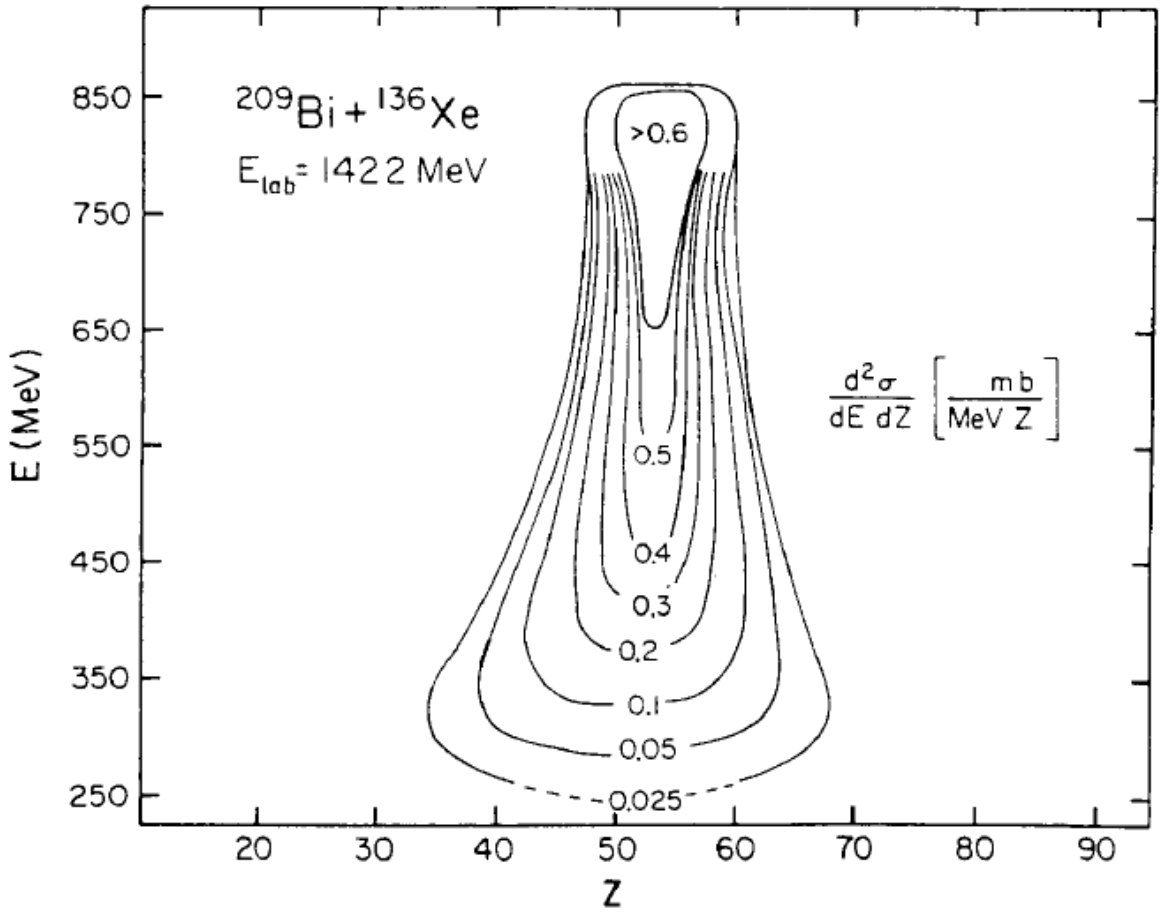
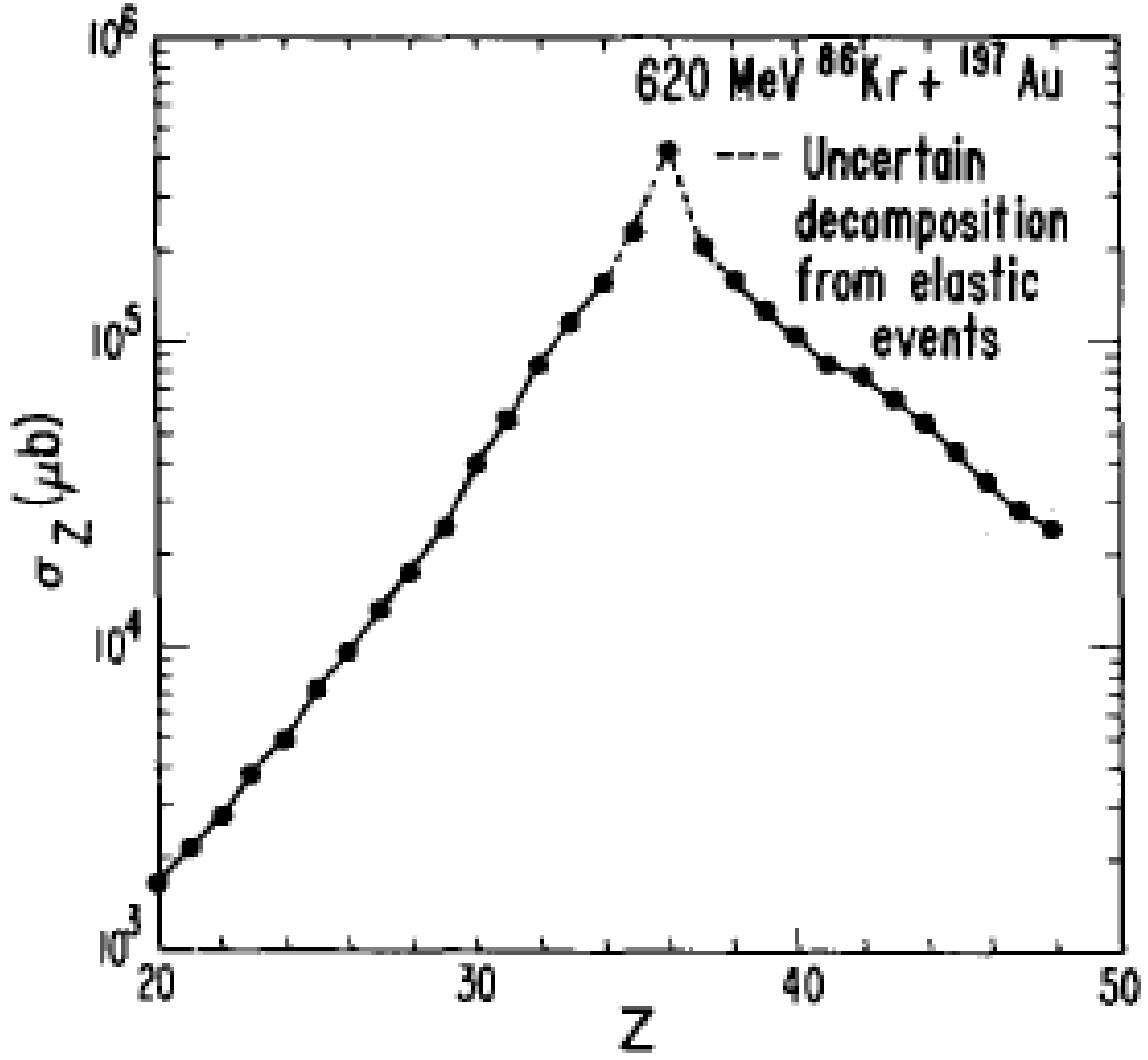
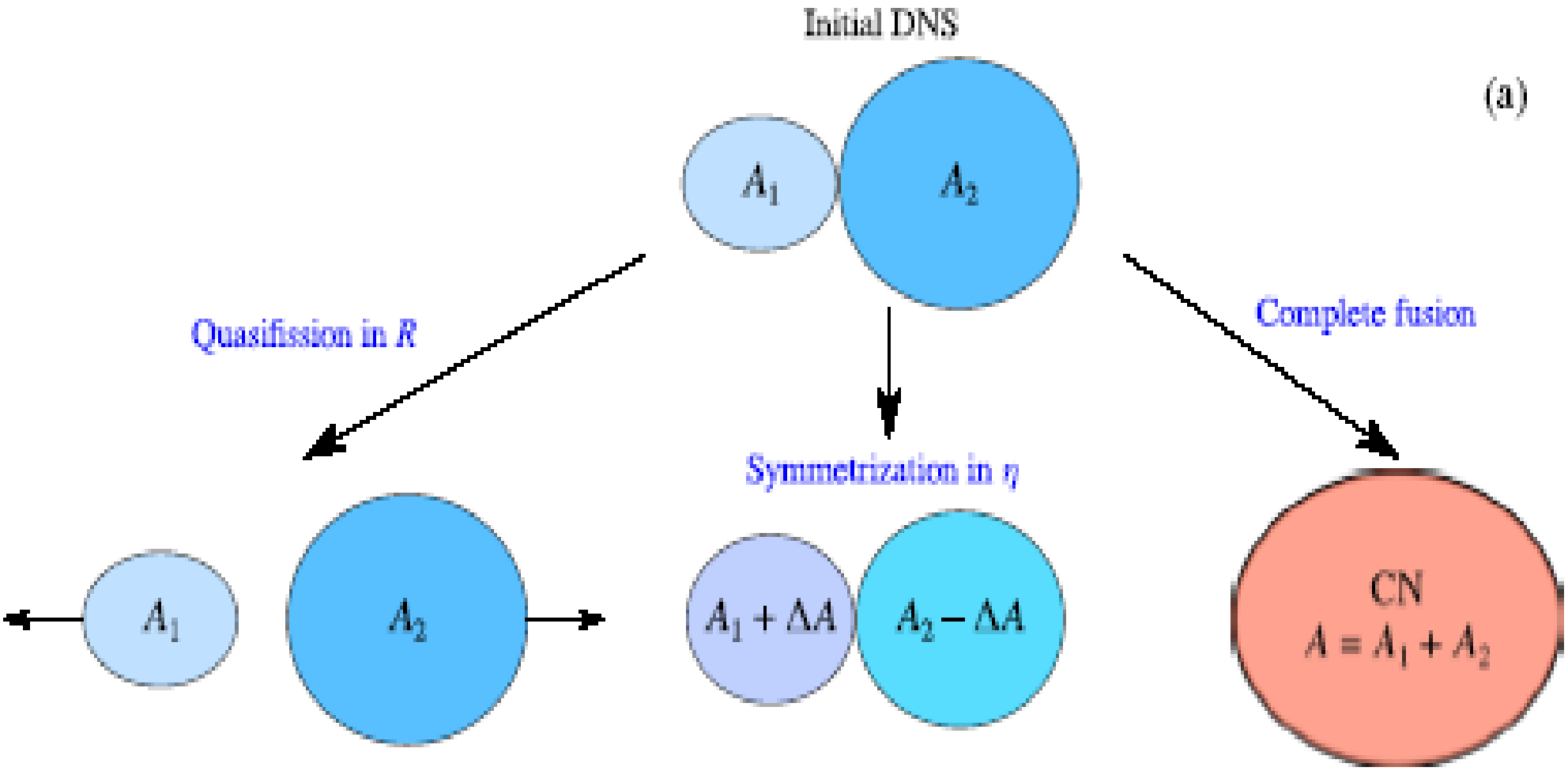


Figure 11.3 The experimental double differential cross section $d^2\sigma/dEdZ$ as a function of the final centre-of-mass energy E and charge Z of the emitted projectile-like fragments for the system ^{136}Xe + ^{209}Bi at E_{lab}(Xe) = 1422 MeV.


620 MeV ^{86}Kr + ^{197}Au
--- Uncertain decomposition from elastic events
σ_Z (μb)
10^6
10^5
10^4
10^3
20
30
40
50
Z

Relevant collective coordinates

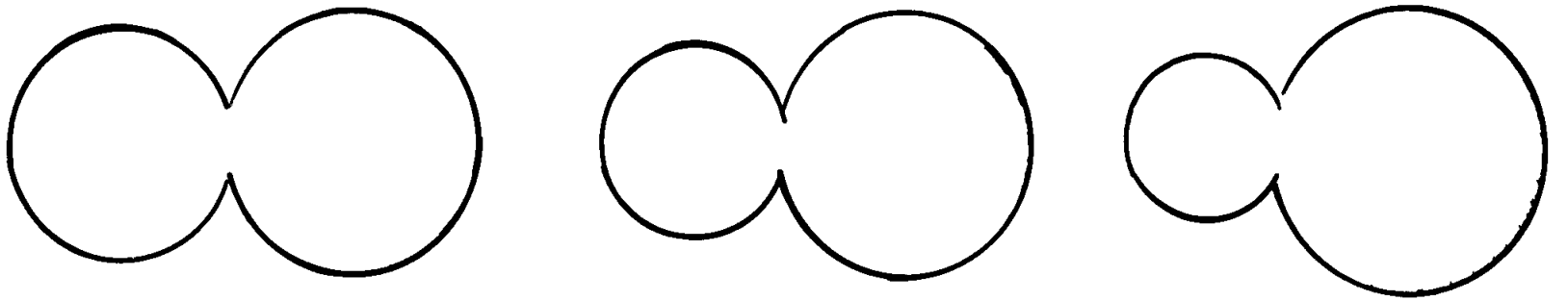


Two main collective coordinates are used for the description of the nuclear reactions:

1. Relative internuclear distance R

2. Mass (charge) asymmetry coordinate η for transfer of nucleons between interacting nuclei

$$\eta=(A_1-A_2)/(A_1+A_2)$$



$\eta \rightarrow 1$

Relative motion of nuclei, capture of target and projectile into dinuclear system,
decay of the dinuclear system: quasifission, deep-inelastic collisions (DIC)

Transfer of nucleons between nuclei, change of mass and charge asymmetries leading to fusion and quasifission (multinucleon transfer), DIC

Langevin description

Two colliding nuclei with reduced mass *M* move in the field of the interaction potential *V(R)*, where *R* is the collective coordinate. Lagrangian

$$\mathcal{L}_0(R, \dot{R}) = \tfrac{1}{2} M \dot{R}^2 - V(R).$$

The internal motion is described by a set of harmonic oscillators of mass m_i and frequency ω_i with internal coordinate q_i.

The internal Lagrangian:

$$\mathcal{L}_{\text{intl}}(q_i, \dot{q}_i) = \sum_i \frac{m_i}{2}(\dot{q}_i^2 - \omega_i^2 q_i^2).$$

The interaction between the collective motion and the internal subsystem is assumed to be separable and linear in coordinate. This drastic assumtion allows us to do analytic.

The full Lagrangian

$$\mathcal{L}(R, \dot{R}; q_i, \dot{q}_i) = \mathcal{L}_0(R, \dot{R}) + \mathcal{L}_{\text{intl}}(q_i, \dot{q}_i) + \sum_i f_i(R) q_i,$$

where $f_i(R)$ is the form factor of the coupling, it vanishes at R beyond which the reaction partners cease to interest and has the same range as the potential $V(R)$. The equations of motion:

$$M\ddot{R} = -\frac{dV(R)}{dR} + \sum_i q_i \frac{df_i(R)}{dR},$$

$$m_i \ddot{q}_i = -m_i \omega_i^2 q_i + f_i(R).$$

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In order to get the equation in *R* alone, we must eliminate the internal coordinates. So,

$$q_i(t) = q_i^0(t) + \int_{t_0}^{t} ds \frac{f_i(R(s))}{m_i \omega_i} \sin \omega_i (t - s),$$

where the first term is the solution of the homogeneous part with $f_i=0$, and has the form

$$q_i^0(t) = q_{i0} \cos \omega_i (t - t_0) + \frac{p_{i0}}{m_i \omega_i} \sin \omega_i (t - t_0);$$

q_{i0} and p_{i0} are the values of the coordinates and momentum of the oscillators of the bath at an initial time t_0. The second term incorporates the effect of coupling.

Substituting the solution for internal coordinates, we obtain the differential equation for R

$$M\ddot{R} = -\frac{dV(R)}{dR} + \sum_i \frac{1}{m_i \omega_i} \int_{t_0}^{t} ds\, f_i(R(s)) \sin \omega_i (t-s) \frac{df_i(R)}{dR}$$

$$+ \sum_i q_i^0(t) \frac{df_i(R)}{dR};$$

Integrating by parts in the second term,

$$\int_{t_0}^{t} ds\, f_i(R(s)) \sin \omega_i (t-s) = \frac{f_i(R(s))}{\omega_i} \cos \omega_i (t-s) \Big|_{s=t_0}^{s=t}$$

$$- \int_{t_0}^{t} ds\, \frac{df_i(R(s))}{dR} \dot{R}(s) \frac{1}{\omega_i} \cos \omega_i (t-s),$$

The surface term contributes only at the upper limit $s=t$

$$\frac{f_i(R(s))}{\omega_i}\cos\omega_i(t-s)\Big|_{s=t_0}^{s=t} = \frac{f_i(R)}{\omega_i},$$

As a result

$$M\ddot{R} = \tilde{F}(R) + F_{\text{frict}}(R, \dot{R}) + F_{\text{L}}(R, t).$$

The renormalized conservative force

$$\tilde{F}(R) = -\frac{d\tilde{V}(R)}{dR}$$

The renormalized potential

$$\tilde{V}(R) = V(R) - \sum_i \frac{1}{2m_i\omega_i^2}[f_i(R)]^2.$$

We have defined the friction force

$$F_{\text{frict}}(R, \dot{R}) = -\sum_i \frac{1}{m_i \omega_i^2} \int_{t_0}^{t} ds \frac{df_i(R(t))}{dR} \cos \omega_i (t-s) \frac{df_i(R(s))}{dR} \dot{R}(s)$$

and the Langevin force

$$F_{\text{L}}(R, t) = \sum_i q_i^0(t) \frac{df_i(R)}{dR}.$$

The renormalization term can be taken away by writing the full Lagrangian in Caderia and Leggett form

$$\mathcal{L}(R, \dot{R}; q_i, \dot{q}_i) = \mathcal{L}_0(R, \dot{R}) + \sum_i \frac{m_i}{2} \dot{q}_i^2 - \sum_i \frac{m_i \omega_i^2}{2} \left(q_i - \frac{f_i(R)}{m_i \omega_i^2} \right)^2$$

The equation for *R* derived from such a Lagrangian contains only the original potential *V(R)*.

The friction force (non-Markovian)

$$F_{\text{frict}}(R, \dot{R}) = -\int_{t_0}^{t} ds\, \gamma(t, s)\dot{R}(s).$$

Here, we introduce the friction kernel (assume, for simplicity, $m_i = m$ and $f_i(R) = f(R)$)

$$\gamma(t, s) = f'(R(t))\, f'(R(s)) \sum_i \frac{1}{m\omega_i^2} \cos\omega_i(t - s),$$

where $f'(R) = df(R)/dR$. The sum over i is a sum of many terms with varying signs which effectively vanishes except when all the cosines have nearly vanishing arguments, i.e. $|t - s| \leq \epsilon$; the small time interval ϵ is the memory time determining the retardation of the friction force, i.e. its length of memory.Therefore,

$$\sum_i \frac{1}{m\omega_i^2} \cos\omega_i(t - s) \approx 2\gamma_0\, \delta_\epsilon(t - s),$$

where $\delta_\epsilon(t - s)$ is a 'smeared-out δ-function with a range ϵ.

Integrating over *t*, we get

$$2\gamma_0 = \int_{-\infty}^{\infty} dt \sum_i \frac{1}{m\omega_i^2} \cos \omega_i t ,$$

where the factor 2 is introduced for convenience. The friction kernel then becomes

$$\gamma(t, s) = 2\gamma(R)\, \delta_\epsilon (t - s)$$

with the friction coefficient

$$\gamma(R) = \gamma_0 [f'(R)]^2$$

The dependence of *R(t)* on *t* is assumed to be weak, so that we can set *R(s)=R(t)* for $|s-t| \le \epsilon$.
Let us introduce the spectral density $g(\omega)$ of the intrinsic excitations, which allows us

$$\sum_i \cdots \rightarrow \int_0^{\infty} d\omega\, g(\omega) \cdots .$$

Langevin force

For simplicity, we assume the same form factors.

$$F_{\mathrm{L}}(R, t) = f'(R)\,\xi(t),$$

where

$$\xi(t) = \sum_i q_i^0(t)$$

The oscillators are assumed to represent a 'heat bath' (Brownian motion). Owing to the implicit interactions of the oscillators of the bath, the coordinates q_{i0} and momenta p_{i0} are treated as random variables whose distributions has mean value zero,

$$\langle q_{i0} \rangle = 0, \qquad \langle p_{i0} \rangle = 0,$$

where $\langle \ldots \rangle$ denotes the average over the ensemble of these variables. They are regarded as uncorrelated,

$$\langle q_{i0}\, q_{j0}\rangle = \delta_{ij}\langle q_{i0}^2\rangle,$$
$$\langle p_{i0}\, p_{j0}\rangle = \delta_{ij}\langle p_{i0}^2\rangle,$$
$$\langle q_{i0}\, p_{j0}\rangle = 0,$$

where the quantities $\langle q_{i0}^2\rangle$ and $\langle q_{i0}^2\rangle$ are the mean-square elongation and momentum of the i-th oscillator, respectively.

$$\langle \xi(t)\rangle = 0,$$

$$\langle \xi(t)\xi(t')\rangle = \sum_i \langle q_{i0}^2\rangle \cos\omega_i(t-t_0)\cos\omega_i(t'-t_0)$$
$$+ \sum_i \frac{1}{m_i^2\omega_i^2}\langle p_{i0}^2\rangle \sin\omega_i(t-t_0)\sin\omega_i(t'-t_0).$$

$$2\cos\omega_i(t-t_0)\cos\omega_i(t'-t_0)=\cos\omega_i(t-t')+\cos\omega_i(t+t'+2t_0),$$
$$2\sin\omega_i(t-t_0)\sin\omega_i(t'-t_0)=\cos\omega_i(t-t')-\cos\omega_i(t+t'+2t_0),$$

Thus,

$$\langle\xi(t)\xi(t')\rangle\approx\sum_i\frac{\langle\epsilon_{i0}\rangle}{m_i\omega_i^2}\cos\omega_i(t-t'),$$

where $\langle\epsilon_{i0}\rangle$ is the mean energy of the i-th oscillator,

$$\langle\epsilon_{i0}\rangle=\frac{\langle p_{i0}^2\rangle}{2m_i}+\tfrac{1}{2}m_i\omega_i^2\langle q_{i0}^2\rangle.$$

We assume that the heat bath is in equilibrium and can be characterized by a temperature T.

$$\langle\epsilon_{i0}\rangle=k_{\mathrm{B}}T,$$

Then

$$\langle \xi(t)\xi(t') \rangle \approx k_B T \sum_i \frac{1}{m_i \omega_i^2} \cos \omega_i (t - t').$$

$m_i = m$

$$\langle \xi(t)\xi(t') \rangle = 2 d_0 \, \delta_\epsilon (t - t')$$

where the *correlation strength* d_0 is given by

$$d_0 = \gamma_0 k_B T.$$

The normalized time-dependent variable

$$\Gamma(t) = \frac{1}{\sqrt{d_0}} \xi(t),$$

with Gaussian distribution.

$$\langle \Gamma(t) \rangle = 0,$$

$$\langle \Gamma(t)\Gamma(t') \rangle = 2\delta_\epsilon(t - t'),$$

The average of the Langevin force is

$$\langle F_L(R(t), t) \rangle = 0.$$

Its correlation function is

$$\langle F_{\mathrm{L}}(R(t), t) F_{\mathrm{L}}(R(t'), t') \rangle = 2D(R)\,\delta_\epsilon(t - t'),$$

where we have introduced the *fluctuation strength coefficient*

$$D(R) = d_0[f'(R)]^2,$$

$$F_{\mathrm{L}}(R, t) = \sqrt{D(R)}\,\Gamma(t).$$

Fluctuation-dissipation theorem

$$D(R) = \gamma(R)\, k_{\mathrm{B}} T,$$

connects the fluctuation strength coefficient *D* of the Langevin force with the friction coefficient γ. It is a consequence of the fact that the friction and Langevin forces have their origin in the coupling between the collective motion and the bath.

At low temperatures

$$\langle \epsilon_i \rangle = \tfrac{1}{2} \hbar \omega_i \coth\left(\frac{\hbar \omega_i}{2 k_{\mathrm{B}} T} \right)$$

Langevin equations, their applicability to DIC

$$M\ddot{R} = \tilde{F}(R) + F_{\mathrm{frict}}(R, \dot{R}) + F_{\mathrm{L}}(R, t)$$

$$F_{\mathrm{frict}}(R, \dot{R}) = -\gamma(R)\,\dot{R},$$

$$F_{\mathrm{L}}(R, t) = \sqrt{D(R)}\,\Gamma(t),$$

$$\dot{R} = \frac{P}{M},$$

$$\dot{P} = \tilde{F}(R) - \gamma(R)\frac{P}{M} + \sqrt{D(R)}\,\Gamma(t).$$

The internal system equlibrates quickly, its equilibration time is smaller than the correlation time ϵ and also smaller than the time scale of collective motion.

Generalization to the multidimensional case.

$$\dot{x}_i = h_i(x) + \sum_j g_{ij}(x)\Gamma_j(t), \qquad i = 1, \ldots, N,$$

where

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

and

$$\langle \Gamma_i(t)\Gamma_j(t') \rangle = 2\delta_{ij}\delta_\epsilon(t - t').$$

The functions $h_i(x)$ contain the conservative and frictional forces, and the functions $g_{ij}(x)$ the fluctuation strength coefficients.

Discretization of the Langevin equations

We introduce the time interval τ and consider the times $t_n = n\tau$. The interval τ is chosen larger than the correlation time ϵ of the random process $\Gamma(t)$, but smaller than the times over which the forces and form factors in the Langevin equation vary appreciably as functions of the coordinate $R = R(t)$. We now integrate eqns (11.64) from t_n to $t_{n+1} = t_n + \tau$. We regard the functions $\tilde{F}(R)$, $\gamma(R)$, and $D(R)$ as constant in this interval and replace them with their values at time t_n. Thus we have, with $R_n = R(t_n)$ and $P_n = P(t_n)$,

$$R_{n+1} = R_n + \frac{P_n}{M}\tau,$$

$$P_{n+1} = P_n + \left(\tilde{F}(R_n) - \gamma(R_n)\frac{P_n}{M}\right)\tau + \sqrt{D(R_n)}\, W_n,$$

where the random variable

$$W_n = W(t_n) = \int_{t_n}^{t_{n+1}} dt'\, \Gamma(t')$$

is a sum of Gaussian-distributed random numbers and is therefore again Gaussian-distributed.

$W_n = a_n w(t_n)$, where $w(t_n)$ is a normalized random variable which satisfies

$$\langle w(t_n) \rangle = 0$$

and

$$\langle w(t_n) w(t_{n'}) \rangle = 2\delta_{nn'}.$$

The coefficient a_n is determined by comparing

$$\begin{aligned} \langle W_n^2 \rangle &= \int_{t_n}^{t_{n+1}} dt' \int_{t_n}^{t_{n+1}} dt'' \, \langle \Gamma(t') \Gamma(t'') \rangle \\ &= 2 \int_{t_n}^{t_{n+1}} dt' \int_{t_n}^{t_{n+1}} dt'' \, \delta_\epsilon(t' - t'') = 2\tau \end{aligned}$$

with

$$\langle W_n^2 \rangle = a_n^2 \langle [w(t_n)]^2 \rangle = 2a_n^2.$$

This yields $a_n = \sqrt{\tau}$.

The discretized form of the Langevin equations

$$R_{n+1} = R_n + \frac{P_n}{M}\tau,$$

$$P_{n+1} = P_n + \left(\widetilde{F}(R_n) - \gamma(R_n)\frac{P_n}{M}\right)\tau + \sqrt{D(R_n)}\sqrt{\tau}\; w(t_n).$$

In the general formulation we then have

$$x_i(t_{n+1}) = x_i(t_n) + h_i[x(t_n)]\,\tau + \sum_j g_{ij}[x(t_n)]\sqrt{\tau}\; w_j(t_n).$$

The Fokker-Planck description

The distribution of the solutions *x(t)* of the Langevin equations, i.e. the distribution function *d(x;t)* of the set of variables x as a function of the time *t*

The distribution function $d(x; t + \tau)$ at time $t + \tau$ is connected with the function $d(x; t)$ at the time t by the relation

$$d(x; t + \tau) = \int dx' \, P(x, t + \tau; x', t) \, d(x'; t),$$

where $P(x, t + \tau; x', t)$ is the *transition probability*. It is defined as the conditional probability density of the variable x at time $t + \tau$ when it is known that this variable has had the sharp value x' at the earlier time t.

It depends only on one previous time, it is called Markovian.

We now introduce the identity

$$P(x, t+\tau; x', t) = \int dy\, \delta(y - x)\, P(y, t+\tau; x', t)$$

and consider the formal expansion of the δ-function into a Taylor series

$$\delta(y - x) = \delta(x' - x + y - x') = \sum_{n=0}^{\infty} \frac{(y - x')^n}{n!} \left(-\frac{\partial}{\partial x}\right)^n \delta(x' - x).$$

For the moment we treat the set of variables $x = \{x_i\}$ as if it were a single variable x;

the transition probability in the form of a moment expansion

$$P(x, t+\tau; x', t) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{\partial}{\partial x}\right)^n \left[M_n(x'; t, \tau)\delta(x' - x)\right]$$

with the moments

$$\begin{aligned} M_n(x'; t, \tau) &= \int dy\, (y - x')^n\, P(y, t+\tau; x', t) \\ &= \langle \left[x'(t+\tau) - x'(t)\right]^n \rangle. \end{aligned}$$

$$d(x;t+\tau)-d(x;t)=\sum_{n=1}^{\infty}\left(-\frac{\partial}{\partial x}\right)^{n}\left(\frac{M_n(x;t,\tau)}{n!}d(x;t)\right)$$

The Kramers-Moyal expansion:

$$\frac{\partial}{\partial t}d(x;t)=\sum_{n=1}^{\infty}\left(-\frac{\partial}{\partial x}\right)^{n}[D^{(n)}(x;t)d(x;t)],$$

$$D^{(n)}(x;t)=\frac{1}{n!}\lim_{\tau\to 0}\frac{M_n(x;t,\tau)}{\tau}=\frac{1}{n!}\lim_{\tau\to 0}\frac{\langle[x(t+\tau)-x(t)]^n\rangle}{\tau}$$

Written explicitly in the N variables

$$x = \{x_i\}$$

$$\frac{\partial}{\partial t} d(x;t) = -\sum_i \frac{\partial}{\partial x_i}[D_i^{(1)}(x;t)d(x;t)] + \sum_{ij} \frac{\partial^2}{\partial x_i \partial x_j}[D_{ij}^{(2)}(x;t)d(x;t)] + \cdots$$

$$D_i^{(1)}(x;t) = \lim_{\tau \to 0} \frac{1}{\tau} \langle [x_i(t+\tau) - x_i(t)] \rangle,$$

$$D_{ij}^{(2)}(x;t) = \frac{1}{2} \lim_{\tau \to 0} \frac{1}{\tau} \langle [x_i(t+\tau) - x_i(t)][x_j(t+\tau) - x_j(t)] \rangle,$$

$$D_{ijk}^{(3)}(x;t) = \cdots;$$

The connection with the Langevin equations

$$x_i(t+\tau) - x_i(t) = \sqrt{\tau}\left(h_i(x)\sqrt{\tau} + \sum_j g_{ij}(x) w_j(t)\right)$$

$$D_i^{(1)}(x;t) = \lim_{\tau\to 0} \frac{1}{\tau}\sqrt{\tau}\left(h_i(x)\sqrt{\tau} + \sum_j g_{ij}(x)\langle w_j(t)\rangle\right) = h_i(x),$$

$$D_{ij}^{(2)}(x;t) = \tfrac{1}{2}\lim_{\tau\to 0}\frac{1}{\tau}\tau\left(h_i(x)h_j(x)\tau + h_i(x)\sum_k g_{jk}(x)\sqrt{\tau}\langle w_k(t)\rangle\right.$$

$$\left. + h_j(x)\sum_l g_{il}(x)\sqrt{\tau}\langle w_l(t)\rangle + \sum_{kl} g_{il}(x)g_{jk}(x)\langle w_k(t)w_l(t)\rangle\right)$$

$$= \sum_k g_{ik}(x)g_{jk}(x),$$

$$D_{ijk}^{(3)}(x;t) = \tfrac{1}{6}\lim_{\tau\to 0}\frac{1}{\tau}\tau^{3/2}(\ldots) = 0,$$

$$D_{ij\ldots}^{(n)}(x;t) = 0 \text{ for } n > 3.$$

Only the first two coefficients are non-vanishing, and they are independent of the time. The first is called the *drift coefficient*

$$v_i(x) = D_i^{(1)}(x),$$

and the second the *diffusion coefficient*

$$D_{ij}(x) = D_{ij}^{(2)}(x).$$

Kramers–Moyal expansion reduces to the

Fokker–Planck equation

$$\frac{\partial}{\partial t} d(x;t) = -\sum_i \frac{\partial}{\partial x_i} v_i(x) d(x;t) + \sum_{ij} \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}(x) d(x;t),$$

where here and in the following the derivatives act on all terms to the right.

Fokker-Planck equation for distribution function

$$\frac{\partial}{\partial t} d(x;t) = -\sum_i \frac{\partial}{\partial x_i} v_i(x) d(x;t) + \sum_{ij} \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}(x) d(x;t),$$

$$v_R = \frac{P}{M},$$

$$v_P = \tilde{F}(R) - \gamma(R)\frac{P}{M},$$

$$D_{RR} = 0,$$

$$D_{PP} = D(R),$$

$$D_{RP} = 0.$$

$$\frac{\partial}{\partial t} d(R, P; t) = \left[-\frac{\partial}{\partial R}\frac{P}{M} - \frac{\partial}{\partial P}\left(\tilde{F}(R) - \gamma(R)\frac{P}{M}\right) + \frac{\partial^2}{\partial P^2} D(R) \right] d(R, P; t).$$

Simple examples
1-dim., const. coefficients

$$\frac{\partial}{\partial t} d(Z;t) = \left(-v \frac{\partial}{\partial Z} + D \frac{\partial^2}{\partial Z^2} \right) d(Z;t).$$

Introducing the new variable $X = Z - vt$ in the place of Z, we obtain the equation

$$\frac{\partial}{\partial t} d(X;t) = D \frac{\partial^2}{\partial X^2} d(X;t).$$

With the initial condition $d(X;0) = \delta(X)$ it has the solution

$$d(X;t) = \frac{1}{\sqrt{4\pi Dt}} e^{-X^2/4Dt},$$

or

$$d(Z;t) = \frac{1}{\sqrt{4\pi Dt}} e^{-(Z-vt)^2/4Dt}.$$

$$\langle 1 \rangle = \int dZ\, d(Z;t) = 1.$$

The mean value and the variance are found from the first and second moments of the distribution function.

$$\bar{Z}(t) = \langle Z \rangle = \int dZ\, Z\, d(Z;t) = vt,$$

$$\sigma_{ZZ}^2 = \langle [Z - \bar{Z}(t)]^2 \rangle = \int dZ\, (Z - vt)^2 d(Z;t) = 2Dt.$$

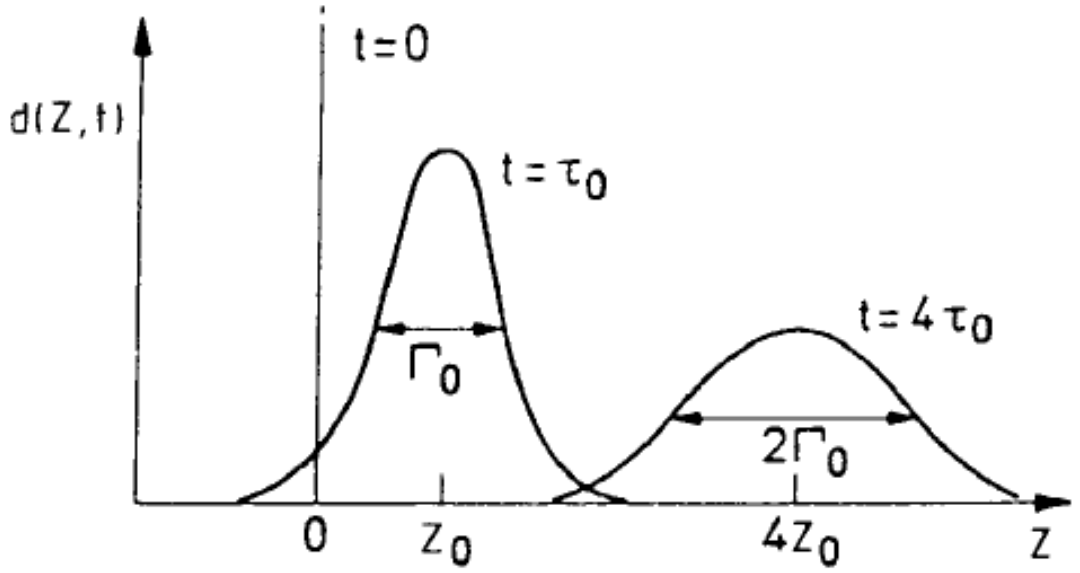


Figure 11.7 The solution (11.96) of the one-dimensional Fokker–Planck equation with constant coefficients at different times. The charge Z and the widths Γ_Z are indicated for two times differing by a factor of four; $Z_0 = Z(\tau_0)$ and $\Gamma_0 = \Gamma_Z(\tau_0)$.

the rate of increase of the variance is called the *diffusion constant*.

The spreading of the distribution function is characterized by the full width at half-maximum Γ_Z which according to eqn (11.96) is defined by

$$\exp\left[-(\Gamma_Z/2)^2/4Dt\right] = \tfrac{1}{2};$$

this yields a width which increases in proportion to the square root of time,

$$\Gamma_Z = \Gamma_Z(t) = 4\sqrt{(\ln 2)\, Dt}. \tag{11.99}$$

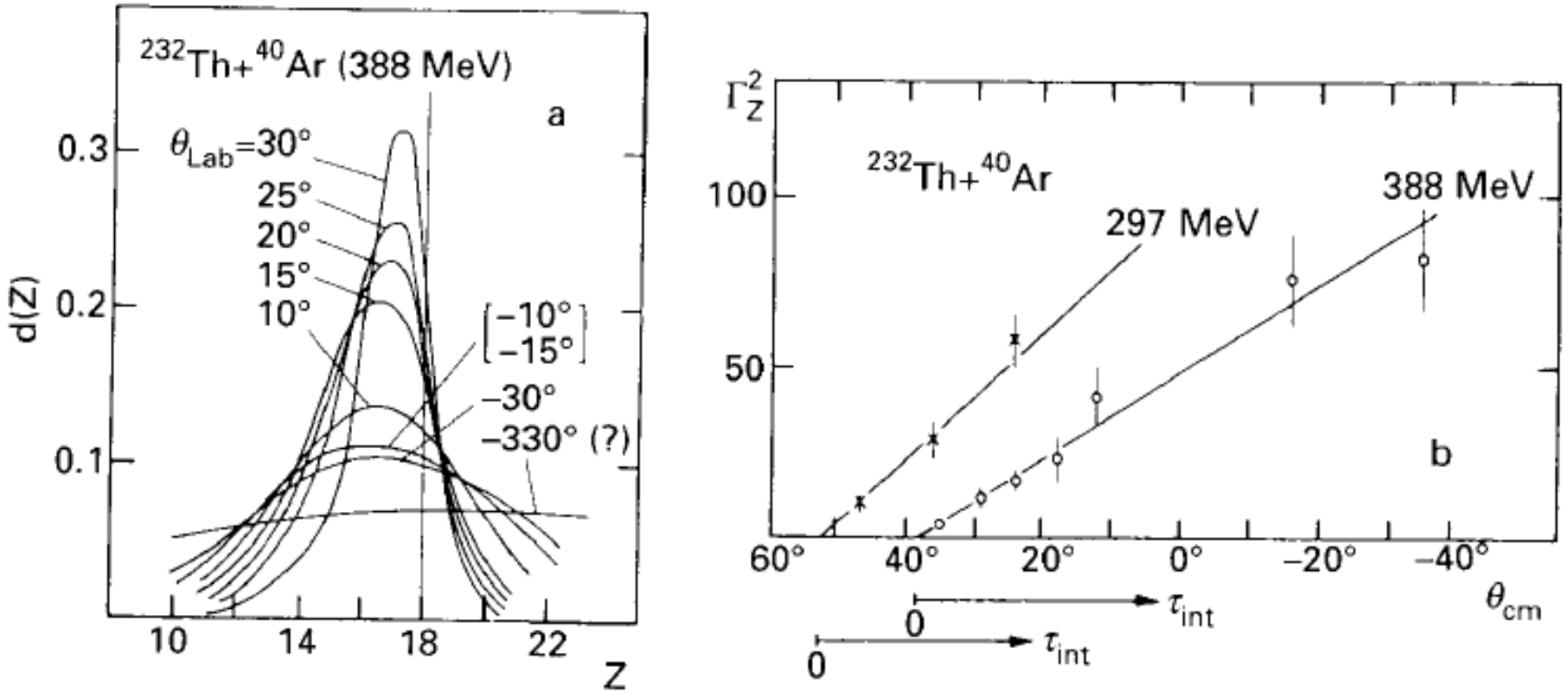


Figure 11.8 Charge transfer in the system ^{232}Th + ^{40}Ar at 388 MeV. (a) Charge distribution $d(Z)$ of the projectile-like fragments ($Z_{proj} = 18$) for different deflection angles Θ_{lab}. (b) The square of the width Γ_Z^2 of the charge distribution as function of the deflection angle (or interaction time τ_{int}) for the same system at the two energies 297 and 388 MeV.

1-dim., variable drift coefficients

$$\frac{\partial}{\partial t} d(Z,t) = \left(-\frac{\partial}{\partial Z} v(Z) + D \frac{\partial^2}{\partial Z^2} \right) d(Z,t).$$

The equilibrium solution ($t \to \infty$) has the form of Boltzmann distribution

$$d(Z) \propto e^{-U(Z)/k_B T},$$

where T is the temperature of the system.

$$\frac{\partial}{\partial Z} \left(-v(Z) + D \frac{\partial}{\partial Z} \right) d(Z,t) = 0,$$

$$v(Z) = \frac{1}{d(Z)} \frac{d}{dZ} D\, d(Z),$$

$$v(Z) = -\frac{D}{k_B T}\frac{\partial U(Z)}{\partial Z}.$$

In the first approximation

$$U(Z) = \frac{C}{Z_{tot}^2}(Z - Z_s)^2.$$

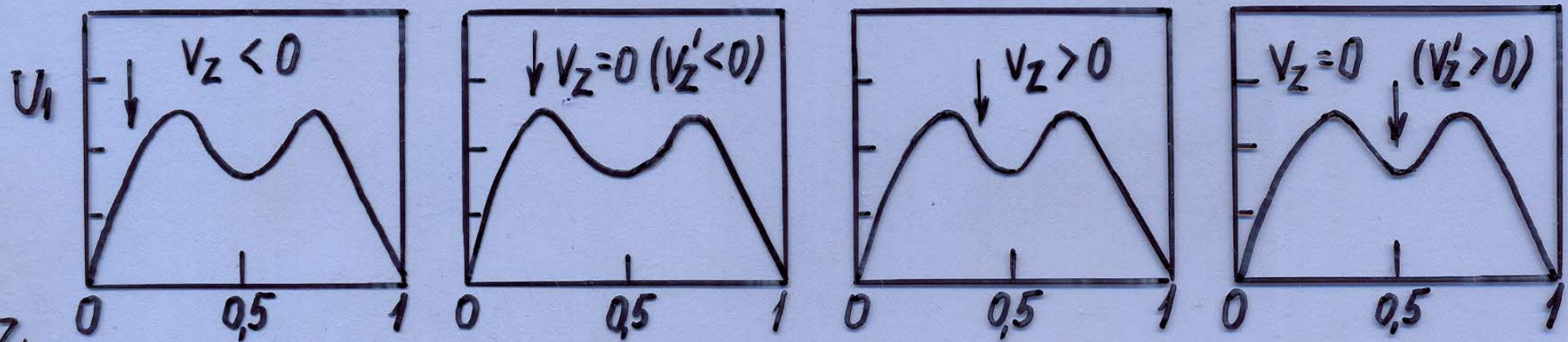
Here Z_{tot} is the total charge of projectile and target, and $Z_s = Z_{tot}/2$. The factor C is the stiffness of the driving potential.

$$\frac{\partial}{\partial t}d(Z,t) = \left(\frac{\partial}{\partial Z}\frac{2CD}{k_B T Z_{tot}^2}(Z - Z_s) + D\frac{\partial^2}{\partial Z^2}\right) d(Z,t).$$

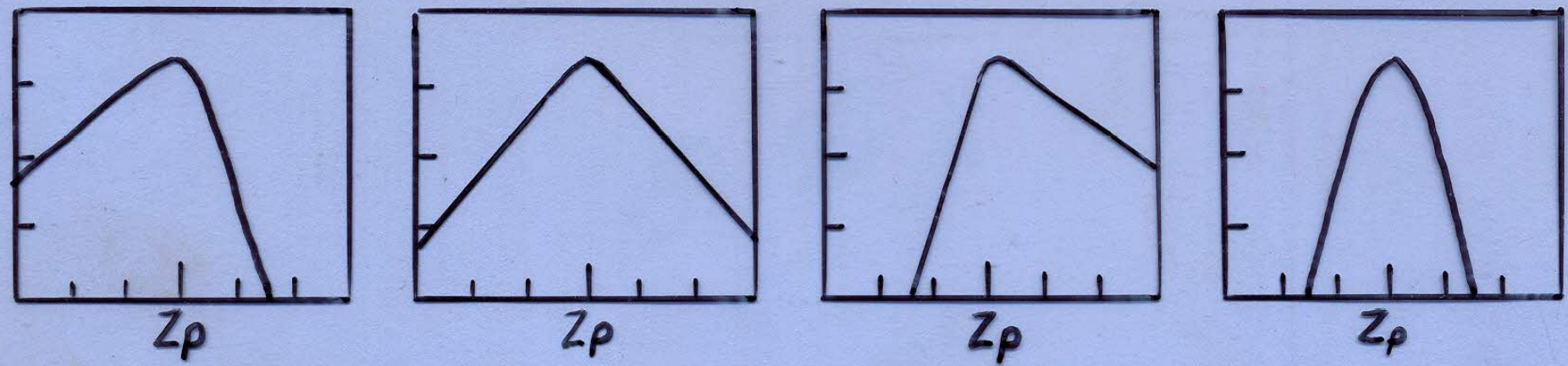
$$d(Z,t) = \frac{1}{\sqrt{2\pi\sigma_{ZZ}^2(t)}}\exp\left(-\frac{[Z - \bar{Z}(t)]^2}{2\sigma_{ZZ}^2(t)}\right),$$

$$\frac{\partial}{\partial t}P(Z_1,t) = -\frac{\partial}{\partial Z_1}(V_Z P) + \frac{\partial^2}{\partial Z_1^2}(D_Z P)$$

$V_Z \sim \frac{\partial U_e}{\partial Z_1}$ $\quad \langle Z_1 \rangle = Z_p + V_Z \cdot t$ $\quad \sigma_Z^2 = 2D_Z \cdot t$



$X = \frac{Z_1}{Z}$



$^{20}Ne + ^{107}Ag$ (252 MeV)

$^{40}Ar + ^{237}Th$ (388 MeV)

$^{86}Kr + ^{166}Er$ (515 MeV)

$^{238}U + ^{238}U$ (1766 MeV)

Two-dimensional Fokker-Planck equation with constant coefficients: Brownian motion

$$\frac{\partial}{\partial t} d(R, P; t) = \left(-\frac{P}{M} \frac{\partial}{\partial R} - \tilde{F} \frac{\partial}{\partial P} + \frac{\gamma}{M} \frac{\partial}{\partial P} P + D \frac{\partial^2}{\partial P^2} \right) d(R, P; t).$$

The distribution function $d = d(R, P; t)$ is normalized to unity in phase space at any time t,

$$\int\int dR\, dP\, d(R, P; t) = 1.$$

$$d(R, P; t) = \frac{1}{(2\pi)^2 (\sigma_{RR}^2 \sigma_{PP}^2 - \sigma_{RP}^2 \sigma_{RP}^2)^{1/2}} \exp\left\{ -\tfrac{1}{2} [(\sigma^2)_{RR}^{-1} (R - \bar{R}(t))^2 \right.$$

$$\left. + 2(\sigma^2)_{RP}^{-1} (R - \bar{R}(t))(P - \bar{P}(t)) + (\sigma^2)_{PP}^{-1} (P - \bar{P}(t))^2] \right\}.$$

General case

d(R,P;t)

$$\bar{R}(t) = \langle R(t) \rangle = \int\int dR dP \; R d(R, P; t),$$

$$\bar{P}(t) = \langle P(t) \rangle = \int\int dR dP \; P d(R, P; t),$$

$$\sigma^2_{RR}(t) = \langle [R - \bar{R}(t)]^2 \rangle = \langle R^2 \rangle - \bar{R}^2(t),$$

$$\sigma^2_{PP}(t) = \langle [P - \bar{P}(t)]^2 \rangle = \langle P^2 \rangle - \bar{P}^2(t),$$

$$\sigma^2_{RP}(t) = \langle [R - \bar{R}(t)][P - \bar{P}(t)] \rangle = \langle RP \rangle - \bar{R}(t)\bar{P}(t).$$

In order to determinate these functions we return to the Fokker–Planck equation (11.111) and derive differential equations for them which can be solved in analytic form.

For example, for the mean value $\bar{P}(t)$ we multiply eqn (11.111) by P on both sides and integrate over the variables R and P. On the left-hand side we have

$$\int\int dR dP\, P \frac{\partial}{\partial t} d(R, P; t) = \frac{d}{dt} \int\int dR dP\, P d(R, P; t) = \frac{d}{dt} \bar{P}(t).$$

Integrating by parts on the right-hand side of eqn (11.111), we find that the term containing the derivative with respect to R vanishes, because all surface terms do so. The same is true for the term containing the second derivative with respect to P. Only the terms containing $\partial/\partial P$ contribute,

$$\int\int dR dP\, P\left(-\tilde{F}\frac{\partial}{\partial P} + \frac{\gamma}{M}\frac{\partial}{\partial P} P\right) d(R, P; t)$$

$$= \int\int dR dP \left(\tilde{F} - \gamma \frac{P}{M}\right) d(R, P, t) = \tilde{F} - \gamma \frac{\bar{P}(t)}{M}.$$

We therefore find

$$\frac{d\bar{P}}{dt} = \tilde{F} - \gamma \frac{\bar{P}}{M}.$$

In a similar fashion one obtains

$$\frac{d\bar{R}}{dt} = \frac{\bar{P}}{M}.$$

The diffusive properties of the system are determined by the variances. We obtain a differential equation for the variance σ_{PP}^2 in the momentum by multiplying the Fokker–Planck equation (11.111) on both sides by the factor $(P - \bar{P})^2$ and observing that again the surface terms vanish after integration by parts. On the left-hand side we have

$$\int\int dR dP\,(P - \bar{P})^2 \frac{\partial}{\partial t} d(R, P; t) = \frac{d}{dt}\sigma_{PP}^2, \tag{11.118}$$

and on the right-hand side,

$$\int\int dR dP\,(P - \overline{P})^2 \left(-\frac{P}{M}\frac{\partial}{\partial R} - \widetilde{F}\frac{\gamma}{M}\frac{\partial}{\partial P} + \frac{\gamma}{M}\frac{\partial}{\partial P}P + D\frac{\partial^2}{\partial P^2}\right) d(R, P; t)$$

$$= -\frac{2\gamma}{M}\sigma_{PP}^2 + 2D. \tag{11.119}$$

Therefore,

$$\frac{d}{dt}\sigma_{PP}^2 + \frac{2\gamma}{M}\sigma_{PP}^2 = 2D. \tag{11.120}$$

Analogously, we derive an equation for the covariance σ_{RP}^2,

$$\frac{d}{dt}\sigma_{RP}^2 + \frac{\gamma}{M}\sigma_{RP}^2 = \frac{1}{M}\sigma_{PP}^2, \tag{11.121}$$

and for the variance σ_{RR}^2,

$$\frac{d}{dt}\sigma_{RR}^2 = \frac{2}{M}\sigma_{RP}^2. \tag{11.122}$$

with the initial conditions $\bar{P}(0) = P_0, \quad \sigma^2_{PP}(0) = \sigma^2_{RR}(0) = \sigma^2_{RP}(0) = 0$

$$\bar{P}(t) = \frac{M\tilde{F}}{\gamma} + \left(P_0 - \frac{M\tilde{F}}{\gamma}\right) e^{-\gamma t/M},$$

$$\sigma^2_{PP}(t) = \frac{MD}{\gamma}\left(1 - e^{-2\gamma t/M}\right),$$

$$\sigma^2_{RR}(t) = \frac{2D}{\gamma^2}t + \frac{DM}{\gamma^3}\left(4e^{-\gamma t/M} - e^{-2\gamma t/M} - 3\right).$$

From these equations we obtain the limits

$$\sigma^2_{PP}(t) \to \begin{cases} 2Dt & \text{for } t \to 0, \\ MD/\gamma & \text{for } t \to \infty, \end{cases}$$

and analogously

$$\sigma^2_{RR}(t) \to \begin{cases} (4D/3M^2)\, t^3 & \text{for } t \to 0, \\ (2D/\gamma^2)\, t & \text{for } t \to \infty. \end{cases}$$

Methods of solving for the distribution function

The Gaussian solution of the Fokker–Planck equation

the 'moment expansion method'.

Computer simulation of the Langevin process

The multi-dimentional Gaussian solution of the Fokker-Planck equation with non-linear coefficients

Gaussian Ansatz (N variables)

$$d(x;t) = A \exp\left(-\tfrac{1}{2} \sum_{i,j=1}^{N} [\sigma^2(t)]_{ij}^{-1} [x_i - \bar{x}_i(t)][x_j - \bar{x}_j(t)]\right)$$

$$A = \frac{1}{\sqrt{(2\pi)^N \det(\sigma_{ij}^2)}}$$

$$\bar{x}_i(t) = \int dx\, x_i d(x,t),$$

$$\sigma_{ij}^2(t) = \int dx\, [x_i - \bar{x}_i(t)][x_j - \bar{x}_j(t)]\, d(x;t)$$

The dynamical variables are $x = r$, p_r, L, and ϕ (relative distance, radial momentum, orbital angular momentum perpendicular to the scattering plane, and conjugate angle), and the Fokker–Planck equation reads

$$\frac{\partial}{\partial t} d(r, p_r, \phi, L; t) = -\left[\frac{p_r}{\mu} \frac{\partial}{\partial r} + \frac{L}{\mu r^2} \frac{\partial}{\partial \phi} + \left(-\frac{dV(r)}{dr} + \frac{L^2}{\mu r^3} \right) \frac{\partial}{\partial p_r} + \frac{\partial}{\partial p_r} \frac{p_r}{\mu} K_r(r) + D_r(r) \frac{\partial^2}{\partial p_r^2} + \frac{\partial}{\partial L} K_\phi(r) \frac{L}{\mu} + D_\phi(r) r^2 \frac{\partial^2}{\partial L^2} \right] d(r, p_r, \phi, L; t).$$

fluctuation-dissipation theorem $D_r(r) = k_B T K_r(r)$ and $D_\phi(r) = k_B T K_\phi(r)$

The equations for the mean values and variances (making use of integration by parts and the vanishing of the surface terms)

$$\frac{d}{dt}\bar{p}_r = \int dr\,dp_r\,d\phi\,dL\; p_r \frac{\partial}{\partial t} d(r, p_r, \phi, L; t)$$

$$= \int dr\,dp_r\,d\phi\,dL\; p_r \left[\left(\frac{dV(r)}{dr} - \frac{L^2}{\mu r^3} \right) \frac{\partial}{\partial p_r} + \frac{\partial}{\partial p_r} \frac{p_r}{\mu} K_r(r) \right] d(r, p_r, \phi, L; t)$$

$$= -\overline{\frac{dV(r)}{dr}} + \overline{\frac{L^2}{\mu r^3}} - \overline{\frac{p_r}{\mu} K_r(r)}.$$

This equation for the mean value $\overline{p}_r$ (the first moment in the variable p_r) contains mean values of the nonlinear and multidimensional functions $dV(r)/dr$, L^2/r^3 and $p_r K_r(r)$.

We are forced to introduce a further approximation, which consists in replacing the mean values of the functions of the dynamical variables with functions of the mean values of these variables,

$$\overline{G(x)} \approx G(\bar{x}). \tag{11.137}$$

This amounts to assuming that the functions in question do not fluctuate appreciably, or that in the expansion

$$\begin{aligned}\overline{G(x)} &= G(\bar{x}) + G'(\bar{x})\overline{(x-\bar{x})} + \tfrac{1}{2}G''(\bar{x})\overline{(x-\bar{x})^2} + \cdots \\ &= G(\bar{x}) + \tfrac{1}{2}G''(\bar{x})\sigma_x^2 + \cdots\end{aligned} \tag{11.138}$$

all terms on the right-hand side but the first can be neglected. This approximation is called the *quasi-linear approximation*. It it is exact for linear functions.

$$\dot{\bar{r}} = \frac{\bar{p}_r}{\mu},$$

$$\dot{\bar{p}}_r = -\frac{dV(\bar{r})}{d\bar{r}} + \frac{\bar{L}^2}{\mu\bar{r}^3} - \frac{K_r(\bar{r})}{\mu}\bar{p}_r,$$

$$\dot{\bar{\phi}} = \frac{\bar{L}}{\mu\bar{r}^2},$$

$$\dot{\bar{L}} = -\frac{K_\phi(\bar{r})}{\mu}\bar{L}.$$

$$\frac{d}{dt}\sigma^2_{\phi\phi} = \frac{2}{\mu\bar{r}^2}\sigma^2_{\phi L},$$

$$\frac{d}{dt}\sigma^2_{\phi L} = \frac{\sigma^2_{LL}}{\mu\bar{r}^2} - \sigma^2_{\phi L}\frac{K_\phi(\bar{r})}{\mu},$$

$$\frac{d}{dt}\sigma^2_{LL} = -2\sigma^2_{LL}\frac{K_\phi(\bar{r})}{\mu} + 2D_\phi(\bar{r})\bar{r}^2.$$

The differential cross section for DIC

$$\left(\frac{d\sigma}{d\theta}\right)_{\mathrm{DIC}} = 2\pi \int_{b_{\mathrm{F}}}^{b_{\mathrm{DIC}}} b\,db\,d_b(\theta).$$

$$d_b(\theta) = \frac{1}{\sqrt{2\pi\,\sigma_b^2}} \exp\left(-\frac{(\theta - \Theta_b)^2}{2\sigma_b^2}\right).$$

Master-equation

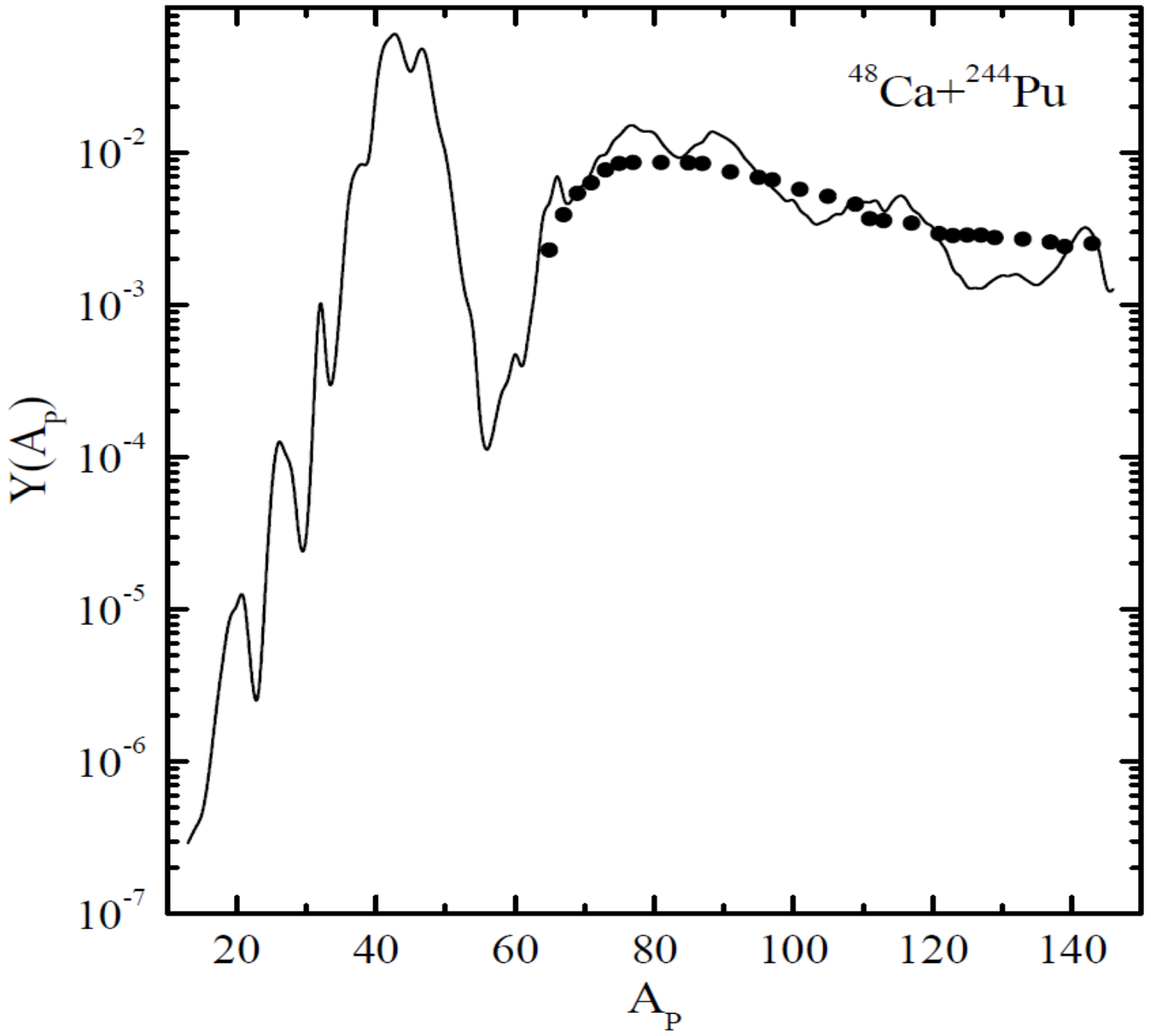
$$\begin{aligned}\frac{d}{dt}P_{Z,N}(t) &= \Delta^{(-,0)}_{Z+1,N}P_{Z+1,N}(t) + \Delta^{(+,0)}_{Z-1,N}P_{Z-1,N}(t) \\ &+ \Delta^{(0,-)}_{Z,N+1}P_{Z,N+1}(t) + \Delta^{(0,+)}_{Z,N-1}P_{Z,N-1}(t) \\ &- \left(\Delta^{(-,0)}_{Z,N} + \Delta^{(+,0)}_{Z,N} + \Delta^{(0,-)}_{Z,N} + \Delta^{(0,+)}_{Z,N}\right) P_{Z,N}(t) \\ &- (\Lambda^{qf}_{Z,N} + \Lambda^{fis}_{Z,N})P_{Z,N}(t)\end{aligned}$$

Rates Δ depend on single-particle energies and temperature related to excitation energy.

Only one-nucleon transitions are assumed.

$\Lambda^{qf}_{Z,N}$: rate for quasifission

$\Lambda^{fis}_{Z,N}$: rate for fission of heavy nucleus


$^{48}Ca+^{244}Pu$
$Y(A_P)$
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
20
40
60
80
100
120
140
A_P

Relation between master-equation and Fokker-Planck equation

In order to describe the charge distribution $P_Z(t)$ in heavy-ion collisions, where Z is the charge of one nucleus in the DNS, the following master equation is often used [23,32]:

$$\frac{dP_Z(t)}{dt} = \Delta_{Z+1}^{(-)} P_{Z+1}(t) + \Delta_{Z-1}^{(+)} P_{Z-1}(t) - [\Delta_Z^{(+)} + \Delta_Z^{(-)}] P_Z(t). \tag{16}$$

The transport coefficients $\Delta_Z^{(+)}$ and $\Delta_Z^{(-)}$ characterize the probability of transitions of a proton from the heavy nucleus to the light one ($\Delta_Z^{(+)}$) and vice versa ($\Delta_Z^{(-)}$). These coefficients can be calculated microscopically [32] or can be parameterized [23] as follows:

$$\Delta_Z^{(+)} = kg \exp\left[\frac{U(Z) - U(Z+1)}{2T}\right], \qquad \Delta_Z^{(-)} = kg \exp\left[\frac{U(Z) - U(Z-1)}{2T}\right]. \tag{17}$$

Here, $U(Z)$ (Z is a function of η) is determined by (13), $g = 2\pi R_{12} d$ is a geometrical factor ($d = 1$ fm), and the value of $k = 10^{21}$ s^{-1} fm^{-2} defines the time scale.

Let us rewrite (16) in the approximate form

$$\frac{dP_Z}{dt} = [\Delta^{(-)}_{Z+1} + \Delta^{(+)}_{Z-1} - \Delta^{(+)}_{Z} - \Delta^{(-)}_{Z}]P_Z(t)$$

$$+[\Delta^{(-)}_{Z+1} - \Delta^{(+)}_{Z-1}]\frac{dP_Z}{dZ} + \frac{1}{2}[\Delta^{(-)}_{Z+1} + \Delta^{(+)}_{Z-1}]\frac{d^2P_Z}{dZ^2}. \tag{18}$$

For large enough temperatures T we obtain the equation

$$\frac{dP_Z}{dt} = \frac{kg}{T}\frac{d}{dZ}\left[\frac{dU(Z)}{dZ}P_Z\right] + \left[kg + \frac{1}{4}\frac{kg}{T}\frac{d^2U(Z)}{dZ^2}\right]\frac{d^2P_Z}{dZ^2}, \tag{19}$$

which is of Fokker–Planck type. The comparison of (19) with the standard form of the FPE in the overdamped limit [41] gives the simple expression for $\gamma_{\eta\eta}$

$$\gamma_{\eta\eta} = \frac{T}{kg}\frac{Z_0^2}{4}, \tag{20}$$

where Z_0 is the total charge of the system. For the system ^{76}Ge + ^{170}Er and $T = 2$ MeV, we obtain $\gamma_{\eta\eta} = 2.9 \times 10^{-19}$ MeV s, which is close to the value obtained from (15). Therefore, the expression (15) can supply realistic values of the friction coefficients.

$$\gamma_{ii'} = \frac{\Gamma}{\hbar}\mu^{-1}_{ii'} \qquad (i, i' = R, \eta)$$

Generation of the random number w

Random number generators usually produce *uniformly distributed* random numbers r in the range $0 \leq r \leq 1$. One can generate Gaussian-distributed random numbers w from a set of uniformly distributed random numbers $\{r_\nu\}$ by defining (cf. Risken 1989, Section 3.6)

$$w = \sqrt{\frac{24}{M}} \sum_{\nu=1}^{M} (r_\nu - \tfrac{1}{2}), \tag{11.151}$$

where an appropriate value for M is $M = 10$. The random numbers w have mean value zero. By virtue of the central-limit theorem (cf. Reif 1965, Chapter 1), the random numbers w, being sums of random numbers, are Gaussian-distributed with mean value zero. Their distribution has a variance equal to 2,

$$\begin{aligned} \langle w^2 \rangle &= \frac{24}{M} \sum_{\nu=1}^{M} \sum_{\mu=1}^{M} \left\langle (r_\nu - \tfrac{1}{2})(r_\mu - \tfrac{1}{2}) \right\rangle \\ &= \frac{24}{M} \sum_{\nu=1}^{M} \langle (r_\nu - \tfrac{1}{2})^2 \rangle \approx \frac{24}{M} M \int_{-1/2}^{1/2} dx\, x^2 = 2. \end{aligned} \tag{11.152}$$

Another method of generating a Gaussian distribution of random numbers is to use the fact that a distribution $p_1(r)$ of a set of random variables r in an interval $a_1 \leq r \leq b_1$ is transformed into a distribution $p_2(w)$ of another set of random variables w in the interval $a_2 \leq r \leq b_2$ if in these regions the two variables are related by the equation

$$p_1(r)dr = p_2(w)dw. \tag{11.153}$$

With the uniform distribution $p_1(r) = 1$ in the interval $0 \leq r \leq 1$ we obtain a distribution $p_2(w)$ for w in another interval $a \leq w \leq b$ by solving $dr/dw = p_2(w)$ for w, which yields $w(r)$ as the inverse of

$$r = r(w) = \int_a^w p_2(w')dw'. \tag{11.154}$$

Choosing for $p_2(w)$ a normalized Gaussian function, we obtain

$$r(w) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{w} e^{-t^2/2}dt, \tag{11.155}$$

whose inverse produces the Gaussian-distributed numbers w in the interval $-\infty < w < \infty$ from the uniformly distributed numbers r in the interval $0 \leq r \leq 1$.

To satisfy the demands for the function $P(\eta, t_0)$ for $\eta > \eta_{BG}$ and in the vicinity of $\bar{\eta}$, we take $P(\eta, t_0)$ as a logistic-type function [39]

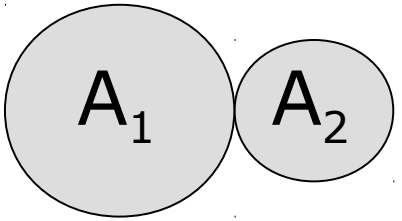
$$P(\eta, t_0) = \frac{\pi \exp\left[-\frac{\pi}{\sqrt{3}} \frac{\eta - \bar{\eta}(t_0)}{\sqrt{\chi_{\eta\eta}(t_0)}}\right]}{\sqrt{3\chi_{\eta\eta}(t_0)}\left(1 + \exp\left[-\frac{\pi}{\sqrt{3}} \frac{\eta - \bar{\eta}(t_0)}{\sqrt{\chi_{\eta\eta}(t_0)}}\right]\right)}. \tag{12}$$

This function practically coincides with the Gaussian in the vicinity of $\bar{\eta}$ and decreases exponentially for $\eta > \eta_{BG}$. We calculate the value of the fusion probability P_{CN} (Eq. (11)) by using (12). We note that a Gaussian distribution function leads to much smaller values of P_{CN} than the ones calculated with the solution of the master equation

Idea of Volkov (Dubna) to describe fusion reactions with the dinuclear system concept:

Fusion is assumed as a transfer of nucleons (or clusters) from the lighter nucleus to the heavier one in a dinuclear configuration.

This process is describable with the mass asymmetry coordinate $\eta=(A_1-A_2)/(A_1+A_2)$.



If A_1 or A_2 get small, then $|\eta|\rightarrow 1$ and the system fuses.