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Solution of a Fokker Planck Equation for Turbulent Diffusion

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Abstract

For investigations on turbulent diffusion /1/ the solution of FOKKER-PLANCK equations with convective terms is needed. In this paper we treat as a 1-dim. example the solutions of the differential equation

$$P_x = P_{ww} + (wP)_w - \frac{P_r}{V(w)} \qquad (2.1)$$

with the initial condition in x

$$P|_{x=0} = \sqrt{\frac{1}{2\pi}}\, exp(-\frac{w^2}{2})\, \delta(r) \;. \qquad (2.2)$$

Doing this, one can see:
For very large x ("far zone") as well as for very small x
P as a function of r is approximatively a GAUSS distribution.
Also the "density"

$$D = D(r;x) = 2\int_0^\infty dw\, \frac{P}{V} \qquad (2.4)$$

as a function of r is a GAUSS distribution, if x is sufficiently large. For

$$V(w) = A + w^2 \qquad (8.1)$$

the "convoluted density"

$$C(g,x) = \frac{1}{\sqrt{2\pi g}} \int_0^\infty dy\, exp\left[-\frac{y^2}{2g}\right]\left[D(y,a_+) + D(y,a_-)\right] , \qquad (8.10a)$$

with

$$a_+ = (1+A)y + x \,, \qquad b)$$

$$a_- = (1+A)y - x \,, \qquad c)$$

is given, which can be used to treat more general velocity fields (s.Ref/1/).

1. Statistical Background

Turbulent diffusion can be decoupled from the whole problem of turbulence by asking for the transition probability of a test particle within a fluid with random velocity field. Approximations on the basis of a BROWNian motion model do not seem to be adequate, especially for the limiting case of "frozen-in- turbulence" (ref/1/), i.e. a situation where the velocity field is irregular but stationary in time. It turns out, however, that the transition probabilities obey a certain kind of FOKKER-PLANCK equation (eq.(2.1) in the 1-dim case) if the velocitiy field $\mathbf{v}(\mathbf{x})$ is modelled by a nonlinear map of a WIENER or ORNSTEIN-UHLENBECK process, e.g. for one dimension one has

$$V(w) = A + w^2 ;$$

see.eq.(8.1).

There is considerable interest in the solution of this equation , which may play a dominant role in understanding the main difference between turbulent diffusion and ordinary BROWNian motion. The results can be extended from the previously treated frozen-in case to a wider class of non-stationary processes, as given in eqs.(8.10)-(8.13).

Aknowledgements

For helpful discussions I thank the Drs. D.PFIRSCH and P.GRAEFF, who has written the sec. "statistical background".

2. Problem

We have to find the solution $P = P(r; w; x)$ of the partial differential equation

$$P_x = P_{ww} + (wP)_w - \frac{P_r}{V(w)} \tag{2.1}$$

with the initial condition in x

$$P|_{x=0} = \sqrt{\frac{1}{2\pi}}\, exp(-\frac{w^2}{2})\, \delta(r) \tag{2.2}$$

where r, w, x are the independent variables;

$V(w)$ is a function that can be chosen almost arbitrarily: the restriction "almost" denotes that the integrals (2.4) and (4.6) must remain finite.

V and P are symmetric in w:

$$V(-w) = V(+w) \tag{2.3}$$

$$P(-w) = P(+w)$$

From P we have to form the "density integral"

$$D = D(r; x) = 2\int_0^\infty dw\, \frac{P}{V} \tag{2.4}$$

and other integrals given in eq.(4.9) and (8.10-13).

The initial condition (2.2) obliges us to introduce a function F with the definition

$$P = \sqrt{\frac{1}{2\pi}}\, exp(-\frac{w^2}{2})\, F \tag{2.5}$$

From eq.(2.1) we than have

$$F_x = F_{ww} - wF_w - \frac{F_r}{V} \tag{2.6}$$

and from eq.(2.2) the initial condition

$$F|_{x=0} = \delta(r)\,. \tag{2.7}$$

3. Basic Equations

In this section we write down the general equations required for representing the solution; proofs and explanations are left aside till Appendix.

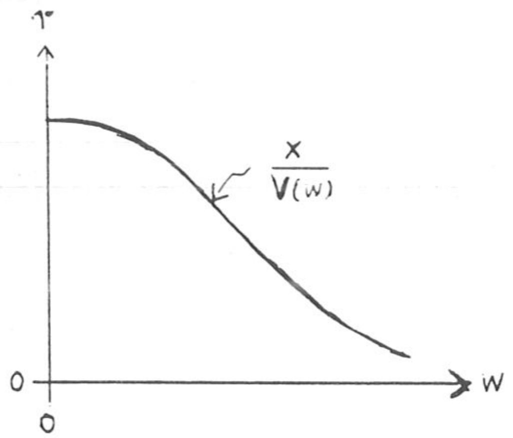


FIG. 3-1

For very small x one gets approximately

$$F = \delta(r - \tfrac{x}{V}) \,. \tag{3.1}$$

(PFIRSCH's approximation - see Sec. 6).

If x is interpreted as "time", eq. (3.1) describes a single wave front with maximum at

$$r = \tfrac{x}{V} \tag{3.2}$$

which propagates in the positive x-direction (see FIG. 3.1).

The term with $\partial^2/\partial w^2$ in eq.(2.6) generally causes the wave front (3.1) to spread in the course of "time" x, leaving

$$\int_{-\infty}^{\infty} F \, dr = 1 \quad \text{for all} \quad x, w. \tag{3.3}$$

F (as a function of r) may therefore be interpreted as the distribution of a random variable r, and one may use the formulae of, for example, M. Fisz (Ref. /3/). According to Ref. /3/ it follows from $\int F dr = 1$ that there exists an expansion

$$ln \, \Phi = \sum_{n=1} \frac{(i\lambda)^n}{n!} \kappa_n \tag{3.4}$$

for the FOURIER transform

$$\Phi = \Phi(\lambda; w; x) = \int_{-\infty}^{\infty} dr \; F(r; w; x) \; e^{i\lambda r} \quad , \tag{3.5}$$

where the

$$\kappa_n = \kappa_n(w, x)$$

are the semi-invariants. Equations (3.4+5) are equivalent to

$$F = \frac{1}{\sqrt{2\pi\kappa_2}}\, exp(-\frac{Z^2}{2})\left[1 + \sum_{n=3}^{\infty} k_n He_n\right] \tag{3.6a}$$

with

$$Z = (r - \kappa_1)/\sqrt{\kappa_2} \tag{b}$$

$$k_n = \kappa_n/[n!\ \kappa_2^{n/2}] \tag{c}$$

$$He_0 = 1 \tag{d}$$

$$He_1 = Z$$

$$He_2 = Z^2 - 1$$

$$He_3 = Z^3 - 3Z$$

$$He_4 = Z^4 - 6Z^2 + 3$$

He_n= HERMITE polynomial of order n with normalization

$$\int_{-\infty}^{\infty} dZ\ exp(-\frac{z^2}{2})\ He_L\ He_M = \sqrt{2\pi}L! \qquad for\ L = M$$

The integral vanishes for $L \neq M$.

The semi-invariants κ_n are given by the differential equations

$$\kappa_{1,x} = \kappa_{1,ww} - w\ \kappa_{1,w} + \frac{1}{V} \tag{3.7a}$$

$$\kappa_{2,x} = \kappa_{2,ww} - w\ \kappa_{2,w} + 2\kappa_{1,w}^2 \tag{b}$$

$$\kappa_{3,x} = \kappa_{3,ww} - w\ \kappa_{3,w} + 6\kappa_{1,w}\kappa_{2,w} \tag{c}$$

$$\kappa_{4,x} = \kappa_{4,ww} - w\ \kappa_{4,w} + 8\kappa_{1,w}\kappa_{3,w} + 6\kappa_{2,w}^2 \tag{d}$$

$$\kappa_{n,x} = \kappa_{n,ww} - w\ \kappa_{n,w} + \sum_{m=1}^{n-1} \frac{n!}{m!(n-m)!}\kappa_{m,w}\kappa_{n-m,w} \tag{e}$$

with the initial condition

$$ln\Phi|_{x=0} = \kappa_n|_{x=0} = 0; \quad n \geq 1\ . \tag{3.8}$$

Every κ_n is determined by a linear inhomogenous equation because in the n-th equation the κ_m's with $m \leq n-1$ are already known. For $n = 1$ the inhomogeneity is given by the function V from eq.(2.1).

The homogeneous equation is of the type

$$h_x = h_{ww} - w h_w \tag{3.9a}$$

and has the solution

$$h = \int_{-\infty}^{\infty} dv \, \frac{G(v)}{2\sqrt{\pi\eta}} \, exp\left[-\frac{(v-\xi)^2}{4\eta}\right] \qquad b)$$

with

$$\xi = w e^{-x} \qquad c)$$

$$\eta = \frac{1}{2}\left[1 - e^{-2x}\right] \qquad d)$$

(PFIRSCH transform).

$G(v)$ is a arbitrarily choosable function. For large x we have

$$\xi = 0. \qquad f)$$

$$\eta = \frac{1}{2} \qquad g)$$

It follows that for large x

$$h = const. \qquad h)$$

The density D (see eq.(2.4)) satisfies the conservation laws

$$\int_0^{\infty} dr \, D(r,x) = c_1 \tag{3.10}$$

$$\int_0^{\infty} dx \, D(r,x) = 1. \tag{3.11}$$

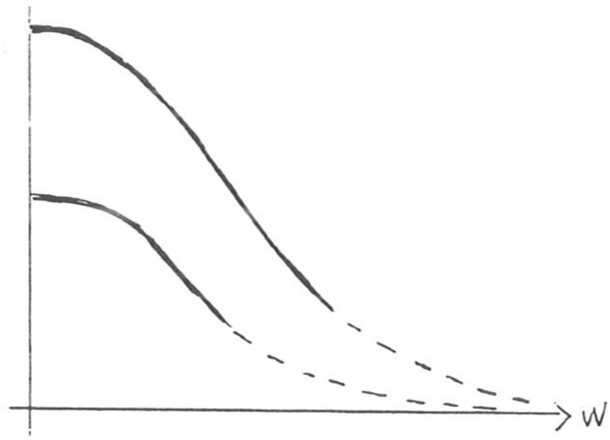
with

$$c_1 = \sqrt{\frac{2}{\pi}} \int_0^{\infty} dv \, \frac{exp(-\frac{v^2}{2})}{V(v)} \, . \tag{3.12}$$

Template Model for Large x

With sufficiently large x and w, the semi-invariants κ_n separate into a term which grows linearly as x and does not depend on w, and a term which only depends on w:

$$\kappa_n(w, x) \;=\; c_n x \;+\; S_n(w) \tag{4.1}$$



If x is interpreted as "time", κ_n behaves like a template, which in the w-diagram in FIG. 4.1 is pulled upwards with constant velocity, hence the name "template model".

FIG. 4-1

κ_n versus w for two x-values $x_2 \geq x_1$, schematic.

Solid curve: template solution (4.1) valid.

Dashed curve: template solution (4.1) not valid.

In the case $n = 1$ we can understand the template behaviour as follows: Equation (4.1) exactly solves the differential equation (3.7a) for κ_1, but not for the desired boundary condition $\kappa_1|_{x=0} \;=\; 0$. We now write the exakt solution which is valid for all x in the form

$$\kappa_1 \;=\; c_1 x \;+\; S_1 \;+\; h \quad , \tag{4.2}$$

where h is the homogeneous solution (3.9) with $G(v) \;=\; -S_1(v)$. Equation (4.2) solves the differential equation (3.7a) exactly for the boundary condition $\kappa_1|_{x=0} \;=\; 0$. Large x results in

$$\xi \rightarrow 0$$

$$\eta \rightarrow 1/2$$

and hence $h \to const,$

which shows that the template solution (4.1) for large x is a good approximation. For the case $n \geq 2$ we require the differential equations for the $S_n(w)$. Substituting the template solution (4.1) in the partial differential equations (3.7) yields

$$c_1 = S_1'' - wS_1' + \frac{1}{V} \tag{4.3a}$$

$$c_2 = S_2'' - wS_2' + 2S_1'^2 \tag{b}$$

$$\dots$$

$$c_n = S_n'' - wS_n' + \sum_{m=1}^{n-1} \frac{n!}{m!(n-m)!} S_m' S_{n-m}' \ , \tag{c}$$

with

$$S_m' = \frac{d}{dw} S_m \quad . \tag{d}$$

The solution according to KAMKE (see Ref. /4/) is

$$S_1' = exp(\frac{w^2}{2}) \int_0^w dv\ exp(-\frac{v^2}{2}) \left[c_1 - \frac{1}{V}\right] , \tag{4.4a}$$

$$S_2' = exp(\frac{w^2}{2}) \int_0^w dv\ exp(-\frac{v^2}{2}) \left[c_2 - 2S_1'^2\right] , \tag{b}$$

$$\dots$$

$$S_n' = exp(\frac{w^2}{2}) \int_0^w dv\ exp(-\frac{v^2}{2}) \left[c_n - \sum_{m=1}^{n-1} \frac{n!}{m!(n-m)!} S_m' S_{n-m}'\right] . \tag{c}$$

We now postulate something which, though plausible, is somewhat arbitrary:
S_n' must not grow proportionally to $exp(+w^2/2)$ for large w.
It thus follows that the integrals on the right-hand side of eq. (4.4) have to vanish for $w \to \infty$

$$c_1 = \sqrt{\frac{2}{\pi}} \int_0^\infty dv\ exp(-\frac{v^2}{2}) \quad \frac{1}{V(w)} , \tag{4.6a}$$

$$c_2 = \sqrt{\frac{2}{\pi}} \int_0^\infty dv\ exp(-\frac{v^2}{2}) \quad 2S_1'^2 , \tag{b}$$

$$\dots$$

$$c_n = \sqrt{\frac{2}{\pi}} \int_0^\infty dv\, exp(-\frac{v^2}{2}) \quad \sum_{m=1}^{n-1} \frac{n!}{m!(n-m)!} S'_m S'_{n-m} \ . \qquad \text{(c)}$$

We learn from eq. (4.6) that $V(w)$ must be so constituted that the integrals (4.6) remain finite.

We can now prove for $n \geq 2$ as well that the semi-invariants for large x are of the template type (4.1): In the case $n= 2$ we consider, besides the original differential equation (3.7b), the solution a_2 for the diff. eq.:

$$a_{2,x} = a_{2,ww} - w\, a_{2,w} + 2S^2_{1,w} \qquad (4.7)$$

a_2 is of the template type, because it is obtained from κ_1 simply by replacing $V(w)$ by another function of w.

For large x one gets

$$\kappa_{1,w} \rightarrow S_{1,w}$$

so that the homogeneous equation (3.9a) is valid for the difference $\kappa_2 - a_2$. The solution acc.to eq.(3.9h)is

$$\kappa_2 - a_2 = const \ ,$$

irrespective of the initial condition. Eq.(4.1) is thus also valid for the case n=2 and analogous for $n \geq 3$.

Eq.(4.4) gives the first derivatives S'_n, but this makes S_n known except for an additive constant. The latter is defined by the requirement that

$$\kappa_n = c_n x + S_n \qquad (4.1)$$

be satisfied as well as possible, where κ_n on the left-hand side denotes the exact solution of the partial differential eq.(3.7) and the right-hand side is the asymptotic approximation for large x.

It follows that

$$\int_0^\infty dw\ S_1\ exp(-\frac{w^2}{2}) = 0 \tag{4.8a}$$

$$\int_0^\infty dw\ S_2\ exp(-\frac{w^2}{2}) = \left[\frac{1}{2}\ t^2\ - \sqrt{\frac{\pi}{2}}\ c_2 x\right]_{x\to\infty} \tag{b}$$

$$t^2 = 2\int_0^\infty dw\ \kappa_2\ exp(-\frac{w^2}{2}) \tag{4.9}$$

t^2 has to be calculated numerically from the exact κ_2 - see, for example, FIG.8-6 - and has nothing to do with the template model.

5. Far Zone

The far zone is the x region in which the term S_n in the template solution

$$\kappa_n = c_n\, x + S_n(w) \qquad s.(4.1)$$

can be neglected in relation to $c_n x$: this leaves

$$\kappa_n = c_n\, x\,. \qquad (5.1)$$

Substituting eq.(5.1) in the semi-invariant expansion (3.6) yields

$$k_3 \; prop \; x^{-0.5}\,, \qquad (5.2a)$$

$$k_4 \; prop \; x^{-1}\,, \qquad (5.2b)$$

....

$$F = \frac{1}{\sqrt{2\pi c_2 x}}\, exp\Big[- \frac{(r - c_1 x)^2}{2 c_2 x} \Big]\,. \qquad (5.3)$$

In the far zone F as a function of r is a GAUSSian distribution which is (almost) independent of w.

Calculating the density integral (2.4) one may therefore put F in front of the integral to yield

$$D = 2 \int_0^\infty dw\, \frac{F}{V} \sqrt{\frac{1}{2\pi}}\; exp(-\frac{w^2}{2}) \qquad (2.4)+(2.8)$$

$$D = F\, c_1 \qquad (4.6a)$$

$$D = \frac{c_1}{\sqrt{2\pi c_2 x}}\, exp\Big[- \frac{(r - c_1 x)^2}{2 c_2 x} \Big]\,. \qquad (5.4)$$

D, too, is a GAUSSian distribution; $F$and D are completely determined in the far zone by specifying c_1 and c_2 in eqs. (4.6a,b).

6. Near Zone

The near zone is the x region in which PFIRSCH's approximation (3.1) is valid. The δ symbol in eq.(3.1) denotes a continuously differentiable function of the type (3.6) whose width $\sqrt{\kappa_2}$ is very small compared with the location κ_1 of the maximum:

$$\sqrt{\kappa_2} << \kappa_1 \; . \tag{6.1}$$

In order to show this for small x, let us consider the differential equations (3.7) for the semi-invariants κ_n. The terms

$$\kappa_{n,ww} \quad - \quad w \; \kappa_{n,w}$$

are one order smaller than $\kappa_{n,x}$, if x is sufficiently small. In the near zone one can therefore neglect $\kappa_{n,ww} - w\kappa_{n,w}$ and integrate the differential equations (3.7). This yields

$$\kappa_n \quad prop \quad x^{2n-1} \; . \tag{6.2}$$

From eq.(6.2) it follows that the above-mentioned ratio of width to location of the maximum

$$\frac{\sqrt{\kappa_2}}{\kappa_1} \quad prop \quad \sqrt{x} \tag{6.3}$$

goes to zero with x, thus proving PFIRSCH's ansatz (3.1). Furthermore, the factors k_n in the expansion (3.6) also tend to zero with x, as can be seen from eq.(6.2), leaving the GAUSS distribution

$$F \;=\; \frac{1}{\sqrt{2\pi\kappa_2}} exp(-\frac{(r-\kappa_1)^2}{2\;\kappa_2}) \tag{6.4}$$

in the near zone as well as in the far zone.

The proportionality factor in eq.(6.2) rapidly increases with n; in the Appendix, eq.(A.13), we give an example.

Finally, let us calculate the density integral (2.4) for very small x. According to eq.(2.4+5) one has

$$D = \sqrt{\frac{2}{\pi}} \int_0^\infty dw \, \frac{F}{V} \, exp(-\frac{w^2}{2}) \, . \qquad (6.5)$$

We introduce PFIRSCH's ansatz (3.1) into eq.(6.5),

define $\hat{w}$ by $$\kappa_1(\hat{w}) = r,$$

expand $$\kappa_1 - r = \kappa_{1,w}(\hat{w}) \cdot (w - \hat{w})$$

and get

$$D = \sqrt{\frac{2}{\pi}} \frac{exp(-\hat{w}^2/2)}{V(\hat{w}) \, \kappa_{1,w}(\hat{w})} \, , \qquad (6.6)$$

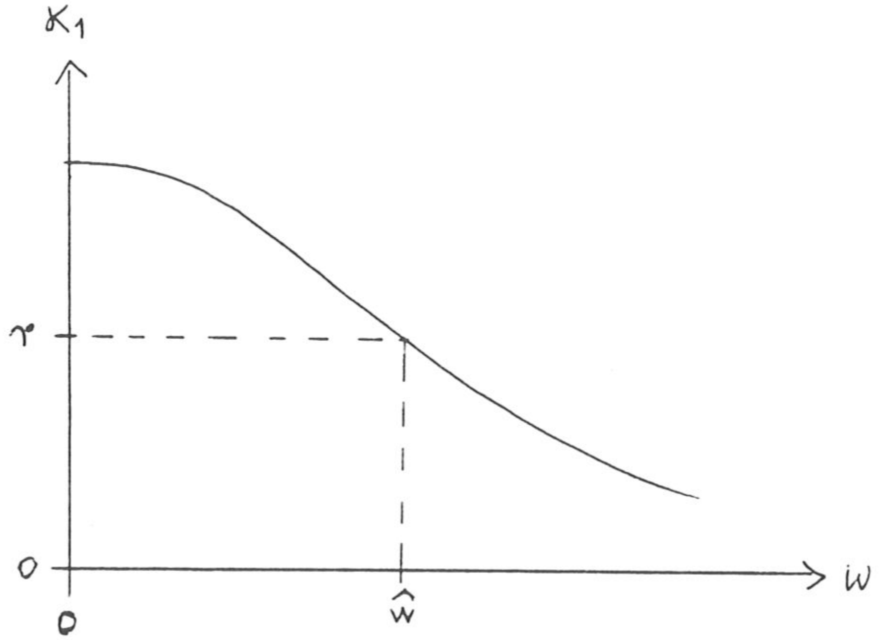
see example in eq.(8.9).

FIG.6-1

κ_1 versus w

with r and $\hat{w}$

schematic



7. The example V = const

In the case

$$V = const \tag{7.1}$$

one has PFIRSCH's solution

$$F = \delta(r - \frac{x}{V}) \qquad s.(3.1)$$

for all x.

The maximum is located at

$$r = \kappa_1 = \frac{x}{V}\ ; \tag{7.2}$$

the moments are

$$m_n = \kappa_1^n \quad n \geq 1\ ; \tag{7.3}$$

the semi-invariants are

$$\kappa_1 = x/V \qquad s.(7.2)$$

$$\kappa_n = 0 \quad n \geq 2\ ; \tag{7.4}$$

the density integral (2.4) is

$$D = 2 \int_0^\infty dw\ \frac{P}{V} = \frac{1}{V}\ \delta(r - \frac{x}{V})\ , \tag{7.5}$$

and the FOURIER transform is

$$\Phi = exp(-i\kappa_1\lambda)\ . \tag{7.6}$$

If λ is interpreted as "time", the real and imaginary parts of Φ behave like the two coordinates of a 2-Dim pendulum moving on the unit circle with constant angular frequency. If V is allowed to be dependent on w, the motion is damped due to $\kappa_2 > 0$ and the pendulum spirals inwards; see FIG.8-1.

8. Numerical examples

In this section the formulae and results are applied to the case

$$V = 1/(A + w^2) \quad ; \quad A \leq 1 . \tag{8.1}$$

If analytical results were not available, we carried out numerical computations. From these we learn that, approximately,

sec.6 for the near zone is valid for $0 \leq x \leq 0.5A$;

sec.4 for the template model is valid for $x \geq 0.5(1 + |w|)$;

sec.5 for the far zone is valid for $x \geq 3/\sqrt{A}$.

The range of validity is chosen somewhat arbitrarily; for example, eq.(8.13) for the convoluted density in the far zone can also be used for small x-values; see FIG.8-8. From this rough survey we learn that there is a "middle x region" between the near zone and the range of validity of the template model. In this "middle x region" the semi-invariant expansion (3.6) is of no use and we computed F from the FOURIER transform Φ by back transformation:

$$F = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\lambda \; \Phi \; e^{-i\lambda r} \; ;$$

see FIGs.8-1; 8-2; 8-3.

In the following we present

in FIG.8-1 the FOURIER transform Φ , which behaves like a damped 2-Dim pendulum if λ is interpreted as "time";

in FIG.8-2 and 8-3 examples of F(r) at various w values;

in FIG.8-4 and 8-5 the semi-invariants κ_1 and κ_2 according to the template model;

in FIG.8-6 the quantity t^2 , as defined in eq.(4.9) , versus x;

in FIG.8-7 the density integral (2.4) and, finally,

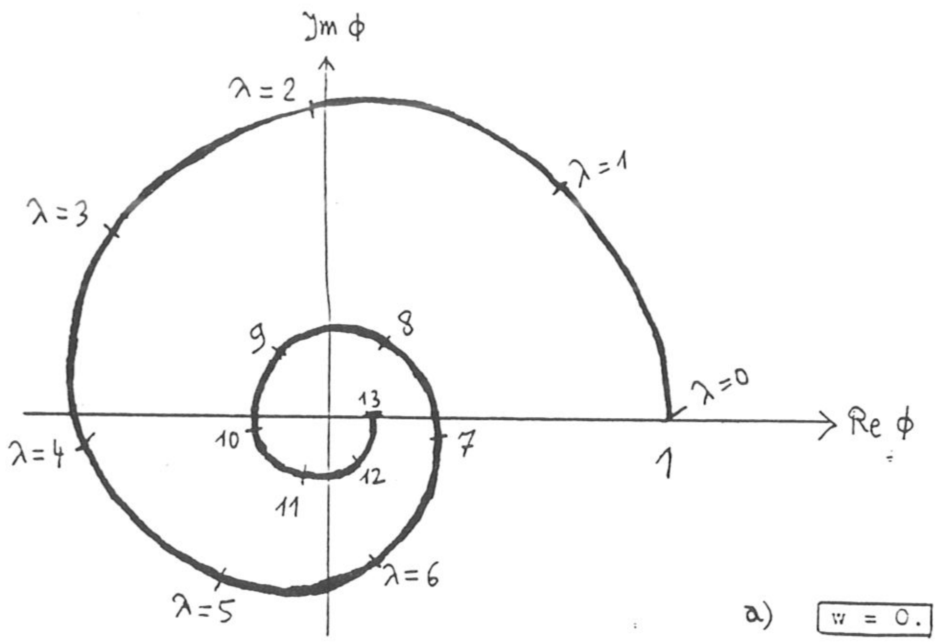
in FIG.8-8 the convoluted density C according to eq.(8.13).

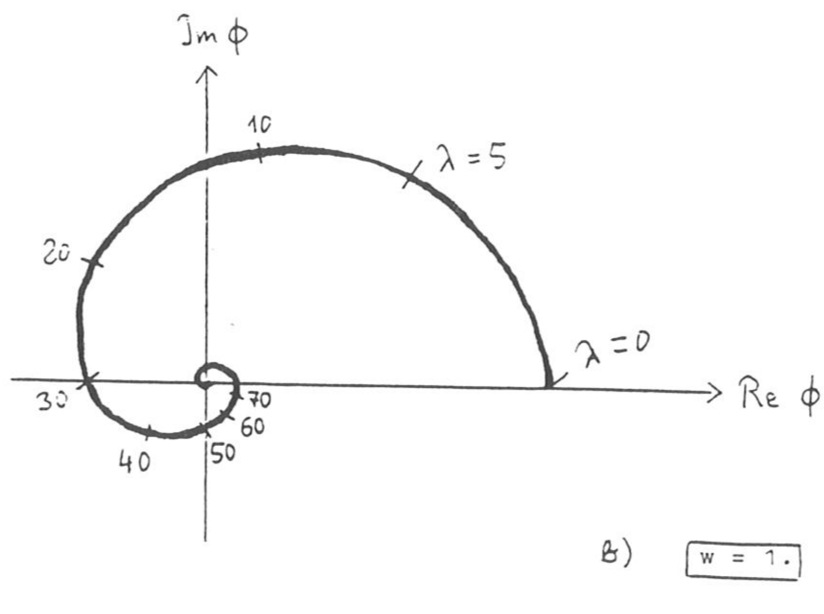
The FOURIER Transform

FIG.8-1

Φ versus λ

for $A = 0.1$ and $x = 0.12$





Next we present three examples for F.

$F(r)$ is asymmetric:

in the case w $= 0$ the third semi-invariant κ_3 is negative;

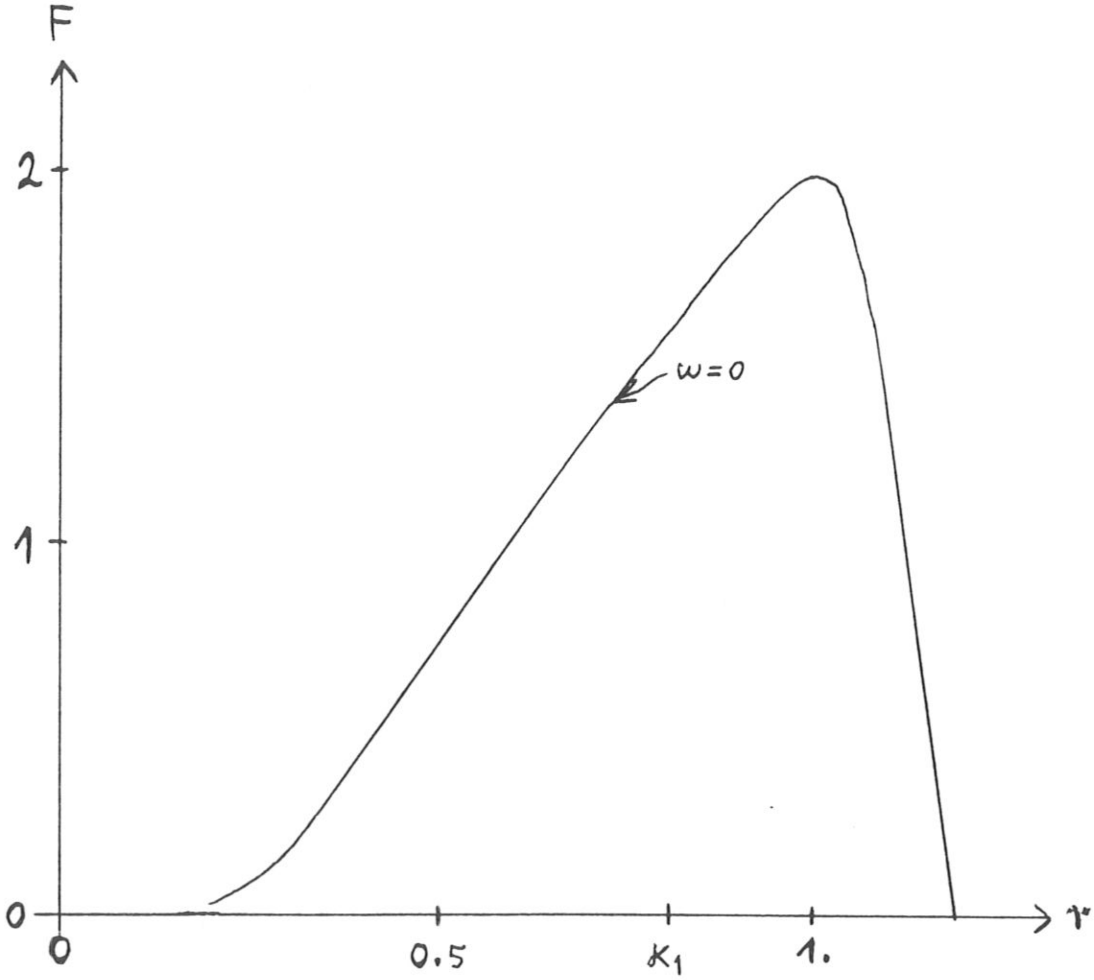
in the case $w \geq 1$ the third semi-invariant κ_3 is positive;

the maximum is shifted accordingly away from κ_1.

FIG. 8-2

F versus r, numerical

for **A** $= 0.1$ and x $= 0.12$



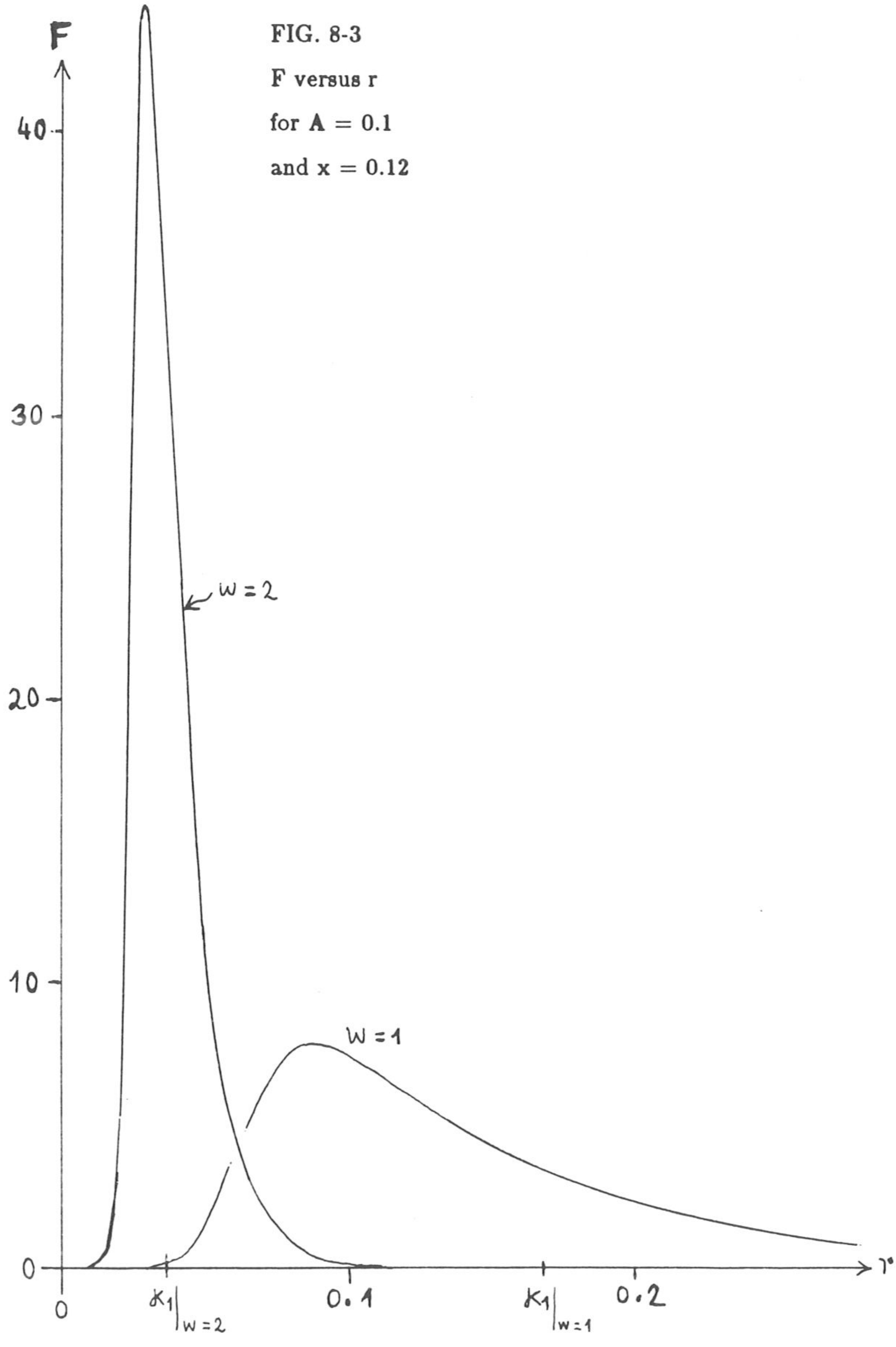


FIG. 8-3
F versus r
for **A** = 0.1
and x = 0.12

The examples shown in FIGs. 8-1 to 8-3 are taken from a "medium" x range in which the semi-invariant expansion (3.6) is useless. F then has to be calculated from the FOURIER transform Φ by back transformation

$$F = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\lambda \, \Phi \, e^{-i\lambda r} \quad .$$

As x increases - roughly for $x \geq 0.5(1+|w|)$ - the template model gradually becomes usable; examples are presented in FIGs. 8-4 and 8-5. Table 8-4 shows c_1 versus A according to eq. (4.6a). The integration in eq. (4.6a) can be performed analytically for $V = A + w^2$; according to Ref. /2/ one has

$$c_1 = \sqrt{\frac{\pi}{2A}} \; exp\left(\frac{A}{2}\right) \; erfc\left(\sqrt{\frac{A}{2}}\right) \tag{8.2a}$$

with

$$erfc(y) = \frac{2}{\sqrt{\pi}} \int_{y}^{\infty} e^{-t^2} \, dt. \tag{b}$$

The derivative of the template solution for n = 1 converges for small A towards the envelope

$$\left.\frac{S_1'}{c_1}\right|_{A\to 0} = -\sqrt{\frac{\pi}{2}} \; erfc\left(\frac{w}{\sqrt{2}}\right) \; exp\left(\frac{w^2}{2}\right) \; . \tag{8.3a}$$

For large w one gets

$$\left.\frac{S_n'}{c_n}\right|_{w\to\infty} = -\frac{1}{w} \tag{b}$$

not only for n = 1, but also for arbitrary n, because the differential equation (4.3) reduces to $c_n = -w \; S_n'$ for large w. Equation (8.3) is important for the numerical calculations: S_n' has to be specified for a large w value (*e.g.* $S_n' = -1/8$ *at* $w = 8$.) and calculated back. If one were to start at w = 0 and calculate forward, i.e. in the positive w direction, the numerical solution would run away proportionally to exp $(w^2/2)$ roughly as of $w \geq 3$ (see eq. (4.4)).

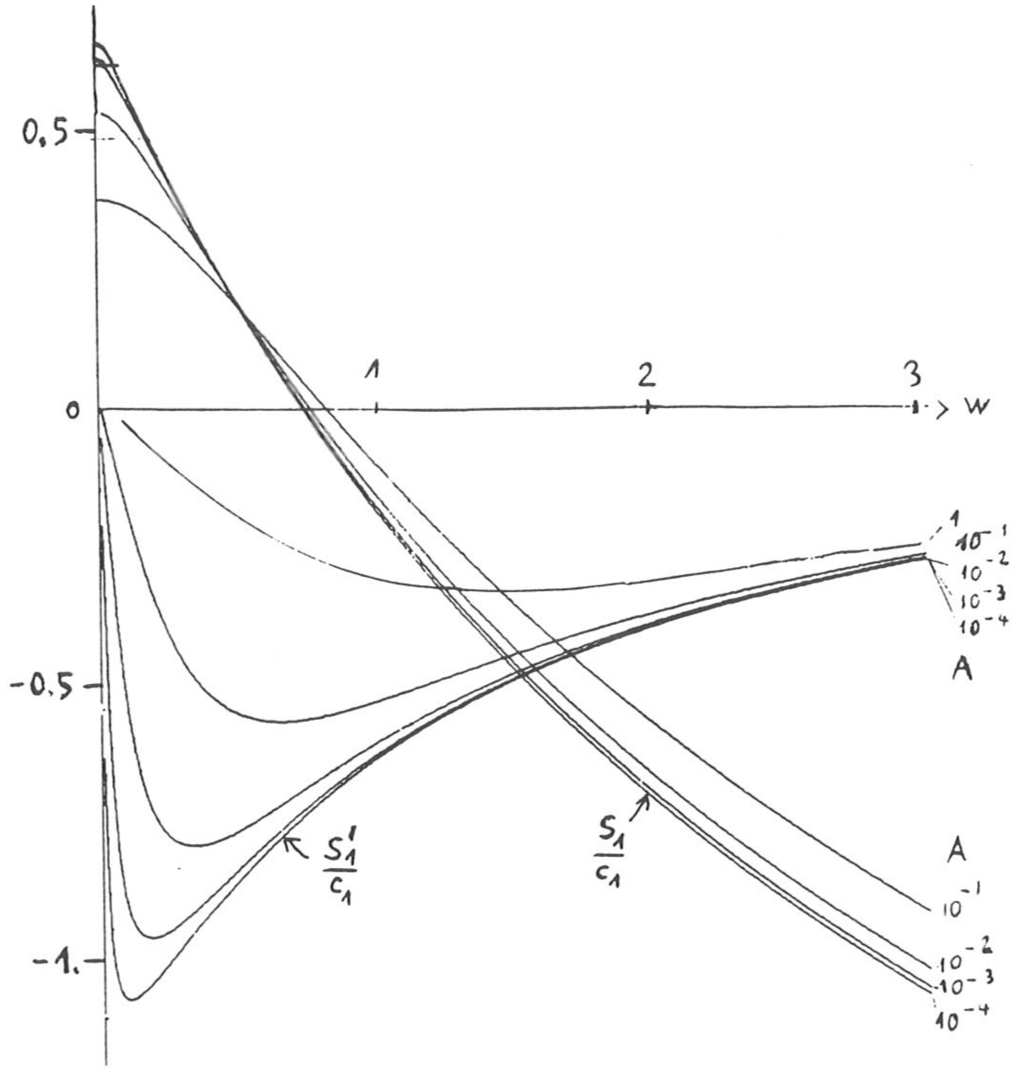


FIG.8-4

$\frac{S_1}{c_1}$ **and** $\frac{S_1'}{c_1}$ **versus w for five A-values**

Tab.8-4	A	$c_1 = \sqrt{\frac{\pi}{2A}}\, exp(\frac{A}{2})\, erfc(\sqrt{\frac{A}{2}})$
c_1 **versus** A	10^{-4}	124.3
	10^{-3}	38.65
	10^{-2}	11.59
	10^{-1}	3.153
	1	0.6557

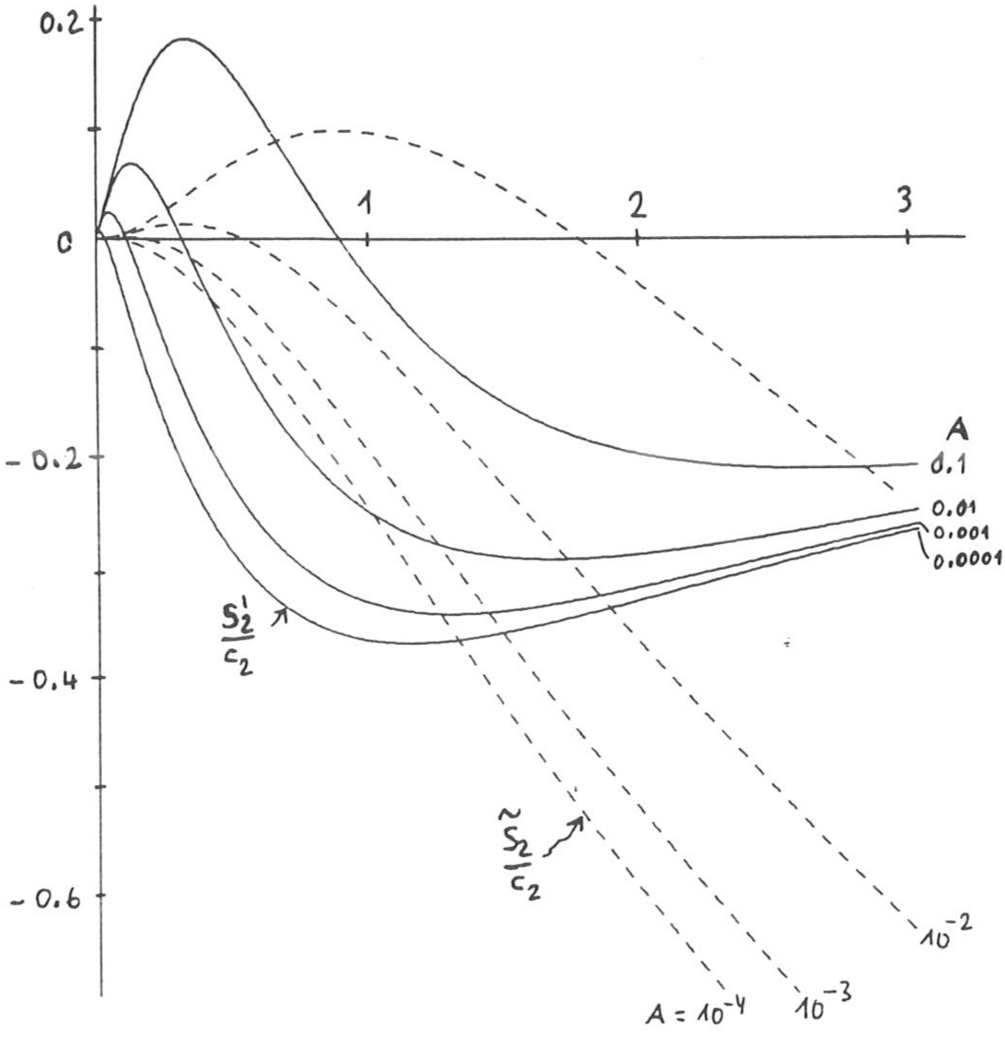


FIG.8-5

$\frac{\tilde{S}_2}{c_2}$ and $\frac{S_2'}{c_2}$ versus w for five A-values; $\tilde{S}_2 = S_2 - S_2|_{w=0}$

Tab.8-5	A	c_2	$S_2\|_{w=0}$
c_2 versus A	10^{-4}	19615.	4500.
	10^{-3}	1678.	440.
	10^{-2}	115.	46.
	10^{-1}	4.66	3.0
	1	0.0573	0.11

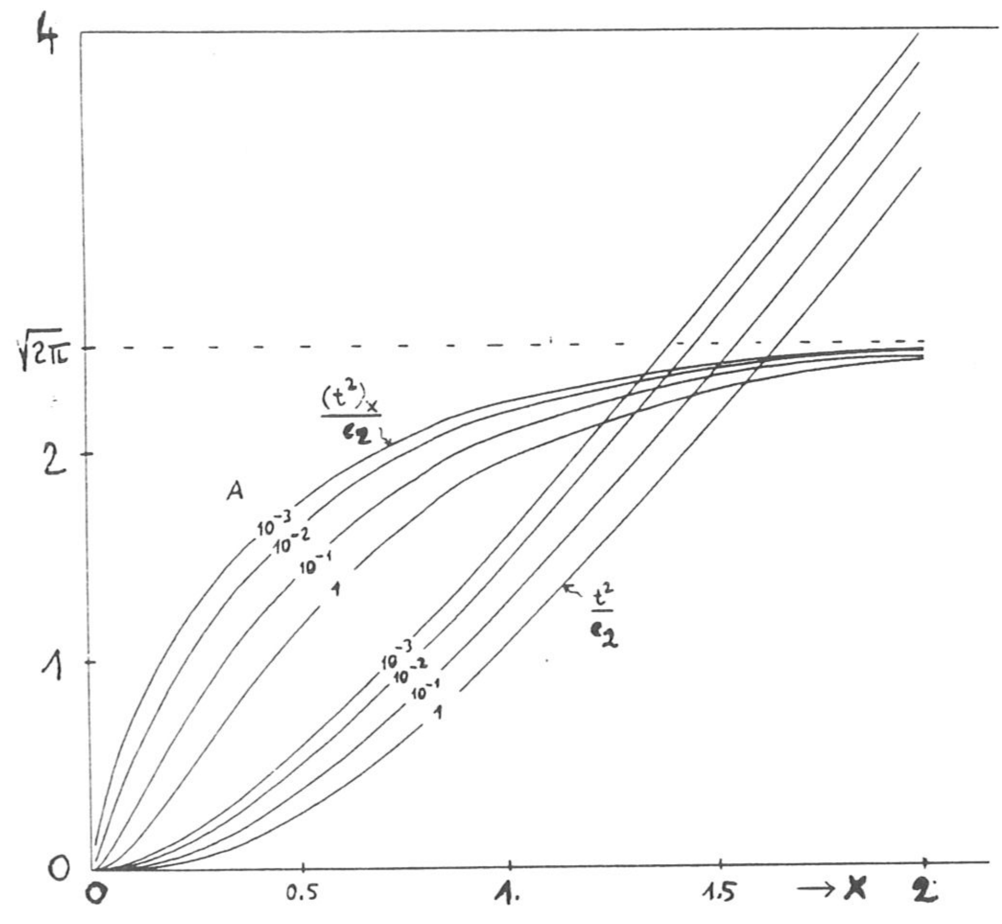
We now present in Fig. 8-6 numerical calculations of t^2 and $(t^2)_x = \frac{\partial}{\partial x}(t^2)$ for $V(w) = A + w^2$.

For large x one gets

$$\left(t^2\right)_x = \sqrt{2\pi}\, c_2. \tag{8.6}$$

FIG.8-6

t^2/c_2 and $\left(t^2\right)_x/c_2$ versus x



Density

First let us consider extremely small x. We transform eq. (6.6) for the case

$$V = A + w^2 \qquad s. (8.1)$$

and obtain

$$\kappa_1 = \frac{x}{A + w^2}$$

$$\hat{w} = \sqrt{\frac{x}{r} - A}$$

$$D = \sqrt{\frac{1}{2\pi}} \frac{exp\,[\frac{1}{2}(A - \frac{x}{r})]}{r\sqrt{\frac{x}{r} - A}} \quad .$$

This equation is only valid if r is also small,

$$r < \frac{x}{A} \quad ,$$

so that the root is real.

For an imaginary root,

$$r > \frac{x}{A} \quad or\ r < 0 \qquad (8.7)$$

one has according to GRAEFF

$$D = 0.$$

If one introduces

$$\tilde{D} = x\ D\ instead\ of\ D\ , \qquad (8.8a)$$

$$y = \frac{r}{x}\ instead\ of\ r \quad , \qquad b)$$

one obtains

$$\tilde{D} = \sqrt{\frac{1}{2\pi}} \frac{exp[\frac{1}{2}(A - \frac{1}{y})]}{y\sqrt{\frac{1}{y} - A}} \quad . \qquad (8.9)$$

In the near zone $\tilde{D}$ depends on the coordinates r, x via y only. If x is allowed to grow, $\tilde{D}$ remains of the order of unity till about $x \leq 2$, so that densities can readily be compared for various x-values in the y-$\tilde{D}$ diagram.

Figure 8-7 shows examples of the density integral (2.4); the curves for x = 0.01, 0.1 and 1 were calculated numerically; the curve marked by eq. (8.9) was calculated according to eq. (8.9).

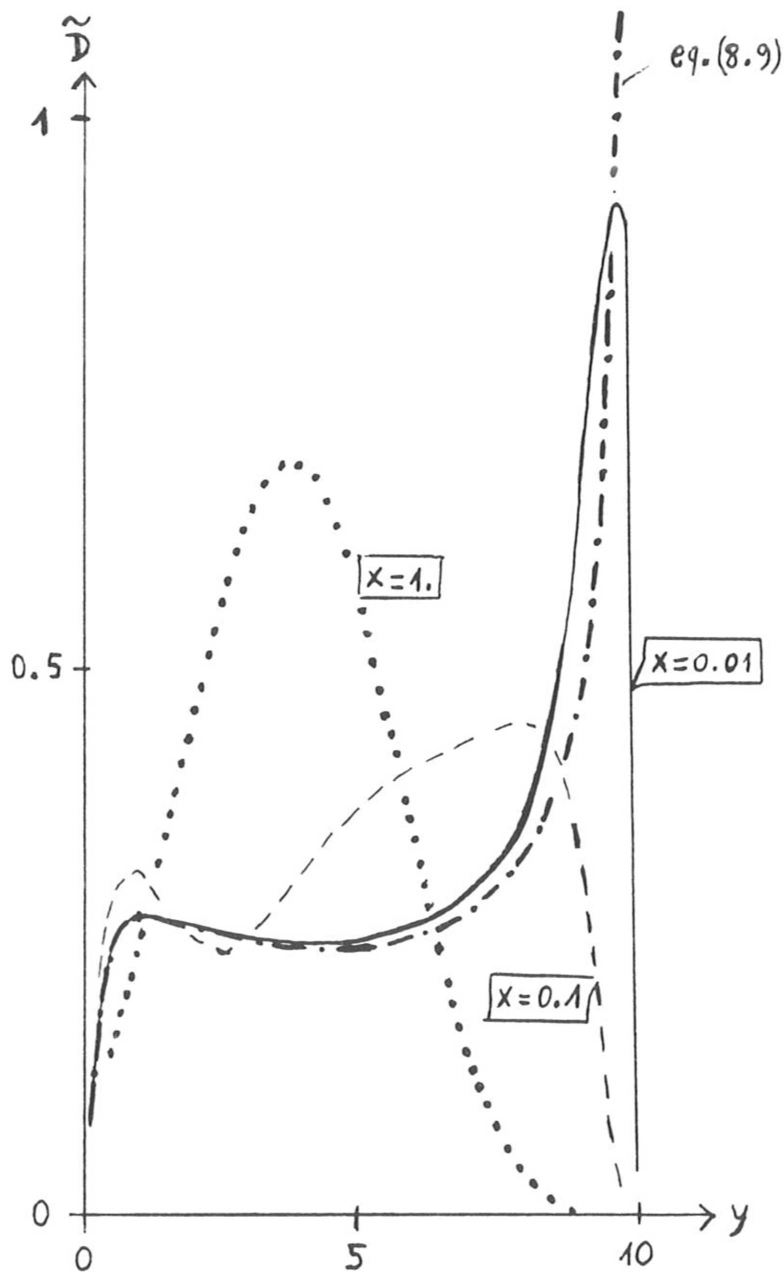
FIG.8-7

$\tilde{D} = xD$

versus

$y = r/x$

for $A = 0.1$



Convoluted Density

If $V = A + w^2$ is valid (see eq. (8.1)), one can form the "convoluted density"

$$C(g,x) = \frac{1}{\sqrt{2\pi g}} \int_0^\infty dy \; exp\left[-\frac{y^2}{2g}\right]\left[D(y,a_+) + D(y,a_-)\right] , \tag{8.10a}$$

where

$$a_+ = (1+A)y + x , \tag{b)}$$

$$a_- = (1+A)y - x , \tag{c)}$$

and

$$D(r,x) = 0 \quad for \quad r \le 0 \quad and/or \quad x \le 0. \tag{d)}$$

C is symmetric in x:

$$C(g,-x) = C(g,x) . \tag{8.11}$$

C satisfies the conservation law

$$\int_0^\infty dx \; C(g,x) = \frac{1}{2}. \tag{8.12}$$

For very large x, i.e. in the "far zone" (see Sec. 5), the integration can be performed approximately; it follows that

$$C = \frac{1}{\sqrt{2\pi\hat{g}}} \, exp\left(-\frac{x^2}{2\hat{g}}\right) , \tag{8.13a}$$

with

$$\hat{g} = \left[1 + A - \frac{1}{c_1}\right]^2 g \tag{b)}$$

(see Appendix).

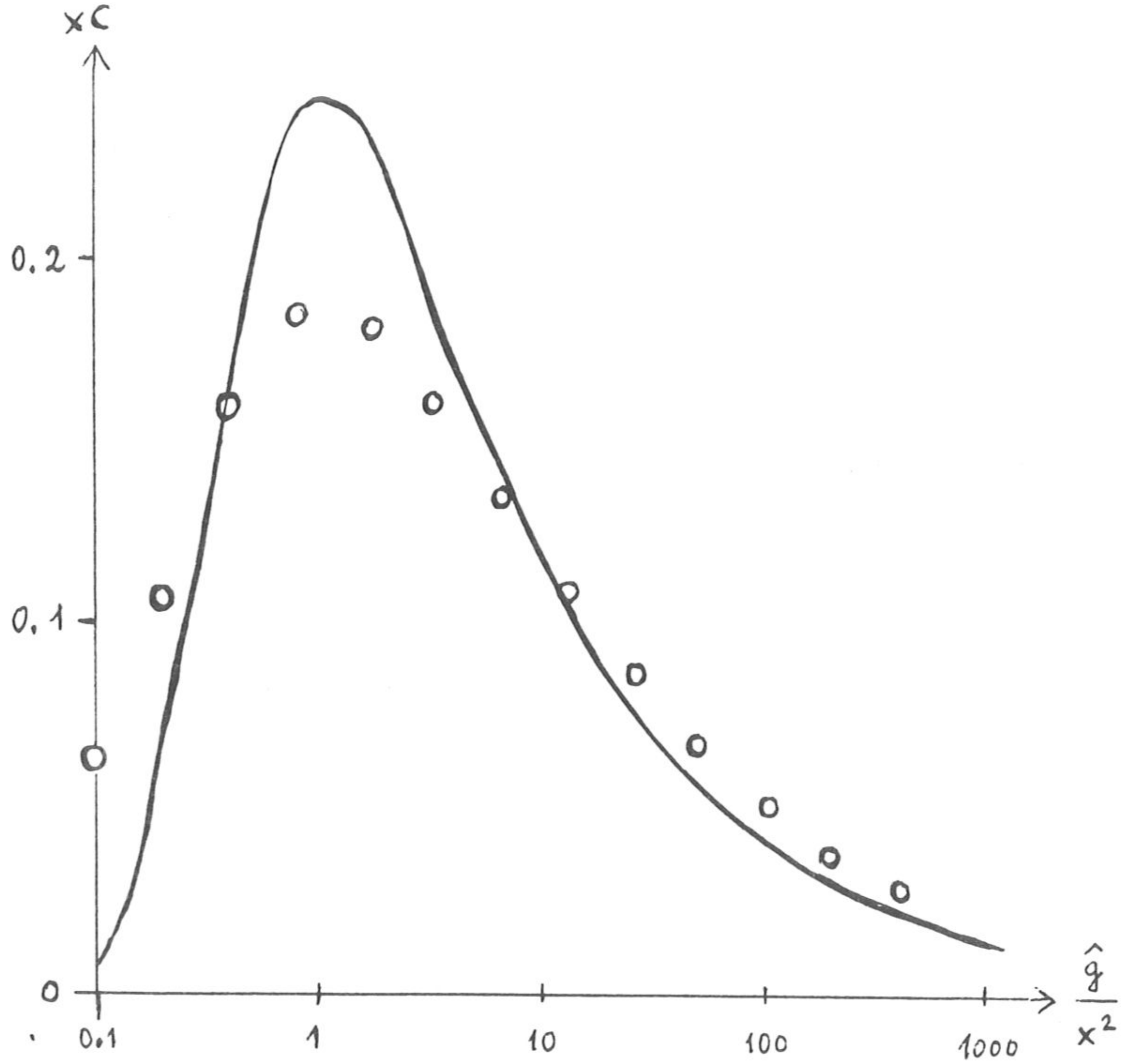
xC thus depends approximately on the parameters A, x, g via $\hat{g}/x^2$ only. To estimate the range of validity, in FIG.8-8 we compare C according to eq.(8.13) with numerical results. It can be seen that eq.(8.13) is also useful for small x.

FIG.8-8

xC versus $\hat{g}/x^2 \;=\; (1 + A - \frac{1}{c_1})^2\; g/x^2$

Solid: according to eq.(8.13)

oooo: numerical for $A = 0.1 \quad x = 0.16$



Appendix

Comments on the equations

Re. eq.(3.3)

Let

$$m_0 = \int_{-\infty}^{\infty} F \, dr \qquad (A.1)$$

be the 0-th moment of the function F. We now calculate m_0 as a function of w and x by integrating the differential equation (2.6) and the initial condition (2.7) over dr:

$$\int_{-\infty}^{\infty} dr \left[F_x = F_{ww} - w F_w - \frac{F_r}{V} \right] \qquad s.(2.6)$$

$$m_{0,x} = m_{0,ww} - w \, m_{0,w} \qquad (A.2)$$

The solution

$$m_0 = 1 \qquad s.(3.3)$$

satisfies both the differential eq.(A.2) and the initial condition

$$m_0|_{x=0} = 1 \, , \qquad s.(2.7)$$

q.e.d.

Re. eq.(3.6)

Calculating the moments of F according to ansatz (3.6) yields

$$\int_{-\infty}^{\infty} dr\, F = 1 \tag{A.3}$$

$$\int_{-\infty}^{\infty} dr\, F\, r = \kappa_1$$

$$\int_{-\infty}^{\infty} dr\, F\, r^2 = \kappa_2 + \kappa_1^2$$

$$\int_{-\infty}^{\infty} dr\, F\, r^3 = \kappa_3 + 3\,\kappa_1\,\kappa_2 + \kappa_1^3$$

$$\int_{-\infty}^{\infty} dr\, F\, r^4 = \kappa_4 + 6\,\kappa_1^2\,\kappa_2 + 4\,\kappa_1\,\kappa_3 + 3\,\kappa_2^2 + \kappa_1^4\,.$$

The same relations (A.3) are valid for moments and semi-invariants according to M.FISZ (ref./3/); this demonstrates the equivalence of eqs.(3.4+5) and (3.6), q.e.d.

The factor $n!$ in eq.(3.6c) is obtained from the normalization (3.6f) of the HERMITE polynomials;

The factor $\kappa_2^{n/2} = (dr/dn)^{n/2}$ results from the transition from r to Z as integration variable.

Re. eq.(3.7)

First we determine the differential equation for Φ. This is done by multiplying the differential eq.(2.6) for F by $exp(i\lambda r)$ and integrating over r:

$$\int_{-\infty}^{\infty} dr \left[F_x = F_{ww} - w\, F_w - \frac{F_r}{V} \right] exp(i\lambda r) \,, \qquad s.(2.6)$$

yielding

$$\Phi_x = \Phi_{ww} - w\, \Phi_w - \frac{i}{V} \lambda \Phi \qquad (A.4)$$

according to the rule

$$\int_{-\infty}^{\infty} dr\, F_r\, G = - \int_{-\infty}^{\infty} dr\, G_r\, F \qquad (A.5)$$

applied to

$$G = exp(i\lambda r) \,.$$

Defining

$$\psi = ln\, \Phi \,, \qquad (A.6)$$

we have

$$\psi_x = \psi_{ww} - w\, \psi_w + \psi_w^2 + \frac{i}{V} \lambda \,. \qquad (A.7)$$

Substituting the semi-invariant expansion (3.4) in the differential eq. (A.7) yields the differential eqs.(3.7) for the semi-invariants, q.e.d. We learn from this that the bilinear inhomogenities come from the quadratic term from eq.(A.7).

Re. eq.(3.9)

Substituting ξ, η (see eq. (3.9c,d) for the independent variables w, x in the homogenous eq.(3.9a) yields

$$\hat{h}_\eta = \hat{h}_{\xi\xi} \,, \qquad (A.8)$$

where

$$\hat{h}(\xi;\eta) = h(w;x) \,;$$

this states that the use of PFIRSCH's transformation (3.9c+d) "transforms away" the term wh_w in eq.(3.9a). The solution (3.9b) is a superposition of GAUSS distributions with weighting G(v) dv.

Re. eq.(3.10)

$$\int_{-\infty}^{\infty} dr\ D \;=\; \underbrace{\int_{-\infty}^{\infty} dw \underbrace{\int_{-\infty}^{\infty} dr\ F}_{1} \sqrt{\frac{2}{\pi}}\,\frac{1}{V}\, exp(-w^2/2)}_{c_1}$$

see(3.1)

see(4.6a)

Re. eq.(3.11)

We consider the derivative with respect to r;

all integrals run from $-\infty$ to $+\infty$.

From eq.(2.4) for D and diff.eq.(2.1) for P we have

$$\frac{\partial}{\partial r}\int dx\ D \;=\; \int dx \int dw\ \frac{P_r}{V}$$

$$= \int dx \int dw \left(P_{ww} \;+\; (wP)_w \;-\; P_x\right)$$

$$= \int dx \left(P_w \;+\; wP\right)\Big|_{w=-\infty}^{w=+\infty} \;+\; \int dw\ P\Big|_{x=-\infty}^{x=+\infty}$$

$$= 0\ .$$

It follows that

$$\int dx\ D(r,x) \quad is \quad independent \quad on \quad r\ .$$

Inserting eq.(5.4) for the far zone gives

$$\int dx\ D \;=\; 1\ ;$$

q.e.d.

Re. eq.(4.8a)

We multiply the differential eqs.(3.7) by $exp(-w^2/2)$ and integrate over w. As a result, the derivatives with respect to w drop out according to the rule

$$\int\limits_{-\infty}^{\infty} dw \; w \; f_w \; exp(-w^2/2) \;=\; \int\limits_{-\infty}^{\infty} dw \; f_{ww} \; exp(-w^2/2) \; . \qquad (A.9)$$

Because f is an even function of w (see eq.(2.3)), this also applies to w integrals from 0 to ∞.

From the differential eqs.(3.7) it therefore follows that

$$\frac{\partial}{\partial x} \int\limits_{0}^{\infty} dw \; \kappa_1 \; exp(-w^2/2) \;=\; \int\limits_{0}^{\infty} dw \; \frac{1}{V} \; exp(-w^2/2) \; , \qquad (A.10a)$$

$$\frac{\partial}{\partial x} \int\limits_{0}^{\infty} dw \; \kappa_2 \; exp(-w^2/2) \;=\; \int\limits_{0}^{\infty} dw \; 2 \; \kappa_{1,w}^2 \; exp(-w^2/2) \; . \qquad (b)$$

....

The right-hand-side of eq.(A.10a) is $\propto c_1$ from eq.(4.6a); integrating eq.(A.10a) from 0 to x with the initial condition (3.8) yields

$$\sqrt{\frac{2}{\pi}} \cdot \int\limits_{0}^{\infty} dw \; \kappa_1 \; exp(-w^2/2) \;=\; c_1 x \qquad (A.11)$$

for all $x \geq 0$, both for large and for small x.

For large x one has the template solution (4.1); substituting eq.(4.1) in eq.(A.11) yields eq.(4.8a), q.e.d.

Re. eq.(4.8b)

We put the template solution for $n = 2$,

$$\kappa_2 \;=\; c_2 x \;+\; S_2 \,, \qquad \text{s.(4.1)}$$

into the defining eq.(4.9) for t^2 and obtain

$$\int_0^\infty dw\ \kappa_2\ exp(-w^2/2) \;=\; \frac{1}{2}\ t^2 \qquad \text{(s.4.9)}$$

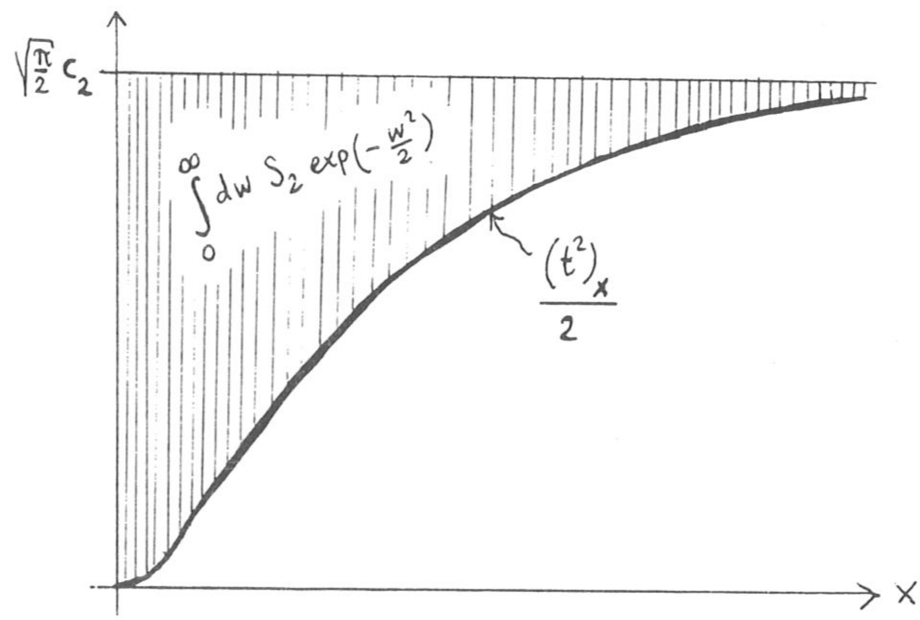
$$\int_0^\infty dw\ S_2\ exp(-w^2/2) \;=\; \frac{1}{2}\ t^2 \;-\; \sqrt{\frac{\pi}{2}}\ c_2 x\ |_{x->\infty} \qquad \text{(s.4.8b)}$$

$$\int_0^\infty dw\ S_2\ exp(-w^2/2) \;=\; \int_0^x dx' \left(\frac{1}{2}\ (t^2)_{x'} \;-\; \sqrt{\frac{\pi}{2}}\ c_2\right)|_{x->\infty}\ . \qquad \text{(A12)}$$

The integral (A.12) denotes the hatched region in FIG.A-1.

FIG.A-1

$\frac{1}{2}(t^2)_x$ versus x for the special case $V = 1/(1 + w^2)$; see FIG.8-6.



Re. sec.5 Far Zone

It should be mentioned that inserting eq.(5.3) for F into the diff. eq.(2.1) gives no mind, because the w-derivatives in eq.(2.1) are of the same order of magnitude as the x-derivative on the left-hand side. Inserting the GAUSS approximation

$$F = \frac{1}{\sqrt{2\pi\kappa_2}} exp\left(-\frac{(\kappa_1 - r)^2}{2\kappa_2}\right)$$

into eq.(2.1) gives eq.(3.7a+b) for $\kappa_{1,2}$ which can be solved by the template eq.(4.1); the term $S_n(w)$ gives the correct w-derivatives when F is inserted into diff.eq.(2.1). However, the neglection of $S_n(w)$ for very large x can be justified by FIG.A-2, which shows schematically κ_1 versus w (solid line) for two different values of x. The hatched area $\sim \sqrt{\kappa_2} \sim \sqrt{x}$ describes the spreading of the wave front with increasing x.

It follows:

for very large x and $w < 3$

$S_1 << \sqrt{\kappa 2}$

and can be neglected.

The region $w > 3$ is of no interst due to the factor $exp(-w^2/2)$ in eq.(2.5) for P.

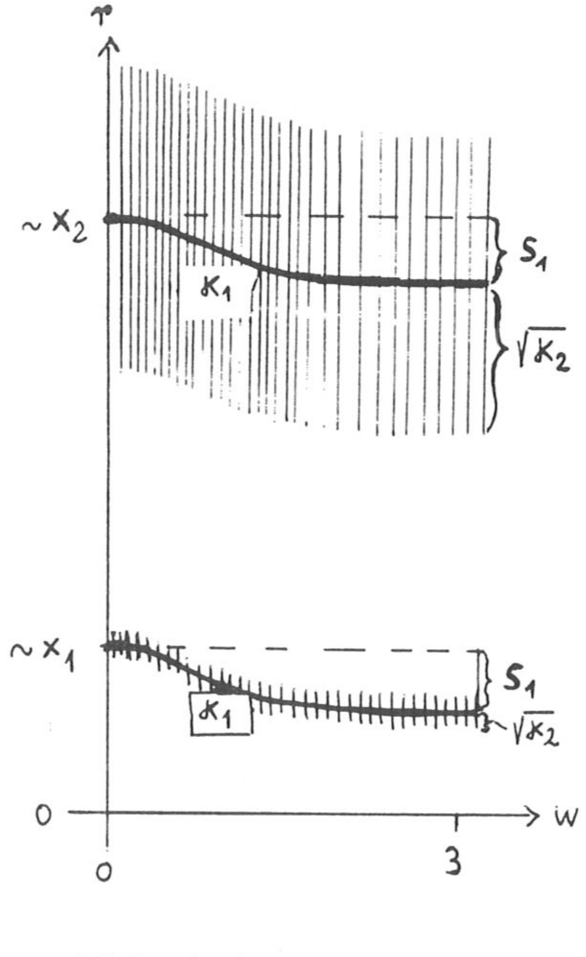


FIG. A-2

Re. eq.(6.2)

Let us consider eqs.(3.7) for the semi-invariants κ_n for very small x.

Neglecting $\kappa_{n,ww} - w\ \kappa_{n,w}$

we have

$$\kappa_{1,x} = \frac{1}{V} \tag{3.7a}$$

$$\kappa_{2,x} = 2\ \kappa_{1,w}^2 \tag{b}$$

$$\kappa_{3,x} = 6\ \kappa_{1,w}\ \kappa_{2,w} \tag{c}$$

$$\kappa_{4,x} = 8\ \kappa_{1,w}\ \kappa_{3,w} + 6\ \kappa_{2,w}^2\ . \tag{d}$$

Introducing the special example

$$V = 1/w^2$$

yields

$$\begin{aligned} \kappa_1 &= \frac{x}{w^2} \\ \kappa_2 &= \frac{8}{3}\ \frac{x^3}{w^6} \\ \kappa_3 &= \frac{192}{5}\ \frac{x^5}{w^{10}} \\ \kappa_4 &= \frac{7680}{7}\ \frac{x^7}{w^{14}}\ . \end{aligned} \tag{A.13}$$

The proportionality factor increases with n more strongly than $n!$ thus causing the expansion (3.6) to be semi-convergent.

With increasing x, the terms with large n become dominant in expansion (3.6); this GRAEFF has called "explosion of the moments". Furthermore, with increasing x the terms $\kappa_{n,ww} - w\ \kappa_{n,w}$ damp the high-n-terms more strongly than the low-n-terms, and, finally, in the far zone cut off all terms with $n \geq 3$ thus leaving a GAUSS distribution (5.3) for F.

Re. eq.(8.13)

Owing to the symmetry (8.11) we have two far zones

one at , say, $x < -100$, and

the other at $x > 100$.

We are only interested in positive large x.

$D(y, a_+)$ is very small compared with $D(y, a_-)$; in order to get $D(y, a_-)$, we apply eq.(5.4) for the density in the far zone to $x = a_-$ and $r = y$ and obtain

$$D(y, a_+) = 0,$$
$$D(y, a_-) = \frac{c_1}{\sqrt{2\pi c_2 a_-}} \, exp\left[-\frac{(y - c_1 a_-)^2}{2c_2 a_-} \right].$$

Inserting this into eq.(8.10) for the convoluted density C gives

$$C(g, x) = \frac{c_1}{2\pi\sqrt{c_2 g}} \int_{y_{min}}^{\infty} dy \; a_-^{-1/2} \; exp(-arg) \qquad (A.14)$$

with

$$y_{min} = x/(1 + A)$$

and

$$arg = \frac{y^2}{2g} + \frac{(y - c_1 a_-)^2}{2c_2 a_-} \qquad (A.15)$$

The main contribution to the integral (8.14) stems from the y-interval in which arg is minimal. In the far zone the minimum of arg is approximately reached, if the numerator in eq.(A.15) vanishes: from

$$y_0 - c_1 a_- = 0$$

and eq.(8.10c) we have

$$y_0 = \frac{x}{1 + A - 1/c_1}.$$

Let us consider the y-dependence of the terms in eq.(A.15).

g is very large in y-intervals with considerable contributions to the integral (8.14) .

The first term $y^2/2g$ - and analog a_- - weakly depend on y, in contrast to the numerator

$(y - c_1 a_-)^2$, which strongly depends on y. Replacing y by y_0 in the terms depending weakly on y gives

$$arg = \frac{y_0^2}{2g} + \frac{\left([c_1(1+A) - 1]y - c_1 x\right)^2}{2c_2[(1+A)y_0 - x]} . \tag{A.16}$$

Inserting eq.(A.16) into eq.(A.14) gives eq.(8.13), q.e.d.

Acknowledgements

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