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Volterra's Functional Integral Equations of the Statistical Theory of Damage

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In the statistical theory of damage, the following functional equation plays a role:

$$\mu(x) = \int_0^x K(x, y)[\mu(y) + \mu(x - y - 1)]\, dy,\ x > 0, \tag{1}$$

where the kernel K is a positive and twice continuously differentiable function for $0 < y \leqslant x$ with the property that

$$\int_0^x K(x, y)\, dy = 1,\ x > 0. \tag{2}$$

The unknown function satisfies the following initial conditions:

$$\mu(x) = 0, \qquad x < 0,$$
$$\mu(x) = 1, \qquad 0 \leqslant x \leqslant 1.$$

This functional equation gives rise to many analytical solutions using Tauberian theorems.

In addition to these solutions, we intend to show the numerical aspect of the problem. We will study the boundary and the asymptotic behavior of $\mu(x)$ for a given class of kernels

$$\lim_{x\to\infty} \mu(x) = A(1 + x) + 0(1),$$

as well as the approximation of $\mu(x)$ for small values of x using cubic cardinal spline functions.

Numerical examples are given to illustrate the method and to define the shape of the distribution of damage for special cross-sections.

INTRODUCTION

Starting with the work undertaken by Snyder and Neufeld, Seitz, Kinchin and Pease, Lindhard, and Robinson [35], one can elaborate the calculation of the number of atoms displaced in a solid subjected to neutron irradiation. The simplest model to describe an elastic collision between atoms is that of free isotropic diffusion. When an atom undergoes a series of elastic shocks, a model such as this enables us to simulate the loss of energy of a primary atom by a well known stochastic process [14], since the problem is reducible to a Markoff chain with a continuous space state whose recurrency relation is easily integrated.

Unfortunately this model only partially expresses the experimental results obtained for solids. Hence, the modification brought about in the formulation of the problem by the addition of the hypothesis that atoms diffused by a primary atom are linked in a lattice is studied. Moreover, since these atomic collisions are anisotropic, the form of the cross-section for the transfer of energy must be improved upon for the calculation of the number of displacements created by a primary [24, 25].

1. Model for an Atomic Cascade Induced by Fast Neutrons in a Solid

A fast neutron of energy E_n scatters elastically on an atom in the lattice. During the collision it transmits an energy E_m between 0 and $(4mM/(m + M)^2)\, E_n$ with probability $P(E_m)$, obtained with the help of the cross-section of elastic diffusion (m: neutron mass, M: mass of the atom of the solid). The atom thus displaced loses its energy in different ways [14]; when the atom's energy is larger than E_0 (Ionization energy threshold), the energy is lost through ionization and excitation. When the energy is less than E_0, the energy is lost principally through atomic shock with other atoms of the lattice, who, in their turn, displace others. An atomic cascade, thus, results.

The displacement of the atoms creates a series of pairs of atom vacancies and interstitial atoms. To evaluate the number of defects thus created, we must know the number of displaced atoms per primary atom.

There is a delicate problem in evaluating the energy threshold E_0 and the displacement (or binding) energy E_d. Fein [11] weights E_d with a probability. The statistical fluctuations in the number of displacements created by a primary are negligible as Pal and Nemeth [21] have shown in their hard sphere hypotheses. Gaussian representation of the distribution of the number of displacements $N(\mu, \sigma^2)$ is probably sufficient; however, we propose to calculate the cumulants of this distribution, because for collision other than those of hard spheres the contribution of cumulants of an order larger than two can become relatively important. All effects of channeling and focusing have been eliminated.

2. Study of the Integral Equation of the Statistical Theory of Damage

a. *General Characteristics*

By a Volterra equation [19, 31, 32] the calculation of $\mu(x)$, the average number of displacements created by a primary of energy E in a solid, is carried out. For each displacement the energy E_d is lost by the secondary in order to free itself from the binding energy which hold it in its potential well.

Let $p_m(x)$ be the probability for a primary of energy x displacing m atoms, where $x = E/E_d$. Assuming $p_m(x) = 0$ for $x < 0$, this gives

$$p_m(x) = \int_{x-1}^{x} K(x, y)\, p_m(y)\, dy + \sum_{m'=0}^{m} \int_0^{x-1} K(x, y)\, p_{m-m'}(y)\, p_{m'}(x - y - 1)\, dy. \tag{2.1}$$

Assume that $g(x, t)$ is the generating function

$$g(x, t) = \sum_{m=0}^{\infty} e^{mt} p_m(x). \tag{2.2}$$

Thus,

$$g(x, t) = \int_{x-1}^{x} K(x, y)\, g(y, t)\, dy + \int_0^{x-1} K(x, y)\, g(y, t)\, g(x - y - 1, t)\, dy. \tag{2.3}$$

The kernel $K(x, y)$ of this integral equation represents the normalized cross-section of atomic collision,

$$K(x, y) = \frac{\sigma(x, y)}{\int_0^x \sigma(x, y)\, dy},$$

$$\int_0^x K(x, y)\, dy = 1 \qquad \begin{aligned} K(x, y) &\geqq 0, \qquad 0 \leqslant y \leqslant x, \\ &= 0, \qquad \text{elsewhere}. \end{aligned} \tag{2.4}$$

The initial conditions imposed on $g(x, t)$ are

$$\begin{aligned} g(x, 0) &= 1, \qquad x \geqslant 0, \\ g(x, t) &= 0, \qquad x < 0, \\ g(x, t) &= e^t, \qquad 0 \leqslant x \leqslant 1, \end{aligned} \tag{2.5}$$

since $p_m(x) = \delta_{m,1}$ and $p_m(x) \equiv 0$ for $x < 0$, ($\delta_{i,j}$: Kronecker symbol).

In the absence of these conditions we know that the functional equation

$$f(x) = f(y) f(x - y - 1), \tag{2.6}$$

where $f(0) = e^c$ and c is a constant, admits the unique solution: $f(x) = e^{c(x+1)}$.

PROPOSITION I. *The integral equation* (2.3), *where* $K(x, y)$ *is a frequency function defined in* (2.4), *and the initial conditions are defined in* (2.5), *admits one and only one solution.*

Proof. Suppose $n \leqslant x \leqslant n+1$, $n = 1, 2, \ldots$. Then we rewrite the equation as follows:

$$g(x, t) = \int_0^{x-1} K(x, y)\, g(y, t)\, g(x-y-1, t)\, dy + \int_{x-1}^{n} K(x, y)\, g(y, t)\, dy + \int_n^x K(x, y)\, g(y, t)\, dy. \tag{2.7}$$

This is a linear Volterra integral equation of the form

$$g(x, t) = g_n(x, t) + \int_n^x K(x, y)\, g(y, t)\, dy, \qquad n \leqslant x \leqslant n+1, \tag{2.8}$$

for which it is well known that it has a unique solution if $g_n(x, t)$ is known.

Now, $g_1(x, t)$ is known, hence $g(x, t)$ can be determined for $1 \leqslant x \leqslant 2$ by the integral equation for $n = 1$. Then we can determine $g_2(x, t)$ and $g(x, t)$, for $2 \leqslant x \leqslant 3$, and so on.

PROPOSITION II. $p_m(x)$ *generating function is bounded*;

$$e^t \leqslant g(x, t) \leqslant e^{t(1+x)}, \qquad x > 0. \tag{2.9}$$

Proof. Using the Picard's method of successive approximation, we may deduce the proof of consistency between the mathematical model and the physical rule of energy conservation. Let

$$F_m(x) \leqslant e^{t(1+x)} \quad \text{for} \quad n \leqslant x \leqslant n+1, \qquad n = 1, 2, \ldots,$$

$$F_{m+1}(x) \leqslant \int_0^{x-1} K(x, y)\, g(y, t)\, g(x-y-1, t)\, dy + \int_{x-1}^{n} K(x, y)\, g(y, t)\, dy + \int_n^x K(x, y)\, e^{t(1+y)}\, dy, \tag{2.10}$$

$$g(x, t) \leqslant e^{t(1+x)}, \qquad \text{since} \quad g(x, t) = e^t \quad \text{for} \quad 0 \leqslant x \leqslant 1.$$

However, if $F_m(x) \geqslant e^t$ for $n \leqslant x \leqslant n+1$, $n = 1, 2, \ldots$,

$$F_{m+1}(x) \geqslant \int_0^{x-1} K(x, y)\, g(y, t)\, g(x-y-1, t)\, dy + \int_{x-1}^{n} K(x, y)\, g(y, t)\, dy + \int_n^x K(x, y)\, e^t\, dy. \tag{2.11}$$

Therefore, $g(x, t) \geqslant e^t$ since $g(x, t) = e^t$ for $0 \leqslant x \leqslant 1$. It may be easily deduced that

$$1 \leqslant \mu_m(x) = \left(\frac{\partial^m g(x, t)}{\partial t^m}\right)_{t=0} \leqslant (1 + x)^m, \qquad x > 0, \tag{2.12}$$

where the $\mu_m(x)$ are the $p_m(x)$ moments, and particularly the average number of displacements,

$$1 \leqslant \mu(x) \leqslant 1 + x \qquad \text{for} \quad x > 0, \tag{2.13}$$

$$\mu(x) = \int_0^x K(x, y)[\mu(y) + \mu(x - y - 1)]\, dy. \tag{2.14}$$

Palasti [22] uses a theorem of Hyers [13] when studying a problem of random filling of a car-park. This problem, introduced by Renyi [23], is analogous to the problem of atomic or electronic cascades, as noted by Ney [20] and Van Roosbroeck [24] (when studying the Fano factor).

Hyers' theorem concerns the stability of a functional linear equation; the transformation f of the Banach space E into the Banach space E' is called a δ linear transformation if it satisfies the following inequality:

$$\| f(x + y) - f(x) - f(y)\|_{E'} \leqslant \delta \tag{2.15}$$

for all $x, y \in E$. For every δ linear transformation of E into E' there is one and only one linear transformation l, which satisfies

$$\| f(x) - l(x)\|_{E'} \leqslant \delta. \tag{2.16}$$

If E and E' represent both the set of real numbers, and if f is a function, l must be a linear function. It is, therefore, interesting to know for which $K(x, y)$ class the following conjecture is verified, taking the norm

$$\begin{gathered} \sup_{0 \leqslant y \leqslant x} | \mu(x) - \mu(y) - \mu(x - y - 1)| \\ \| \mu(x) - \mu(y) - \mu(x - y - 1)\| \leqslant 1, \qquad 0 \leqslant y \leqslant x, \end{gathered} \tag{2.17}$$

we have

$$\sup_{x \geqslant 0} | \mu(x) - A(1 + x)| \leqslant 1, \tag{2.18}$$

which implies

$$\lim_{x \to \infty} \frac{\mu(x)}{1 + x} = A, \tag{2.19}$$

where A is a constant $\in (0, 1)$.

The equation (2.14) may be resolved by the iterated kernels method as Corciovei and others [7, 33] have noted.

PROPOSITION III. *If*

$$\mu(x) = 0, \qquad x < 0,$$
$$\mu(x) = 1, \qquad 0 \leqslant x \leqslant 1,$$

and $K(x, y) \in C^n$ $(0 < y \leqslant x < \infty)$, $n = 0, 1, 2,\ldots$ *we have* $\mu(x) \in C^m[m, \infty)$, $m = 0, 1, 2,\ldots, n+1$.

Proof. $\mu(x)$ will be continuous in all the intervals $(n, n+1)$, $n = 1, 2,\ldots$. Continuity is assured at the boundary of these intervals, and $\mu(x) \in C[0, \infty)$

$$\begin{aligned} &\mu'(x) = \phi(x) + \delta(x),\\ &\phi(x) \text{ continuous; } \phi(x) = 0,\ x < 1,\\ &\delta(x)\text{: Dirac "function."}\end{aligned} \tag{2.20}$$

Differentiating (2.14) with respect to x, we get

$$\begin{aligned}\mu'(x) = K(x, x)\,\mu(x) + \int_0^x K(x, y)\,\mu'(x - y - 1)\,dy + \int_0^x \frac{dK(x, y)}{dx}\\ \cdot [\mu(y) + \mu(x - y - 1)]\,dy, \qquad x > 1.\end{aligned} \tag{2.21}$$

If $K(x, y) \in C\,(0 < y \leqslant x < \infty)$

$\mu'(x)$ will be continuous except where $x = 1$,

$\mu'(1_-) = 0$,

$$\lim_{x \downarrow 1} \mu'(x) = \lim_{x \downarrow 1} |\, K(x, x - 1)| = K(1, 0).$$

Thus, $\mu(x) \in C^1[1, \infty)$.

By successive differentiations $\mu^{(n)}(x)$ adopts the form due to the Leibnitz rule for $x > n$, then it will be easily proved by induction that

$$\mu(x) \in C^m[m, \infty), \qquad m = 0, 1,\ldots, n+1,$$

if

$$K(x, y) \in C^n \quad (0 < y \leqslant x < \infty), \qquad n = 0, 1, 2,\ldots. \tag{2.22}$$

Much stricter boundaries may be found for $\mu(x)$ for a more reduced $K(x, y)$ class using for the proof an analogy with the Gronwall's lemma.

PROPOSITION IV. *If K is a Goursat kernel of rank* 1:

$$K(x, y) = n(y)\, g(x), \qquad 0 \leqslant y \leqslant x < \infty, \qquad n'(y) \geqslant 0. \tag{2.23}$$

$\mu(x)$ follows the Hölder continuity for $x > 1$.

Proof. Let

$$\begin{aligned} F_m(x) &\leqslant \mu(n) + x - n \qquad \text{for} \quad n \leqslant x \leqslant n+1, \qquad n = 1, 2, \ldots, \\ F_{m+1}(x) &\leqslant \int_0^n K(x, y)[\mu(y) + \mu(x - y - 1)]\, dy + \int_n^x K(x, y)(\mu(n) + y - n)\, dy \\ &\leqslant \mu(n) + x - n, \end{aligned} \tag{2.24}$$

since $\mu(x - y - 1) - \mu(n - y - 1) \leqslant x - n$ and

$$g(x) \int_0^n n(y)[\mu(n - y - 1) + \mu(y) - \mu(n)]\, dy = 0.$$

Let

$$\begin{aligned} F_m(x) &\geqslant \mu(n) \qquad \text{for} \quad n \leqslant x \leqslant n+1, \qquad n = 1, 2, \ldots, \\ F_{m+1}(x) &\geqslant \int_0^n K(x, y)[\mu(y) + \mu(x - y - 1)]\, dy + \int_n^x K(x, y)\, \mu(n)\, dy \\ &\geqslant \mu(n), \end{aligned} \tag{2.25}$$

since $\mu(x - y - 1) - \mu(n - y - 1) \geqslant 0$. Therefore,

$$0 \leqslant \mu(x) - \mu(n) \leqslant x - n \qquad \text{for} \quad n \leqslant x \leqslant n + 1, \qquad n > 0. \tag{2.26}$$

The Hölder continuity is, thus, assured.

Note. For a Goursat kernel, due to the iterated kernels method, we easily obtain

$$\mu(x) = h(x) + \int_0^x R(x, y)\, h(y)\, dy, \tag{2.27}$$

where $R(x, y) = n(y) \cdot g(y)$ and

$$h(x) = \int_0^x K(x, x - z)\, \mu(z - 1)\, dz.$$

After differentiation with respect to x of (2.14) we get, $x > 1$

$$\mu'(x) = \int_0^x K(x, x - z)\, \mu'(z - 1)\, dz + \phi_1(x), \tag{2.28}$$

where

$$\phi_1(x) = \int_0^x (\mu(y) + \mu(x - y - 1))(K(x, y)\, K(x, x) + dK(x, y)/\overline{dx})\, dy,$$

$$\phi_1(x) = 0 \text{ if } K(x, y) \text{ is a Goursat kernel } (\alpha \text{ condition}). \tag{2.29}$$

We can differentiate (2.14) once more. The integral equation is transformed into a differential-difference equation [2], for $x > 2$

$$\mu''(x) + K(x, 0)(\mu'(x) - \mu'(x - 1)) = \phi_1'(x) + K(x, 0)\, \phi_1(x) + \phi_2(x), \tag{2.30}$$

where

$$\phi_2(x) = \int_0^x \mu'(z - 1) \left[K(x, 0)\, K(x, x - z) + \frac{dK(x, x - z)}{dx}\right] dz, \tag{2.31}$$

$$\phi_2(x) = 0 \quad \text{if} \quad \underset{(\beta \text{ condition})}{K(x, x - z) = s(z)\, t(x)}, \quad 0 \leqslant z \leqslant x < \infty. \tag{2.32}$$

PROPOSITION V. *If $K(x, y)$ is a degenerated kernel satisfying the α and β conditions and*

$$K(x, x) = \sup_{0 \leqslant y \leqslant x} K(x, y) < \infty,$$

$$K(x, 0) = \inf_{0 \leqslant y \leqslant x} K(x, y) > 0,$$

$$\lim_{x \to \infty} \frac{\mu(x)}{1 + x} \text{ exists.}$$

Proof. Some conditions are analogous to those of the Ney's theorem [20], but the essential difference consists in the fact that Ney imposes symmetry for the kernel $K(x, y)$, when a cross-section of atomic collision is monotonically decreasing.

To demonstrate the existence of the $\lim_{x \to \infty} \mu'(x) = A$ a De Bruijn theorem [8, 9] will be used, whose hypotheses are reproduced below. A completion of this theorem has just been given by Brands [3]. If

$$\omega(x) > 0 \quad \text{and} \quad \sum_{n=1}^{\infty} \exp\left\{-\int_{n-1}^{n} \frac{dt}{\omega(t)}\right\} = \infty,$$

$$\phi(x) \downarrow 0 \quad \text{for} \quad x \to \infty,$$

$$\phi(1) < \infty \quad \text{and} \quad \int_1^\infty \phi(x)\, dx < \infty,$$

where

$$p(x) = 1 + O(\phi(x)),$$
$$q(x) = 1 + O(\phi(x)),$$
$$z(x) = O(\phi(x)),$$

and if for $x > 0$, $u(x)$ satisfies

$$\omega(x)\, u'(x) + p(x)\, u(x) - q(x)\, u(x-1) = z(x), \qquad \lim_{x\to\infty} u(x) \text{ exists.} \tag{2.33}$$

Also

$$B(x) = |\, u(x) - \lim_{x\to\infty} u(x)| \leqslant \delta_1 \prod_{n=1}^{(x)} \left| 1 - \exp\left\{ - \int_n^{n+1} \frac{dt}{\omega(t)} \right\} \right|$$
$$+ 2MC \sum_{n=1}^{(x)} \phi(n) \left| \prod_{j=n+1}^{(x)} \left| 1 - \exp\left\{ - \int_j^{j+1} \frac{dt}{\omega(t)} \right\} \right| \right|$$
$$+ MC \sum_{j=(x)+1}^{\infty} \phi(j), \tag{2.34}$$

where $M = \max_{0\leqslant x<\infty} |\, u(x)|$, cf. (9) for the significance of the constants C and δ_1.

In our case $\omega(x) = 1/K(x, 0) \geqslant x$. Therefore

$$\sum_{n=1}^{\infty} \exp\left\{ - \int_{n-1}^{n} K(t, 0)\, dt \right\} = \infty. \tag{2.35}$$

If the β condition is satisfied we get

$$\sum_{n=1}^{\infty} \frac{K(n, 1)}{K(n-1, 0)} = \infty.$$

The convergence of $\mu'(x)$ to a limit is given below, if the α and β conditions are satisfied,

$$B(x) = |\, \mu'(x) - \lim_{x\to\infty} \mu'(x)\,| \leqslant \prod_{n=1}^{(x)} \left| 1 - \frac{K(n+1, 1)}{K(n, 0)} \right|. \tag{2.36}$$

We, thus, have a method for determining the approximate value of $A = \mu'(x) + O(B(x))$ for all the cross-sections belonging to the $K(x, y)$ class following the α and β conditions. When $\mu'(x)$ and $B(x)$ can be calculated for a given x, the number of displacements may be deduced from as follows:

$$| \mu(x) - A(x+1) | \leqslant \left| 1 - 2A + 0 \left(\int_1^x B(t)\, dt \right) \right| \leqslant | e - 1 - 2A |, \quad (2.37)$$

since

$$\int_1^\infty B(t)\, dt \leqslant \int_1^\infty \prod_{n=1}^{(t)} \left| 1 - \exp \left\{ - \int_n^{n+1} K(v, 0)\, dv \right\} \right| dt$$
$$\leqslant \int_1^\infty \prod_{n=1}^{(t)} \left| 1 - \exp \left\{ - \int_n^{n+1} \frac{dv}{v} \right\} \right| dt = \int_1^\infty \frac{dt}{\Gamma(t+2)} \leqslant e - 2. \quad (2.38)$$

Sigmund's result for the equation of the Kinchin and Pease [29, 30] type is, thus, verified for the Snyder model (32)

$$\lim_{x \to \infty} \mu(x) = A(x+1) + 0(1). \quad (2.39)$$

So that, we may apply the De Bruijn theorem, when the α, β conditions are approximately verified, we must have

$$\int_1^\infty \left(\phi_1(x) + \frac{\phi_1'(x)}{K(x, 0)} + \frac{\phi_2(x)}{K(x, 0)} \right) dx < \infty. \quad (2.40)$$

b. *Numerical Approximation Using the Cubic Splines Method*

The speed of convergence being known, Eq. (2.14) admits a solution which tends to become linear as x increases. The practical method used is, thus, justified. $\mu(x)$ is determined by the Monte-Carlo method for a certain number of values of x, such that $B(x)$ is negligible compared with the statistical fluctuations inherent in this method. Next, the straight line $\mu(x)$ is passed through the points obtained, by the least-square criterion.

The Monte-Carlo method has the advantage of giving in one calculation all the first cumulants of the distribution of the number of displacements. However, in order to give more precise results, the splines method may be used to integrate Eq. (2.14). The $N + 1$ cardinal splines may be introduced as defined by the boundary conditions

$$\begin{aligned} &\mathscr{A}_j''(x_0) = \mathscr{A}_j''(x_1) \qquad \text{and} \qquad \mathscr{A}_j''(x_{N-1}) = \mathscr{A}_j''(x_N), \\ &\mathscr{A}_j(x_i) = \delta_{i,j} \qquad (i, j = 0, 1, \ldots, N). \end{aligned} \quad (2.41)$$

LEMMA.

$$| \mu^{(p)}(x) - S^{(p)}(x)| \leqslant O(h^{2-p}), \qquad x > 1 \qquad p = 0, 1, 2, \tag{2.42}$$

provided the kernel $K(x, y)$ belong to $(\alpha, \beta)'$ class.

Proof. h is the grid size, and $S(x)$ the interpolating spline.

$$\mu(x) \in C^1[1, \infty) \qquad \text{and} \qquad K(x, y) \in C \quad (0 < y \leqslant x < \infty).$$

In addition,

$$\lim_{x \to \infty} \mu''(x) \to 0 \qquad \text{and} \quad \mu(x) = S(x) \qquad \text{as} \quad x = 1_+ .$$

$\mu''(x)$ is discontinuous as $x = 2$ but $L^2[1, \infty)$, since

$$\mu''(x) = K(x, 0)[\mu'(x - 1) - \mu'(x)] + \Phi(x), \tag{2.43}$$

where

$$\int_1^\infty \frac{\phi(x)}{K(x, 0)} dx < M_1, \qquad 0 \leqslant \mu'(x) < M_2$$

and

$$K(x, 0) = \inf_{0 \leqslant y \leqslant x} K(x, y) \leqslant 1/x.$$

Thus,

$$\int_1^\infty \mu''^2(x)\, dx \leqslant \int_1^\infty \frac{dx}{x^2} + 2 \int_1^\infty \frac{dx}{x} \phi(x)\, dx + \int_1^\infty \phi^2(x)\, dx < \infty.$$

Hence,

$$\mu(x) \in H^2[1, \infty),$$

where $H^n(a, b) = C^{n-1}(a, b) \cap L_2{}^n(a, b)$. In addition, $\mu(x)$ satisfies Hölder continuity, which must give

$$| \mu^{(p)}(x) - S^{(p)}(x)| \leqslant O(h^{2-p}), \qquad p = 0, 1, 2.$$

The interpolating spline has the form

$$S(x) = \sum_{j=0}^{N} \mu_j \mathscr{A}_j(x), \qquad \text{where} \quad \mu_j = \mu(x_j). \tag{2.44}$$

Representative numerical results obtained for the hard spheres model will be found in Table I.

TABLE I

$\mu(x)$ exact value	$x(h = 0.025)$	Value calculated by the splines method
1.0953	1.1	1.0948
1.1823	1.2	1.1819
1.2624	1.3	1.2620
1.3337	1.4	1.3336
1.4055	1.5	1.4052
1.4700	1.6	1.4698
1.5306	1.7	1.5304
1.5878	1.8	1.5876
1.6419	1.9	1.6417
1.6931	2.0	1.6430
1.7443	2.1	1.7441
1.7973	2.2	1.7971
1.8516	2.3	1.8515
1.9069	2.4	1.9067
1.9629	2.5	1.9627
2.0193	2.6	2.0191
...	...	...
$\sigma^2(x)$	$x(h = 0.01)$	
0.086	1.1	0.086
0.149	1.2	0.153
0.194	1.3	0.201
0.223	1.4	0.234
0.241	1.5	0.254
0.249	1.6	0.265
...	...	...

3. Cross-Section of Elastic Collision

We must choose between a sophisticated model where the finer points are met lost by imprecise calculations, and a cruder model where errors in calculation are completely overcome [4]. We have prefered the second type of model to provide an example which may be studied by analytical methods, the Monte-Carlo method and the cubic splines method, so as to have some idea of the effectiveness of this method for more complex cross-sections.

For $K(x, y)$, the exponential form studied by Lehmann [16] has been chosen. He calculates the number of displacements by the Kinchin and Pease hypotheses.

Sigmund used it to study channeling [28]. In fact it is the result of some sort of screened potential.

$$K(x, y) = \frac{e^{ay}a}{e^{ax} - 1}; \qquad a \geqslant 0; \qquad 0 \leqslant y \leqslant x < \infty, \\ = 0 \qquad \text{elsewhere.} \tag{3.1}$$

This choice is justified if we take as solution of the problem of diffusion [24].

$$K(x, y) = \frac{1}{x}\left[1 + 2 \sum_{k=1}^{\infty} D_k(x)\, P_k\left(1 - \frac{2z}{x}\right)\right], \tag{3.2}$$

where $z = x - y$.

Expanding $e^{-az}a/(1 - e^{-ax})$ in Legendre polynomials, after a change of variables

$$u = \frac{2z}{x}; \qquad b = \frac{ax}{2} : H(x, u) = \frac{1}{x} \sum_{k=0}^{\infty} B_k(b)\, P_k(1 - u).$$

This gives

$$B_0(b) = 1, \\ B_1(b) = 3(\coth b - 1/b), \\ B_2(b) = 5(1 - B_1(b)/b), \tag{3.3}$$

The cross-section selected will enable a description of "*d* wave" collisions. The parameter a will be defined by $D_1(x)$ and $D_2(x)$ obtained either theoretically (using the collision phase-shifts) or by expanding the experimental cross-section into Legendre polynomials.

The odd coefficients of such an expansion tend to become zero where the primary's energy has a small value [24]. This truncated exponential distribution comprises the idealized model of hard spheres collision. If

$$a \to 0 \qquad K(x, y) = 1/x \qquad y \in (0, x), \tag{3.4}$$

then, of course, $a \to \infty$, $K(x, y) = \delta(x - y)$.

Zero energy is transferred by elastic shock. Hence, we consider a as a constant, even though this is a restrictive condition. The conditions of the preceding paragraph are fulfilled by K, which is L^2 integrable with the norm

$$Ln\left(\frac{Sh(ah/2)}{Sh(a/2)}\right).$$

After differentiating (2.14) with respect to x, we get

$$\frac{e^{ax}-1}{a}\mu''(x)+\mu'(x)=\mu'(x-1) \qquad \text{for} \quad x>2,$$
$$\lim_{x\to\infty}\mu'(x) \text{ exists if } \omega(x)=\frac{e^{ax}-1}{a}, \tag{3.5}$$

where

$$B(x,a)\leqslant\prod_{n=1}^{(x+1)}\frac{e^{a}-1}{e^{an}-1}. \tag{3.6}$$

In particular

$$B(x,0)\leqslant\frac{1}{\Gamma(x+2)}, \tag{3.7}$$

which gives

$$\mu(x)=A(0)(x-1)+\mu(1)+0\left[\int_1^x\frac{ds}{\Gamma(s+2)}\right]. \tag{3.8}$$

When the function $\nu(t,n)$ is introduced [6] we get

$$|\mu(x)-e^{-\gamma}(x+1)|\leqslant|e-1-2e^{-\gamma}|<1,$$

where

$$\nu(t,n)=\int_0^\infty\frac{t^{n+x}\,dx}{\Gamma(n+x+1)},$$

since $A(0)=e^{-\gamma}$, where $\gamma=0.577215$ is the Euler's constant.

This was already a classical result in the analytical theory of prime numbers [10] before being used in the statistical theory of damage. $\mu(x)$ for $x\leqslant 4$ may be explicitly calculated [5], $\mu(4)=2.8072708$ and $\overline{\mu(x)}=e^{-\gamma}(1+x)=2.8072974$ for $x=4$, from which

$$\left|\frac{\mu(4)-\overline{\mu(4)}}{\mu(4)}\right|\simeq 10^{-5}.$$

This justifies the use of the asymptotic formula given by Seitz [27] even where x is of small value. Indeed, most of the asymptotic formula of the theory of damage have been given without defining the area in which they are acceptable; certain cross-sections offer asymptotic results which are not valid for primaries of very low energy. Only Frey [12] uses De Bruijn results [9] in the case of hard spheres shocks, but unfortunately his results do not agree with the Pal and Nemeth results, since the equations used do not represent moments of the order >2 for the distribution of damage.

$$\text{When } a \text{ is very large } B(x,a)\lesssim e^{-ax(x+1)/2} \tag{3.9}$$

$$\mu(x)=\mu(1)+A(a)(x-1)+0\left(\int_1^x e^{-as(s+1)/2}\,ds\right). \tag{3.10}$$

The equation may be written under the form

$$\frac{1-e^{-ax}}{a}\mu'(x) = e^{-ax}\mu(x-1) + e^{-a}\int_{-1}^{x-1} ae^{-ay}\mu(y)\,dy \qquad \text{for} \quad x > 1. \tag{3.11}$$

Integrating by parts, then making $x \to \infty$

$$A(a) = \mu'(x) = ae^{-a}\left(1 + \int_1^{\infty} e^{-ay}\mu'(y)\,dy\right). \tag{3.12}$$

But $\mu'(x)$ is bounded on $[1, \infty)$, thus,

$$A(a) = ae^{-a} + 0(ae^{-2a}), \qquad a \to \infty, \qquad \text{from which } a \to \infty \tag{3.13}$$

$$\left|\mu(x) - \frac{a}{e^a - 1}(x+1)\right| \leqslant \left|1 - \frac{2a}{e^a - 1} + \frac{2e^{-a}}{3a}\right| < 1. \tag{3.14}$$

This result may be usefully compared to that obtained by Lehmann [16] with the Kinchin and Pease hypotheses

$$A(a) = \frac{ae^{-a}}{1 - e^{-a}}, \qquad a \geqslant 0. \tag{3.15}$$

Thus, where a is large, the mean of the two models converge. This fact is shown by comparing the two results in Fig. 1. In the same figure the results obtained by

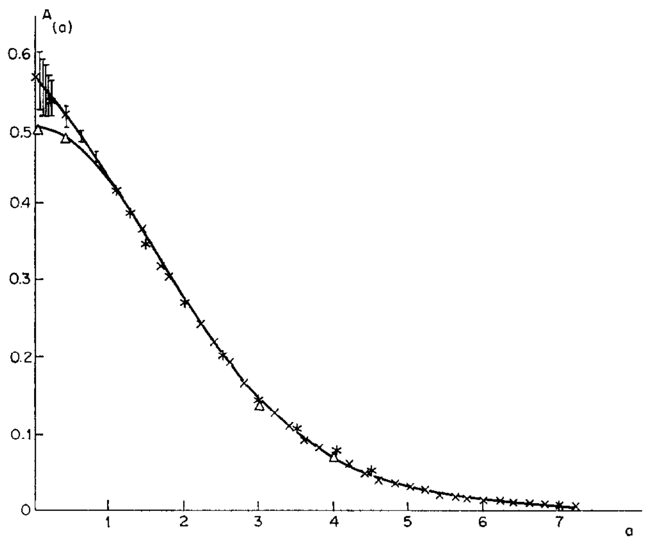

FIG. 1. $A_{(a)}$ displacements factor. (*) Monte-Carlo results. (·) Approximate results. (Δ) Lehmann results. (I) Error bars corresponding to $B(x, a)$ (for $x = 3$).

the Monte-Carlo method are shown to closely agree with analytical results which have been obtained in the following way:

$$\mu(x) = 1 + e^{-a}Ln\left(\frac{e^{ax}-1}{e^{a}-1}\right), \qquad 1 \leqslant x \leqslant 2, \tag{3.16}$$

$$\begin{aligned}\mu(x) = 1 + e^{-a}Ln\left(\frac{e^{ax}-1}{e^{a}-1}\right) + e^{-2a}\Big\{\frac{1}{2}\left(Ln^2\left(\frac{e^{ax}-1}{e^{a}-1}\right) - Ln^2\left(\frac{e^{2a}-1}{e^{a}\quad 1}\right)\right)\\ + \left(L_2\left(\frac{e^{a}-1}{e^{ax}-1}\right) - L_2\left(\frac{e^{a}-1}{e^{2a}-1}\right)\right) + \frac{1}{2}\left(Ln^2\left(\frac{e^{2a}-1}{e^{a}}\right) - Ln^2\left(\frac{e^{ax}-1}{e^{a}}\right)\right)\\ + \left(L_2\left(-\frac{1}{e^{2a}-1}\right) - L_2\left(-\frac{1}{e^{ax}-1}\right)\right)\Big\}, \qquad 2 \leqslant x \leqslant 3.\end{aligned}$$

$L_2(x)$ is the dilogarithm function [18] calculated using Kölbig's algorithm [15].

If $A(a)$ represents $\lim_{x\to\infty} \mu'(x)$, the exact value $\mu'(x)$, for a given x, gives estimate with an error less than $B(x, a)$. Figure 1 represents the graph of $A(a)$ obtained in this way, the errors bars correspond to $B(x, a)$. The calculation was made using $\mu'(3) \pm B(3, a)$; we may observe that $A(a)$ decreases monotonically from $e^{-\gamma}$ to zero as $x \to \infty$ and

$$|\, \mu(x) - A(a)(1 + x)| \leqslant |\, 1 - 2A(a) + O(1)| < 1. \tag{3.17}$$

4. Study of the Cumulants of the Distribution of the Number of Displacements

The equation governing the moment of order 2 is written with the help of

$$\mu_2(x) = \left[\frac{\partial^2 g(x,t)}{\partial t^2}\right]_{t=0},$$

$$\mu_2(x) = \int_0^x K(x,y)[\mu_2(y) + \mu_2(x-y-1)]\,dy + 2\int_0^x K(x,y)\,\mu(y)\,\mu(x-y-1)\,dy, \tag{4.1}$$

$$\mu_2(x) = \sigma^2(x) + \mu^2(x),$$

where $\sigma^2(x)$ is the variance. The integral equation may be written as

$$\begin{aligned}\sigma^2(x) - \int_0^x K(x,y)(\sigma^2(y) + \sigma^2(x-y-1))\,dy\\ = \int_0^x K(x,y)|\,\mu(x) - \mu(y) - \mu(x-y-1)|^2\,dy \leqslant 1.\end{aligned} \tag{4.2}$$

For the $K(x, y)$ class to be introduced, the following asymptotic result is obtained using the De Bruijn theorem after having differentiated the preceding equation twice for $x > 2$.

$$\lim_{x\to\infty} \sigma^2(x) = A_2(a)(1 + x) + 0(1). \tag{4.3}$$

Figure 2 shows the variation of $A_2(a)/A(a)$ as a function of a (for $x = 3$), as

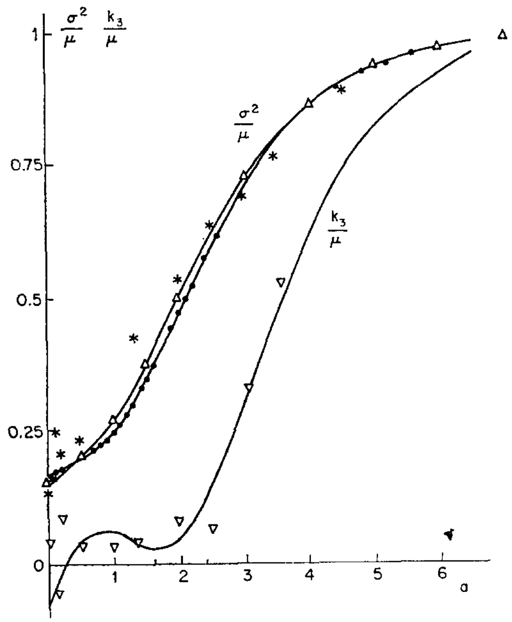

FIG. 2. σ^2/μ (a) k_3/μ (a). (*, ∇) Monte-Carlo results. (·) Approximate results calculated for $x = 3$. (Δ) Lehmann results.

well as Lehmann's results with the Kinchin and Pease's hypotheses. It will be seen that for $a \to \infty$, the variances of the two models become the same. Besides we have

$$\sigma^2(x) \simeq |\, 2A(a) - 1 \,|\, \mu(x) \qquad \text{for} \quad \begin{array}{l} x \to \infty \\ a \to \infty \end{array} \tag{4.4}$$

as is verified by the approximated calculation. We may, thus, state that for $a \to \infty$: $A(a) \to 0$ and $\sigma^2(x) \to \mu(x)$. The Monte-Carlo method provides values for the variance (Fig. 2) in accordance with the analytical results.

The equation governing the moment of order 3

$$\begin{aligned}\mu_3(x) &= \int_0^x K(x, y)\{(\mu_3(y) + \mu_3(x - y - 1)) \\ &\quad + 3(\mu(y)\,\mu_2(x - y - 1) + \mu(x - y - 1) \cdot \mu_2(y))\}\,dy = 0, \qquad (4.5) \\ K_3(x) &= \mu_3(x) - 3\sigma^2(x)\,\mu(x) - \mu^3(x).\end{aligned}$$

The results obtained for cumulants of order less than 3 are extended to the cumulant of order 3 in the example chosen

$$\lim_{x\to\infty} K_3(x) = A_3(a)(1 + x) + 0(1). \qquad (4.6)$$

Figure 2 shows the variation of $A_3(a)/A(a)$, as a function of a

$$K_3(x) = (\tfrac{15}{2}A^2(a) - 6A(a) + 1)\,\mu(x) \qquad \text{for } \begin{array}{l} x \to \infty \\ a \to \infty \end{array} \qquad (4.7)$$

as justified by the approximate calculation.

Thus, for $a \to \infty$, $A(a) \to 0$ and $K_3(x) \to \mu(x)$, the Monte-Carlo method provides the correct values of the cumulant showing asymmetry only when this cumulant is not too weak and not masked by the asymmetry inherent in the distribution of the pseudo-random numbers. Notice that the statistical fluctuations of the displacement factor $A(a)$ are particularly felt as a is large. What is more, we have shown the result to be

$$\sigma^2(x) \to \mu(x), \qquad K_3(x) \to \mu(x) \quad \text{as} \quad a \to \infty. \qquad (4.8)$$

The property $K_n = K_{n-1}$, $n = 2, \ldots$ typifies Poisson's law, i.e., a highly dispersive law or a "small numbers law." Thus, for $a \to \infty$, we will get

$$p_m(x) = \frac{(ae^{-a}(x + 1))^m}{m!} \exp\{-ae^{-a}(x + 1)\}. \qquad (4.9)$$

Leibfreid's conjecture is, thus, verified [17]. For $a \to 0$, $p_m(x)$ has a strongly Gaussian appearance. Between these extreme zones, $p_m(x)$ could be represented by an Airy function to take the asymmetry into account, or by an Edgeworth expansion in terms of the first cumulants to take the skewness into account.

Conclusion

Figure 3 gives the number of displacements as a function of energy in the hard sphere example and for different values of a. These results were calculated by the cubic splines method. The comparison with the explicit solution enables us to judge the precision of this method (Table I).

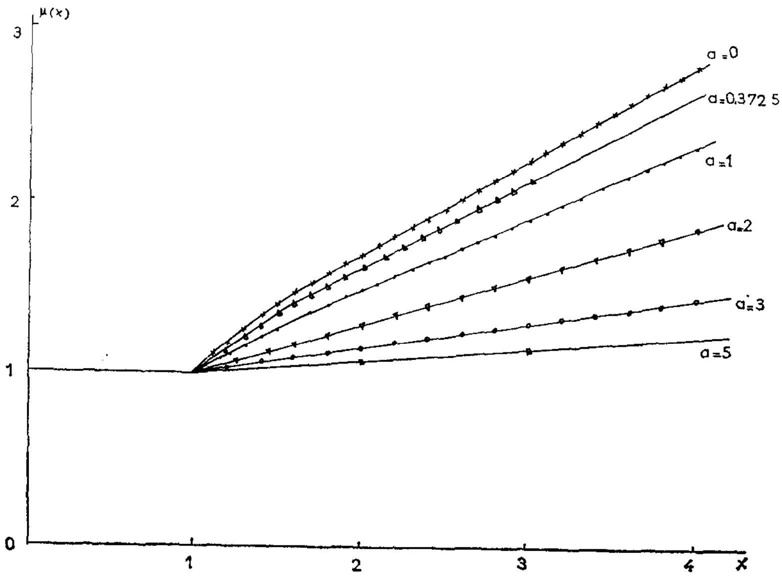

FIG. 3. Number of displacements $\mu(x) = A_{(a)}x + ct$ (by splines method).

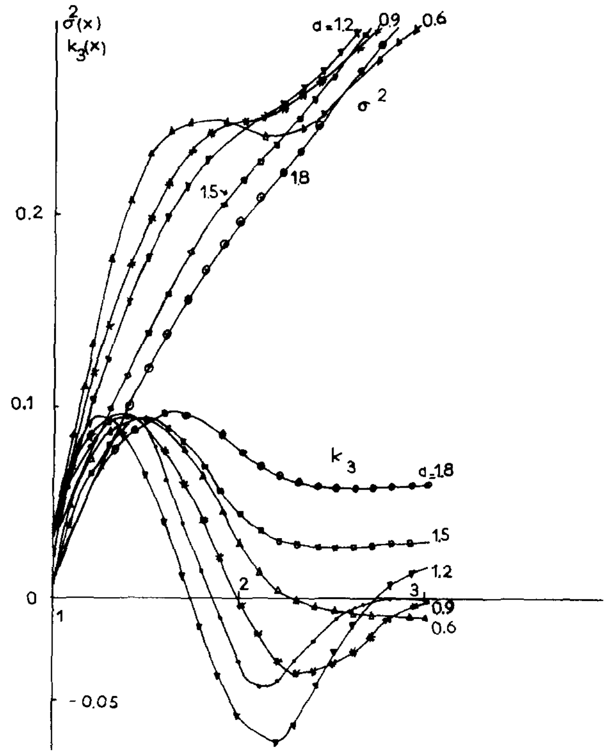

FIG. 4. $\sigma^2(x)$ variance and $k_3(x)$.

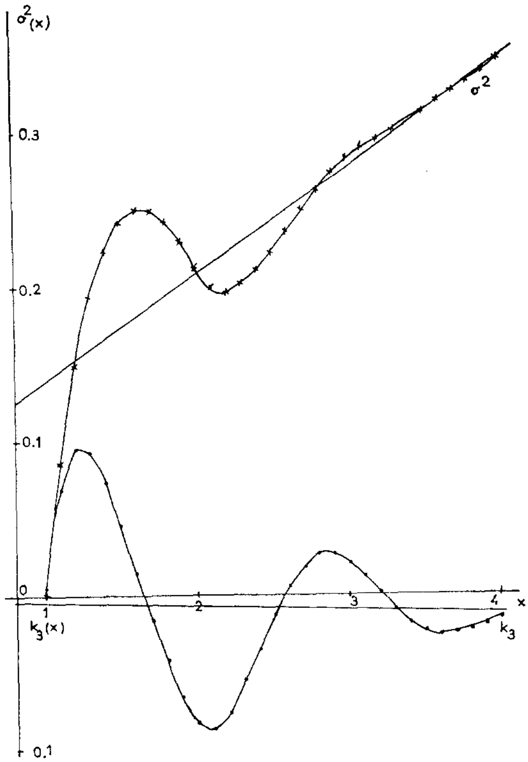

FIG. 5. Variance and k_3 $a = 0$.

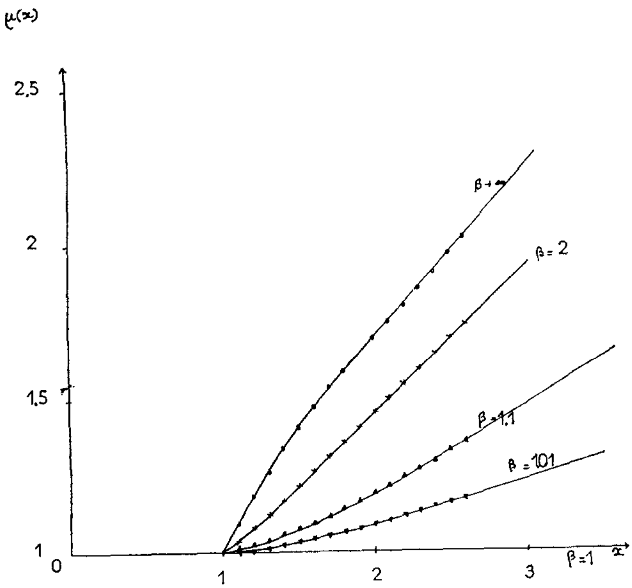

FIG. 6. Number of displacements by splines method for truncated Coulomb cross section $K(x, x - z) = (\beta^2 - 1)/x(\beta - 1 + 2z/x)^2$.

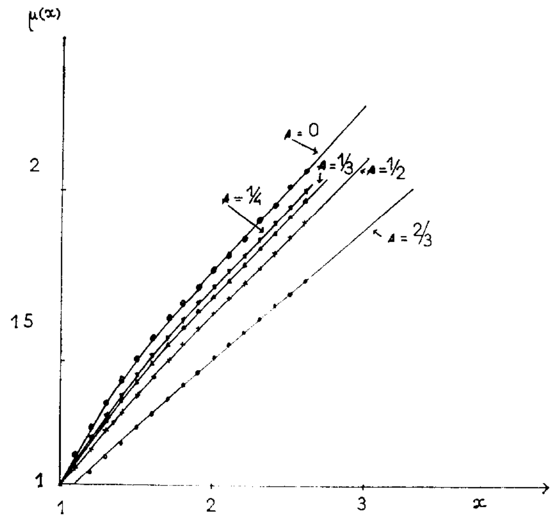

FIG. 7. Number of displacements by splines method for Firsov potential $K(x, x - z) = ((1 - s)/x)(x/z)^s$; $0 \leqslant s < 1$.

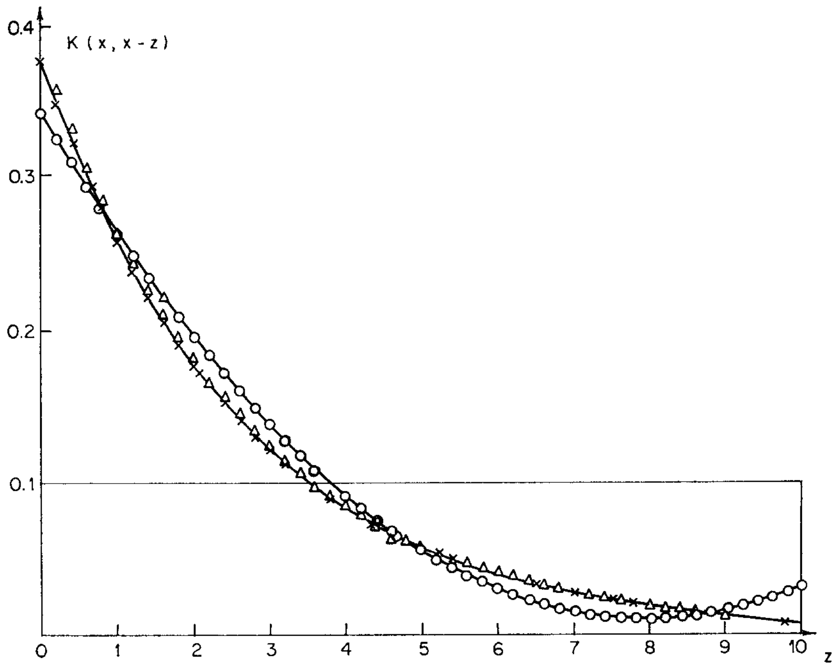

FIG. 8. Elastic collisions cross sections. (—) Hard spheres. (Δ) Truncated exponential, $a = 0.372507$ ($x = 10$). (○) Legendre polynomials expansion (order 2).

In Fig. 4 and 5 we observe the variance of the number of displacements and the cumulant of order 3. These two cumulants enable us to observe the asymptotic properties for the solutions of the equations studied and their stability.

Lehmann's exponential cross-section [16] permits us to vary considerably the number of displacements, taking into account the anisotropy introduced by the first coefficients of the expansion in Legendre polynomials of the cross-section. The results obtained for $A(a)$ are likely to provide theoretical results comparable to the experimental results [25]. Further, the distribution of the number of displacements is highly Gaussian for a primary of low energy, whereas it is Poissonian for a primary of high energy whose loss of energy due to the binding energy is not very important.

Figures 6 and 7 give the number of displacements as a function of energy for the truncated Coulomb cross-section and for the Firsov potential for different values of the parameters β and s.

$$K(x, x-z) \notin L_2[0, h) \qquad \text{if} \quad s \geqslant \tfrac{1}{2},$$

so that the splines method is poorly accurate.

Figure 8 gives the truncated exponential cross-section and its Legendre polynomials expansion (order 2); Table II gives the corresponding values of $\mu(x)$.

TABLE II

$\mu(x)$ truncated exponential (exact)	x	$\mu(x)$ Legendre polynomials expansion (order 2) (by splines method)
1	1.0	1
1.0793	1.1	1.0802
1.1530	1.2	1.1539
1.2220	1.3	1.2229
1.2870	1.4	1.2878
1.3485	1.5	1.3493
1.4070	1.6	1.4078
1.4629	1.7	1.4636
1.5165	1.8	1.5172
1.5681	1.9	1.5687
1.6178	2.0	1.6184
1.6705	2.1	1.6680
1.7219	2.2	1.7182
1.7732	2.3	1.7691
1.8247	2.4	1.8204
1.8763	2.5	1.8720
1.9282	2.6	1.9238

$a = 0.372507.$

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