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LANGEVIN'S SIMULATION IN DIC

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ABSTRACT:

A numerical test is made of the Gaussian approximation to the Fokker-Planck equation for a Hamiltonian with two degrees of freedom and potentials and friction coefficients appropriate for the description of the deep inelastic collision of the system $^{90}\text{Zr} + ^{232}\text{Th}$ at $E_{\text{lab}} = 279$ MeV. The exact solution is constructed with the Langevin's simulation method. The failure of the gaussian approximation is discussed and exhibit separately its sources from (i) diffusion coefficients, the linearization (ii) of the potentials and (iii) of the friction forces.

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1. INTRODUCTION

The Fokker-Planck equation has been shown to be relevant for the description of fluctuations in heavy ion collisions. Solutions to it by conventional numerical methods are limited to phase spaces of dimensions smaller than four, which obliges restricted use for heavy ion collisions where much larger dimensioned phase spaces are required [1,2]. Approximate solutions for many degrees of freedom can be obtained by assuming the Fokker-Planck equation as linear in the phase space coordinates. In this case, the solution is well known to be a Gaussian distribution with convenient ordinary differential equations for the first and second moments [3]. This property has been endowed with slight modifications, to heavy ion collisions to obtain a description of the fluctuations of the collective variables involved [4-6].

A connection between Langevin's and Fokker-Planck equations has been well described by Chandrasekhar [7]. More recently Langevin's simulation has been used in Lattice Q.C.D. calculations [8] in which the time variable is fictitious. The aim is to reach, by convenient "viscous" field, the static equilibrium which is the correct probability distribution required by quantum field theory [9].

The use of Langevin's equations in heavy ion collisions is more direct and simpler. Here the Langevin

time is the actual time and since one expects that the reaction takes place in a time smaller than or of the order of 5×10^{-21} s, the interest lies in the transient phenomena predicted by the theory. The first application of Langevin's simulation to D.I.C. has been done by Barbosa et al. [10] for calculating both the angular momentum transfer and its fluctuation in the $^{14}\text{O} + ^{138}\text{Ba}$ collision with $^{17}\text{O} + ^{138}\text{Ba}$ and $^{15}\text{O} + ^{138}\text{Ba}$ at 1400 MeV and the reaction $^{86}\text{Kr} + ^{138}\text{Ba}$ at 610 MeV. Later, the method was applied independently by Rbe et al. [11] to the fission decay of ^{235}U .

In this paper we calculate and compare different moments of the distribution in phase space as: (i) predicted by the Gaussian approximation to the Fokker-Planck equation as proposed by Feldmeier and Spangenberg [5] and (ii) predicted by the Langevin's equation. We represent D.I.C. by the simple four dimensional phase space model of Gross and Kalinowski [12]. In section 2 we describe the details of the two approaches. In section 3 the results are compared and the main conclusions are drawn.

2. THE PROBLEM

Given Hamilton's function $H(p, q)$ for the collective degrees of freedom involved in D.I.C., the Fokker-Planck equation describing the distribution in phase space is:

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial p_i} \left[(F_i - \frac{\partial H}{\partial q_i}) f \right] + \frac{\partial}{\partial q_i} \left(\frac{\partial H}{\partial p_i} f \right) = D_{ij} \frac{\partial^2 f}{\partial p_i \partial p_j} \quad (1)$$

where F_i is the friction force and D_{ij} the diffusion tensor. The corresponding Langevin's equations are:

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \quad (2)$$

$$\dot{p}_i = - \frac{\partial H}{\partial q_i} + F_i + \ell_i$$

where ℓ_i are random white noises satisfying

$$\langle \ell_j \rangle = 0$$

and

$$\langle \ell_i(t) \ell_j(t') \rangle = 2D_{ij} \delta(t-t') \quad (3)$$

The gaussian approximation to the Fokker-Planck eq. is based on the following result. Let ω_α stands for either p or q ($\omega_i = p_i$ and $\omega_{n+i} = q_i$, $i=1, \dots, n$) and let us assume that the Fokker-Planck equation takes the following linear form:

$$\frac{\partial t}{\partial t} + \frac{\partial}{\partial \omega_\alpha} (\dot{\omega}_\alpha + A_{\alpha\beta} (\omega_\beta - \bar{\omega}_\beta)) = D_{\alpha\beta} \frac{\partial^2 f}{\partial \omega_\alpha \partial \omega_\beta} \quad (4)$$

where $\bar{\omega}_\alpha$, $A_{\alpha\beta}$ and $D_{\alpha\beta}$ are functions of time only and $\dot{\omega}_\alpha = d\omega_\alpha/dt$. One may prove by substitution that the above equation has a fundamental solution in the form of a gaussian distribution [3].

$$f = N \exp[-\frac{1}{2} \sigma_{\alpha\beta}^{-2} (\omega_\alpha - \bar{\omega}_\alpha)(\omega_\beta - \bar{\omega}_\beta)] \quad (5)$$

with

$$N = [(2\pi)^n \det(\sigma_{\alpha\beta}^2)]^{-1/2}$$

and

$$\sigma_{\alpha\beta}^2 = A_{\alpha\gamma} \sigma_{\gamma\beta}^2 + A_{\beta\gamma} \sigma_{\gamma\alpha}^2 + 2D_{\alpha\beta} \quad (6)$$

Therefore, the gaussian approximation to equation (1) is obtained by expanding its coefficients up to linear terms in the neighborhood of the classical orbit. Thus we obtain

$$\begin{aligned} A_{ij} &= [\frac{\partial}{\partial p_j} (F_i - \frac{\partial H}{\partial q_i})]_{cl} \\ A_{i,n+j} &= [\frac{\partial}{\partial q_j} (F_i - \frac{\partial H}{\partial q_i})]_{cl} \\ A_{n+i,j} &= (\frac{\partial}{\partial p_j} \frac{\partial H}{\partial p_i})_{cl} \\ A_{n+i,n+j} &= (\frac{\partial}{\partial q_j} \frac{\partial H}{\partial q_i})_{cl} \end{aligned} \quad (7)$$

where the left hand side is calculated on the classical orbit. Also we must have

$$D_{ij} = [D_{ij}]_{cl} \quad (8)$$

From now on we consider the specific model given by

$$H = \frac{p^2}{2\mu} + \frac{l^2}{2\mu r^2} + V(r) \quad (9)$$

where (r, θ) are the polar coordinates describing the relative motion of the two ions, p and l are their canonical conjugate momenta and $V(r)$ the nuclear plus Coulomb potential. As our system we consider the $^{40}\text{Ar} + ^{232}\text{Th}$ collision at $E_{lab} = 279$ MeV observed by Wilczynski [13] and analysed by Gross and Kalinowski [12] with a similar model. We take the point charge approximation for the Coulomb potential and for the nuclear interaction we assume $V(r)$ in MeV:

$$V(r) = \begin{cases} 157.22 \exp(-\xi/a) & \xi > 3.05 \\ -3.29\xi^2 + 26.013\xi - 54.10 & \xi < 3.05 \end{cases} \quad (10)$$

with $\xi = (r - C_1 - C_2)/b$ with $b = 1$ fm, $a = 0.903$ and C_1, C_2 the half density nuclear radius.

We further assume the friction force to be linear in the velocities:

$$F_i = \Gamma_{ij} \partial H / \partial p_j \quad (11)$$

and Einstein's relation

$$D_{ij} = T F_{ij} \quad (12)$$

where T is the temperature of the system. We also assume friction coefficients to be diagonal, with the tangential equal to 1/400 times the radial coefficient as used in ref. [12]. The radial dependence of $\Gamma(r)$ is of the form:

$$1.831 \times 10^{-18} \exp(-\xi/a_1) \quad \xi > 2.75 \quad (13)$$

$\Gamma(r) =$

$$8.006 \times 10^{-21} + 2.572 \times 10^{-21} \xi, \quad \xi < 2.75$$

with $a_1 = 0.363$ and Γ given in units of $\text{MeV} \cdot \text{s} \cdot \text{fm}^{-2}$. With such a model we are able to describe the orbiting phenomena observed in this reaction, with a grazing angular momentum, $l_{gr} = 220 \hbar$, and a critical one, $l_{cr} = 80 \hbar$. The reason for using form factors for both the potential and friction coefficient different from reference [12] is to favor the gaussian approximation. We observe that our form factors give a linear nuclear force and friction coefficient over most of the surface region.

Making use of equations (11) and (12) into equations (7) and (8) and changing to a self-explained index notation, we arrive at the explicit equations for the gaussian approximation:

$$\dot{r} = \frac{1}{\mu} p$$

$$\dot{\theta} = \frac{l}{\mu r^2}$$

$$\dot{p} = -V' + \frac{l^2}{\mu r^3} - \Gamma_r \frac{p}{\mu}$$

$$\dot{l} = -\Gamma_\theta \frac{l}{\mu r^2}$$

$$\dot{\sigma}_{rr}^2 = \frac{2}{\mu} \sigma_{pr}^2$$

$$\dot{\sigma}_{\theta\theta}^2 = \frac{2}{\mu r^2} \sigma_{l\theta}^2 - \frac{4l}{\mu r^3} \sigma_{r\theta}$$

$$\dot{\sigma}_{pp}^2 = -2 \left(\frac{3l^2}{\mu r^4} + V'' \right) \sigma_{rp}^2 + \frac{4l}{\mu r^3} \sigma_{pl}^2 - 2\Gamma_r \frac{\sigma_{pp}^2}{\mu} + 2\Gamma_r T - 2\Gamma_r' \frac{p}{\mu} \sigma_{rp}^2$$

$$\dot{\sigma}_{ll}^2 = -2\Gamma_\theta \frac{\sigma_{ll}^2}{\mu r^2} + \Gamma_\theta \frac{4l}{\mu r^3} \sigma_{lr}^2 + 2\Gamma_\theta T - 2\Gamma_\theta' \frac{l}{\mu r^2} \sigma_{lr}^2$$

$$\dot{\sigma}_{r\theta}^2 = \frac{\sigma_{p\theta}^2}{\mu} + \frac{1}{\mu r^2} \sigma_{lr}^2 - \frac{2l}{\mu r^3} \sigma_{rr}^2$$

$$\dot{\sigma}_{rp}^2 = - \left(\frac{3l^2}{\mu r^4} + V'' \right) \sigma_{rr}^2 + \frac{2l}{\mu r^3} \sigma_{rl}^2 + \frac{\sigma_{pp}^2}{\mu} - \Gamma_r \frac{\sigma_{rp}^2}{\mu} - \Gamma_\theta' \frac{p}{\mu} \sigma_{rr}^2$$

$$\dot{\sigma}_{rl}^2 = \frac{\sigma_{pl}^2}{\mu} - \Gamma_\theta \frac{\sigma_{lr}^2}{\mu r^2} + 2\Gamma_\theta \frac{l}{\mu r^3} \sigma_{rr}^2 - \Gamma_\theta' \frac{l}{\mu r^2} \sigma_{rr}^2$$

$$\dot{\sigma}_{p\theta}^2 = - \left(\frac{3\ell^2}{\mu r^4} + V'' \right) \sigma_{r\theta}^2 + \frac{2\ell}{\mu r^3} \sigma_{\ell\theta}^2 + \frac{\sigma_{p\ell}^2}{\mu r^2} - \frac{2\ell}{\mu r^3} \sigma_{pr}^2 - \Gamma_r \frac{\sigma_{p\theta}^2}{\mu} - \Gamma_r' \frac{p}{\mu} \sigma_{r\theta}^2$$

$$\dot{\sigma}_{\ell\theta}^2 = \frac{\sigma_{\ell\ell}^2}{\mu r^2} - \frac{2}{\mu r^3} \sigma_{\ell r}^2 - \Gamma_\theta \frac{\sigma_{\ell\theta}^2}{\mu r^2} + 2\Gamma_\theta \frac{\ell}{\mu r^3} \sigma_{r\theta}^2 - \Gamma_\theta' \frac{\ell}{\mu r^2} \sigma_{r\theta}^2$$

$$\begin{aligned} \dot{\sigma}_{p\ell}^2 = & - \left(\frac{3\ell^2}{\mu r^4} + V'' \right) \sigma_{\ell r}^2 + \frac{2\ell}{\mu r^3} \sigma_{\ell\ell}^2 - \Gamma_r \frac{\sigma_{p\ell}^2}{\mu} - \Gamma_\theta \frac{\sigma_{p\ell}^2}{\mu r^2} + \Gamma_\theta \frac{2\ell}{\mu r^3} \sigma_{pr}^2 \\ & - \Gamma_r' \frac{p}{\mu} \sigma_{\ell r}^2 - \Gamma_\theta' \frac{\ell}{\mu r^2} \sigma_{pr}^2 \end{aligned} \quad (14)$$

3. COMPARISON OF THE RESULTS

We calculated the first and second moments in the Gaussian approximation, eq. (14), and integrated Langevin's equations (2) for the ${}^4\text{He} + {}^{232}\text{Th}$ system with $E_{\text{lab}} = 279$ MeV using two values for the initial angular momentum: (i) $\ell_0 = 180 \hbar$ (near ℓ_{gr}) and $\ell = 90 \hbar$ (near ℓ_{cr}). For Langevin's simulation we employed 1000 orbits for each initial value of the angular momentum. We note that the orbits are strictly Coulombian up to the point where the two ions are 22.75 fm apart. At this distance we set the time $t=0$ and measured it in units of 10^{-23} s. Figure 1 exhibits σ_{pp} and $\sigma_{\theta\theta}$ for $\ell_0 = 180 \hbar$ in the time interval from zero to 500×10^{-23} s. σ_{pp} is measured in units of $\hbar^2 \text{fm}^{-2}$ with vertical scale on the left and $\sigma_{\theta\theta}$ in radians with vertical scale on the right. We observe the very good agreement of the gaussian and Langevin's results. We must mention that Langevin's simulation has two main sources of error. First due to the finite step Δt of integration. This error is equivalent to a correction of the order of $\Delta t/\tau$ to the coefficients of Fokker-Planck equation, where τ is a characteristic time of the system. We have used $\Delta t = 0.2 \times 10^{-23}$ s and if we take $\tau \approx 20 \times 10^{-23}$ s a typical collision time for such orbits we get 1% of error from this source. The second source of error is due to the size of the sample used. For the 1000 orbits we considered we expect errors of 3%. Therefore, the discrepancies between

the two estimatives of σ_{pp} exhibited in Figure 1 may be due entirely to the Langevin's simulation. We notice that the agreement for σ_{00} was such that in figure 1 the two curves coincide. Similar results were observed for other moments calculated. It is interesting to mention that the fourth moments estimated by the Langevin's simulation agrees with the predicted by the gaussian within 7% for σ_{pp} and σ_{ll} what shows that the distributions in p and l have good gaussian shapes.

The situation changes completely for the $\ell_0=90 \text{ \AA}$ case. Figure 2 exhibits Langevin's result for σ_{pp} (solid curve) and Figure 3 the gaussian one (solid curve). The vertical scale is in units of $\text{\AA} \text{ fm}^{-1}$ and the horizontal scale in 10^{-23} s . We observe the totally different results of the two methods with the gaussian approximation giving results of one order of magnitude larger than the Langevin's simulation for $t=340 \times 10^{-23} \text{ s}$. To understand the large error in the gaussian approximation, we simulated different intermediate approximations to exhibit its main sources: (a) the linearization of the potential forces (nuclear, Coulomb and centrifugal)

$$F_p(r) \approx F_p(\bar{r}) + \frac{\partial F_p}{\partial r} \Big|_{\bar{r}} (r - \bar{r}) \quad (15)$$

(b) the linearization of the friction force

$$F_f(r, p) \approx F_f(\bar{r}, \bar{p}) + \frac{\partial F_f}{\partial p} (p - \bar{p}) + \frac{\partial F_f}{\partial \bar{r}} (r - \bar{r}) \quad (16)$$

and (c) the neglect of space dependence of the diffusion coefficient

$$D_{ij}(r) \approx D_{ij}(\bar{r}) \quad (17)$$

In simulating these different approximations we used for the mean values of the variables that calculated one step earlier. Figure 2 exhibits the results of these three approximations for σ_{pp} treated separately. Curve (a) resulting from approximation given by equation (15) and curves (b) and (c) those given by equations (16) and (17), respectively. We notice that the main source of error comes from equations (15) and (16). Figure 3 exhibits σ_{pp} calculated with the two approximations given by equations (15) and (16) together (dashed curve), and all three together the (triangular dots). We notice that with the three together we obtain a very good agreement with the gaussian approximation as expected. Equations (15) and (16) are responsible for the reproduction of the large peak at $350 \times 10^{-23} \text{ s}$ but fails the fast drop of σ_{pp} for large times. This comes from the approximation given by equation (17). Figure 4 exhibits $F(t)$. The vertical scale is in fm and horizontal scale in 10^{-23} s . Curves (a) and (b) correspond to approximations given by equations (15) and (16), respectively. The gaussian, (a) + (b) and (a) + (b) + (c) approximations coincide within the scale of the graph (curve

G). Curve (L) is the Langevin's simulation, equation (2). We observe that the mean value $\bar{r}(t)$ is far from being given by the classical orbit (gaussian approximation) near ℓ_{cr} . Figure 5 exhibits σ_{rr} for the Langevin's simulation (L), gaussian approximation (G), Langevin's simulation with approximations given by eqs. (15) and (16) (a) and by eq. (18) only (b). We notice the very large value of σ_{rr} predicted by the gaussian approximation. The vertical scale is in fm and the horizontal scale in 10^{-22} s. With such large value of σ_{rr} one may understand why approximation given by equation (17) plays an important role even when the two ions are 30 fm apart as observed in figure 3. As a concluding remark we observe that the gaussian approximation gives good results near the grazing angular momentum but fails substantially near the critical angular momentum.

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FIGURE CAPTIONS

- Figure 1. σ_{pp} and $\sigma_{\theta\theta}$ as indicated for $\ell_0=180$ Å. The solid line is Langevin's simulation and dashed line the gaussian results. Horizontal scale represents the time t in units of 10^{-23} s; the vertical scale on the left in units of Å \cdot fm $^{-1}$ for the σ_{pp} curve and on the right in units of radians for $\sigma_{\theta\theta}$.
- Figure 2. σ_{pp} for $\ell_0=90$ Å. The solid line is Langevin's simulation and curves (a), (b) and (c) correspond to intermediate approximations as explained in the text. Horizontal scale in units of 10^{-23} s, vertical scale for solid curve and curve (c) is on the left and for curves (a) and (b) on the right, both in units of Å \cdot fm $^{-1}$.
- Figure 3. σ_{pp} calculated with the gaussian approximation (solid curve). The dashed curve is the simulation with approximation (a) + (b) and the triangular points are the gaussian approximation calculated by Langevin's simulation. Vertical scale in units of Å \cdot fm $^{-1}$ and horizontal scale in units of 10^{-23} s.
- Figure 4. The mean value of the relative distance between the ions $r(t)$ as a function of the time. Vertical scale in units of fm and horizontal scale in units of 10^{-23} s for Langevin's simulation (L), gaussian approximation (G) and intermediate approximations (a) and (b) as explained in the text.
- Figure 5. σ_{pp} for the Langevin's simulation (L), the gaussian approximation (G) and the two intermediate approximations (a) and (b). Vertical and horizontal scales the same as in figure 4.

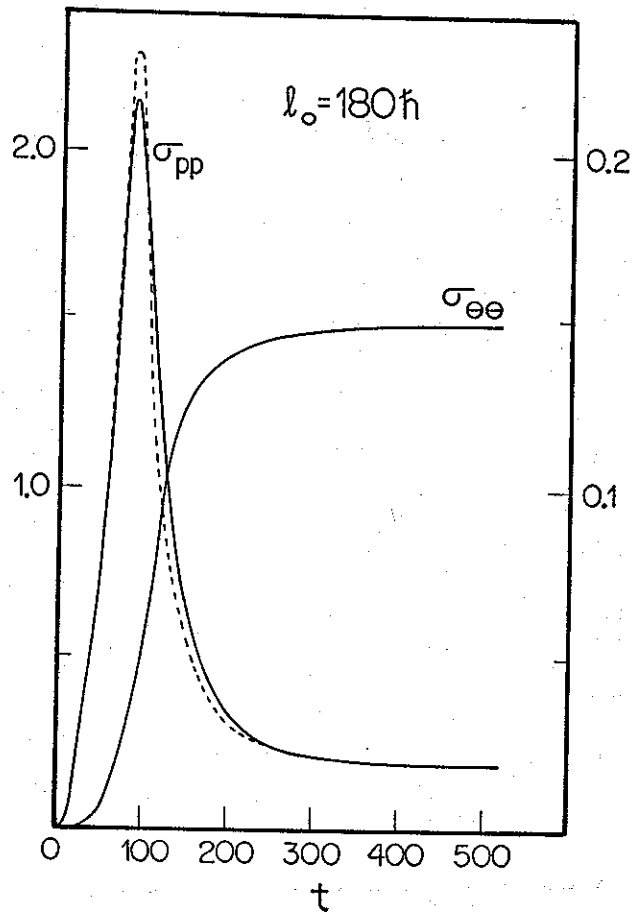


Figura 1

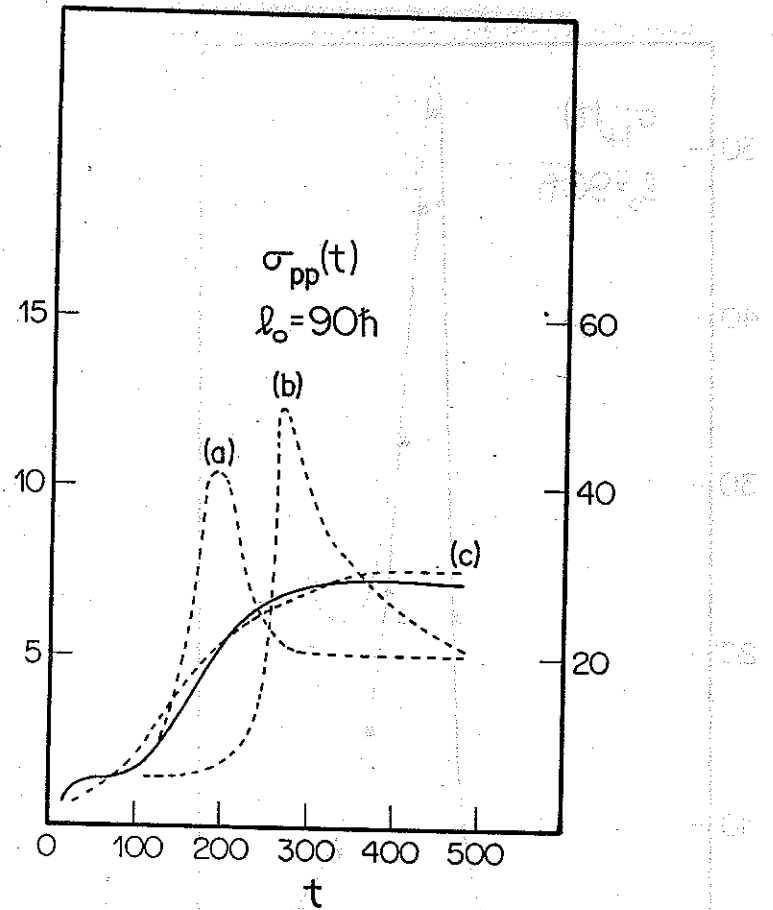


Figura 2

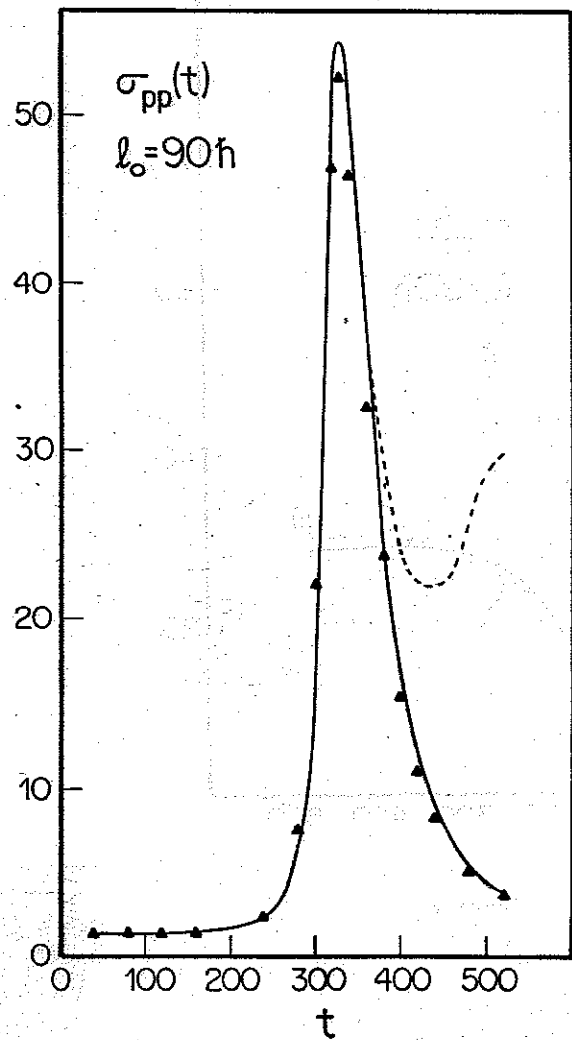


Figura 3

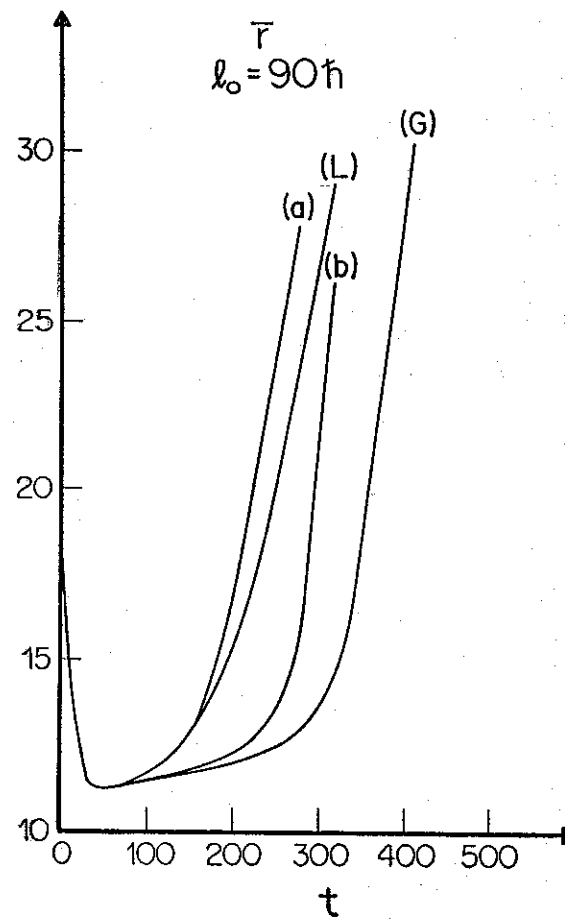


Figura 4

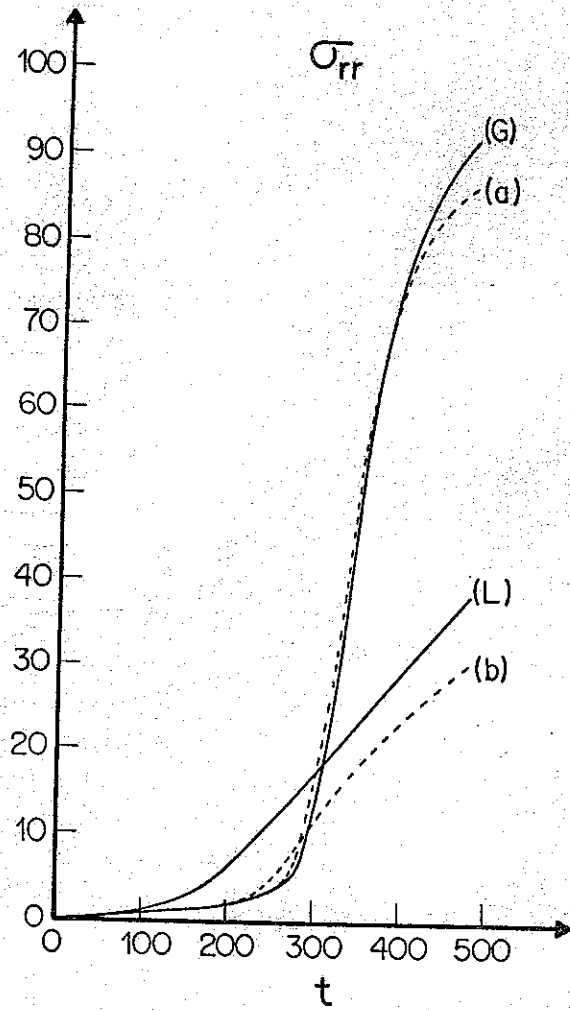


Figura 5