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**MORE ABOUT THE TIME ANALYSIS
OF TUNNELLING PROCESSES**

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and
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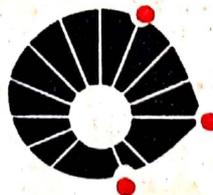
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**Instituto de Matemática
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ABSTRACT - In a recent review paper [*Phys.Reports* 214(1992)339] we proposed new definitions for the sub-barrier tunnelling and reflection times, which seem to be meaningful and acceptable within conventional quantum mechanics. Aims of the present note are: (i) to show that our definition $\langle \tau_T \rangle$ of the average transmission time results to constitute an *improvement* upon the ordinary dwell-time $\bar{\tau}^{Dw}$ formula; (ii) to propose new definitions also for the variances (or dispersions) $D\tau_T$ and $D\tau_R$ of the transmission and reflection times; (iii) to reply to some recent comments by C.R.Leavens [*Solid State Commun.* 85(1993)115], which were uncorrectly based *not* on our own equations, but on different formulae (with integrations, in particular, running from 0 to ∞ [Leavens'] instead of running from $-\infty$ to ∞ [ours]). We take advantage of such opportunity for *confirming* that our approach predicts the existence of the *Hartman effect*, an effect that in these days, at Cologne and at Berkeley, is receiving very interesting and intriguing experimental verifications.

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B I E L I O T E C A

MORE ABOUT THE TIME ANALYSIS
OF TUNNELLING PROCESSES^(*)

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Abstract – In a recent review paper [*Phys.Reports* 214(1992)339] we proposed new definitions for the sub-barrier tunnelling and reflection times, which seem to be meaningful and acceptable within conventional quantum mechanics. Aims of the present note are: (i) to show that our definition $\langle \tau_T \rangle$ of the average transmission time results to constitute an *improvement* upon the ordinary dwell-time $\bar{\tau}^{Dw}$ formula; (ii) to propose new definitions also for the variances (or dispersions) $D\tau_T$ and $D\tau_R$ of the transmission and reflection times; (iii) to reply to some recent comments by C.R.Leavens [*Solid State Commun.* 85(1993)115], which were uncorrectly based *not* on our own equations, but on different formulae (with integrations, in particular, running from 0 to ∞ [Leavens'] instead of running from $-\infty$ to ∞ [ours]). We take advantage of such opportunity for *confirming* that our approach predicts the existence of the *Hartman effect*, an effect that in these days, at Cologne and at Berkeley, is receiving very interesting and intriguing experimental verifications.

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In our review article¹ [*Phys.Rep.* 214 (1992) 339] we put forth an analysis of the main theoretical definitions of the sub-barrier tunnelling and reflection times, and proposed new definitions for such durations which seem to be self-consistent within conventional quantum mechanics. This research field, however, is developing so rapidly, and in such a controversial manner, that during the last year several new papers already did appear, which demand a further critical analysis.

(i) First of all, let us mention that we had overlooked a new expression for the dwell-time $\bar{\tau}^{Dw}$ derived by Jaworsky and Wardlaw²

$$\bar{\tau}^{Dw}(x_i, x_f; k) = \left(\int_{-\infty}^{\infty} dt t J(x_f, t) - \int_{-\infty}^{\infty} dt t J(x_i, t) \right) \left(\int_{-\infty}^{\infty} dt J_{in}(x_i, t) \right)^{-1}, \quad (1)$$

which is indeed equivalent² to our eq.(16) of ref.¹ (all notations being defined there):

$$\bar{\tau}^{Dw}(x_i, x_f; k) = \left(\int_{-\infty}^{\infty} dt \int_{x_i}^{x_f} dx \rho(x, t) \right) \left(\int_{-\infty}^{\infty} dt J_{in}(x_i, t) \right)^{-1}. \quad (2)$$

This equivalence *reduces* the difference between our definition $\langle \tau_T \rangle$ of the average transmission time and quantity $\bar{\tau}^{Dw}$ to the difference between the average made with use of the positive-definite probability density $dtJ_+(x, t) / \int_{-\infty}^{\infty} dt J_+(x, t)$ and the average made with use of the ordinary "probability density" $dtJ(x, t) / \int_{-\infty}^{\infty} dt J(x, t)$. Generally speaking, the last expression is *not* always positive definite, as it was explained at page 350 of ref.¹, and hence does not possess any direct physical meaning. A clear physical meaning can be attributed to the dwell-time expressions (1)-(2) only when¹ $x_i \rightarrow -\infty$ and $x_f \geq a$.

(ii) In ref.³ an attempt was made to analyze the evolution of the wave-packet mean position $\langle x(t) \rangle$ ("center of gravity"), averaged over ρdx , during its tunnelling through a potential barrier. Let us here observe that the conclusion to be found therein, about the absence of a causal relation between the incident space centroid and its transmitted equivalent, holds *only* when it is negligible the contribution coming from the barrier region to the space integral.

(iii) Let us also add that in ref.⁴ it was analyzed the *distribution* of the transmission time τ_T in a rather sophisticated way, which is very similar to the dwell-time approach, however with an *artificial* (not self-consistent) abrupt switching on of the initial wave-packet.

We propose, on the contrary, and in analogy with our eqs. (30)-(31) of ref.¹, the following expressions as physically adequate definitions for the *variances* (or dispersions) $D\tau_T$ and $D\tau_R$ of the transmission and reflection time, respectively:

$$D\tau_T = Dt_+(x_f) + Dt_+(x_i) \quad (3)$$

and

$$D\tau_R = Dt_-(x_i) + Dt_-(x_i), \quad (4)$$

where

$$Dt_{\pm}(x) = \frac{\int_{-\infty}^{\infty} dt t^2 J_{\pm}(x, t)}{\int_{-\infty}^{\infty} dt J_{\pm}(x, t)} - \left(\frac{\int_{-\infty}^{\infty} dt t J_{\pm}(x, t)}{\int_{-\infty}^{\infty} dt J_{\pm}(x, t)} \right)^2. \quad (5)$$

These equations (3)-(5) are based on the formalism expounded in ref.⁵ as well as on our definitions in ref.1 for $J_{\pm}(x, t)$. Of course, we are supposing that the integrations over $J_+(x_f) dt$, $J_+(x_i) dt$ and $J_-(x_i) dt$ are independent from one another.

(iv) At last, very recently it appeared a paper by C.R.Leavens⁶ claiming our definitions (30)-(31) from ref.¹ to be "seriously flawed", on the basis of some numerical calculations for the average transmission times. We have nothing to object to those Leavens' calculations; except that they, simply, do *not* refer to our approach. In fact, they are based on equations *different* from the formulae proposed by us; so that Leavens' conclusions might be valid only for theories *different* from our one. Below, we are going to show how further calculations, based on *our own* equations, *do confirm* that our approach is physically acceptable. Moreover, we shall answer and comment on Leavens' criticism⁶ on our analysis¹ of the dwell-time approaches⁷⁻¹¹.

To begin with, let us recall that, in our eqs.(30)-(31) for the *average* transmission and reflection times, $\langle \tau_T \rangle$ and $\langle \tau_R \rangle$, the related, temporal integrations¹ had to run from $-\infty$ to $+\infty$. [For example, eq.(30) read:¹

$$\langle \tau_T(0, a) \rangle = \frac{\int_{-\infty}^{\infty} dt t J_+(a, t)}{\int_{-\infty}^{\infty} dt J_+(a, t)} - \frac{\int_{-\infty}^{\infty} dt t J_+(0, t)}{\int_{-\infty}^{\infty} dt J_+(0, t)}, \quad (6)$$

and analogously for eq.(31); where J_{\pm} were the flux densities relative to positive and negative direction, respectively, while $x = 0$ and $x = a$ were the coordinates of the first and second wall of the rectangular barrier (in the incident wave-packet direction)].

On the contrary, in ref.⁶ they were replaced by time integrals running only from zero to ∞ : see eqs.(4)-(5) and (12) therein. This is not admissible in our approach—which does of course deal with a collision process,— for the following reasons. First of all, to assume that the incident wave-packet is prepared strictly at a finite time $t = 0$, *i.e.* starts passing through the point x_i at an instant $t = 0$, means to introduce a sharp forward front, getting a certain contribution from large *above-barrier* speeds (which ought to be cut off, according to condition (7) in our ref.¹). Even more important, such a "preparation" is incompatible even with choice (7), adopted by Leavens himself in ref.⁶

for the initial wave-packet, since in any self-consistent formalism a wave-packet with tails infinitely extended in space (namely, for $|x - x_0| \rightarrow \infty$) does inevitably possess tails infinitely extended also in time (i.e., for $|t - t_0| \rightarrow \infty$). With that choice, therefore, the substitution of integrals of the type $\int_0^\infty dt$ for our integrals $\int_{-\infty}^\infty dt$ does mean cutting off the temporal extension for $t < 0$ of the wave-packet moving along the x -axis; and this artificial, and physically unjustified, cut-off does even depend on x . No wonder, therefore, that in ref.⁶ unphysical results were obtained when calculating the average transmission times inside the barrier by his (but not our!) equation (12). Let us recall that we are not interested only in the centroids, but rather in the full extension (around their centroid) of the wave-packets: in particular, in integrating over their whole temporal extension. [Actually, we¹ make recourse to time *distributions* (and not only to an arrival time!) in order to evaluate e.g. the (average) time-instant at which a wave-packet passes through a certain position along the x axis].

We can here stress, at variance with the author of ref.⁶, that the evaluations performed by Zakhariev (briefly presented by us in ref.¹², and qualitatively depicted in ref.¹) show clearly enough that a noticeable contribution to all time averages comes just from the integration from $-\infty$ to zero. Moreover, we did re-check by numerical calculations (in collaboration with A.K. Zaichenko, at the I.N.R. of Kiev) the behaviour of the (average) transmission time $\langle \tau_T \rangle$ just on the basis of our eq.(30) of ref.¹ as a function of the penetration depth x_f (with $x_i = 0$ and $0 < x_f < a$). By using parameters very near to the ones^(**) adopted by Leavens for his Figs.3 and 4 in ref.⁶, we verified once more—contrarily to Leavens' claim—that *physical*, causal results are obtained for $\langle \tau_T(x_f) \rangle$, whose value does increase with increasing x_f . If the penetration depth is expressed in Å, and the penetration time in seconds, with $a = 5$ Å one gets for example:

$$\begin{array}{lll}
0.1 \text{ \AA} \longrightarrow 0.760 \times 10^{-17} \text{ s}; & 0.5 \text{ \AA} \longrightarrow 0.465 \times 10^{-16} \text{ s}; & 1.0 \text{ \AA} \longrightarrow 0.161 \times 10^{-15} \text{ s}; \\
1.5 \text{ \AA} \longrightarrow 0.511 \times 10^{-15} \text{ s}; & 2.0 \text{ \AA} \longrightarrow 0.159 \times 10^{-14} \text{ s}; & 2.5 \text{ \AA} \longrightarrow 0.336 \times 10^{-14} \text{ s}; \\
3.0 \text{ \AA} \longrightarrow 0.430 \times 10^{-14} \text{ s}; & 3.5 \text{ \AA} \longrightarrow 0.463 \times 10^{-14} \text{ s}; & 4.0 \text{ \AA} \longrightarrow 0.474 \times 10^{-14} \text{ s}; \\
4.5 \text{ \AA} \longrightarrow 0.478 \times 10^{-14} \text{ s}; & 5.0 \text{ \AA} \longrightarrow 0.479 \times 10^{-14} \text{ s}. &
\end{array}$$

One can observe that the absolute values of our results are roughly twice as big as those in ref.⁶; this too shows that the contribution of the wave-packet tail for negative times is not at all negligible.

In Fig.1 and Fig.2 we show the plots corresponding to $a = 5$ Å and to $a = 7.5$ Å, respectively. The penetration time $\langle \tau_T \rangle$ rapidly increases for few, initial ångstroms of the penetration depth x_f , tending afterwards to a saturation value. This, incidentally, confirms the existence of the so-called Hartman effect;¹³ an effect that, due to the theoretical connections between tunnelling and evanescent-wave propagation,¹⁴ seems to be

^{0(**)} In the relation $G(k - \bar{k}) = C \exp[-(k - \bar{k})^2 / (\Delta k)^2]$ we choose $\Delta k = 0.02 \text{ \AA}^{-1}$, and then we set $\bar{E} \equiv \hbar^2 \bar{k}^2 / 2m = 5 \text{ eV}$ and $V_0 = 10 \text{ eV}$, quantity C being the normalization constant and m the electron mass.

receiving (indirect) experimental verifications.^{15,16}

Let us stress that, when varying the parameter Δk between 0.01 and 0.03 \AA^{-1} and increasing a up to 10 \AA (and more), practically the same results have been got, in the sense that the numerical values of $\langle \tau_T \rangle$ change very little for x_f in the range 0 to 3 \AA , while the length only of the subsequent plateau does increase. Similar calculations have been performed (always with physically acceptable results) also for many energies \bar{E} in the range 1 to 10 eV. In Fig.3 we present, *e.g.*, the result of the same calculations as in Fig.1 (with $a = 5 \text{\AA}$), but for $\bar{E} = 1 \text{ eV}$.

For the interested reader, let us add that our integrations over dk [as well as over dt] were performed both by the simple summation method and by the Simpson method, obtaining the same results within a 10^{-5} accuracy (for the elementary integration-step δk used by us). We choose $\delta k = \Delta k/10$, while integrating from $\bar{k} - 5\Delta k$ to $\bar{k} + 5\Delta k$. To check our results, we also adopted $\delta k' = \Delta k/8$, and then integrated from $\bar{k} - 4\Delta k$ to $\bar{k} + 4\Delta k$. The correction term resulted to be of the order of 10^{-6} times the main term. When integrating over dt , we used the interval -10^{-13}s to $+10^{-13}\text{s}$ (symmetrical with respect to $t = 0$), very much larger than the temporal wave-packet extension. [Recall that the extension in time of a wave-packet is of the order of $1/(\bar{v} \Delta k) = (\Delta k \sqrt{2\bar{E}/m})^{-1} \simeq 10^{-16}\text{s}$]. The step δt was chosen to be 10^{-17}s . As a check, also the choice $\delta t = 10^{-16}\text{s}$ was made, with corrections of the order of 10^{-5} . Our "centroid" has been always $t_0 = 0$; $x_0 = 0$.

For clarity's sake, let us underline again that in our approach the initial wave-packet $\Psi_{\text{in}}(x, t)$ is not regarded as prepared at a certain instant of time, but it is expected to flow through any (initial) point x_i during the infinite time interval $(-\infty, +\infty)$, even if with a finite time-centroid t_0 . The value of such centroid t_0 is essentially defined by the phase of the weight amplitude $G(k - \bar{k})$, and in our case is equal to 0 when $G(k - \bar{k})$ is real. Actually, it is an usual procedure in the collision theory (differently from the case of the decay theory!) to assume the initial packet to be prepared during a rather long (ideally infinite) time interval, in a remote past; see, *e.g.*, sect.1 of Chapter 5 in Golberger and Watson's book, ref.⁹; assuming such a physically clear initial condition is an improved way for implementing the so-called adiabatic hypothesis. In conclusion, in our formalism a finite time-instant (for instance, $t = 0$) can be associated with the passage of the initial wave-packet through a point x_i only via an average operation; so that $t = 0$ can be its time-centroid relative to x_i ; but $t = 0$ cannot be considered as the beginning of the initial wave-packet preparation.

At last, let us stress that the fact that in our eqs.(1)-(3) it enters the flux $J(x, t)$, instead of $\rho(x, t)$, is a consequence of the standard postulates of quantum mechanics, as it was shown in the papers cited under refs.(6) in our Phys.Rep. article:¹ namely, of the continuity equation $\partial\rho/\partial t + \text{div}J = 0$ and of the ordinary probabilistic interpretation of $\rho(x, t) dx$; cf. *e.g.* ref.⁵. It should be also recalled that the probability densities we have been dealing with, in the case of unidirectional motion (*i.e.*, for instance, quantity

$J_+(x, t) dt / \int_{-\infty}^{\infty} J_+(x, t) dt$, are evidently always *positive*.

In ref.⁶ it has been critically commented also on our view about performing actual averages over the physical time. We cannot agree with those comments. Let us re-emphasize that, within conventional quantum mechanics, the time $t(x)$ at which a particle (wave-packet) passes through the position x is “statistically distributed” with the probability densities $dt J_{\pm}(x, t) / \int_{-\infty}^{\infty} dt J_{\pm}(x, t)$, as we explained at page 350 of ref.¹. This distribution meets the requirements of the time–energy uncertainty relation.

The last object of the criticism in ref.⁶ refers to the impossibility, in our approach, of distinguishing between “to be transmitted” and “to be reflected” particles at the leading edge of the barrier. Actually, we do *distinguish* them; only, we cannot —of course— *separate* them, due to the obvious presence of the related interference terms in $\rho(x, t)$, in $J(x, t)$ and even in $J_{\pm}(x, t)$. This is known to be an inevitable consequence of the superposition principle, valid for wave functions in conventional quantum mechanics. That last objection, therefore, should be addressed to quantum mechanics, rather than to us.

Let us end by observing that Leavens’ criticism on our paper¹ seems to be merely due to incorrect interpretation of our formulas and reasoning. On the other hand, his aim of comparing the definitions proposed by us for the tunnelling times not only with conventional, but also with non–standard quantum mechanics *might* be regarded a priori as stimulating and possibly worth of further investigation.

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Figure Captions

Fig.1 - Behaviour of the average transmission time $\langle \tau_T \rangle$ (expressed in seconds) as a function of the penetration depth x_f (expressed in ångstroms) through a rectangular barrier with width $a = 5 \text{ \AA}$, for the average wave-packet energy $\bar{E} = 5 \text{ eV}$. The other parameters are listed in footnote (**). It is worthwhile to notice that $\langle \tau_T \rangle$ rapidly increases for the first, few initial ångstroms ($\sim 2.5 \text{ \AA}$), tending afterwards to a saturation value. This seems to confirm the existence of the so-called "Hartman effect".

Fig.2 - The same plot as in Fig.1, except that now the barrier width is $a = 7.5 \text{ \AA}$. Let us observe that the numerical values of $\langle \tau_T \rangle$ change very little for x_f in the range 0 to 3 \AA , while only the length of the subsequent plateau does increase.

Fig.3 - Again the same plot as in Fig.1, this time —however— with the new energy $\bar{E} = 1 \text{ eV}$. When re-doing the calculations represented in Figs.1 and 2 with average wave-packet energies \bar{E} between 1 and 10 eV, we always obtained the same qualitative behaviour.

$E=5$ eV $a=5$ Å $V=10$ eV
 $dk=0.02$

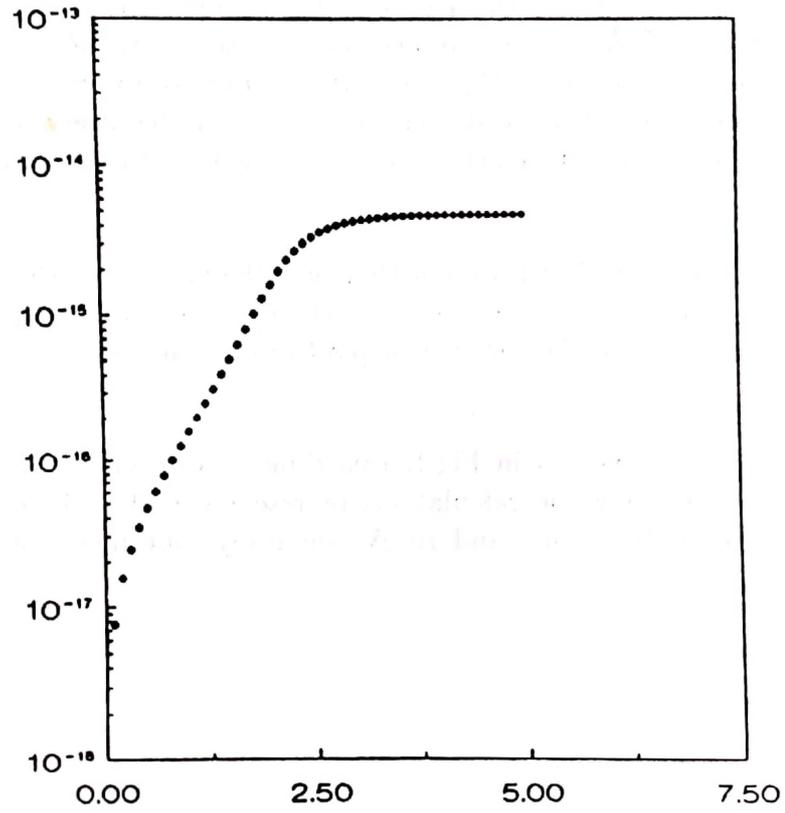


FIG. 1

$E=5$ eV $a=7.5$ Å $V=10$ eV
 $dk=0.02$

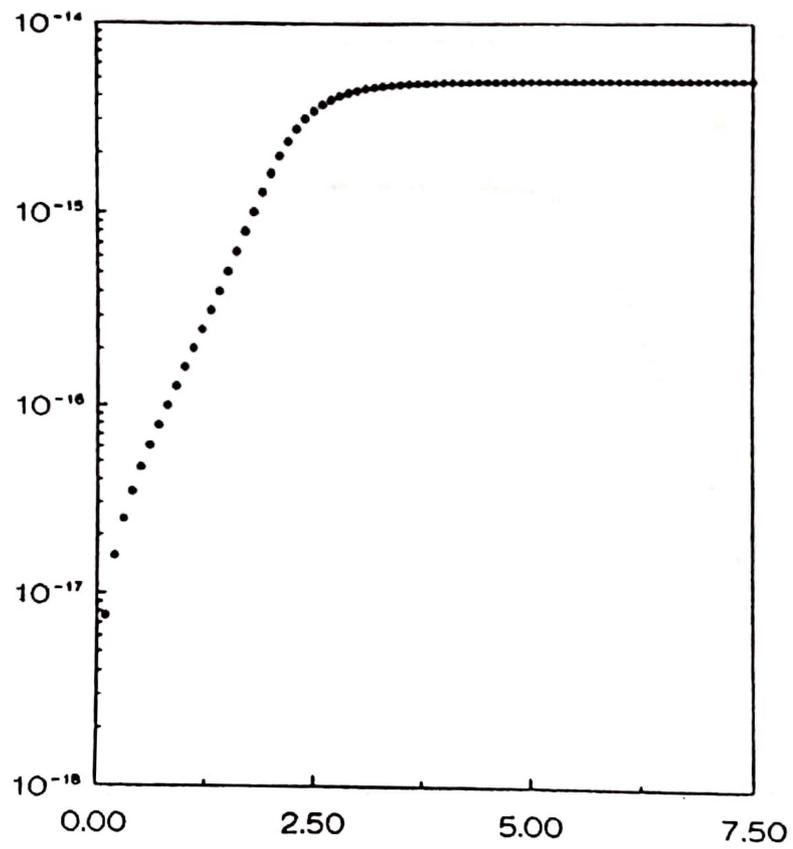


FIG. 2

$E=1$ eV $a=5$ Å $V=10$ eV
 $dk=0.02$

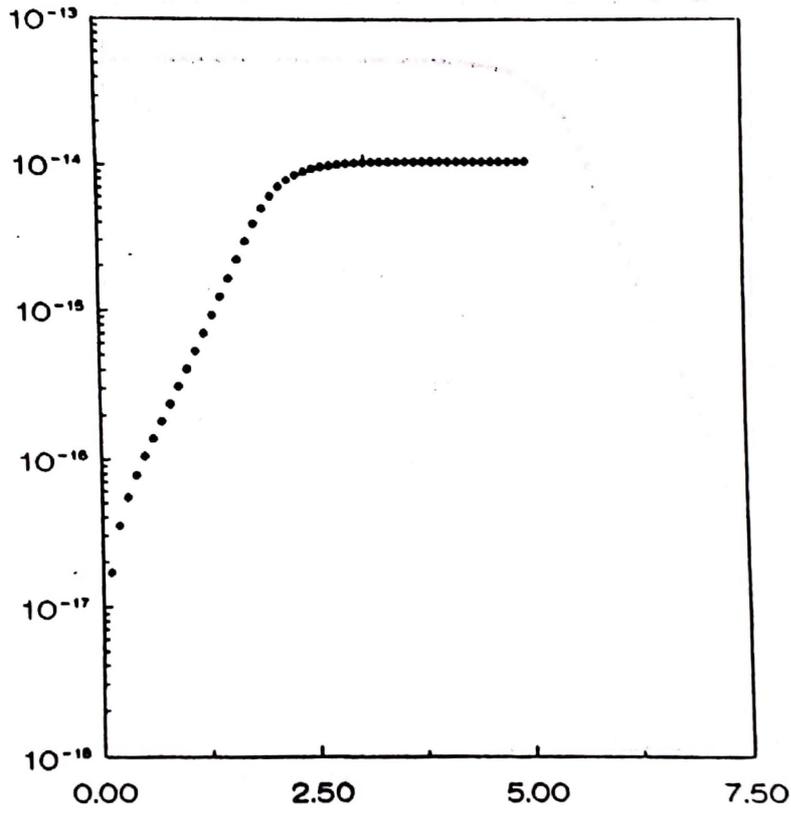


FIG. 3

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