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EXPONENTIAL PHOTONIC LOCALIZATION FOR THE HYDROGEN ATOM IN A MONOCHROMATIC FIELD

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НОВОСИБИРСК

Exponential Photonic Localization for the Hydrogen Atom in a Monochromatic Field

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ABSTRACT

We present theoretical and numerical results according to which the distribution on energy levels of highly excited Hydrogen atoms produced by a monochromatic field should be exponentially localized in the number of absorbed photons. These results allow for a new interpretation of underthreshold ionization and also for an estimate of the ionization rate.

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The behaviour of highly excited Hydrogen atoms in monochromatic microwave field is currently the object of intense theoretical and experimental investigations [1—6]. The observed strong underthreshold ionization has been related to the onset of chaotic motion in the classical atom and, indeed, a good agreement has been found between experimental data and numerical results of computer simulations of classical dynamics [4]. At the same time, however, it is known that quantum interference effects may place strong limitations on chaotic motion. This was numerically demonstrated and theoretically justified on simple models [7, 8, 11, 12] for which, in contrast to the unlimited diffusion taking place in classical action space, the quantum distribution over unperturbed levels stays localized, with a localization length l that under semiclassical conditions is roughly equal to the classical diffusion coefficient. If the latter is constant, then the time-averaged steady-state distribution is approximately $\bar{f}_n \propto \exp(-2|n-n_0|/l)$, n_0 being the initially excited level. This phenomenon of «quantum limitation of classical chaos» was then numerically detected even in the 1-dimensional Hydrogen atom in a monochromatic electric field, that provides a model for the study of excitation and ionization of atoms initially prepared in extended states along the field [9, 10]. The important difference from previous models being that the classical diffusion coefficient increases with n. Due to this peculiarity, under appropriate conditions, also delocalization and unlimited diffusion close to the classical one may occur, which explains the observed agreement between experiments and classical computations. Anyway, the nonconstancy of the

localization length in n did not allow for a theoretical prediction of the distribution on levels in the localized case. As a matter of fact, this distribution displays, on high n-values, a characteristical peak structure, produced by multiphoton transitions, the explanation of which seemed out of the reach of localization theory, which seemed therefore unable to achieve a complete description of the excitation process, nor a determination of the ionization rate.

In this paper we show that localization theory can actually be modified, so as to indicate these eventual details of the excitation process. The basic result will be that an approximately exponential distribution is again obtained, by just the plotting the quasi stationary localized distribution against the number of absorbed photons (and not, as previously, against the state number n). We shall demonstrate this on numerical simulations of the quantum Hydrogen atom and by two independent theoretical arguments.

The first of these is of a general nature, and in principle it may be applied to widely different quantum systems. Let us consider a quantum system with a density of unperturbed levels ρ which is acted upon by an external monochromatic perturbation. Then the system initially concentrated on some unperturbed level will start diffusing in energy. This may happen due to an irregular distribution of levels*), or also when the perturbation is strong enough to give rise to a chaotic diffusion in the classical limit. However, quantum effects will lead this diffusion to a halt after a time t_D that can be estimated as $4\pi^2/(\omega\Delta\nu)$. Here $\Delta\nu$ is the average spacing of quasi-energy eigenvalues significantly contributing in the evolution ($\hbar=1$ here and in the following, $0\leqslant\nu\leqslant 2\pi$). In estimating $\Delta\nu$ we shall distinguish between two opposite situations, according to whether all unperturbed levels take part in the diffusion process, or not (a quantitative condition discriminating these two cases will be given below). In the former case, $\Delta\nu\sim 2\pi/\Delta n$ [8, 12, 13] where Δn is the spread over unperturbed levels at time t_D: $\Delta n=\rho\Delta E\sim$ $\sim\rho(Dt_D)^{1/2}$, with $D=\langle(\Delta E)^2\rangle/\Delta t$ the diffusion coefficient in energy. From $\frac{2\pi}{\omega}\rho(Dt_D)^{1/2}\sim t_D$ we then get t_D and the localization length in energy, $l\approx\Delta n/\rho\approx 2\pi\alpha\rho D/\omega$. According to numerical experiments, the numerical factor α can be given the value 1 [12, 15]. The localization length in the number of absorbed photons is then $l_\Phi=2\pi\rho D/\omega^2$. Now, the change in energy due to one-photon transition is ω, so that $D=2\omega^2 W$, where W is the one-photon transition rate. According to Fermi's golden rule, $W=\frac{\pi}{2}|\mu_{E,E+\omega}|^2\varepsilon^2\rho$ where $\mu_{E,E+\omega}$ is the relevant dipole matrix element, and ε is field strength. Thus we finally get [16]

$$l_\Phi\approx 2\pi^2\mu^2\varepsilon^2\rho^2. \tag{1}$$

The assumption that all levels are involved in the diffusion process is satisfied for $\mu\varepsilon\geqslant\omega$. Indeed, $\mu\varepsilon$ is an estimate for the critical detuning from the resonant Rabi frequency [14]. In the opposite case, $\mu\varepsilon\ll\omega$, only levels close to resonance will be excited. Then the above argument is not valid, and we instead proceed as follows. First we estimate the number of excited levels at time t by $\Delta n\sim N_\Phi\Delta n_\Phi$ where N_Φ is the number of absorbed photons and Δn_Φ is the number of excited levels in each resonant zone. N_Φ grows diffusively in time, and from the above written transition rate we get $N_\Phi\sim(\pi\mu^2\varepsilon^2\rho t)^{1/2}$, while $\Delta n_\Phi\sim\mu^2\varepsilon^2\rho^2$. Since all excited levels lie in zones of width $\sim\mu^2\varepsilon^2\rho$ around resonant levels, then the quasi-energy eigenvalues can also be assumed to lie in an interval $\sim 2\pi\mu^2\varepsilon^2\rho/\omega$ in $(0, 2\pi)$. Therefore their spacing is $\Delta\nu\sim 2\pi\mu^2\varepsilon^2\rho/(\omega\Delta n)$. Upon substituting the above estimates for $l_\Phi\sim N_\Phi$, Δn_Φ in $t_D\sim 4\pi^2/(\omega\Delta\nu)$ we finally get the previous estimate (1). However, the structure of the steady state distribution will now exhibit a chain of peaks, with gaps between them. If l_Φ is but weakly dependent on energy, the probability within these peaks will decay exponentially $\sim\exp(-2|N_\Phi|/l_\Phi)$.

We shall now apply these considerations to the particular case of a 1-dimesional atom in a microwave field. The classical Hamiltonian for this system in action-angle variables (n,λ) and in atomic units is [5, 13, 17]:

$$H=-\frac{1}{2n^2}+\varepsilon n^2\cos\omega t\left[\frac{3}{2}-2\sum_{s=1}^{\infty}\frac{J_s'(s)}{s}\cos s\lambda\right], \tag{2}$$

where J_s are Bessel functions. Using asymptotic expansions for these functions with $s\approx\omega n^3$, $s\to\infty$ we get the semiclassical expansion for dipole matrix elements [18]:

$$\mu\approx\frac{0.411}{\omega^{5/3}n^3}. \tag{3}$$

*) Such case when the frequency $\omega\gg\rho^{-1}$ has been considered in Ref. (14).

On the other hand, $\rho = n^3$. Then (1) shows that the localization is homogeneous in the number of absorbed photons, with a length given by

$$l_\Phi \approx 3.33 \frac{\varepsilon^2}{\omega^{10/3}}. \qquad (4)$$

On multiplying this value by ωn^3, i. e., the number of unperturbed levels in a one-photon interval of energy, we obtain the previously derived [10, 13] value of the localization length. The slight difference in the numerical factor is due to the particular choice of the numerical factor in the classical diffusion coefficient in Ref. [10], as explained in Ref. [13]. We wish to emphasize, however, that the previous theory was only able to justify the form of the steady state distribution in a restricted neighbourhood of the initially excited level. Instead, we have now an approximate description for the overall distribution, including its peak structure. If the photonic localization length is large enough, then this peak structure will produce a plateau in the distribution [10, 13]. If, moreover, l_Φ is comparable with the number of photons required for ionization $N_I = 1/(2n_0^2\omega)$ then strong ionization will occur. This is the delocalization phenomenon described in Refs [10, 13], which leads to diffusive ionization like in the classical atom. As a matter of fact, the condition $l_\Phi \sim N_I$ yields the same expression for the delocalization border as in [10, 13]. We also remark that for typical experimental conditions [1—4] $\omega \sim 0.5$, $\varepsilon_0 \sim 0.04$, $n_0 \sim 66$ the equation (4) yields $l_\Phi \sim 230 \gg N_I \sim 66$, indicating that experiments took place in the delocalization regime and explaining the agreement with classical data.

The above theoretical prediction was checked bv us on numerical data from extensive numerical simulations of the quantum Hydrogen atom that are fully reported elsewhere [13]. In Fig. 1 a time-averaged distribution is plotted versus the number of photons $N_\Phi = N_I - \frac{1}{2n^2\omega}$. An approximately exponential behaviour is here evident. We determined the value of l_Φ by dividing the explored range of values of N_Φ (to the right of 0) in one-photon intervals, and by taking the maximum of the distribution $\bar{f}_n$ in each interval. A least-squares fit of the plot of these values in semi-logarithmic scale with a straight line yielded the localization length. The ratio of the l_Φ thus obtained to the theoretical value (4) was here 1.6.

The results of several such determinations of l_Φ for different parameter values ($1 \leqslant \omega_0 \leqslant 3$; $0.02 \leqslant \varepsilon_0 \leqslant 0.16$; $n_0 = 30, 45, 66, 100$) are shown in Fig. 2. Here $\ln \bar{f}_N$ is plotted versus the number of photons $X = 2N_\Phi/l_\Phi$ with this rescaling, pure exponential localization in all cases would yield the solid line. In all the considered cases but 3, the theoretical value of $l_\Phi > 1$, and ε_0 was larger than the classical chaotic border, $\varepsilon_c = (50\omega_0^{1/3})^{-1}$. The dependence of l_Φ on ε predicted by (4) can be checked on Fig. 3. The theoretical formula correctly works in a range of 5 orders of magnitude of ε^2. Fig. 4 gives an overall comparison of theoretical to numerical values of l_Φ in all the considered cases. The spreading of points may be due to large fluctuations in the steady state distribution (cf. Fig. 1).

We can give another independent theoretical justification for photonic exponential localization. First we reduce the classical dynamics described by (2) to a mapping. To this end, we integrate the Hamiltonian equations of motion over an orbital period of the electron, substituting unperturbed motion in the field-dependent terms and keeping just the resonant term $s \sim \omega n^3$. We find that the variables N (energy divided by ω) and $\Phi = \omega t - s\lambda$ during an orbital period change to

$$\bar{N} = N + k \sin \Phi,$$
$$\bar{\Phi} = \Phi + 2\pi\omega(-2\omega\bar{N})^{-3/2}, \qquad (5)$$

where $k = 0.822\pi\varepsilon/\omega^{5/3}$. The equations (5) give a «Kepler map» that approximately describes the motion of the classical electron. It is defined for all bound states ($N < 0$) but carries some of them into the positive energy region, where it is not defined. The real trajectory then goes to infinity, and its energy is determained by the last «kick» (term $k \sin\Phi$ in (5)). It is important remark that (5) can be locally approximated by a standard map [19] with parameters k, $T \approx 6\pi\omega^2 n_0^5$ and stochasticity parameter $K = kT = \frac{\varepsilon_0}{\varepsilon_c}$, as follows from linearization. Thus (5) shows again that global diffusion is to be expected for $K \geqslant 1$, i. e. $\varepsilon_0 \geqslant \varepsilon_c$.

Now we quantize the map (5). Since this map describes an unbounded motion in Φ under a periodic perturbation, a new integral of motion will appear («quasi-impulse»), besides quasi-energy. For a given unperturbed level n_0, it will be just the fractional part of $N_0 = -n_0/2\omega_0 = -N_I$. Then putting $N_\Phi = N - N_0$, we can represent N_Φ by the operator $\hat{N}_\Phi = -i\frac{\partial}{\partial\Phi}$, and the quantized version of (5)

will be:

$$\bar{\psi} = e^{-i\hat{H}_0}\,\hat{P}\,e^{-ik\cos\Phi}\,\psi, \tag{6}$$

where the operator $\hat{H}_0 = 2\pi[-2\omega(N_0+\hat{N}_\Phi)]^{-1/2}$, and $\hat{P}$ is the projection operator on bounded states ($N_\Phi < N_l$). By iterating (6) we get the distribution on the number of photons that follows from a given initial condition N_0. The classical diffusion coefficient (in number of iterations) for (5) is constant, and for $K \gg 1$ is given by $D \approx k^2/2$. According to existing estimates [12, 15] the localization length for the steady state distribution is, under semiclassical conditions, $l_\Phi \approx D$, i. e., the same obtained above (4). From the numerical data of Ref. [12] it follows, that the steady-state distribution can be satisfactory described by the formula

$$\bar{f}_{N_\Phi} \approx \frac{1}{2\,l_\Phi}\left(1+\frac{2|N_\Phi|}{l_\Phi}\right)\,\exp\left(-\frac{2|N_\Phi|}{l_\Phi}\right). \tag{7}$$

The results of a numerical simulation of (6) are reported in Fig. 1, where the numerically obtained populations of N_Φ eigenstates (points) gotten from (6) are compared with the probabilities in one-photon intervals of energy gotten from the numerical simulation of the Schrödinger equation (crosses). The two sets of data are not very close, but there is an average agreement, espesially in a neighbourhood of the initial peak.

The map (6) also allows for the determination of the ionization rate. This is particularly simple for one-photon ionization with $k \ll 1$: then the ionization rate in number of iterations is $\gamma_\Phi = (k/2)^2$. In real physical time, the rate is $\Gamma_\Phi = \gamma_\Phi/(2\pi n_0^3)$ which is the standard result [6, 13]. In general, in the localized regime the ionization rate should be

$$\gamma_\Phi \sim \sum_{N=N_l-k}^{N_l} \bar{f}_N \sim k\,f_{N_l}$$

when $N_l > l_\Phi > k > 1$. In physical time, this gives

$$\Gamma_\Phi \sim k\,\bar{f}_{N_l}\,(k\omega)^{3/2} \sim \frac{\omega^3}{\varepsilon^{3/2} n_0^2}\,\exp\left(-\frac{0.3\,\omega^{7/3}}{\varepsilon^2 n_0^2}\right). \tag{8}$$

Also, if as in the classical case, the destribution in the continuous part of the spectrum is essentially determined by the effect of a single kick on states close to the ionization border, then from (6)

we get that for $k \gg 1$ this distribution should be $\propto J^2_{N_\Phi}(k)$, in agreement with results obtained in Ref. [20].

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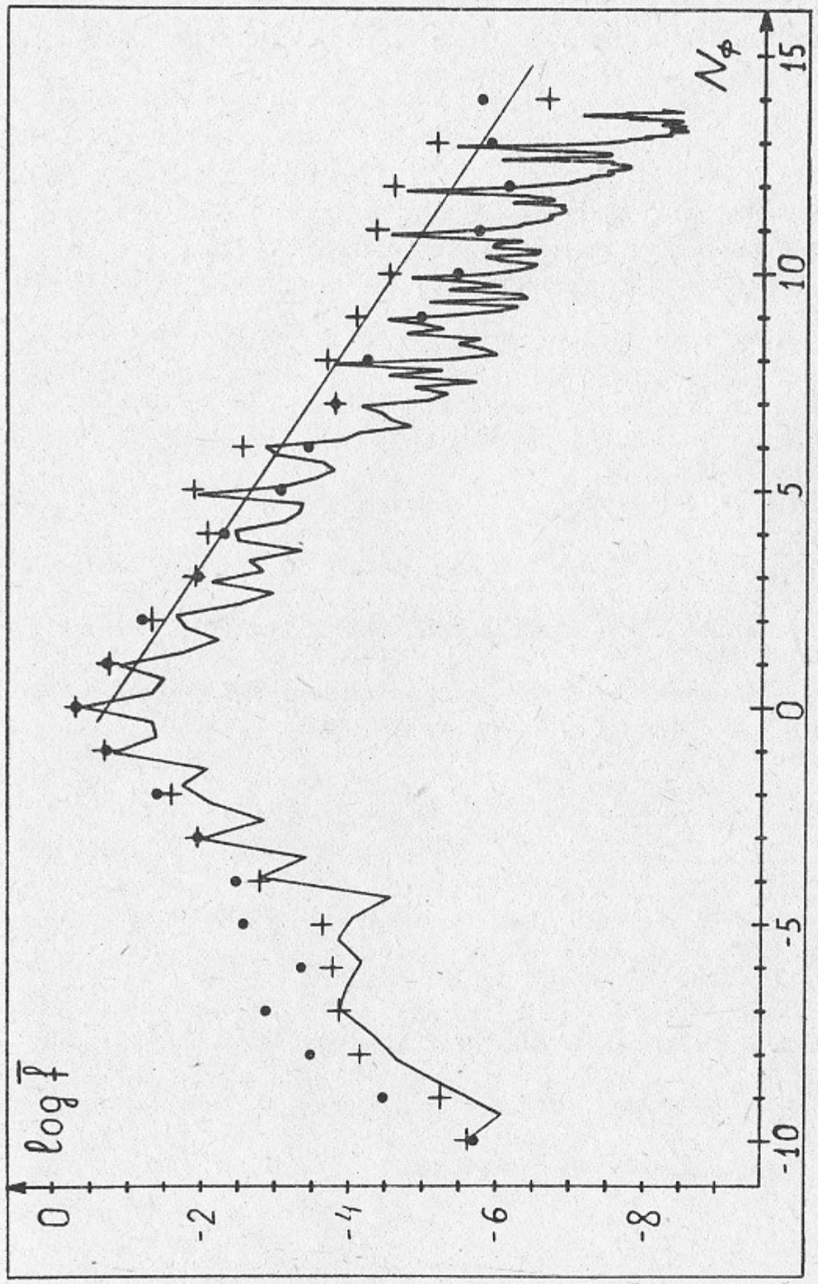

Fig. 1. The distribution, averaged from 80 to 120 periods of the external field, versus the number of photons $N_\phi = N_l - \frac{1}{2n^2\omega}$. Here $n_0 = 100$, $\varepsilon_0 = \varepsilon n_0^4 = 0.04$, $\omega_0 = \omega n_0^3 = 3$. For each integer value of N_ϕ crosses (+) indicate the probability in the interval $N_\phi - \frac{1}{2}$, $N_\phi + \frac{1}{2}$. The straight line is the result of a least-square fitting. Points were obtained by iterating the quantum map (6).

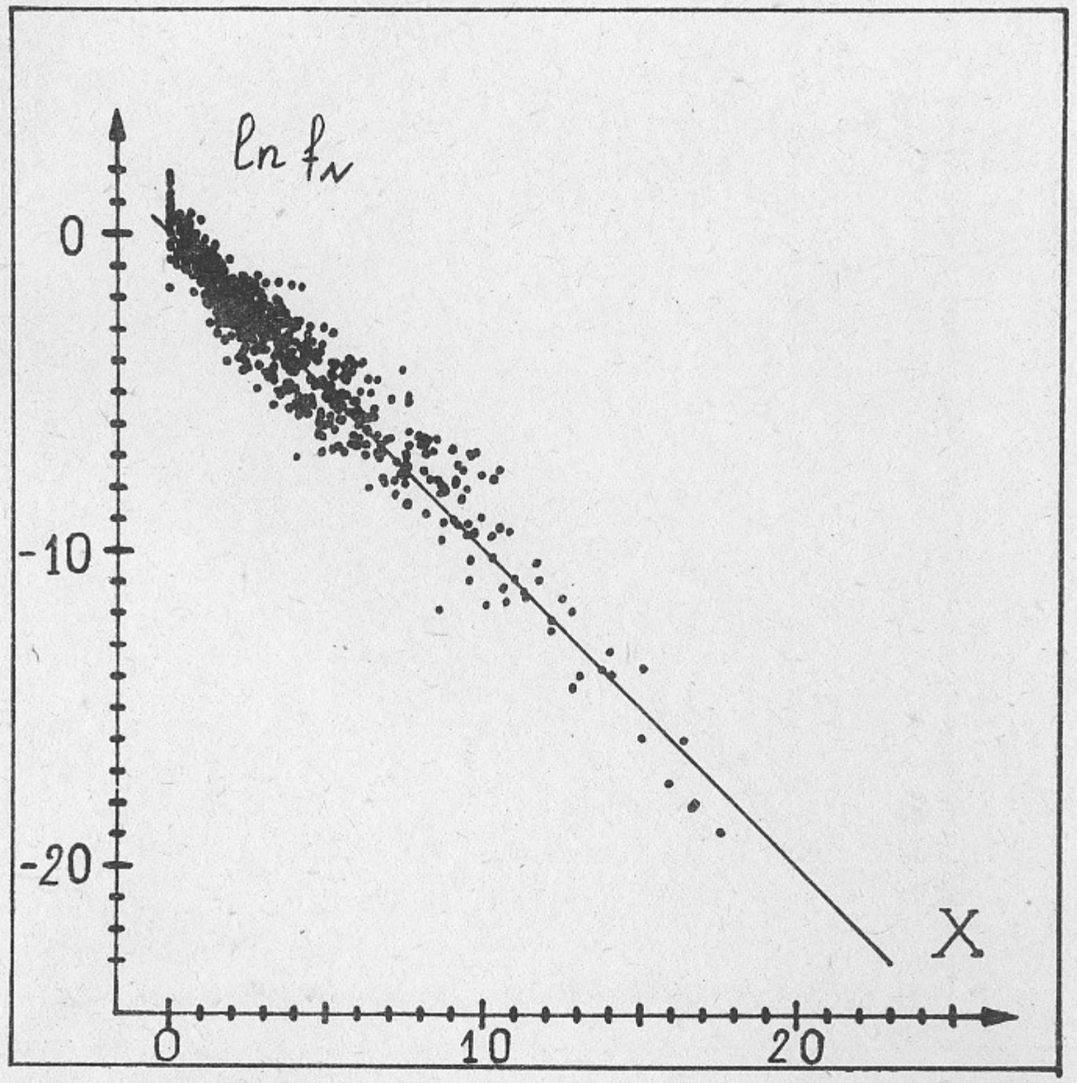

Fig. 2. The dependence of $\ln f_N$ on $X = \frac{2N_\phi}{l_\phi}$, where l_ϕ is the experimental value, obtained by least-squares fits on 41 distributions, as described in Fig. 1, for different values of ε_0, ω_0, n_0. The constant parts in $\ln f_N$ have been subtracted, so that perfect exponential localization would correspond to $\ln f_N = -X$ which is also drawn in figure (full line).

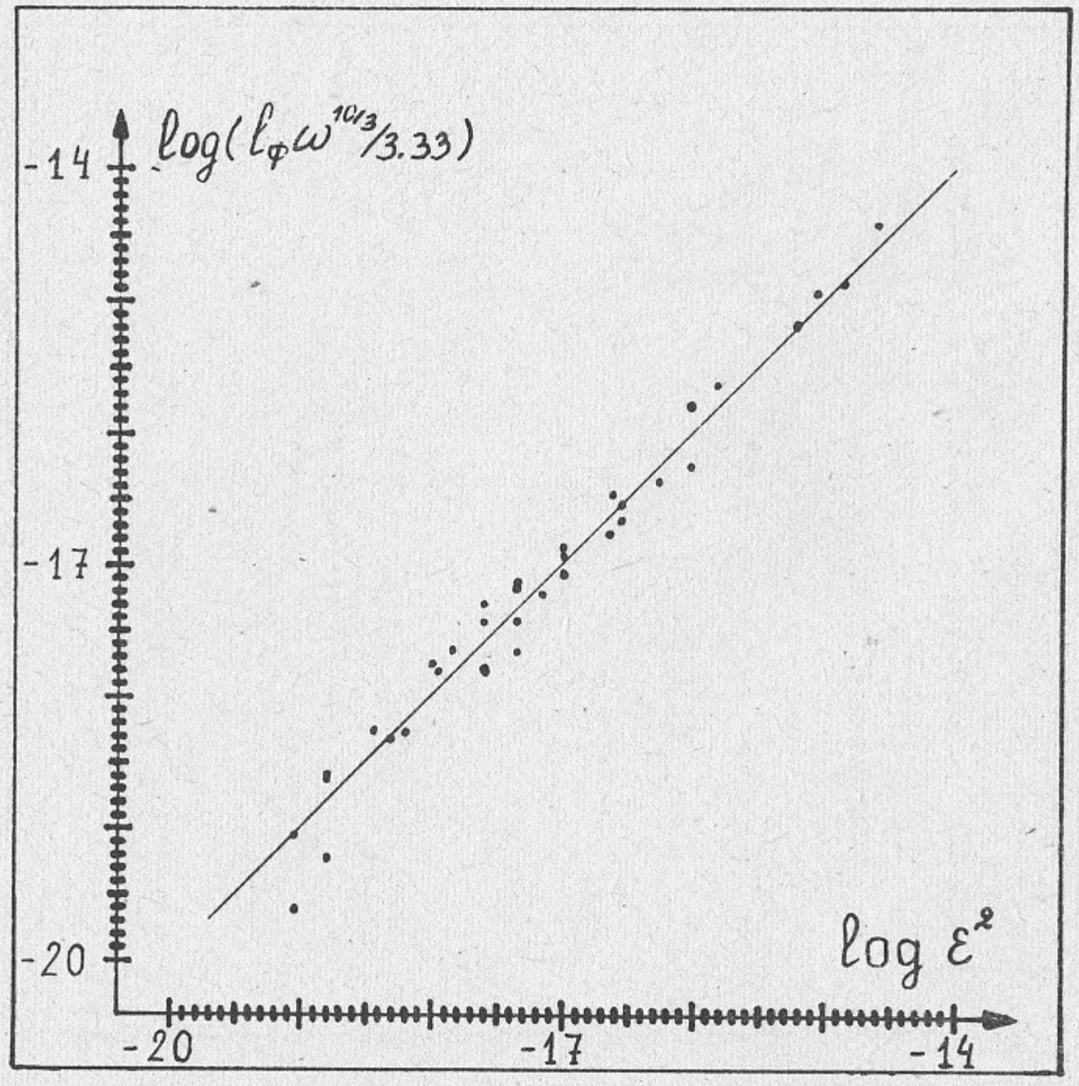

Fig. 3. Plot of the logarithm of the rescaled experimental localization length $\log (l_\Phi \omega^{10/3}/3.33)$ versus $\log \varepsilon^2$. The solid line is the theoretical dependence from formula (4). Experimental data from 38 different distributions with $l_\Phi > 1$.

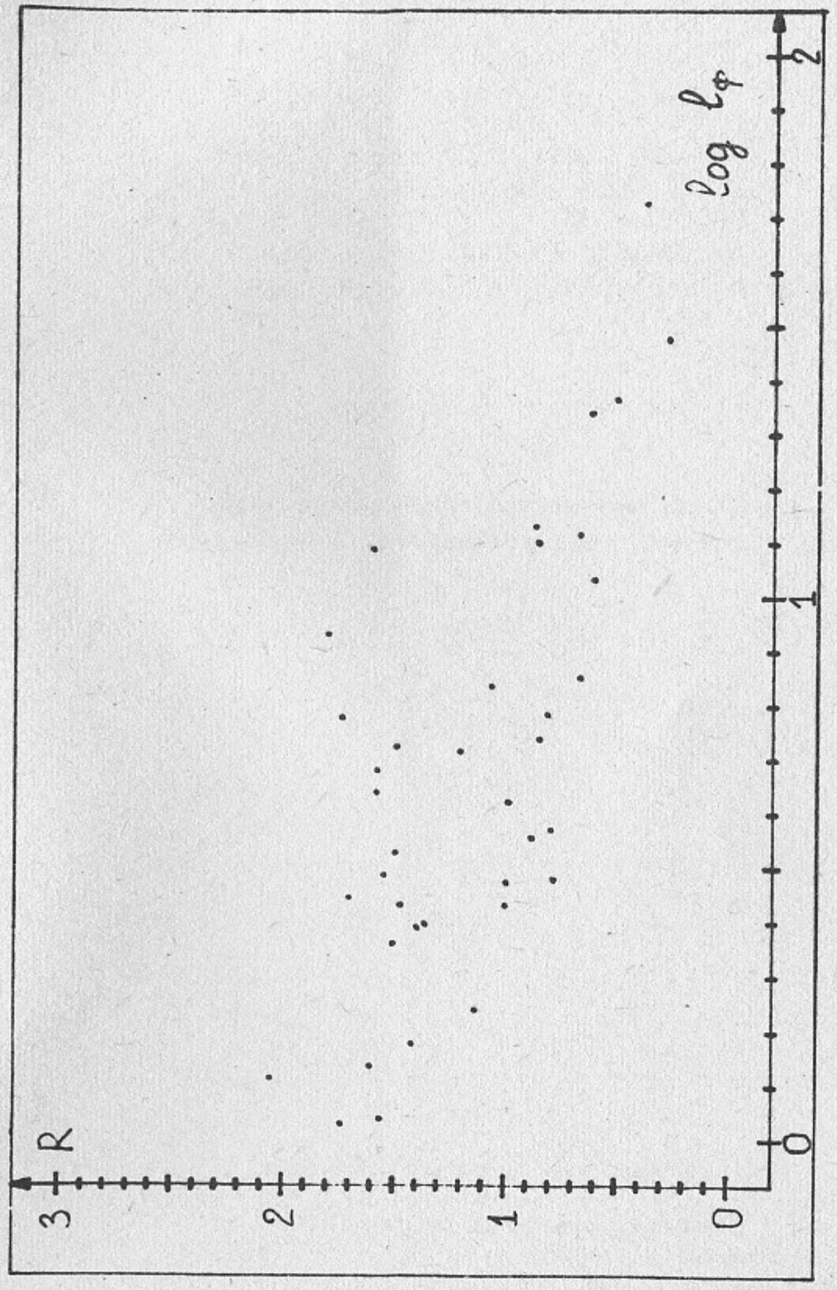

Fig. 4. The ratio $R = l_\Phi^E / l_\Phi^T$ of the experimentally obtained l_Φ^E to its theoretical value l_Φ^T from formula (4) versus $\log l_\Phi^T$ from the same 38 cases used in Fig. 3. The average value $\langle R \rangle = 1.17 \pm 0.07$.

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