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Modelling the Plasma-Sheath Boundary for Plasmas with Warm-Ion Sources

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ABSTRACT

In this paper we present a new approach how to solve the plasma equation for the case of Maxwellian ion source of a finite-temperature distribution. This problem is an old one which assumes solving an integral equation of Fredholm or, alternatively, Volterra type with a particular bell-shaped kernel. Due to mathematical difficulties with such physically very important kernel choice its shape was in the past approximated in several ways yielding approximate numerical solutions. Unfortunately, these solutions are valid only in limited ranges of ion temperature. In our approach we work with *exact* kernel, so we are capable to obtain the results which are, in principle, of arbitrary precision in an arbitrary range of the ion source temperatures. Precise solution of plasma-equation with finite temperature ion-source is extremely important in determining the plasma parameters for determining the plasma sheath boundary. In this paper we obtain the ion velocity distribution at arbitrary point in a plane-parallel discharge, which enable ones to calculate its moments (density, temperature and higher order moments) also at the edge of the system, where boundary conditions for a discharge should be known with a high degree of accuracy. We present here our results obtained both with PIC simulation and analytic-numerical method.

1 INTRODUCTION

Defining the edge of quasi-neutral plasma, i.e., the plasma-sheath boundary is an old but still not definitely solved problem which is of high relevance for fusion, laboratory and space plasmas. The plasma-sheath boundary is a surface up to which plasma can be considered as quasi-neutral, so that plasma can be modelled by using fluid approximation (instead of employing demanding kinetic model) by using the plasma-sheath boundary as a relevant boundary condition. However, this surface is still impossible to find with high accuracy. The plasma-sheath boundary can be rather precisely defined only in the asymptotic two-scale limit. In such an approximation the plasma-sheath boundary can be identified either from the plasma side (infinitely thin sheath) as a point of electric field singularity (famous Tonks-Langmuir model from 1929 [1]), or from the sheath side (infinitely large sheath) as the point of vanishing electric field (famous Bohm model from 1949 [2]). Both models were originally

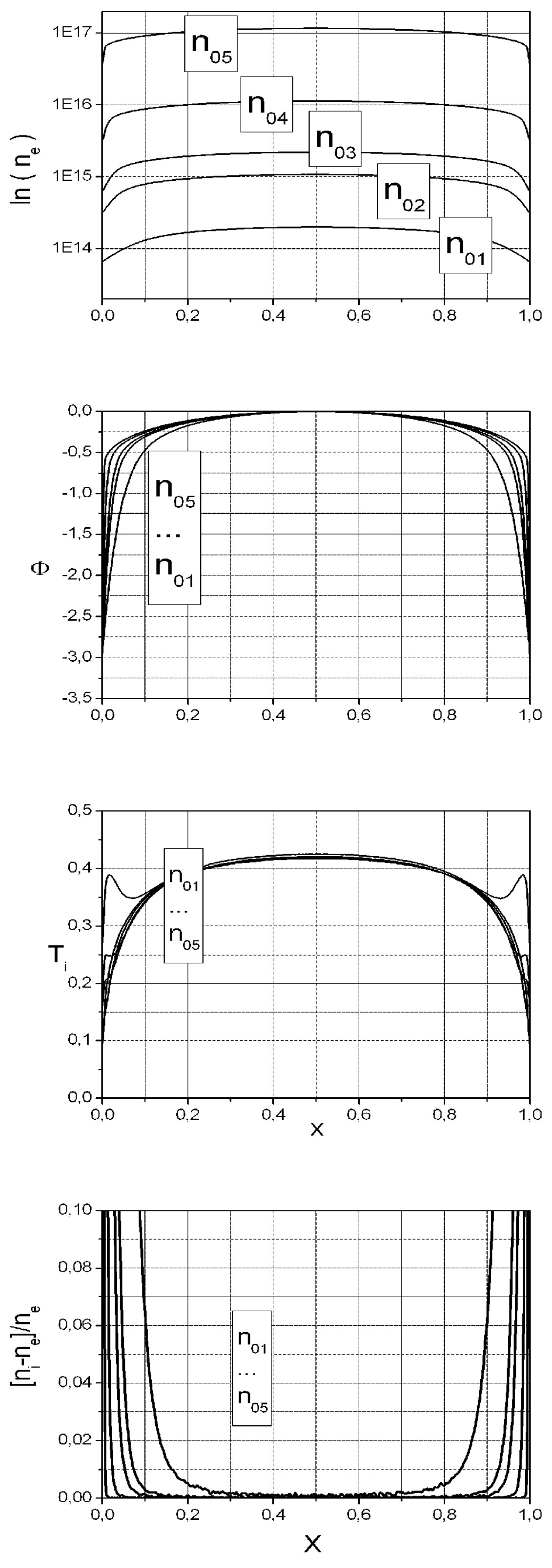

Fig. 1: Illustration of some basic plasma parameters, i.e., the plasma density, potential profile, ion temperature, local values of γ_i and charge imbalance for various source strengths obtained from one set of our numerical plasma "experiments" by using PIC simulations with finite ε

developed for the case of cold ion sources (ions created in plasma with *negligible ion source velocities* in comparison with electron velocities) and latter were generalized in a commonly adopted expression saying that the plasma-sheath is a place at which the ion average directional velocity in direction "z" normal to the plasma sheath surface is

$$u_i \geq \sqrt{k\left(T_e^* + \gamma T_i\right)/m_i},$$

where k is Boltzmann's constant, m_i is the ion mass, T_e^* is the electron so-called "screening" temperature($T_e^* = en_e/(kdn_e/d\Phi)$), T_i is the ion effective temperature, Φ is the local plasma potential, and γ is the ion "polytropic" coefficient (defined by $dp_i/dx = \gamma kT_i dn_i/dx$), with all quantities taken at the plasma-sheath boundary.

While during the last half-century γ was assumed to be constant in all fluid plasma models, it has been recognized only recently that γ is a spatially varying quantity (depending on position x in the one-dimensional case) rather than a global constant. Kuhn et al. (2006) [3] have shown by predominantly analytical means that in the asymptotic two-scale limit γ_i (subscript "i" means - ions) exhibits a sharp peak exactly at the plasma-sheath boundary. Jelić at al. (2007) [4], performed both analytic calculations and numerical particle-in-cell (PIC) simulations in the finite ε plasmas confirming the results of Kuhn et al for the "cold" ion velocity distribution ($T_i \ll T_e$). However, the analytic results obtained for cold ion-sources results are only of limited importance for fusion plasmas.

In order to extend the validity of Tonks-Langmuir model to the case of finite ion temperature source Bissell and Johnson in 1987 [5] developed an appropriate model (as shortly described bellow). However, their solution to the model was not enough reliable i.e., fails for small ion-source temperatures as a consequence of their choice of the kernel approximation in integral equation. Secondly, Bissell and Johnson imposed the boundary condition at the plasma-sheath boundary *in* *advance*, based on so called “marginal generalized Bohm criterion”. This assumption was recently explicitly disproved to be valid in general plasmas (se Riemann [6] and references therein).

On the other hand Scheuer and Emmert in 1988 [7] used a better kernel approximation enabling them to extend the validity of Bissell-Johnson model also for negligible ion-source temperatures, thus fitting excellent the original Tonks-Langmuir model. Secondly, they did not impose plasma-sheath boundary in advance but instead they calculated it a’posteriori.

However due to *kernel approximations* both above solutions remain limited either for small or for large temperatures. In the present work we present the method how to obtain the results for arbitrary T_i / T_e in an arbitrary wide range. This is done by employing the exact kernel of integral equation and solving it numerically. In addition we present the results of our PIC simulations as a reference highly reliable reference investigation.

2 THEORETICAL BACKGROUNDS

The geometry of the problem is symmetric one-dimensional plan-parallel as illustrated in Fig. 1 where we show some basic plasma parameters, i.e., the plasma density, potential profile, ion temperature and charge imbalance for various source strengths obtained from one set of our numerical plasma “experiments” by using PIC simulations with finite ε. Plasma is bounded between two perfectly absorbing walls biased at the same external electric potential. In simulation as well as in the theoretical model the electron velocity distribution function (VDF) is assumed to be Maxwellian with uniform electron temperature T_e. Consequently the electron density over the system is Boltzmann–distributed. The influence of the cut-off of the tail of electron velocity distribution (which yields the “screening” temperature) is assumed to be negligible (although it is trivial to take this effect into account whenever necessary). The ions are produced by ionization of neutrals with *finite* initial velocities, and the pre-sheath constitutes the entire quasi-neutral plasma. The ion VDF $f_i(x,v)$ in phase-space is calculated from Boltzmann’s equation:

$$v\frac{\partial f_i}{\partial x} - \frac{e}{m_i}\frac{d\Phi}{dx}\frac{\partial f_i}{\partial v} = S_i(x,v) \qquad (1)$$

with x the Cartesian space coordinate, v the particle velocity, e the positive elementary charge, m_i the ion mass, $\Phi(x)$ the electrostatic potential at position x. The discharge is symmetric about the position $x = 0$, with $\Phi(0) = 0$. The ionization rate in general depends on local coordinate. A formal solution of the above equation can be found along the characteristics in the form:

$$\frac{e}{m_i}\frac{d\Phi}{dx}\frac{1}{v} = \frac{dv}{dx} \qquad (2)$$

Source velocity distribution is bell-shaped (here it is Maxwellian) in velocity space. After introducing new variables:

$$x' = x$$
$$v'^2 = v^2 - \frac{2e}{m_i}(\Phi' - \Phi) \qquad (3)$$

the Boltzmann equation transforms into:

$$\frac{df_i}{dx'} = \frac{1}{v'(x')} S_i\left(x', v'^2 + \frac{2e}{m_i}(\Phi' - \Phi) \right) \qquad (4)$$

with a formal solution:

$$f_i(x, v(x)) = \int_x \frac{1}{v'} S_i\left(x', v'^2 + \frac{2e}{m_i}(\phi' - \phi) \right) dx' \tag{5}$$

where integration should be performed over all the space. As we pointed out the choice of the limits of integration depends on the model e.g., Bissell and Johnson used the marginal generalized Bohm criterion in advance as the boundary condition of the problem, while Scheuer and Emmert, instead, used the wall potential as the boundary condition and found *a posteriori* that the singularity of solution coincides with the place where generalized Bohm criterion holds, with rather high degree of accuracy.

Having in mind that we look at a monotonic potential $\Phi(x)$ the last solution takes the form appropriate for finding the velocity distribution:

$$f_i(\Phi, v) = \int_\Phi \frac{1}{v'} S_i\left(\Phi', v' + \frac{2e}{m_i}(\phi' - \phi) \right) \frac{dx'}{d\Phi'} d\Phi' \tag{6}$$

For some particular source distributions a step further can be performed like in work of Emmert and al [8] for the artificial velocity distribution, and in Bissell and Johnson [5] and Scheuer and Emmert [6] works with the Maxwelian ion-source velocity distribution.

On the other hand the Poisson's equation states:

$$-\frac{d^2\Phi}{dx^2} = \frac{e}{\varepsilon_0}(n_i - n_e), \tag{7}$$

where ε_0 is the vacuum dielectric constant and $n_{i,e}$ are the ion and electron densities, respectively.

In non-dimensional form the space coordinate is normalized to a suitable characteristic length ℓ of the plasma, i.e., the physical extension L of the system or the ionization length ℓ. In present investigation we are interested primarily in fusion plasmas where ℓ or L is much larger than the Debye length defined as

$$\lambda_D = \sqrt{\frac{\varepsilon_0 k T_e}{n_0 e^2}}, \tag{8}$$

Here n_0 is the electron density in the center of the plasma. Normalized quantities of interest are as follows:

$$\frac{e\Phi}{kT_e} \to \Phi\,,\ \frac{x}{\ell} \to x(\Phi)\,,\ \frac{n_{i,e}}{n_0} \to n_{i,e,}\,,\ \frac{T_i}{T_i} \to \tau\,,\ \frac{S_i \ell}{\sqrt{2} c_s n_0} \to S_i\,,\ \frac{c_{s0} f_i}{\sqrt{2} n_0} \to f_i\,,\ \frac{\lambda_D}{\ell} \to \varepsilon \tag{9}$$

where $c_{s0} \equiv \sqrt{kT_e/m_i}$ represents so called "cold-ion sound velocity". Since we assume that the potential profile $\Phi(x)$ is monotonic, so that the inverse function $x(\Phi)$ is monotonic as well, the mathematic rule: $d^2y/dx^2 = -(d^2x/dy^2)/|(dx/dy)|^3$ holds. The Poisson equation (Eq. (8)) in normalized variables thus reads

$$\int f_i(\Phi, v) dv = n_e + \varepsilon^2 \frac{d^2x/d\Phi^2}{|(dx/d\Phi)|^3}. \tag{10}$$

Esq. (10) and (6) provide a complete description of the finite-ε discharge. The central quantity of interest is obviously inverse electric field $dx/d\Phi$. Once this quantity is found the ion VDF can be calculated self-consistently from Eqs.(10) and Eq (6), depending on assumption of vanishing or non-vanishing ε respectively. Then, the moments of the VDF can be calculated as functions of the potential Φ or, equivalently, of the position x.

Once a numerical solution of the system (10) and (6) is obtained, it is straightforward to calculate the ion velocity distribution and all their moments i.e. density ($n = \int f(v) dv$), directional velocity ($u = \int f(v) v dv$), and ion temperature $T = \int f(v)(v-u)^2 dv$ and all higher moments like heat flux, energy flux etc. at any location,

The special quantity of our interest is the polytropic coefficient $\gamma_i(x)$ (or equivalently $\gamma_i(\Phi)$) which can be found by using the expression

$$\gamma_i = 1 + \frac{n_i}{T_i}\frac{dT_i}{dn_i} \equiv 1 + \frac{n_i}{T_i}\frac{dT_i/d\Phi}{dn_i/d\Phi} \tag{11}$$

with previously calculated moments of ion VDF.

3 RESULTS

Particle in cell method

For *quasi-neutral* models ($\varepsilon = 0$) solutions can be obtained analytically only in some special cases. Solving above problem for finite T_i and $\varepsilon > 0$ is a very non-trivial one, even via numerical-computation method and still is a considerable challenge which is waiting for a reliable algorithm to be used. Fortunately, we can instead use Particle in Cell numerical simulation (PIC) method [9, 10] which is full kinetic and inherently requires $\varepsilon > 0$ while the ion temperature is arbitrary. The shape of the velocity distribution obtained by us from PIC simulations is illustrated in Fig 2. On the other hand the fluid quantities in PIC simulations must not be calculated a'posteriori from such velocity distribution but, instead, the number of particles with certain properties (density, directional velocity, temperature, heat and energy fluxes) are "counted" within each discretization cell during the simulation.

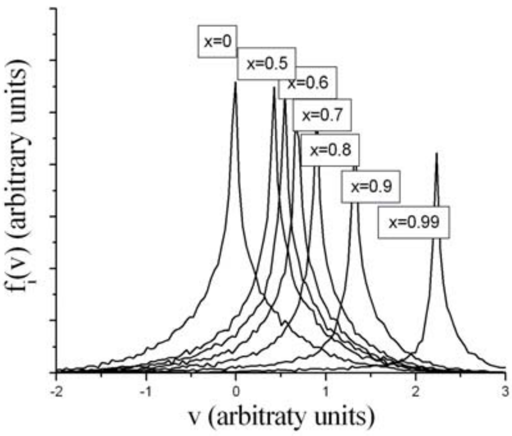

Fig. 2: Ion velocity distribution as obtained at various places by using PIC simulation experiments and corresponding polytropic coefficient as a function of local potential

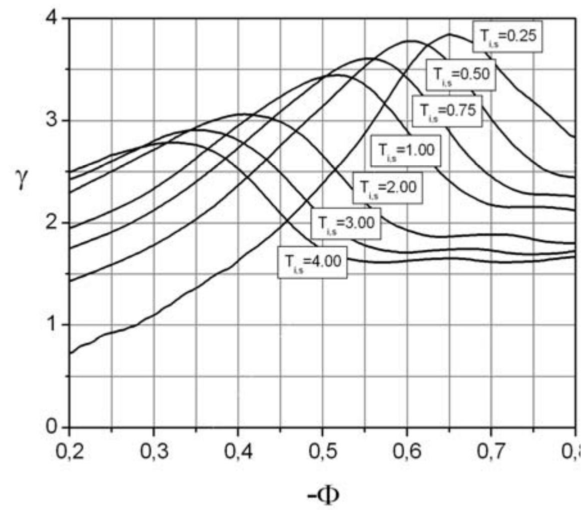

Fig. 3 Ion polytropic coefficients as obtained from PIC simulations

In Figure 3 we show also the ion poly-tropic coefficient obtained in our PIC simulations as function on local potential. Simulations were performed with care by using huge computer resources and can be considered as highly reliable regarding ion velocity distribution ever done for Tonks-Langmuir model with finite ion temperature.

However, a big problem of performing PIC simulations is the high cost of simulation. In addition the shape of our velocity distributions from PIC simulations is just a result of a very demanding "experiment". The results from such experiments are characterized by experimental or numerical noise which can be removed with highly increased cost. Finally, it is difficult to derive some possible semi-empiric physical laws from simulation results.

Therefore, our next step in the near future is to calculate corresponding curves from analytic-numerical ion velocity distributions for $\varepsilon > 0$, with even higher degree of accuracy than from PIC simulations. As an intermediate step, however, here we present our improvements of the existing analytic-numerical method for finite ion temperature and $\varepsilon = 0$, which is extremely important in the theory of two-scale and intermediate scale plasmas (see [6]), before the problem with $\varepsilon > 0$ will be finally also solved via this method.

Analytic-numerical approach

In the analytic numerical method here we use the procedure described above with ε=0. This approximation is perfect for fusion plasmas which are so dense that the sheath region can be neglected as a source of particles. The basic equation in this case is:

$$n_i = \int f_i(\Phi, v)dv \tag{12}$$

In the case of Maxwellian ion source Eq. (13) can be transformed into the form (see [6, 7]):

$$\frac{1}{B} = \int_0^1 dx' \exp[(1+\frac{\tau}{2})(\Phi' - \Phi)]\mathrm{K}_0(\frac{\tau}{2}|\Phi - \Phi'|) \;, \tag{13}$$

where K_0 is the modified Bessel function (see e.g., [11]), primed quantities represent dummy variables and

$$B = \frac{1}{2\pi}\sqrt{\frac{\tau m_i}{m_e}}\frac{n_0}{n_{average}}\exp(\Phi_{wall}) \tag{14}$$

depends on the kind of gas and the ratio of the electron over the ion temperature $\tau = T_e / T_i$. The wall potential is denoted by Φ_{wall} and $n_{average}$ is the average density of the electron (i.e., ion) population.

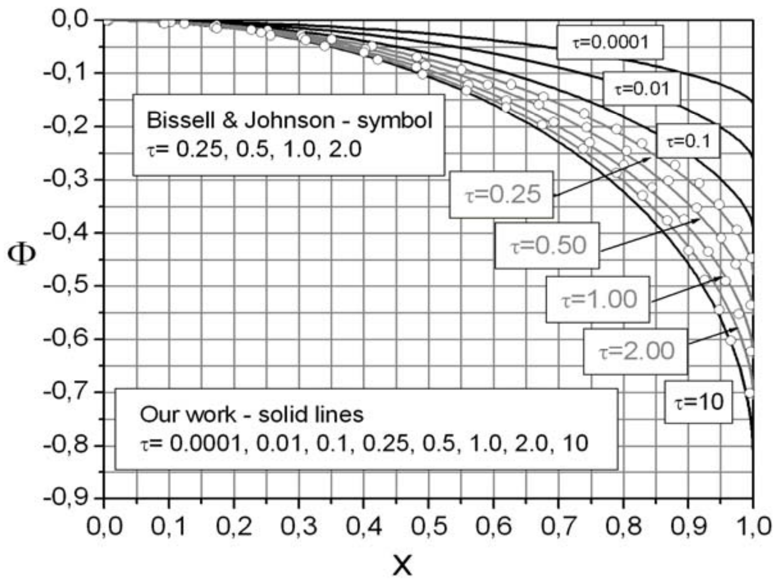

Fig. 4: Potential profiles as calculated from plasma-equation via our method. The range of the ratio of electron to ion temperature is practically unlimited and the solution is exact one within the numerical errors, but without any approximation of original formulas.

We solve Eq. (13) with finite difference mesh with varying density at x positions. The location of the i-th mesh point is given by

$$x_i = 1 - \left[1 - \frac{i-1}{n-1}\right]^{\lambda},$$

with n mesh points and $\lambda \geq 3$ to control higher density when x is approaching one. At each x_i we position unknown normalized potential Φ_i that is initialized as monotone function with shape similar to expected result. Each zone between points x_i and x_{i+1} is assumed to be linear variation of Φ and integrated as integral with singularity.

Equation (13) is rearranged to discrete version as

$$\exp[(1+\frac{\tau}{2})\Phi] = B\int_0^1 dx' \exp[(1+\frac{\tau}{2})\Phi']\mathrm{K}_0(\frac{\tau}{2}|\Phi-\Phi'|) \tag{15}$$

On each iteration, the right side of Eq. (15) is calculated and new Φ_i is corrected with a soft step of 5% to a new position. Constant *B* is also adjusted with the soft step strategy at the middle (x=0.5). To assure stable convergence, each approximation of Φ is additionally shifted and smoothed for next initialization In Fig 3. we show the potential profiles for varying the ion source temperature with other parameters fixed constant. We show the results of Bissell and Johnson presented by circles in the range of validity of their kernel approximation with our exact calculation in *grey color*. There is a nice qualitative and quantitative agreement within this range (τ =0.25, 0.5, 1.0, 2) .

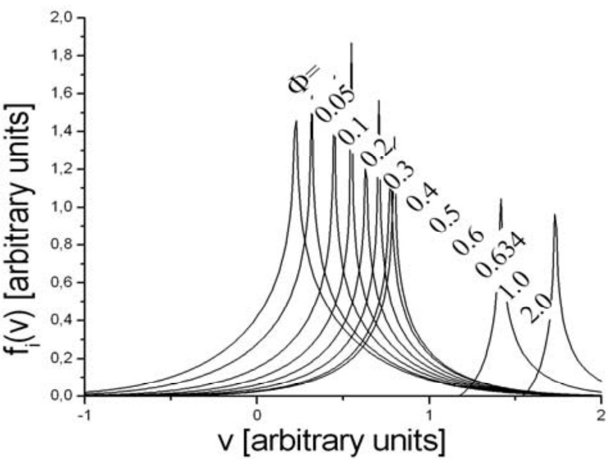

Fig. 5: Ion velocity distribution as obtained at various places by using our theoretical-numerical solution with exact kernel

Slight deviations should be ascribed not to our model but rather to the model of Bisell and Johnson. In black color we present our solution extended for some arbitrary ion temperatures (τ =0.0001, 0.01, 0.1, 10), where Bissel&Johnson and Scheuer&Emmert models are not valid.

. In Fig 5 we show the velocity distribution calculated at various location in the plasma discharge for the case τ=1. As mentioned above it is now technically “trivial” task to calculate the velocity distribution and consequently all the plasma parameters at each point of the plasma system.

4 DISCUSSION AND CONCLUSION

Our approach is novel in many aspects. As first by using PIC simulation method we obtained highly reliable potential profiles and ion velocity distribution ever done for Tonks-Langmuir model with finite ion temperature and with finite ε. In addition we obtained the profiles of a recently defined quantity ion polytropic coefficient as a function of local plasma potential (or equivalently as a function of local space coordinate). This investigation can be regarded as a reference one for comparing with results obtained via other alternative methods. Secondly, by using analytic-numeric approach for the case $\varepsilon = 0$ we obtained the solution with exact integral equation kernel. The advantage of our solution is advantageous at least at next aspects, i.e., (i) that our solution is exact in the sense that the original analytic kernel (modified Bessel function is not approximated as in previous works), so the results can be obtained for any combination of discharge parameters with arbitrary accuracy, and (ii) that the range of ion temperatures is not anymore limited like in previous works. The results appear to be very clear qualitatively. Quantitative comparison of the basic quantity, i.e., potential profile obtained with our method shows nice agreement with the results of Bissell and Johnson in the range of validity of their results. New results, obtained by us outside this range are presented as well. Our next step will be to extend our analytic-numerical calculations to the case of finite ε, for comparing with PIC simulations, which are applicable to real system without dividing the problem into plasma and sheath scale a-priori.

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