



Quasiclassical Theory of Tunnel Ionization of an Atom by the Perpendicular Electric and Magnetic Fields

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Abstract

The method of quasiclassical localized states is developed for the stationary Schrödinger equation with the potentials of the atomic field and perpendicular electric and magnetic fields. Using this method quasiclassical wave functions for an arbitrary atom are constructed in classically forbidden and allowed regions. The general analytical expression for leading term of the asymptotic (at small intensities of electrostatic \mathcal{E} and magnetic H fields when $H/(c\mathcal{E}) \ll 1$) behaviour of ionization rate of an atom in such electromagnetic field is found. Various limiting cases of the expression obtained are analysed.

1 Introduction

The problem of an atom in electric and magnetic fields has fundamental meaning for the quantum mechanics and atomic physics and has many applications (see, for example, [1, 2, 3] and the references therein). Since the twenties [4], properties of an energy spectrum of hydrogen atom and other atoms in external fields were rather intensively studied in the framework of the Schrödinger equation.

In order to construct a consistent theory of tunnel ionization of atoms one should solve the problem of electron motion in the field created by nucleus and constant uniform electric and magnetic fields. Since the Schrödinger equation with such superpositional potential does not permit complete separation of variables in any orthogonal system of coordinates, the given problem has no exact analytical solution, and numerical methods are still demand significant computational efforts.

The quasiclassical theory of atomic particles decay elaborated in sixties (see for instance [3]) has allowed obtaining useful analytical formulae for ionization rate which are asymptotic in the limit of “weak” fields. Both neutral atom [1, 5, 6, 7] and negative ions like H^- , J^- etc. [5, 8] (the first of these problems is more complicated due to necessity of taking into account the Coulomb interaction between outgoing electron and atomic core) were considered.

Subsequently (see papers [9, 10] and references therein) the imaginary time method (ITM) was elaborated for study ionization of atoms by electric and magnetic fields where classical trajectories are used with imaginary time. Although

this method is physically obvious it is not able to take into account the Coulomb interaction between an atom and outgoing electron consequently. Second limitation of this method is accounting only s -states.

Among the quantum-mechanical methods for studying the processes of interaction of atomic particles with electrical and magnetic fields, $1/n$ -expansion method (n – principal quantum number), which is quite effective for highly excited (Rydberg) states of atoms and molecules, including the consideration of effects in strong external fields (see, for instance, [11]) occupies a special place.

Additionally, of practical interest is the case when the intensities of the external electric and magnetic fields are much smaller than the intensity of the characteristic atomic fields. If this condition is satisfied the breakup of the atomic particle occurs slowly compared to the characteristic atomic times and the leaking out of the electron takes place primarily in directions close to the direction of the electric field. Therefore, in order to determine the frequency of the passage of the electron through the barrier it is convenient to solve the Schrödinger (or Dirac) equation near an axis directed along the electric field and passing through the atomic nucleus. This idea was used for solving the relativistic two-center problem at large intercenter distances [12], for calculating the leading term (in intensity of electric field F) of the tunnel ionization rate of an atom in a constant uniform electric field in non-relativistic [5, 13] and relativistic [14, 15, 16, 17] cases, and first two terms in non-relativistic case [18]. Also, we have calculated the leading term of the tunnel ionization rate of an atom in parallel electric field and magnetic field both non-relativistic [19, 20] and relativistic [21]. In our papers such method called “*the method of quasiclassical localized states*” (MQLS) is shown to be free from limitations of ITM.

In the present paper, our aim is to apply the method of quasiclassical localized states to solve the problem of an atom in the perpendicular constant uniform electric and magnetic field.

The paper is organized as follows. In section 2, the problem of the the atom in the perpendicular electric and magnetic fields is formulated. In section 3, we seek solutions of the stationary Schrödinger equation for an atom in the perpendicular constant uniform electric and magnetic fields in the form of the WKB expansion. In section 4, we find the solution of the problem in the domain $2Z/\gamma^2 \ll r \leq r_m$ where the atomic potential prevails electric and magnetic ones. In section 5, we find the solution in the domain $r \geq r_m$ using the idea of localized states. In section 6, we find the wave function in classically forbidden and allowed regions, calculate the leading term of tunnel ionization rate, and compare our results with ones of other authors in some limiting cases. In the last section of the paper, we discuss advantages of the elaborated method and further perspectives concerning its evolution.

2 The problem formulation

Consider an arbitrary non-relativistic atom placed in the constant uniform electric (the intensity \vec{E} is directed oppositely to z axis) and magnetic (the intensity \vec{H} is directed oppositely to y axis). The Hamiltonian for an electron in the

electromagnetic field is ($m_e = |e| = 1$)

$$\hat{\mathcal{H}} = \frac{1}{2} \left(\hat{\vec{p}} - \frac{1}{c} \vec{A} \right)^2 + V, \quad (1)$$

where $\hat{\vec{p}} = -i\hbar\vec{\nabla}$, \vec{A} and V are the vector and electrostatic potentials, respectively, c is the speed of light, \hbar is the reduced Planck constant, which will be turned later to unity. For the vector potential we use the Coulomb gauge:

$$\vec{A} = \frac{1}{2} \vec{H} \times \vec{r}.$$

The electrostatic potential is equal

$$V = V_{atom} - \mathcal{E}z, \quad V_{atom} \xrightarrow[r \rightarrow \infty]{} -Z/r.$$

The spectrum of such quantum-mechanical problem is quasistationary. The energy of an electron is complex

$$E_c = E - i\Gamma/2, \quad (2)$$

where E gives a position of quasistationary level, $\Gamma = w/\hbar$ is its width.

Considering all the above mentioned, we obtain the following wave equation:

$$\Delta\Psi + \frac{iH}{\hbar c} \left(z \frac{\partial\Psi}{\partial x} - x \frac{\partial\Psi}{\partial z} \right) + \frac{1}{\hbar^2} \left[2(E - V) - \frac{H^2}{4c^2} (x^2 + z^2) \right] \Psi = 0, \quad (3)$$

unpermitting the separation of variables in any orthogonal system of coordinates.

3 WKB expansion

We seek a solution of equation (3) in the form of the WKB expansion:

$$\Psi = e^{S/\hbar} \sum_{n=0}^{\infty} \hbar^n \psi_n. \quad (4)$$

Having substituted (4) into (3) and equated to zero the coefficients of each power of \hbar , we arrive at the hierarchy of equations

$$(\vec{\nabla}S)^2 + \frac{iH}{c} \left(z \frac{\partial S}{\partial x} - x \frac{\partial S}{\partial z} \right) = 2 \left(V - E + \frac{H^2}{8c^2} (x^2 + z^2) \right); \quad (5)$$

$$2\vec{\nabla}S\vec{\nabla}\psi_0 + \frac{iH}{c} \left(z \frac{\partial\psi_0}{\partial x} - x \frac{\partial\psi_0}{\partial z} \right) + \Delta S \psi_0 = 0; \quad (6)$$

$$2\vec{\nabla}S\vec{\nabla}\psi_{n+1} + \frac{iH}{c} \left(z \frac{\partial\psi_{n+1}}{\partial x} - x \frac{\partial\psi_{n+1}}{\partial z} \right) + \Delta S \psi_{n+1} = -\Delta\psi_n, \quad (7)$$

where $n = 0, 1, 2, \dots$

Unfortunately, equations (5)–(7), similarly to the initial equation (3), do not permit an exact separation of variables. In order to solve them we shall use the

idea of splitting the whole configuration space into domains, where in each of them only the dominating interaction type is taken into account exactly while the other interaction types are treated as perturbations.

Note that the conditions of applicability of the quasiclassical approximation used are ($m_e = |e| = \hbar = 1$)

$$\mathcal{E} \ll \gamma^3, \quad H/c \ll \gamma^2, \quad \gamma = \sqrt{-2E}. \quad (8)$$

For such intensities, the domain $2Z/\gamma^2 \ll r \ll r_m$ of space exists where the atomic field prevails the external ones, and in the zero approximation the wave function Ψ coincides with the leading term of the asymptotic behavior (at large r) of the unperturbed (atomic) wave function

$$\Psi_0^{(as)} = R^{(as)}(r)Y_{lm}(\theta, \varphi), \quad R^{(as)}(r) \simeq ar^{Z/\gamma-1} \exp(-\gamma r). \quad (9)$$

Here $r_m = r_m(\theta, \varphi)$ is the equation of the surface of space points in which the atomic potential is equal to the potential of the external superpositional (electromagnetic) field (for a rough estimate we can assume $r_m \sim \sqrt{Z}/\max(\mathcal{E}, H/c)$), $Y_{lm}(\theta, \varphi)$ is the spherical harmonics, l and m are respectively the orbital quantum number and its projection onto the quantization axis, a is the asymptotic coefficient of the radial wave function $R(r)$.

This fact allows us to formulate the following boundary condition for the equation (3)

$$\Psi \Big|_{2Z/\gamma^2 \ll r \ll r_m} \simeq \Psi_0^{(as)}. \quad (10)$$

Further, we shall solve the equations (5)–(7) in two domains: $2Z/\gamma^2 \ll r \leq r_m$ and $r \geq r_m$. In the first domain, it is worth to use the spherical coordinates while in the second domain – the Cartesian ones.

4 The solutions in the domain $2Z/\gamma^2 \ll r \leq r_m$

In the spherical coordinates (r, θ, φ) , the equation (5) is of the form

$$\begin{aligned} (\vec{\nabla}S)^2 + \frac{iH}{c} \left(\cos \varphi \frac{\partial S}{\partial \theta} - \frac{\cos \theta \sin \varphi}{\sin \theta} \frac{\partial S}{\partial \varphi} \right) = & \gamma^2 - \frac{2Z}{r} - 2\mathcal{E}r \cos \theta \\ & + \frac{H^2}{4c^2} r^2 (\sin^2 \theta \cos^2 \varphi + \cos^2 \theta). \end{aligned} \quad (11)$$

In the domain $2Z/\gamma^2 \ll r \leq r_m$, the coordinate $r^{-1} \ll 1$ is a small parameter, and the angular dependence of S is weak. Therefore, we seek the solution of (11) in the form of series

$$S = s_0(r) + s_1(r, \theta, \varphi) + s_2(r, \theta, \varphi) + \dots, \quad (12)$$

where each term is r times smaller than a previous one. Having substituted (12) into (11), and equated to zero the terms of each order of r , we arrive at the

hierarchy of equations

$$(s'_0)^2 = \gamma^2; \quad (13)$$

$$2s'_0 \frac{\partial s_1}{\partial r} = -\frac{2Z}{r} - 2\mathcal{E}r \cos \theta, \dots \quad (14)$$

Having solved the first two equations of this system with the boundary condition (10), we obtain

$$S = -\gamma r + \frac{Z}{\gamma} \log r + \frac{\mathcal{E}}{2\gamma} r^2 \cos \theta + O(r^{-1}). \quad (15)$$

In the same way, one can get the solution of the equation (6):

$$\psi^{(0)} = \frac{a}{r} Y_{lm}(\theta, \varphi) [1 + O(r^{-1})]. \quad (16)$$

5 The solutions in the domain $r \geq r_m$

5.1 The localized states

Let us now find solutions of the equations (5) and (6) in the domain $r \geq r_m$, where the Coulomb interaction can be considered as a perturbation. We seek the solution of (5) in the form

$$S = S_0 + S_1 + S_2 + \dots, \quad (17)$$

where S_0 is the solution of (5) without the Coulomb potential, S_1, S_2, \dots are the correction taking into account the Coulomb interaction:

$$\left(\frac{\partial S_0}{\partial x} + \frac{iH}{2c} z \right)^2 + \left(\frac{\partial S_0}{\partial y} \right)^2 + \left(\frac{\partial S_0}{\partial z} - \frac{iH}{2c} x \right)^2 = \gamma^2 - 2\mathcal{E}z; \quad (18)$$

$$\left(\frac{\partial S_0}{\partial x} + \frac{iH}{2c} z \right) \frac{\partial S_1}{\partial x} + \frac{\partial S_0}{\partial y} \frac{\partial S_1}{\partial y} + \left(\frac{\partial S_0}{\partial z} - \frac{iH}{2c} x \right) \frac{\partial S_1}{\partial z} = -\frac{Z}{\sqrt{x^2 + y^2 + z^2}}, \dots \quad (19)$$

In order to solve this system of equation we shall use the idea of the localized states consisting in the following.

There are many cases when for solving quantum mechanical problem it is sufficient to find a wave function not in the whole configurational space but in the neighbourhood of manifold M of less dimension. States described by such wave functions are called ‘‘localized states’’. It is natural to expand all the quantities in inseparable equations including their solutions in this vicinity. This idea was founded by Fock and Leontovich [22] and employed at solving diffraction problems [23] (the boundary-layer method), some quantum mechanical problems [24] (the parabolic equation method), and, finally, in the MQLS [14, 17, 19, 20, 21]. Here we apply this idea to the equations (18), (19).

As it is known [25] the classical trajectory of the charged particle in the perpendicular electric and magnetic field is located in the plane being perpendicular to the intensity of the magnetic field and containing the intensity of the electric field. In our field configuration, it is the plane xOz . Thus, we seek the solutions S_i of equation (18) in the form of the series in even powers of y :

$$S_i = S_{i0}(x, z) + S_{i1}(x, z)y^2 + \dots, \quad i = 0, 1, 2, \dots \quad (20)$$

Having substituted (20) into (18), (19) and equated to zero the coefficients of each power of y , we arrive at the hierarchy of equations for the functions S_{ij} . In order to find the wave function in zero approximation, it is sufficient to find S_{00} , S_{01} , and S_{10} which satisfy the equations

$$\left(\frac{\partial S_{00}}{\partial x} + \frac{iH}{2c}z\right)^2 + \left(\frac{\partial S_{00}}{\partial z} - \frac{iH}{2c}x\right)^2 = \gamma^2 - 2\varepsilon z; \quad (21)$$

$$\left(\frac{\partial S_{00}}{\partial x} + \frac{iH}{2c}z\right) \frac{\partial S_{01}}{\partial x} + \left(\frac{\partial S_{00}}{\partial z} - \frac{iH}{2c}x\right) \frac{\partial S_{01}}{\partial z} + 2S_{01}^2 = 0; \quad (22)$$

$$\left(\frac{\partial S_{00}}{\partial x} + \frac{iH}{2c}z\right) \frac{\partial S_{10}}{\partial x} + \left(\frac{\partial S_{00}}{\partial z} - \frac{iH}{2c}x\right) \frac{\partial S_{10}}{\partial z} = -\frac{Z}{\sqrt{x^2 + z^2}}. \quad (23)$$

5.2 The solutions of the equation (21)

The equation (21) is the non-linear but it can be ‘‘linearized’’ in the following way. Rewrite it in the form:

$$\frac{\partial S_{00}}{\partial z} - \frac{iH}{2c}x = \pm \sqrt{\gamma^2 - 2\varepsilon z - \left(\frac{\partial S_{00}}{\partial x} + \frac{iH}{2c}z\right)^2} \quad (24)$$

and make substitutions

$$\frac{\partial S_{00}}{\partial x} = P(x, z), \quad \frac{\partial S_{00}}{\partial z} = Q(x, z). \quad (25)$$

Then equation (24) is of the form

$$Q - \frac{iH}{2c}x = \pm q, \quad q(P, z) = \sqrt{\gamma^2 - 2\varepsilon z - \left(P + \frac{iH}{2c}z\right)^2}. \quad (26)$$

After differentiating (26) in x and taking into account the relation $\partial Q/\partial x = \partial P/\partial z$, we obtain the quasi-linear partial differential equation of the 1-st order for the unknown function $P(x, z)$:

$$\pm \left(P + \frac{iH}{2c}z\right) \frac{\partial P}{\partial x} + q \frac{\partial P}{\partial z} = \frac{iH}{2c}q. \quad (27)$$

The equation (27) can be solved by the method of characteristics and together with the boundary condition

$$P \underset{r \sim r_m}{\simeq} -\gamma \left(1 - \frac{\varepsilon z}{2\gamma^2}\right) \frac{x}{\sqrt{x^2 + z^2}}, \quad (28)$$

choosing the lower sign in (26) and (27), yields to the algebraic equation for P

$$\sqrt{\gamma^2 - 2\mathcal{E}z - \left(P + \frac{iH}{2c}z\right)^2} - \sqrt{\gamma^2 - \left(P - \frac{iH}{2c}z\right)^2} + \frac{\mathcal{E}c}{H} \log \frac{\frac{\mathcal{E}c}{H} - \sqrt{\gamma^2 - 2\mathcal{E}z - \left(P + \frac{iH}{2c}z\right)^2} + i\left(P + \frac{iH}{2c}z\right)}{\frac{\mathcal{E}c}{H} - \sqrt{\gamma^2 - \left(P - \frac{iH}{2c}z\right)^2} + i\left(P - \frac{iH}{2c}z\right)} = \frac{iH}{c}x. \quad (29)$$

As it is seen, an analytical solution of the equation (29) could allow us to find

$$S_{00} = \frac{iH}{2c}xz - \int qdz + f_0(x), \quad (30)$$

where $f_0(x)$ is defined by matching S with the expression (15) when $r \sim r_m$, and, therefore, to solve all the equations (22)-(23) and (6) by means of the method of characteristics. However, the equation (29) is transcendent and can be solved only approximately. For this, in the next section, we shall limit ourselves by the case when the the electric field prevails the magnetic one.

6 Approximation of the “weak” magnetic field

6.1 The wave function in the under-the-barrier region

Let us the situation when $H/(c\mathcal{E}) \lesssim \sqrt{\mathcal{E}} \ll 1$ when the classical trajectory is located in the vicinity of the z axis.

The asymptotic solution of the equation (29) is of the form

$$P(x, z) = -\frac{iH(\gamma - q_0)^2}{12c\mathcal{E}} - \frac{(\gamma + q_0)x}{2z}, \quad q_0(z) = \sqrt{\gamma^2 - 2\mathcal{E}z}. \quad (31)$$

Having calculated the integral in (30), solved the equations (22)-(23) and (6) by means of the method of characteristics and matching S and ψ_0 when $r \sim r_m$ with (15) and asymptotic (at $\theta \ll 1$) behavior of (16), respectively, we obtain the functions S_{00} , S_{01} , S_{10} , and ψ_0 . Finally, gathering all formulas together, we obtain the following solution of the equation (3):

$$\Psi = \psi_0 e^S, \quad (32)$$

$$S = \frac{q_0^3 - \gamma^3}{3\mathcal{E}} + \frac{Z}{\gamma} \log \frac{4\gamma^2 z}{(\gamma + q_0)^2} - \frac{H^2(\gamma - q_0)^3}{72c^2\mathcal{E}^3} \left[\frac{4}{5}(\gamma - q_0)^2 + 3\gamma q_0 \right] - \frac{iHx(\gamma - q_0)^2}{12c\mathcal{E}} - \frac{\gamma + q_0}{4z}(x^2 + y^2), \quad (33)$$

$$\psi_0 = \frac{\sqrt{\gamma} a A_{lm}}{\sqrt{q_0}} \left(\frac{\gamma + q_0}{2\gamma z} \right)^{|m|+1} \left[\left(x - \frac{iH z q_0}{3c\mathcal{E}} \right)^2 + y^2 \right]^{|m|/2} \times \exp \left(im \arctan \frac{y}{x - \frac{iH z q_0}{3c\mathcal{E}}} \right), \quad (34)$$

$$A_{lm} = (-1)^{\frac{m+|m|}{2}} \frac{1}{2^{|m|} (|m|)!} \sqrt{\frac{2l+1}{4\pi} \frac{(l+|m|)!}{(l-|m|)!}}. \quad (35)$$

Note that the expression (32) for the wave function is valid only in the classically forbidden (under-the-barrier) region $z < z_1$, where $z_1 = \gamma^2/(2\mathcal{E})$ is the turning point in which the quasiclassical momentum $q_0 = 0$.

6.2 The wave function in the classically allowed region. The tunnel ionization probability

Continuing Ψ to classically allowed region $z > z_1$, we find $(p_0(z) = iq_0(z) = \sqrt{2\mathcal{E}z - \gamma^2})$

$$\tilde{\Psi} = \tilde{\psi}_0 e^{\tilde{S}}, \quad (36)$$

$$\tilde{S} = \frac{ip_0^3 - \gamma^3}{3\mathcal{E}} + \frac{Z}{\gamma} \log \frac{4\gamma^2 z}{(\gamma - ip_0)^2} - \frac{H^2(\gamma + ip_0)^3}{72c^2\mathcal{E}^3} \left[\frac{4}{5}(\gamma + ip_0)^2 - 3\gamma ip_0 \right] - \frac{iHx(\gamma + ip_0)^2}{12c\mathcal{E}} - \frac{\gamma - ip_0}{4z}(x^2 + y^2), \quad (37)$$

$$\tilde{\psi}_0 = e^{i\pi/4} \frac{\sqrt{\gamma} a A_{lm}}{\sqrt{p_0}} \left(\frac{\gamma - ip_0}{2\gamma z} \right)^{|m|+1} \left[\left(x - \frac{H z p_0}{3c\mathcal{E}} \right)^2 + y^2 \right]^{|m|/2} \times \exp \left(im \arctan \frac{y}{x - \frac{H z p_0}{3c\mathcal{E}}} \right). \quad (38)$$

As it is known [1], the ionization probability (rate) is equal to

$$w = \int_S \vec{j} d\vec{s}, \quad \vec{j} = \frac{i}{2} \left(\tilde{\Psi} \vec{\nabla} \tilde{\Psi}^* - \tilde{\Psi}^* \vec{\nabla} \tilde{\Psi} \right). \quad (39)$$

Here S is the plane perpendicular to axis z and located at $z > z_1$.

Substituting (36) into the formula (39) one can calculate the leading term of the ionization rate

$$w = \frac{a^2(2l+1)}{2^{|m|+1}|m|!|\gamma|^{|m|}} \frac{(l+|m|)!}{(l-|m|)!} \left(\frac{2\gamma^2}{\mathcal{E}} \right)^{2Z/\gamma - |m| - 1} \exp \left(-\frac{2\gamma^3}{3\mathcal{E}} - \frac{H^2\gamma^5}{45c^2\mathcal{E}^3} \right). \quad (40)$$

For s -states ($l = m = 0$) formula (40) coincides with the result [26] obtained by ITM.

When $H \rightarrow 0$ the expression (40) is transformed into well-known result of Smirnov and Chibisov [5] for ionization rate of an atom in electrostatic field.

For finding the tunnel ionization rate of one time charged negative ions (i.e. H^- , J^- etc.), in (40) it is necessary to put $Z = 0$. If the particle is in weakly bound states in the central field with small radius of action r_0 then beyond this radius the asymptotic behaviour of the unperturbed ($\mathcal{E} = 0$) radial wave function is of the form [1]

$$R^{(as)}(R) = br^{-1}e^{-\gamma r}, \quad (41)$$

where b is determined by means of normalization. When $r_0 \ll 1$ the behaviour of the wave function within the potential well $0 \leq r \leq r_0$ is inessential because the particle stands basically beyond the well. This gives that $b \approx \sqrt{2\gamma}$ and the ionization rate of negative ion with the given energy E in the perpendicular electric and magnetic fields is equal to

$$w = \frac{2\gamma^2(2l+1)(l+|m|)!}{|m|!(l-|m|)!} \left(\frac{\mathcal{E}}{4\gamma^3}\right)^{|m|+1} \exp\left(-\frac{2\gamma^3}{3\mathcal{E}} - \frac{H^2\gamma^5}{45c^2\mathcal{E}^3}\right). \quad (42)$$

For s -states the formula (42) coincides with the result [26] obtained by ITM which at $H = 0$ transforms into the famous result of Demkov and Drukarev [1, 8].

Summary

The method of quasiclassical localized states is elaborated to solve asymptotically the Schrödinger equation with barrier-type potentials which do not permit a complete separation of variables. It is based on physically clear ideas, applicable to arbitrary states (not only s -states as ITM) and takes into account the Coulomb interaction between the outgoing electron and atomic core during tunneling consistently. This method has allowed us to obtain for the first time the wave function and general analytical expressions for leading term of the asymptotic behaviour of ionization rate of an arbitrary atom (and negative ion) in the perpendicular constant uniform electric and magnetic fields whose intensities \mathcal{E} and H are much smaller than intensity of intra-atomic field but $H/(c\mathcal{E}) \lesssim \sqrt{\mathcal{E}} \ll 1$.

Our next tasks are generalizations of MQLS on other configurations of electric and magnetic fields (perpendicular fields for the case $H/(c\mathcal{E}) \gg 1$, fields of arbitrary orientations, ununiform fields, non-stationary fields, strong laser field of various polarizations, etc.) and obtaining higher orders of ionization probability expansions in powers of \mathcal{E} and H in both the non-relativistic and relativistic cases.

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