Electronic Structure of Superheavy Atoms. Revisited.

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The electronic struture of an atom with $Z \leq Z_{\rm c} = 137$ can be described by the Dirac equation with the Coulomb field of a point charge Ze. It was believed that the Dirac equation with $Z > Z_{\rm c}$ is inconsistent and physically meaningless because the formula for the lower energy level of the Dirac Hamiltonian formally gives imaginary eigenvalues. But a strict mathematical consideration shows that difficulties with the electronic spectrum for $Z > Z_{\rm c}$ do not arise if the Dirac Hamiltonian is correctly defined as a self-adjoint operator, see [1]. In this article, we briefly summarize the main physical results of that consideration in a form suitable for physicists with some additional new details and numerical calculations of the electronic spectra.

I. INTRODUCTION

The question of electronic structure of an atom with large number Z of the nucleus, especially with Z that is more than the critical value $Z_{\rm c} = \alpha^{-1} \simeq 137,04$, where α is the finite structure constant, is of fundamental importance. The formulation of QED cannot be considered really completed until an exhaustive answer to this question is given. Although nuclei with overcritical charges can hardly be synthesized (at present, the maximum is $Z = 118$), the existing heavy nuclei can imitate the supercritical Coulomb fields at collision. Nuclear forces can hold the colliding nuclei together for $10^{-19}s$ or more. This time is enough to effectively reproduce the experimental situation where the electron experiences the supercritical Coulomb field [2]. The electronic structure of an atom with $Z \leq Z_{\rm c}$ can be described by the Dirac equation, which gives relativistic electronic spectra in agreement with experiment [3]. For such Z a complete set of solutions of the Dirac equation exists, and a relativistic quantum mechanics of an electron in such a Coulomb field can be constructed. As for the Dirac equation with the Coulomb field with $Z > Z_{\rm c}$, it was considered inconsistent and physically meaningless [4–6]. One of the standard arguments is that the formula for the lower energy level,

$$E = mc^2\sqrt{1-(Z\alpha)^2}\,, \qquad (1)$$

formally gives imaginary result for $Z > Z_{\rm c}$. This difficulty of the imaginary spectrum was attributed to an inadmissible singularity of the supercritical Coulomb field at the origin for a relativistic electron, see [7]. It was believed that this difficulty can be eliminated if a nucleus of some finite radius R is considered. It was shown that with cutting off the Coulomb potential with $Z < 173$ at a radius $R \sim 1,2 \times 10^{-12}$cm, the Dirac Hamiltonian has physically meaningful spectrum and eigenstates [8, 9]. But even in the presence of the cutoff, another difficulty arises at $Z \sim 173$. Namely, the lower bound state energy descends to the upper boundary $E = -mc^2$ of the lower continuum, and it is generally agreed that in such a situation, the problem can no longer be considered a one-particle one because of the electron-positron pair production, which, in particular, results in a screening of the Coulomb potential of the nucleus.

Not disputing the fact that taking account of a finite size of the nucleus corresponds to a more realistic setting up the problem, we do not agree with the assertion that the Dirac Hamiltonian with the Coulomb field of overcritical point-like nucleus charge is inconsistent. The abovementioned difficulties with the spectrum for $Z > Z_{\rm c}$ do not arise if the Dirac Hamiltonian is correctly defined as a self-adjoint (s.a.) operator. A rigorous mathematical treatment of all the aspects of this problem including a spectral analysis of the Hamiltonian based on the theory of s.a. extensions of symmetric operators and the Krein method of guiding functionals was presented in [1, 10, 11]. It was demonstrated that from a mathematical standpoint, a definition of the Dirac Hamiltonian as a s.a. operator presents no problem for arbitrary Z. A specific feature of the overcritical charges is a nonuniqueness of the s.a. Dirac Hamiltonian, but this non uniqueness is characteristic even for $Z > Z_{\rm s} = \left(\sqrt{3}/2\right)\alpha^{-1} \simeq 118,68$. For each $Z \geq Z_{\rm s}$, there exist a family of s.a. Dirac Hamiltonians parametrized by a finite number of extra parameters (and specified by additional boundary conditions at the origin). The existence of these parameters is a manifestation of a nontrivial physics inside the nucleus. A real spectrum and a complete set of eigenstates can be evaluated for each Hamiltonian, so that a relativistic quantum mechanics for an electron in such a Coulomb field can be constructed. In the present article, we briefly summarize all the previously obtained formal results in a form more suitable for physicists with some additional details and numerical calculations of the electronic spectra.

II. DIRAC HAMILTONIAN WITH COULOMB FIELD

We consider an electron of charge $-e < 0$ and mass m moving in the Coulomb field of a charge $Ze > 0$. We describe this field by a scalar electromagnetic potential of the form $A^0 = Zer^{-1}$, we set $\hbar = c = 1$ in what follows. A behavior of the electron in the Coulomb field is governed by the Dirac Hamiltonian $\hat{H}\,(Z)$ that is a

s.a. operator in the Hilbert space of square-integrable bispinors $\Psi(\mathbf{r})$. On its domain $\hat{H}(Z)$ acts by the differential operation

$$\check{H}(Z)=\gamma^0(\boldsymbol{\gamma}\check{\mathbf{p}}+m)-qr^{-1},\ \check{\mathbf{p}}=-i\nabla,\ r=|\mathbf{r}|,\ q=Z\alpha.$$

In the problem under consideration there are three commuting s.a. operators $\hat{\boldsymbol{J}}^2$, $\hat{J}_z$, and $\hat{K}$, where $\hat{\boldsymbol{J}}$ the total angular momentum, and $\hat{K}$ a spin operator,

$$\hat{\boldsymbol{J}}=\hat{\boldsymbol{L}}+\boldsymbol{\Sigma}/2,\ \hat{\boldsymbol{L}}=[\mathbf{r}\times\hat{\mathbf{p}}],\ \hat{K}=\gamma^0\left[1+\left(\boldsymbol{\Sigma}\hat{\boldsymbol{L}}\right)\right].$$

All they commute with $\hat{H}(Z)$. Any bispinor $\Psi(\mathbf{r})$ can be represented as $\Psi(\mathbf{r})=\sum_{j,M,\zeta}\Psi_{j,M,\zeta}(\mathbf{r})$, where $\Psi_{j,M,\zeta}$ are bispinors of the form

$$\Psi_{j,M,\zeta}(\mathbf{r})=\frac{1}{r}\begin{pmatrix}\Omega_{j,M,\zeta}(\theta,\varphi)f(r)\\ i\Omega_{j,M,-\zeta}(\theta,\varphi)g(r)\end{pmatrix},$$

$\Omega_{j,M,\zeta}$ are spherical spinors, $f(r)$ and $g(r)$ are radial functions, and $j=1/2,3/2,...,\ M=-j,-j+1,...,j$, $\zeta=\pm1$. Bispinors $\Psi_{j,M,\zeta}$ are eigenvectors of $\hat{\boldsymbol{J}}^2$, $\hat{J}_z$, and $\hat{K}$,

$$\hat{\boldsymbol{J}}^2\Psi=j(j+1)\Psi,\ \hat{J}_z\Psi=M\Psi,\ \hat{K}\Psi=-\zeta(j+1/2)\Psi\ .$$

The stationary Schrödinger equation $\hat{H}(Z)\Psi(\mathbf{r})=E\Psi(\mathbf{r})$ is reduced to a radial equation $\hat{h}(Z,j,\zeta)F(r)=EF(r)$, where F are doublets (with components $f(r)$ and $g(r)$) from the Hilbert space $\mathbb{L}^2(\mathbb{R}_+)=L^2(\mathbb{R}_+)\oplus L^2(\mathbb{R}_+)$ and $\hat{h}(Z,j,\zeta)$ are some s.a. radial Hamiltonians acting on the doublets $F(r)$ by radial differential operations

$$\check{h}(Z,j,\zeta)=-i\sigma_2d_r+\zeta(j+1/2)r^{-1}\sigma_1-qr^{-1}+m\sigma_3\ . \quad (2)$$

On basis of the differential operations $\check{h}(Z,j,\zeta)$ one can construct all possible corresponding s.a. radial Hamiltonians $\hat{h}(Z,j,\zeta)$ using von Neumann theory of s.a. extensions of symmetric operators. All the s.a. operators $\hat{h}(Z,j,\zeta)$ are defined by their definition domains $D_{\hat{h}(Z,j,\zeta)}$ where they act by the same differential operations (2). By the way of construction, all these s.a. operators $\hat{h}(Z,j,\zeta)$ represent s.a. extensions of the corresponding so-called initial symmetric operators $\hat{h}_{\rm in}(Z,j,\zeta)$ with the definition domains $D_{\hat{h}_{\rm in}(Z,j,\zeta)}=\mathcal{D}(\mathbb{R}_+)\oplus\mathcal{D}(\mathbb{R}_+)$, where $\mathcal{D}(\mathbb{R}_+)$ is a space of smooth functions $f(r)$ with a compact support on the interval $\mathbb{R}_+$. At the same time, all these s.a. operators $\hat{h}(Z,j,\zeta)$ represent s.a. restrictions of the operators $\hat{h}^+_{\rm in}(Z,j,\zeta)$ that act on the so-called natural domains $D^*_{\hat{h}(Z,j,\zeta)}(\mathbb{R}_+)$ of doublets $F\in\mathbb{L}^2(\mathbb{R}_+)$ that are absolutely continuos in $\mathbb{R}_+$ and, in addition, $\check{h}(Z,j,\zeta)F\in\mathbb{L}^2(\mathbb{R}_+)$. Thus, $D_{\hat{h}^+_{\rm in}(Z,j,\zeta)}=D^*_{\hat{h}(Z,j,\zeta)}(\mathbb{R}_+)$. The above mentioned restrictions are given by some s.a. boundary conditions such that $D_{\hat{h}(Z,j,\zeta)}\subseteq D^*_{\hat{h}(Z,j,\zeta)}(\mathbb{R}_+)$. Just after all $\hat{h}(Z,j,\zeta)$ are defined as s.a. operators a corresponding s.a. Dirac Hamiltonian can be restored in a unique way. A result of constructing s.a. radial Hamiltonians $\hat{h}(Z,j,\zeta)$ essentially depends on the values of the parameters Z and j. There are two regions of these parameters in the semiplane j,Z, we call them nonsingular and singular ones, where the problem of s.a. extensions has principally different solutions. These regions are separated by the singular curve $Z=Z_{\rm s}(j)$, where

$$Z_{\rm s}(j)=\sqrt{j(j+1)}\alpha^{-1}$$

such that the nonsingular and singular regions are defined by the respective inequalities $Z\leq Z_{\rm s}(j)$ and $Z>Z_{\rm s}(j)$. The values $Z_{\rm s}(j)=118,68;\ 265,37;\ ...$, can be called the singular Z-value for a given j. Below, we consider s.a. radial Hamiltonians $\hat{h}(Z,j,\zeta)$ and their spectra in the nonsingular and singular regions separately. Here we list common for both regions properties of these Hamiltonians. It turns out that the spectrum of each s.a. Hamiltonian $\hat{h}(Z,j,\zeta)$ is simple (nondegenerate) and contains a continuous part occupying the two semiaxis $E\leq-m$ and $E\geq m$ and a discrete part $\{E_{n_\zeta}(Z,j,\zeta)\}$ located in the interval $|E|\leq m$. The quantum numbers n_ζ take the values: $n_1=1,2,...;\ n_{-1}=0,1,2,....$ The discrete spectrum is always accumulated at the point $E=m$, and asymptotic form of the difference $E_{n_\zeta}(Z,j,\zeta)-m$ as $n_\zeta=n\to\infty$ is given by the well-known non-relativistic formula $E^{\rm nonrel}_n=-mq^2\left(2n^2\right)^{-1}$. Eigenfunctions of the discrete spectrum and generalized eigenfunctions of the continuous spectrum form a complete orthonormalized system in $\mathbb{L}^2(\mathbb{R}_+)$.

III. NONSINGULAR REGION

In the nonsingular region, $Z\leq Z_{\rm s}(j)$, deficiency indices of each operator $\hat{h}_{\rm in}(Z,j,\zeta)$ are zero and the operator $\hat{h}(Z,j,\zeta)=\hat{h}^+_{\rm in}(Z,j,\zeta)$ is a unique s.a. extension of $\hat{h}_{\rm in}(Z,j,\zeta)$ with the definition domain $D_{\hat{h}(Z,j,\zeta)}=D^*_{\hat{h}(Z,j,\zeta)}(\mathbb{R}_+)$. The functions belonging to $D^*_{\hat{h}(Z,j,\zeta)}(\mathbb{R}_+)$ have the following asymptotic behavior

$$F(r)=O(r^{1/2}),\ r\to0;\ F(r)\to0,\ r\to\infty.$$

A discrete spectrum $\{E_{n_\zeta}(Z,j,\zeta)\}$ of each Hamiltonian $\hat{h}(Z,j,\zeta)$ has the form

$$E_{n_\zeta}(Z,j,\zeta)=\frac{m(n_\zeta+\gamma)}{\sqrt{q^2+(n_\zeta+\gamma)^2}},\ \gamma=\sqrt{(j+1/2)^2-q^2}, \quad (3)$$

which is the well-known Sommerfeld spectrum of the Dirac electron in the Coulomb field with Z in the nonsingular region. This result justifies the standard formal treatment of the Dirac Hamiltonian with Z in the nonsingular region in the physical literature where the Dirac Hamiltonian is identified with the differential operation $\check{H}_D(Z)$ and the natural domain is implicitly assumed.

IV. SINGULAR REGION

In the singular regions, $Z > Z_{\rm s}\,(j)$, the deficiency indices of the operator $\hat{h}_{\rm in}\,(Z,j,\zeta)$ are $(1,1)$, and therefore, there exists a family $\{\hat{h}_\nu\,(Z,j,\zeta)\}$ of s.a. extensions of $\hat{h}_{\rm in}\,(Z,j,\zeta)$ parametrized by a parameter $\nu \in [\,-\pi/2,\pi/2]$, $-\pi/2 \sim \pi/2$. At the same time, each $\hat{h}_\nu\,(Z,j,\zeta)$ is a nontrivial restriction of $\hat{h}^+_{\rm in}\,(Z,j,\zeta)$, such that $D_{\hat{h}_\nu(Z,j,\zeta)} \subset D^*_{\hat{h}(q,\varkappa)}\,(\mathbb{R}_+)$. The position of the discrete energy levels $E^{(\nu)}_{n_\zeta}\,(Z,j,\zeta)$ essentially depends on ν, in particular, there exists a value $\nu = \nu_{-m}$, for which the lower energy level coincides with the boundary $E = -m$ of the lower continuous spectrum.

Technically, it is convenient to divide the singular region into three subregions, we call them subcritical, critical, and overcritical regions. The subregions are distinguished by a character of asymptotic boundary conditions at the origin specifying the domains $D_{\hat{h}_\nu(Z,j,\zeta)}$ of the operators $\hat{h}_\nu\,(Z,j,\zeta)$ and providing their self-adjointness. The boundary conditions are similar in each subregion, which provides similar solutions of the corresponding spectral problems. In what follows, we describe these subregions, the domains $D_{\hat{h}_\nu(Z,j,\zeta)}$ in these subregions, and some details of discrete spectra.

A. Subcritical regions

The subcritical region is defined by the inequality $Z_{\rm s}\,(j) < Z \le Z_{\rm c}\,(j)$, where

$$Z_{\rm c}\,(j) = (j+1/2)\,\alpha^{-1} = 137,04;\ 274,08;\ \ldots\ . \qquad (4)$$

In the subcritical region, the s.a. radial Hamiltonians $\hat{h}_\nu\,(Z,j,\zeta)$ are specified by s.a. boundary conditions,

$$F(r) = c[(mr)^\gamma d_+\cos\nu + (mr)^{-\gamma} d_-\sin\nu] + O(r^{1/2}),\ r\to 0,$$

where $0 < \gamma = \sqrt{(j+1/2)^2 - q^2} < 1/2$, c is an arbitrary complex number, and $d_\pm$ some constant doublets. The discrete spectrum consists of the points $\{E^{(\nu)}_{n_\zeta}\,(Z,j,\zeta)\}$ that obey the equation

$$\frac{\omega(E)\cos\nu + \Gamma(1-2\gamma)\sin\nu}{\omega(E)\sin\nu - \Gamma(1-2\gamma)\cos\nu} = 0,\ \omega\,(E)$$
$$= \frac{\Gamma(1+2\gamma)\Gamma(-\gamma - qE\tau^{-1})[q(m-E) - (\varkappa+\gamma)\tau]}{\Gamma(\gamma - qE/\tau)[q(m-E) - (\varkappa-\gamma)\tau](2\tau/m)^{2\gamma}},$$

where $\varkappa = \zeta(j+1/2)$, and $\tau = \sqrt{m^2 - E^2}$. The spectrum can be evaluated explicitly for the cases of $\nu = \pm\pi/2$ and $\nu = 0$. For $\nu = \pm\pi/2$, we have

$$E^{(\pm\pi/2)}_{n_\zeta}\,(Z,j,\zeta) = \frac{(n_\zeta - \gamma)m}{\sqrt{q^2 + (n_\zeta - \gamma)^2}}\ .$$

For $\nu = 0$, the spectrum $E^{(0)}_{n_\zeta}\,(Z,j,\zeta)$ is given by eq. (3), of course, with new values of γ. Thus, the known textbook results (in particular the Sommerfeld spectrum) correspond to $\nu = 0$.

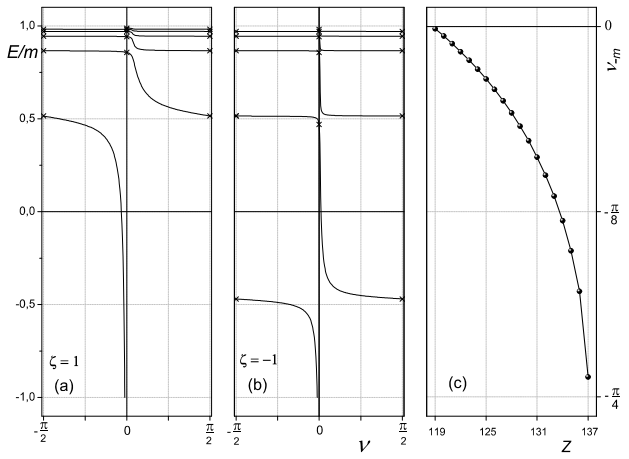

FIG. 1. ν-dependence of energy levels $E^{(\nu)}_{n_\zeta}\,(121,1/2,\zeta=\pm1)$ and Z-dependence of ν_{-m}, $j = 1/2$.

B. Critical region

The critical region is the critical curve $Z = Z_{\rm c}\,(j)$. For integer Z, this region does not exist if the finite structure constant α is an irrational number, see (4). In particular, this region certainly is absent for $j = 1/2$. In the critical region, the s.a. radial Hamiltonian $\hat{h}_\nu\,(Z,j,\zeta)$ is specified by s.a. boundary conditions at the origin of the form

$$F(r) = c\,[d_0(r)\cos\nu + d_+\sin\nu] + O(r^{1/2}\ln r),\ r\to 0,$$

where $d_0(r)$ are some doublet with the asymptotic behavior $d_0(r) = O\,(\ln mr)$ as $r\to 0$. Here the discrete spectrum $\{E^{(\nu)}_{n_\zeta}\,(Z,j,\zeta)\}$ is determined by the equation

$$\frac{f(E)\cos\nu - \sin\nu}{f(E)\sin\nu + \cos\nu} = 0,\ f(E) = \ln(2\tau/m)$$
$$+\,\psi(-\,(j+1/2)\,E/\tau) + \frac{\zeta - (\tau+\zeta m)\,/E}{2\,(j+1/2)} - 2\psi(1),$$

where $\psi(x) = \Gamma'(x)\Gamma^{-1}(x)$. The spectrum can be explicitly evaluated in the case of $\nu = \pm\pi/2$, where we have

$$E^{(\pm\pi/2)}_{n_\zeta}\,(Z,j,\zeta) = \frac{mn_\zeta}{\sqrt{(j+1/2)^2 + n_\zeta^2}}\ , \qquad (5)$$

which is eq. (3) with $\gamma = 0$.

C. Overcritical region

The overcritical region is defined by the inequality $Z > Z_{\rm c}\,(j)$. In this region, the s.a. radial Hamiltonians $\hat{h}_\nu\,(Z,j,\zeta)$ are specified by s.a. boundary conditions at the origin of the form

$$F(r) = c\left[{\rm e}^{i\nu}(mr)^{i\sigma}\rho_+ + {\rm e}^{-i\nu}(mr)^{-i\sigma}\rho_-\right] + O(r^{1/2}),\ r\to 0,$$

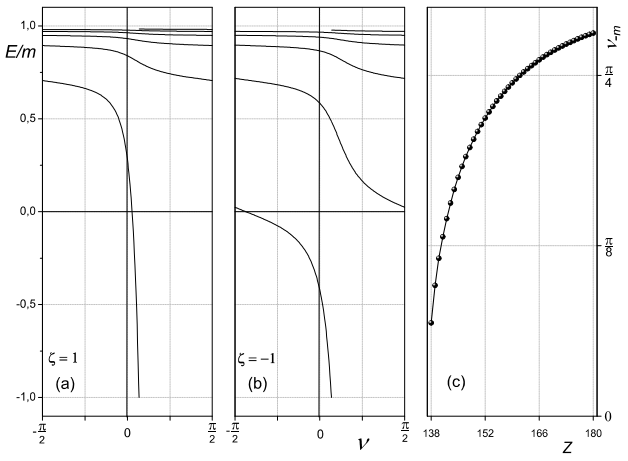

FIG. 2. ν-dependence of energy levels $E_{n_\zeta}^{(\nu)}(138, 1/2, \zeta = \pm 1)$ and Z-dependence of ν_{-m}, $j = 1/2$.

where $\sigma = \sqrt{q^2 - (j+1/2)^2} > 0$, c is an arbitrary complex number, and $\rho_\pm$ some constant doublets. Its discrete spectrum $\{E_{n_\zeta}^{(\nu)}(Z, j, \zeta)\}$is determined by the equation

$$\cos\left[\frac{1}{2i}\sum_{a=1}^{3}\left[\ln\left(B_a\right) - \ln\left(B_a^*\right)\right] + \sigma \ln\frac{2\tau}{m} - \nu\right] = 0,$$

where $B_1 = -2i\sigma$, $B_2(E) = i\sigma - Eq\tau^{-1}$, and $B_3(E) = \tau(j + 1/2 - i\zeta\sigma) - \zeta q(m - E)$.

V. CONCLUDING REMARKS

The total s.a. Dirac Hamiltonian $\hat{H}(Z)$ with $Z \leq 118$ is defined uniquely.For $Z \geq 119$, there is a family $\{\hat{H}_{\nu_1,...,\nu_\Delta}(Z)\}$ of possible total s.a. Dirac Hamiltonians.

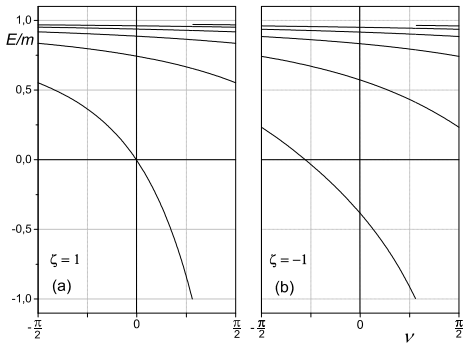

FIG. 3. ν-dependence of energy levels $E_{n_\zeta}^{(\nu)}(180, 1/2, \zeta = \pm 1)$.

The family is parametrized by the parameters $\nu_i \in [-\pi/2, \pi/2]$, $-\pi/2 \sim \pi/2$, $i = 1, ..., \Delta$. The number Δ of the parameters is given by $\Delta = 2k(Z)$, where the integer $k(Z) = (1/4 + Z^2\alpha^2)^{1/2} - \delta$, $0 < \delta \leq 1$. Any specific s.a. Dirac Hamiltonian $\hat{H}_{\nu_1,...,\nu_\Delta}(Z)$ corresponds to a certain prescription for a behavior of an electron at the origin. The general theory thus describes all the possibilities that can be offered to a physicist for his choice. This choice is a completely physical problem. We believe that each s.a. Dirac Hamiltonian with superstrong Coulomb field can be understood through an appropriate regularization of the potential and a subsequent limit process of removing the regularization. We recall that a physical interest in the electronic structure of superheavy atoms was mainly motivated by a possible pair creation in the superstrong Coulomb field. Consideration of this effect in the framework of the most simplest model of a point-like nucleus was accepted to be impossible due to the conclusion (which is wrong as it is clear now) that this model is mathematically inconsistent [7]. We believe that the described rehabilitation of the model allows returning to a consideration of the particle creation in this model that provide great scope for analytical studies.

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