Nuclear Polarization Study: New Frontiers for Tests of QED in Heavy Highly Charged Ions

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A systematic investigation of the nuclear polarization effects in one- and few-electron heavy ions is presented. The nuclear polarization corrections in the zeroth and first orders in $1/Z$ are evaluated to the binding energies, the hyperfine splitting, and the bound-electron g factor. It is shown that the nuclear polarization contributions can be substantially canceled simultaneously with the rigid nuclear corrections. This allows for new prospects for probing the QED effects in a strong electromagnetic field and the determination of fundamental constants.

The enormous progress made in experimental investigations of heavy highly charged ions during the last decades (see, e.g., Refs. [1–5] and references therein) has triggered the vigorous development of *ab initio* QED theory in the presence of strong nuclear fields. The relativistic behavior of electrons in highly charged ions requires a fully relativistic description from the very beginning, i.e., nonperturbative in the αZ parameter, where Z is the nuclear charge number. This plays a key role in contrast to QED theory for light atomic systems, where the parameter αZ is employed as an expansion parameter. Over the last decades essential progress has been achieved in theoretical calculations of various spectroscopic properties of highly charged ions, such as transition energies, hyperfine splitting (HFS), and the g factor (see Refs. [6–8] for reviews). In many cases, further improvement of the achieved theoretical accuracy seems strongly limited by the lack of knowledge of the nuclear properties. For example, in the case of the g factor of the H-like lead ion the uncertainty of the nuclear charge distribution correction is the main source of the total uncertainty, and in the case of the HFS in the H-like bismuth ion the uncertainty of the nuclear magnetization distribution correction (the so-called Bohr-Weisskopf effect) strongly masks the QED contributions. In Ref. [9] it was proposed to consider a specific difference of the HFS values of H- and Li-like ions with the same nucleus, where the uncertainty of the Bohr-Weisskopf effect is significantly reduced and the QED effects can be tested on the level of a few percent. In the case of the g factor, similar cancellations of the finite nuclear size corrections have been recognized for the specific differences of the g factors of H- and Li-like ions in Ref. [10] and of H- and B-like ions in Ref. [11], respectively. These differences can be calculated with a substantially higher accuracy, which opens excellent perspectives for a test of the QED effects and even provides a possibility for an independent determination of the fine structure constant from the strong-field QED theory.

Another nuclear effect appears due to the intrinsic nuclear dynamics, where the nucleus interacting with electrons via the radiation field can undergo real or virtual electromagnetic excitations. The latter effect leads to the nuclear polarization (NP) correction, e.g., to the binding energy of the electrons. Being restricted to phenomenological descriptions of the nucleon-nucleon interaction, the NP correction sets the ultimate accuracy limit up to which QED corrections can be tested in highly charged ions. Therefore, an important question should be addressed: To which extent can NP corrections be canceled in specific differences? In this Letter, we rigorously examined the NP and the screened NP corrections to the binding energies, HFS, and the g factor of heavy highly charged ions. We analyze the ratio of the finite nuclear size and the NP corrections and consequently evaluate the NP contribution to the specific differences, designed for the cancellation of the finite nuclear size and the Bohr-Weisskopf effect.

In Refs. [12,13] a relativistic field theoretical approach to the NP corrections in electronic atoms incorporating the effects due to virtual collective nuclear excitations within the framework of bound-state QED for atomic electrons was developed. This approach was successfully applied in calculations of NP corrections to the binding energies [12–16], to the HFS [17], and to the bound-electron g factor [18].

The lowest-order diagrams describing the NP effect are depicted in Fig. 1. As virtual nuclear excitations, we account for the dominant ones arising from the collective nuclear dynamics, such as rotations of deformed nuclei, harmonic surface vibrations, and giant resonances. Since the velocities associated with the collective nuclear dynamics are nonrelativistic, we can restrict ourselves to the nuclear charge-density fluctuation (electric multipole transitions) and neglect contributions arising from fluctuations of the nuclear vector current (magnetic multipole transitions). It is most suitable to employ the Coulomb gauge and keep the longitudinal component $\tilde{D}_{00}$ of the effective
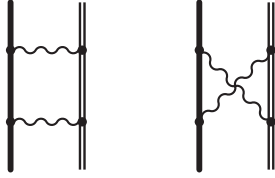
FIG. 1.   Feynman diagrams representing the lowest-order nuclear polarization effect to the electron binding energy. The bound electron (double line) interacts with the nucleus (heavy line) in its ground state via the exchange of virtual photons (wavy lines).

photon propagator $\tilde{D}_{\mu\nu}$ only. It describes the interaction between the electrons and virtual nuclear transitions and takes the form [12,13]

$$
\tilde{D}_{00}(\mathbf{r}_1, \mathbf{r}_2, \omega) = \sum_{LM} B(EL; L \to 0) \frac{2\omega_L}{\omega^2 - \omega_L^2 + i0} \\
\times F_L(r_1) F_L(r_2) Y_{LM}(\Omega_1) Y_{LM}^*(\Omega_2). \quad (1)
$$

Here ω_L is the nuclear excitation energy and $B(EL; L \to 0)$ is the corresponding reduced electric transition probability. This form of the propagator is also very suitable for numerical calculations, since it exclusively depends on phenomenological quantities such as transition energies ω_L, and corresponding electric transition strengths. The radial dependence carried by the functions F_L may be specified utilizing, e.g., a sharp surface model for describing the corresponding collective nuclear multipole transition densities [12–16]. The nuclear ground-state sphere radius R_0 is determined as $R_0 = \sqrt{5/3} \langle r^2 \rangle^{1/2}$, where $\langle r^2 \rangle^{1/2}$ is the root-mean-square charge radius.

The energy shift due to the lowest-order NP effect is given by

$$
\Delta E_{\text{NP}} = e^2 \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \sum_n \frac{\langle an | \tilde{D}_{00}(\omega) | na \rangle}{\varepsilon_a - \omega - \varepsilon_n u}, \quad (2)
$$

where the summation runs over the complete Dirac spectrum, and $u = 1 - i0$ preserves the proper treatment of the poles of the electron propagator. In Table I the leading order NP corrections are presented for the 1s, 2s, and $2p_{1/2}$ binding energies in $^{208}_{82}$Pb and $^{238}_{92}$U ions. For the low-lying rotational and vibrational nuclear excitations, the experimental values for the excitation energies ω_L and electric transition strengths $B(EL; L \to 0)$ are taken from Ref. [19] for the $^{208}_{82}$Pb ion and from Ref. [20] for the $^{238}_{92}$U ion. The corresponding ω_L and $B(EL; L \to 0)$ values for the giant resonances have been estimated employing the phenomenological energy-weighted sum rules [21]. The summation over the spectrum of the Dirac equation has been performed employing the dual-kinetic-balance finite basis set method [22] with basis functions constructed from B splines [23]. The Dirac spectrum is calculated in the field of extended nuclei utilizing nuclear charge-density distributions with recent values for the radii

TABLE I.   Nuclear polarization ΔE_{NP} and finite nuclear size ΔE_{FNS} corrections to the 1s, 2s, and $2p_{1/2}$ binding energies in $^{208}_{82}$Pb and $^{238}_{92}$U ions. The nuclear polarization corrections are compared with the previous calculations [16]. The corresponding ratios of the nuclear polarization and finite nuclear size contributions $\Delta_{\text{NP/FNS}}$ are presented.

State	1s	2s	$2p_{1/2}$
	$^{208}_{82}$Pb nucleus		
ΔE_{NP} (meV)	−28.89	−5.033	−0.4249
	−29.3[a]	−5.0[a]	
	−31.8[b]	−5.5[b]	
ΔE_{FNS} (eV)	67.18	11.66	0.9991
$\Delta_{\text{NP/FNS}}$ (10^{-3})	−0.430	−0.431	−0.425
	$^{238}_{92}$U nucleus		
ΔE_{NP} (meV)	−188.2	−35.88	−4.153
	−197.6[a]	−37.2[a]	−4.2[a]
	−213.4[b]	−40.9[b]	−4.6[b]
ΔE_{FNS} (eV)	198.6	37.73	4.412
$\Delta_{\text{NP/FNS}}$ (10^{-3})	−0.947	−0.951	−0.941

[a]Reference [16]: Direct numerical integration.
[b]Reference [16]: B-spline calculations.

$\langle r^2 \rangle^{1/2} = 5.5010$ fm and $\langle r^2 \rangle^{1/2} = 5.8569$ fm in the case of lead and uranium ions, respectively. As one can see from Table I, the obtained results are in a fair agreement with the previous calculations presented in Ref. [16], and a better agreement is found with the results obtained by the direct numerical integration.

In Table I we also present the corresponding leading order finite nuclear size corrections ΔE_{FNS} together with a ratio of the NP and finite nuclear size terms $\Delta_{\text{NP/FNS}}$ defined as $\Delta_{\text{NP/FNS}} = \Delta E_{\text{NP}} / \Delta E_{\text{FNS}}$. These ratios appear to behave rather similarly for all the considered electron states. This means that when we cancel the finite nuclear size corrections in an energy difference, the NP effect will also be reduced to a large extent.

However, the hydrogenic excited energy states are not always accessible experimentally; e.g., at present, the highest accuracy was achieved in measurements of the $2p_{1/2} - 2s$ transition energy in the heavy Li-like ^{238}U^{89+} ion [24]. Therefore, it becomes of distinct importance to investigate the NP effect in few-electron ions. In the presence of other electrons, in addition to the leading order one-electron NP correction, terms combining the interelectronic-interaction and NP effects appear. In analogy to the corresponding QED corrections we refer to them as the screened NP contribution. The diagrams of the NP corrections to the one-photon exchange are depicted in Fig. 2. Expressions for the energy shift due to this effect can be derived according to the Feynman diagrams depicted but are too lengthy to be presented here. Their evaluations have been performed in both Feynman and Coulomb gauges for the photon propagator describing the electron-electron interaction, thus providing an accurate check of the numerical procedure. The results obtained for the screened
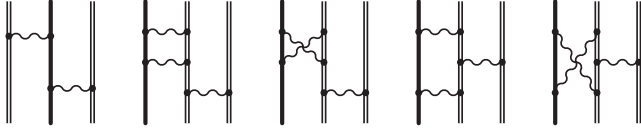
FIG. 2. Feynman diagrams representing the screened nuclear polarization effect to the electron level energy. Notations are the same as in Fig. 1.

NP corrections to the $(1s)^2$ binding energy and to the $(1s)^2 2s$, $(1s)^2 2p_{1/2}$, and $(1s)^2 2p_{3/2}$ ionization energies in $^{208}_{82}$Pb and $^{238}_{92}$U ions are presented in Table II. As one can see, the screened NP correction is comparable with the leading order term, and has to be taken into account in specific differences constructed for eliminating the finite nuclear size effect. In Table II we also present the finite nuclear size effect coming from the first-order interelectronic-interaction correction, the so-called screened finite nuclear size correction ΔE_{SFNS}, together with the corresponding ratio $\Delta_{SNP/SFNS}$ defined as $\Delta_{SNP/SFNS} = \Delta E_{SNP}/\Delta E_{SFNS}$. The ratio of screened NP and finite nuclear size corrections appears to be rather stable for different electronic configurations. This opens a possibility to eliminate in such differences not only the finite nuclear size corrections, but also the NP terms to a rather large extent.

As an example for such a cancellation, let us consider the following difference. One of the most precise measurements was performed for the $1s$ Lamb shift $\Delta E^{(1s)}$ in H-like uranium U^{91+} [25] and for the $2p_{1/2} - 2s$ transition energy $\Delta E^{(2p_{1/2}-2s)}$ in U^{89+} [24]. In both cases the uncertainty of the finite nuclear size correction essentially contributes to the total theoretical error bars. Thus, we can construct the following specific difference: $\Delta' E = \Delta E^{(2p_{1/2}-2s)} + \xi \Delta E^{(1s)} \approx 355.8$ eV, where the parameter $\xi = 0.161\,856$ is chosen in a way to cancel the leading order and the screened finite nuclear size terms. Such a cancellation is also rather stable with respect to the employed nuclear

TABLE II. Screened nuclear polarization and screened finite nuclear size corrections ΔE_{SNP} and ΔE_{SFNS}, respectively, to the $(1s)^2$ binding energy and to the $(1s)^2 2s$, $(1s)^2 2p_{1/2}$, and $(1s)^2 2p_{3/2}$ ionization energies (with the opposite sign) in $^{208}_{82}$Pb and $^{238}_{92}$U ions. The ratio of the screened nuclear polarization and screened finite nuclear size contributions $\Delta_{SNP/SFNS}$ are presented.

State	$(1s)^2$	$(1s)^2 2s$	$(1s)^2 2p_{1/2}$	$(1s)^2 2p_{3/2}$
		$^{208}_{82}$Pb nucleus		
ΔE_{SNP} (meV)	0.8441	0.3017	0.1218	0.0335
ΔE_{SFNS} (eV)	−1.9629	−0.6988	−0.2763	−0.0863
$\Delta_{SNP/SFNS}$ (10^{-3})	−0.430	−0.432	−0.441	−0.388
		$^{238}_{92}$U nucleus		
ΔE_{SNP} (meV)	5.498	2.048	0.9369	0.1793
ΔE_{SFNS} (eV)	−5.802	−2.152	−0.9816	−0.2117
$\Delta_{SNP/SFNS}$ (10^{-3})	−0.948	−0.952	−0.955	−0.847

charge distribution model. The NP corrections are canceled in $\Delta' E$ up to 10^{-4} eV, opening a possibility for unprecedented tests of strong-field QED. Although we have considered here only nuclear excitations of an electric type, this conclusion will hold in general, since the cancellation being discussed is observed for each individual nuclear excitation. In view of this, we can expect that this cancellation will be rather independent from the employed nuclear models.

Let us now go over to the NP effects to the HFS in few-electron ions. The HFS transition line in Li-like Bi^{80+} has been recently observed and directly measured in a laser spectroscopy measurement at GSI [4,5]. This has allowed us, for the first time, to compare experimental and theoretical values for the specific difference between the HFS of H- and Li-like bismuth ions. Although the present experimental accuracy is smaller than the theoretical one [26,27], in the future SPECTRAP Penning trap facility this will be improved by 3 orders of magnitude [28]. Substantial progress in the theoretical calculations of the specific difference [26,27,29,30] allows us to improve the theoretical accuracy by an order of magnitude, and the present uncertainty is partially restricted by the NP correction, which was so far known only for the $1s$ HFS [17].

In this Letter, we present for the first time results for the leading order and the screened NP corrections to the HFS of H-, Li-, and B-like bismuth ions. The leading order and the screened NP effect are given by the diagrams depicted in Figs. 3 and 4, respectively.

The basic expressions for the leading order diagrams are similar to those derived in Ref. [17], and for the screened diagrams they are rather bulky and will be presented elsewhere. The numerical procedure has been accurately checked by employing the Feynman and Coulomb gauges for the photon propagator describing the interelectronic interaction. For the nuclear parameters of low-lying vibrational levels of the nearly spherical odd-even $^{209}_{83}$Bi nucleus, we have employed the corresponding collective vibration levels in the neighboring even-even isotope of $^{208}_{82}$Pb (the weak-coupling limit). Moreover, we have evaluated the effect of single-nucleon excitations and the effect going beyond the weak-coupling limit. Both have been found to be negligible in the case of the $^{209}_{83}$Bi nucleus compared to
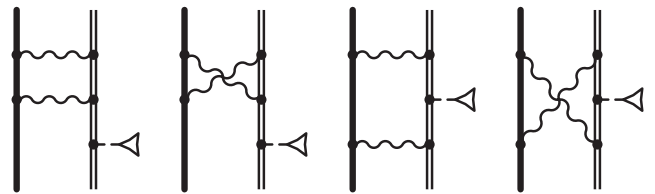

FIG. 3. Feynman diagrams representing the lowest-order nuclear polarization effect in the presence of an external potential. The dashed line terminated with the triangle denotes the interaction with the external magnetic field. Notations are the same as in Fig. 1.
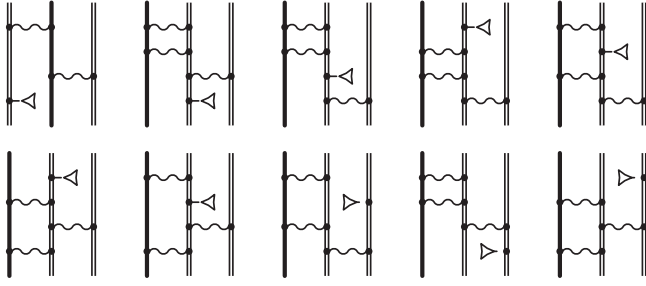
FIG. 4. Feynman diagrams representing the screened nuclear polarization effect in the presence of an external potential. For brevity, we depict here only the direct part of the nuclear polarization correction for all the diagrams except the first one. Notations are the same as in Fig. 1.

the effect of the collective core excitations. The detailed consideration will be presented elsewhere. The obtained results for the leading order and the screened NP corrections, $\Delta E_{\mathrm{HFS,NP}}$ and $\Delta E_{\mathrm{HFS,SNP}}$, respectively, are presented in Table III. Here, we employ the nuclear single-particle model for the description of the Bohr-Weisskopf effect. In the case of the $1s$ state, a fair agreement has been achieved with the previous value [17], which was obtained within the pointlike magnetic moment approximation. Now we introduce two specific differences: The first is between the HFS of H- and Li-like ions $\Delta'_{\mathrm{HL}} E_{\mathrm{HFS}}$ defined as $\Delta'_{\mathrm{HL}} E_{\mathrm{HFS}} = \Delta E_{\mathrm{HFS}}^{[(1s)^2 2s]} - \xi_{\mathrm{HL}} \Delta E_{\mathrm{HFS}}^{[1s]}$, and the second is between the HFS of H- and B-like ions $\Delta'_{\mathrm{HB}} E_{\mathrm{HFS}} = \Delta E_{\mathrm{HFS}}^{[(1s)^2 (2s)^2 2p_{1/2}]} - \xi_{\mathrm{HB}} \Delta E_{\mathrm{HFS}}^{[1s]}$. The parameters ξ_{HL} and ξ_{HB} are chosen in a way to cancel the Bohr-Weisskopf effects, and they appear to be rather stable with respect to variations of the nuclear model of the magnetization distribution [9]. In the case of $^{209}_{83}\mathrm{Bi}$, these parameters are chosen to be $\xi_{\mathrm{HL}} = 0.168\,86$ and $\xi_{\mathrm{HB}} = 0.014\,459$. In Table III we present the obtained results for the total NP contribution to the specific differences under consideration. As we can stress now, the NP effects are essentially reduced in both differences. The obtained results for the $\Delta'_{\mathrm{HL}} E_{\mathrm{HFS,NP}}$ and $\Delta'_{\mathrm{HB}} E_{\mathrm{HFS,NP}}$ appear to be rather stable with respect to the changes of the charge and magnetization

distribution models. In view of this we assign an uncertainty of 50% to the total NP corrections to the specific differences. This result opens the possibility for further theoretical improvements of the HFS specific differences and tests of the magnetic sector of strong-field QED. Moreover, this can lead to the determination of the nuclear magnetic moments from a comparison between the theoretical and experimental values for the specific differences.

We can now also consider the situation for the bound-electron g factor. The leading order and the screened NP corrections are given by the same diagrams as those for the HFS; see Figs. 3 and 4, respectively. In Table IV we present our numerical results obtained for the g factors of H-, Li-, and B-like lead ions. Our values for Δg_{NP} are in a reasonable agreement with the previous calculations of Ref. [18]. We also present the results for the specific differences between the H- and Li-like g factors g'_{HL} defined by $g'_{\mathrm{HL}} = g^{[(1s)^2 2s]} - \xi_{\mathrm{HL}} g^{[1s]}$, and between the H- and B-like g factors $g'_{\mathrm{HB}} = g^{[(1s)^2 (2s)^2 2p_{1/2}]} - \xi_{\mathrm{HB}} g^{[1s]}$. In the case of the Pb ions, the ξ parameters are chosen to be $\xi_{\mathrm{HL}} = 0.167\,026\,4$ [10] and $\xi_{\mathrm{HB}} = 0.009\,741\,6$ [11]. As one can see from the table, the NP corrections are canceled in specific differences by about 2 orders of magnitude. Our conservative estimation of the total uncertainty is of about 50% of the effect. In comparison with the rough estimation of the screened NP correction made in Ref. [11], here we rigorously take into account the first-order interelectronic-interaction correction to the nuclear polarization. We have also evaluated the effect originating from nuclear excitations induced via two types of magnetic interactions: One is due to the interaction with a constant magnetic field, and the other one is due to the magnetic interaction with an electron. In Ref. [31] such corrections were referred to as nuclear magnetic susceptibility corrections to the g factor. The contributions of this effect to the g factor are found to be -6.6×10^{-11}, -1.1×10^{-11}, and -0.4×10^{-11} for the $1s$, $2s$, and $2p_{1/2}$ states, respectively. The corresponding contributions to the specific differences are at least by an order of magnitude smaller than our uncertainty. Thus, we

TABLE III. Individual contributions to the leading order $\Delta E_{\mathrm{HFS,NP}}$ and the screened $\Delta E_{\mathrm{HFS,SNP}}$ nuclear polarization corrections to the ground-state hyperfine splitting of H-, Li-, and B-like $^{209}_{83}\mathrm{Bi}$ ions in $\mu\mathrm{eV}$. The total nuclear polarization contribution to the specific differences, $\Delta'_{\mathrm{HL}} E_{\mathrm{HFS,NP}}$ and $\Delta'_{\mathrm{HB}} E_{\mathrm{HFS,NP}}$, are also presented in $\mu\mathrm{eV}$.

State	$1s$	$2s$	$2p_{1/2}$	$\Delta'_{\mathrm{HL}} E_{\mathrm{HFS,NP}}$	$\Delta'_{\mathrm{HB}} E_{\mathrm{HFS,NP}}$
$\Delta E_{\mathrm{HFS,NP}}$	50.34 55[a]	8.865	0.730		
$\Delta E_{\mathrm{HFS,SNP}}$		−0.340	−0.095		
				0.025(12)	−0.09(5)

[a]Reference [17].

TABLE IV. Individual contributions to the leading order Δg_{NP} and the screened Δg_{SNP} nuclear polarization corrections to the ground-state g factor of H-, Li-, and B-like $^{208}_{82}\mathrm{Pb}$ ions in 10^{-8}. The total nuclear polarization contribution to the specific differences, $\Delta g'_{\mathrm{HL,NP}}$ and $\Delta g'_{\mathrm{HB,NP}}$, are also presented in 10^{-8}. The leading order nuclear polarization corrections are compared with the previous calculations [18].

State	$1s$	$2s$	$2p_{1/2}$	$\Delta g'_{\mathrm{HL,NP}}$	$\Delta g'_{\mathrm{HB,NP}}$
Δg_{NP}	−19.77 −22[a]	−3.444 −3.8[a]	−0.291 −0.32[a]		
Δg_{SNP}		0.129	0.104		
				−0.013(6)	0.006(3) 0.004(6)[b]

[a]Reference [18].
[b]Reference [11].

can state an improvement of the accuracy of the NP correction to the specific difference g'_{HB} by a factor of 2. In view of this new result we can push back the ultimate limit, defined by the NP effects, to the specific difference g'_{HB} and consequently to the possible accuracy of the determination of the fine structure constant. The recommended value of the fine structure constant according to the recent CODATA [32] is $\alpha = 1/137.035\,999\,074(44)$. The corresponding uncertainty in the specific difference $\delta g'_{HB}[\alpha] = 5 \times 10^{-11}$ is 1.5 times larger than the theoretical limit given by the NP uncertainty $\delta g'_{HB,NP} = 3 \times 10^{-11}$. Another principal uncertainty in the specific difference is coming from the remaining finite nuclear size effect. However, this uncertainty can be substantially reduced by employing the more accurate charge distribution parameters obtained from muonic atoms [33,34].

To conclude, we have evaluated the leading order and the screened NP corrections to the binding energies, HFS, and the bound-electron g factor of heavy highly charged ions. The interelectronic-interaction effects have been rigorously evaluated within the QED perturbation theory up to the first order in $1/Z$. The effect of the nuclear polarization has been evaluated for the specific differences constructed in a way to cancel the nuclear size corrections. In all cases considered here it turns out that the NP corrections determining the ultimate accuracy cancel substantially. Therefore, the rigorous investigations of the specific differences provide a unique opportunity to test the strong-field QED with a much higher accuracy than expected before. The ultimate accuracy of the nuclear polarization for the specific difference g'_{HB} has been now improved by a factor of 2. This may clear the way for a more accurate determination of the fine structure constant from the strong-field QED with a precision similar to the one obtained from the investigations of the free-electron g factor.

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