Calculation of the hyperfine structure of the superheavy elements $Z=119$ and $Z=120^+$

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The hyperfine-structure constants of the lowest s and $p_{1/2}$ states of superheavy elements $Z=119$ and $Z=120^+$ are calculated using *ab initio* approach. Core polarization and dominating correlation effects are included to all orders. Breit and quantum electrodynamic effects are also considered. Similar calculations for Cs, Fr, Ba$^+$, and Ra$^+$ are used to control the accuracy. The dependence of the hyperfine-structure constants on the nuclear radius is discussed.

I. INTRODUCTION

The study of the hyperfine structure (hfs) of heavy and superheavy elements is an important source of the information about nuclear structure of these elements (see, e.g., Refs. [1,2]). Hyperfine-structure intervals are proportional to nuclear moments, such as magnetic dipole moment, electric quadrupole moment, etc. The values of these moments can be extracted from the comparison of the calculations and the measurements. Apart from that, the hyperfine-structure intervals are sensitive to electric charge and magnetic moment distributions within the nucleus. Parameters of these distributions can often be extracted from the analysis of the hyperfine structure subject to sufficient experimental data and the accuracy of the calculations.

The hyperfine-structure analysis can be even more important for the superheavy elements ($Z>100$) where sources of the information are very limited. The study of the superheavy elements are motivated by the hypothetical *island of stability* in the region $Z=114$ to $Z=126$ where shell closures are predicted (see, e.g., [3]). Elements up to $Z=118$, excluding $Z=117$, have been synthesized (see, e.g., Refs. [4,5]) and evidence for the naturally occurring element $Z=122$ has been reported [6].

The use of the hyperfine-structure analysis is limited to nuclei with odd number of protons or neutrons. The heaviest examples of such nuclei that can be found in the literature as being already observed include, e.g., $^{288}_{115}$Uup and $^{289}_{114}$Uuq [7]. There are numerous similar examples for smaller Z. The information about nuclear magnetic dipole and electric quadrupole moments, charge, and magnetic moment distribution for these elements is practically absent.

Some standard approaches to the analysis of the hyperfine structure do not work for very high Z. Consider, for example, the Fermi-Segré [2] formula with the Casimir relativistic factor. It expresses the hyperfine-structure constant of the s state of an external electron via its wave function in the origin,

$$A_s = \text{const} \times |\psi(0)|^2 F_{rel}(Z\alpha)(1-\delta)\text{Ry}, \qquad (1)$$

where α is the fine-structure constant, Ry is Rydberg, δ is the correction due to finite nuclear size, and $F_{rel}(Z\alpha)$ is the relativistic factor

$$F_{rel}(Z\alpha) = \frac{3}{\gamma(4\gamma^2 - 1)}, \quad \gamma = \sqrt{1 - Z^2\alpha^2}. \qquad (2)$$

Formulas (1) and (2) are widely used in the hfs analysis; however, they fail at very high Z. It is easy to see that the relativistic factor (2) turns to infinity at $Z=118.7$. Therefore, it is likely to overestimate the relativistic corrections at smaller Z as well. The reason for this is that the formulas treat finite nuclear size as a small correction. Hydrogenlike wave functions for a pointlike nucleus are used to calculate the relativistic factor. However, it is known that the finite nuclear size correction for superheavy elements is not small and cannot be treated as a perturbation (see, e.g., [8]).

A combination of analytical and numerical approaches was recently used in Ref. [9] to study the dependence of the hyperfine-structure intervals on the nuclear radius. A formula was suggested, which is in good agreement with accurate numerical calculations for s states of atoms with $Z<100$. However, this formula also fails at higher Z.

In this Brief Report we do not use any analytical approaches but just perform accurate numerical calculations of the hyperfine-structure constants for superheavy atoms. We demonstrate that the calculation which uses finite-size nuclei with realistic charge and magnetic moment distribution is very similar to the calculations for lighter atoms. We consider elements E119 and E120$^+$. The latter may have hyperfine structure if there is an isotope with odd number of neutrons. Neither of these elements has been synthesized yet. However, the ways of their production and the physics of their nuclei are discussed in the literature [10]. These elements are heavier than any known element. Therefore, if the calculation of the hyperfine structure brings no surprises for them, one can expect no surprises for lighter elements as well. Also, these elements have a very simple electron structure with one external electron above closed shells. Therefore, very accurate calculations are possible for the elements. In our previous work [11] we have calculated the energy levels of E119 and E120$^+$. Apart from some expected relativistic effects such as larger fine structure and stronger attraction of the s states to atomic core, the spectra of these superheavy elements are very similar to the spectra of their lighter analogies, Fr, Ra$^+$, Cs, and Ba$^+$. We expect similar trend for the hyperfine structure and we perform the calculations for the same set of atoms. This gives us an estimate of the accuracy of the results for superheavy elements. We

TABLE I. Isotopes of Cs, Ba, Fr, and Ra for which hyperfine-structure constants have been calculated in the present work. Magnetic moments are in nuclear magnetons; $g_I \equiv \mu / I$.

Isotope	μ	I	g_I	r_N (fm)	rms (fm)[a]
^{133}Cs	2.582024	7/2	0.737721	5.671	4.8041
^{135}Ba	0.837943	3/2	0.558629	5.703	4.8273
^{211}Fr	4.00(8)	9/2	0.889	6.717	5.5545
^{225}Ra	−0.7348(15)	1/2	−1.4696	6.887	5.6781

[a]Reference [17].

stress that, although the calculations bring no major surprise, the dependence of the hyperfine structure on the nuclear radius is significantly stronger for the superheavy elements than for their lighter analogies.

II. METHOD OF CALCULATION

We perform the calculations using a totally *ab initio* method developed in our previous works [11–16]. It starts from the relativistic Hartree-Fock (RHF) calculations for atomic core and includes dominating correlation and all core polarization corrections to all orders.

Single-electron orbitals are found by solving a system of the RHF equations for $N-1$ electrons of the closed-shell core (the V^{N-1} approximation). The RHF Hamiltonian has a form

$$\hat{H}_0 = c\boldsymbol{\alpha} \cdot \mathbf{p} + (\beta - 1)mc^2 + V_{\text{nuc}}(r) + V^{N-1}. \quad (3)$$

Here, α and β are Dirac matrices, $V_{\text{nuc}}(r)$ is the nuclear potential, $V^{N-1} = V_{\text{dir}} + V_{\text{exch}}$ is the sum of the direct and exchange Hartree-Fock potentials, and N is the number of electrons. At distances much larger than the nuclear radius r_N, the nuclear potential is given by $V_{\text{nuc}}(r) = -Ze^2/r$; at short distances $V_{\text{nuc}}(r)$ is obtained by numerical integration of the Fermi distribution of nuclear electric charge. We use $d = 2.3$ fm as the thickness of the distribution and the data from Ref. [17] for the radii (see Table I). We use $r_N = 1.1(2.5Z)^{1/3}$ fm for superheavy elements.

The hyperfine interaction (HFI) is included in a self-consistent way as well. The time-dependent Hartree-Fock (TDHF) method [12], which is equivalent to the well-known random-phase approximation (RPA), is used for this. To take into account finite nuclear size we use a simple model which represents the nucleus as a uniformly magnetized ball. In our calculations the magnetic nuclear radius is the same as the electric one. However, these two parameters can be varied independently.

The HFI Hamiltonian is given by

$$\hat{H}_{hfi} = e\boldsymbol{\mu} \cdot \mathbf{F}(\mathbf{r}), \quad (4)$$

$$\mathbf{F}(\mathbf{r}) = \begin{cases} \dfrac{\mathbf{r} \times \boldsymbol{\alpha}}{r_m^3}, & r < r_m \\[2mm] \dfrac{\mathbf{r} \times \boldsymbol{\alpha}}{r^3}, & r \geq r_m, \end{cases} \quad (5)$$

where r_m is the magnetic nuclear radius.

The TDHF equations have a form

$$(\hat{H}_0 - \epsilon_a)\delta\psi_a = (-F_z - \delta V^{N-1} + \delta\epsilon_a)\psi_a, \quad (6)$$

$$\delta\epsilon_a = \langle \psi_a | F_z + \delta V^{N-1} | \psi_a \rangle. \quad (7)$$

Here, the index a numerates states in the closed-shell core. These equations are solved self-consistently for all states in the core.

States of the valence electron are calculated in the frozen field of atomic core complemented by the *correlation potential* operator $\hat{\Sigma}$ [13],

$$(\hat{H}_0 + \hat{\Sigma} - \epsilon)\psi_v^{BO} = 0. \quad (8)$$

Here, the index v numerates valence states. The correlation potential Σ includes all lowest second-order correlation corrections and dominating higher-order correlation corrections [14,15]. These higher-order correlations include screening of Coulomb interaction and hole-particle interaction. They are taken into account in all orders. Solving Eq. (8) for valence states we find the so-called *Brueckner* orbitals (BOs) for the valence states. This is emphasized by using superscript *BO* for the orbitals.

The total-energy shift for the valence state v due to HFI and correlations is given by

$$\delta\epsilon_v = \langle \psi_v^{BO} | F_z + \delta V^{N-1} + \delta\hat{\Sigma} | \psi_v^{BO} \rangle. \quad (9)$$

Here, $\delta\hat{\Sigma}$ is the change to the correlation potential $\hat{\Sigma}$ due to the hyperfine interaction. The term with $\delta\hat{\Sigma}$ is often called the *structure radiation*. Finally, there is a contribution due to the renormalization of the many-electron wave function (see, e.g., [13])

$$\delta\epsilon_{\text{norm}} = -\langle \psi_v | F_z + \delta V^{N-1} | \psi_v \rangle \langle \psi_v | \partial\hat{\Sigma}/\partial E | \psi_v \rangle. \quad (10)$$

The magnetic dipole hyperfine-structure constant A_v for the valence state v is given by

$$A_v = \frac{\mu e^2}{2m_p I} \frac{\delta\epsilon_v}{\sqrt{j_v(j_v + 1)(2j_v + 1)}}. \quad (11)$$

Breit and quantum electrodynamics corrections

It is hard to claim high accuracy of calculations for superheavy elements without considering Breit and quantum elec-

TABLE II. Hyperfine-structure constants of the lowest $s_{1/2}$ and $p_{1/2}$ states of Cs, Fr, E119, Ba$^+$, Ra$^+$, and E120$^+$ in different approximations in MHz (Cs, Fr, Ba$^+$, Ra$^+$) and $g_I \times$ MHz (E119, E120$^+$).

Atom	State	RHF	RPA	BO	RPA (BO)	Breit	Rad.	Str+norm	Total	Expt.
Cs	$6s$	1425	1718	1970	2325	6	−21	−31	2279	2298.2[a]
	$6p_{1/2}$	161	202	240	294	0	0	5	299	291.89[a]
Fr	$7s$	5791	6875	7716	8967	33	−162	−120	8718	8713.9[b]
	$7p_{1/2}$	623	772	968	1180	−4	−4	8	1180	1142[b]
E119	$8s$	39344	46781	45531	53306	210	−553	−1315	51648	
	$8p_{1/2}$	5141	6165	8751	10506	−65	−41	135	10535	
Ba$^+$	$6s$	2607	3095	3147	3684	8	−42	−82	3568	3591.6706(3)[c]
	$6p_{1/2}$	441	530	568	674	−1	0	4	677	664.2(2.4)[c]
Ra$^+$	$7s$	−21357	−25022	−25114	−28986	92	436	668	−27790	−27684(13)[d]
	$7p_{1/2}$	−3626	−4330	−4746	−5611	19	19	−31	−5604	−5446(7)[d]
E120$^+$	$8s$	74195	86640	80396	92884	352	−837	−2790	89609	
	$8p_{1/2}$	16883	19849	22286	26218	−117	−92	12	26021	

[a]Reference [20].
[b]Reference [21].
[c]Reference [22].
[d]Reference [23].

trodynamics (QED) corrections. We include Breit corrections in a very accurate way described in our previous works [16,18]. The QED corrections are included approximately via the QED potential suggested in Ref. [19].

The Breit operator has the form

$$h^B = -\frac{\alpha_1 \cdot \alpha_2 + (\alpha_1 \cdot \mathbf{n})(\alpha_2 \cdot \mathbf{n})}{2r}, \qquad (12)$$

where $\mathbf{r} = \mathbf{n}r$, r is the distance between electrons, and α is the Dirac matrix. It corresponds to the zero-energy transfer approximation and includes magnetic interaction and retardation.

Similar to the hyperfine interaction, Breit operator induces a correction to the self-consistent Hartree-Fock potential, which is taken into account in all orders in Coulomb interaction by iterating the RHF equations with the potential

$$V^{N-1} = V^C + V^B, \qquad (13)$$

where V^C is the Coulomb potential and V^B is the Breit potential. The same potential (13) goes to the left- and right-hand sides of the TDHF equations (6).

For the QED corrections we use a radiative potential derived in Ref. [19]. This potential was chosen to fit accurate calculations of the QED corrections to the energies. It may give less accurate results for the hyperfine structure. Therefore, we consider current calculations of the QED corrections as rough estimations only.

III. RESULTS

Table I lists isotopes of lighter analogs of the superheavy elements E119 and E120$^+$ for which the hyperfine-structure constants are calculated. The results of the calculations are presented in Table II. Here, RHF corresponds to the $\langle \psi_v | F_z | \psi_v \rangle$ matrix elements with the Hartree-Fock wave func-

tions ψ_v; RPA corresponds to the $\langle \psi_v | F_z + \delta V^{N-1} | \psi_v \rangle$ matrix elements; BO and RPA(BO) columns correspond to the same matrix elements but with Hartree-Fock wave function replaced with Brueckner orbitals; and the "Str+norm" column includes structure radiation and renormalization.

As can be seen from the table the most important corrections are the many-body corrections associated with the core polarization effect (RPA) and with the correlation interaction of the external electron with the core (BO). These effects follow approximately the same pattern when moving from light to heavy atoms. This means that the accuracy of the results should be about the same for all atoms and ions.

Breit contribution is small and can be neglected in all cases. This is because Breit contributions are proportional to lower powers of Z than other relativistic effects. The QED corrections are large for s states. They reduce the hfs constants of these states by about 1%.

We also study the dependence of the hyperfine-structure constants on the nuclear radius. This is done numerically by calculating the hfs constants at different radii and then calculating the derivative dA/dr_n numerically. It is convenient to represent the results in a form of the dimensionless constant κ_{hr} as in Ref. [9],

$$\kappa_{hr} = \frac{\delta A_v / A_v}{\delta r_n / r_n}. \qquad (14)$$

Here, A_V is the hyperfine-structure constant of the valence state v and r_n is the nuclear radius. The results are presented in Table III. There are few things to note here. First, the effect in superheavy elements is much larger than in their lighter analogs. Second, the effects for s and $p_{1/2}$ states are significantly different. This represents an opportunity to use the measurements of the hyperfine structure in superheavy elements not only to extract nuclear magnetic moments but also to get some information about the nuclear radius. Note

TABLE III. Sensitivity of the hyperfine-structure constants to the change in the nuclear radius (κ_{hr}).

		E119		E20$^+$	
Cs 6s	Fr 7s	8s	8$p_{1/2}$	8s	8$p_{1/2}$
−0.024 [a]	−0.11[a]	−0.45	−0.28	−0.46	−0.22

[a]Reference [9].

finally that the analytical formulas describing the dependence of the hyperfine structure on the nuclear radius presented in Refs. [1,9] do not work here. They are not just inaccurate; they give absolutely meaningless results. The reason for this is that the effect is large and cannot be treated perturbatively.

Calculating κ_{hr} we assume that the magnetic and electric radii of the nucleus are the same. However, the program allows us to treat them independently and calculate two partial derivatives $\partial A / \partial r_n$ and $\partial A / \partial r_m$, where r_n is the electric radius and r_m is the magnetic radius. Such calculations show that the hyperfine-structure constants are more sensitive to the change in the electric radius. The corresponding partial derivatives are approximately two times larger than those over the magnetic radius. This is true for both s and $p_{1/2}$ states.

IV. CONCLUSION

The hyperfine structures of lowest s and $p_{1/2}$ states of the superheavy elements $Z=119$ and $Z=120^+$ have been calculated with an uncertainty of a few percent. The dependence of the constants on the nuclear radius is presented. The results may be used for experimental studies of nuclear, spectroscopic, and chemical properties of the elements.

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