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

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I. INTRODUCTION

Study of the hyperfine structure of heavy and superheavy elements is an important source of the information about nuclear structure of these elements (see, e.g., Ref. [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 which can be found in the literature as being already observed include, e.g. $^{288}$Uup and $^{289}$Uuo [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.

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

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

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

Formulæ [12] 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 formulæ treat finite nuclear size as a small correction. Hydrogen-like wave functions for a point-like nucleus are used to calculate 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 an analytical and numerical approaches were recently used in Ref. [9] to study the dependence of the hyperfine structure intervals on 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 paper we don’t use any analytical approaches but just perform accurate numerical calculations of the hyperfine structure constants for superheavy atoms. We demonstrate that the calculation which use finite-size nuclei with realistic charge and magnetic moment distribution are 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 have been synthesized yet. However, the ways of their production and physics of their nuclei are discussed in literature [10]. These elements are heavier than any known element. Therefore, if calculation of the hyperfine structure brings no surprises for them one can expect no surprises for lighter elements as well. Also these elements have 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 energy levels of E119 and E120$^+$. Apart from some expected relativistic effects like larger fine structure and stronger attraction of the $s$-states to atomic core, the spectra of these superheavy elements is 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 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 \[11, 12, 13, 14, 15, 16\]. 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

\[
\hat{H}_0 = c \alpha \cdot \mathbf{p} + (\beta - 1)me^2 + V_{\text{nuc}}(r) + V^{N-1}. \tag{3}
\]

Here \( \alpha \) and \( \beta \) are Dirac matrices, \( V_{\text{nuc}}(r) \) is nuclear potential, \( V^{N-1} = V_{\text{dir}} + V_{\text{exch}} \) is the sum of the direct and exchange Hartree-Fock potentials, \( N \) is the number of electrons. At distances much larger than nuclear radius \( r_N \) 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 \[1\]). 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 method (TDHF) \[12\], 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 an uniformly magnetized ball. In our calculations magnetic nuclear radius is the same as the electric one. However, these two parameters can be varied independently.

The HFI Hamiltonian is given by

\[
\hat{H}_{hf} = \mu \cdot \mathbf{F}(r), \tag{4}
\]

\[
\mathbf{F}(r) = \begin{cases} \frac{r \times \alpha}{r}, & r < r_m \\ \frac{r \times \alpha}{r_m^3}, & r \geq r_m \end{cases} \tag{5}
\]

where \( r_m \) is the magnetic nuclear radius.

The TDHF equations have a form

\[
(\hat{H}_0 - \epsilon_a)\psi_a = (-F_z + \delta V^{N-1} + \delta \epsilon_a)\psi_a \tag{6}
\]

\[
\delta \epsilon_a = \langle \psi_a | F_z + \delta V^{N-1} | \psi_a \rangle. \tag{7}
\]

Here 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 \( \hat{\Sigma} \) \[13\]

\[
(\hat{H}_0 + \hat{\Sigma} - \epsilon)\psi_v^{BO} = 0. \tag{8}
\]

Here index \( v \) numerates valence states. Correlation potential \( \hat{\Sigma} \) 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 equations \(8\) for valence states we find the so called Breit-Bethe orials for the valence states. This is emphasized by using superscript \( BO \) for the orbitals.

Total energy shift for the valence state \( v \) due to HFI and correlations is given by

\[
\delta \epsilon_v = \langle \psi_v^{BO} | F_z + \delta V^{N-1} + \delta \hat{\Sigma} | \psi_v^{BO} \rangle. \tag{9}
\]

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 structure radiation. Finally, there is a contribution due to the renormalization of the many-electron wave function (see, e.g. \[13\])

\[
\delta \epsilon_{\text{norm}} = -\langle \psi_v | F_z + \delta V^{N-1} | \psi_v \rangle \langle \psi_v | \partial \hat{\Sigma} / \partial E | \psi_v \rangle. \tag{10}
\]

Magnetic dipole hyperfine structure constant \( A_v \) for the valence state \( v \) is given by

\[
A_v = \frac{\mu e^2}{2m_p I} \sqrt{J_v(J_v + 1)(2J_v + 1)} \tag{11}
\]

A. Breit and QED corrections

It is hard to claim high accuracy of calculations for superheavy elements without considering Breit and quantum electrodynamics (QED) corrections. We include Breit corrections in a very accurate way described in our previous works \[16, 18\]. The QED correction are included approximately via the QED potential suggested in Ref. \[19\].

The Breit operator has the form:

\[
\gamma = -\frac{\mathbf{1} \cdot \alpha_2 + (\mathbf{1} \cdot \mathbf{n})(\alpha_2 \cdot \mathbf{n})}{2r}, \tag{12}
\]

where \( r = \mathbf{r} \), \( r \) is the distance between electrons, and \( \mathbf{n} \) is the Dirac matrix. It correspond 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
The QED corrections are large for the hfs constants of these states by about 1%. 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 nuclear radius. This is done numerically by calculating the hfs constants at different radius and then calculating the derivative $dA/dr_n$ numerically. It is convenient to represent the results in a form of the dimensionless constant $\kappa_{hr}$ as in Ref. [9]

$$\kappa_{hr} = \frac{\delta A_v/A_v}{\delta r_n/r_n}.$$  

Here $A_v$ is the hyperfine structure constant of the valence state $v$, $r_n$ is 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 analogies. Second, the effect for $s$ and $p_{1/2}$ states is 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 nuclear radius. Note finally that the analytical formulae describing the dependence of the hyperfine structure on 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 $\kappa_{hr}$, we assume that magnetic and electric radii of the nucleus are the same. However, the program allows to treat them independently and calculate two partial derivatives $\partial A/\partial r_n$ and $\partial A/\partial r_m$, where $r_n$ is electric radius and $r_m$ is magnetic radius. Such calculations show that the hyperfine structure constants are more sensitive to the change of the electric radius. Corresponding partial derivative is approximately two time larger than those over the magnetic radius. This is true for both $s$ and $p_{1/2}$ states.

### III. RESULTS

Table I lists isotopes of lighter analogies of the superheavy elements E119 and E120$^+$ for which the hyperfine structure constants are calculated. The results of the calculations are presented in Table I. Here RHF corresponds to the $\langle \psi_v | F_z | \psi_v \rangle$ matrix elements with the Hartree-Fock wave functions $\psi_v$, the RPA corresponds to the $\langle \psi_v | F_z + V^{N-1} \delta V \psi_v \rangle$ matrix elements; BO and RPA(BO) columns correspond to the same matrix elements but with Hartree-Fock wave function replaced by Brueckner orbitals; the “$\text{Str}+$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%.

### IV. CONCLUSION

The hyperfine structure 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 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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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 | Exp. |
|------|-------|-----|-----|----|---------|-------|------|----------|-------|------|
| 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| 1180    | -4    | -4   | 8        | 1180  |       |
| 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 |       |

*aReference. [20]
*bReference. [21]
*cReference. [22]
*dReference. [23]

TABLE III: Sensitivity of the hyperfine structure constants to the change of nuclear radius ($\kappa_{hr}$).

| Atom | State | Sensitivity ($\kappa_{hr}$) |
|------|-------|-----------------------------|
| Cs   | 6s    | -0.024$^a$                 |
|      | 7s    | -0.11$^a$                  |
| Fr   | 8s    | -0.28$^a$                  |
|      | 8p$_{1/2}$ | -0.46$^a$      |

*aReference. [9]

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