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Calculation of the spectrum of the superheavy element $Z=120$

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High-precision calculations of the energy levels of the superheavy element $Z=120$ are presented. The relativistic Hartree-Fock and configuration-interaction techniques are employed. The correlations between core and valence electrons are treated by means of the correlation potential method and many-body perturbation theory. Similar calculations for barium and radium are used to gauge the accuracy of the calculations and to improve the *ab initio* results.

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I. INTRODUCTION

The study of the superheavy elements is now a popular area of research driven by the search for the *island of stability* in the region $Z=114$ to $Z=126$ where shell closures are predicted (see, e.g., [1]). Elements up to $Z=118$ have been synthesized (see, e.g., [2,3]) and evidence for the naturally occurring element $Z=122$ has been reported [4].

Experimental efforts are underway to measure the spectra and chemical properties of the superheavy elements [5]. There are also many theoretical works in atomic physics and quantum chemistry devoted to these studies (see, e.g., the references in [6,7]).

In our previous work [8] we calculated the electronic spectra of the superheavy element $Z=119$ and the singly ionized superheavy element $Z=120$. The nucleus with $Z=120$ protons and $N=172$ neutrons is predicted to be doubly magic in relativistic mean-field nuclear calculations [9]. Moreover, there is evidence from fusion reactions for the enhanced stability of the element $Z=120$ [10].

To our knowledge, the spectrum of the neutral element $Z=120$ has not been calculated. On the other hand, it has a relatively simple electronic structure similar to the structure of its lighter analogs barium and radium. These atoms have two valence electrons above closed shells. High-precision calculations of the spectra of barium and radium have been carried out before [11–13]. In our works [12,13] we used an approach that combines the correlation potential method with many-body perturbation theory and the configuration interaction technique.

In the present work we perform accurate relativistic calculations for the energy levels of the neutral superheavy element 120 applying a similar approach as in our earlier works for barium and radium [12,13].

II. METHOD

Calculations are performed with a method that combines the configuration interaction (CI) technique with many-body perturbation theory (MBPT). It has been described in detail in our previous works [12–16]. Here we repeat the main points, focusing on the details specific to the current calculations.

Calculations are carried out in the V^{N-2} approximation [15]. This means that the initial Hartree-Fock procedure is performed for the doubly ionized ion, with the two valence electrons removed. This approach has many advantages. It simplifies the inclusion of the core-valence correlations by avoiding the so-called *subtraction* diagrams [14,15]. This in turn allows one to go beyond second order in many-body perturbation theory in the treatment of core-valence correlations. Inclusion of the higher-order core-valence correlations significantly improves the accuracy of the results [15,16].

The effective CI Hamiltonian for an atom with two valence electrons is the sum of the two single-electron Hamiltonians and an operator representing the interaction between the valence electrons,

$$H^{\text{eff}} = h_1(r_1) + h_1(r_2) + h_2(r_1,r_2). \tag{1}$$

The single-electron Hamiltonian for a valence electron has the form

$$h_1 = h_0 + \Sigma_1, \tag{2}$$

where h_0 is the relativistic Hartree-Fock Hamiltonian,

$$h_0 = c\boldsymbol{\alpha}\cdot\mathbf{p} + (\beta-1)mc^2 - \frac{Ze^2}{r} + V^{N-2}, \tag{3}$$

and Σ_1 is the correlation potential operator, which represents the correlation interaction of a valence electron with the core.

The interaction between valence electrons is given by the sum of the Coulomb interaction and the correlation correction operator Σ_2,

$$h_2 = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} + \Sigma_2(r_1,r_2). \tag{4}$$

The operator Σ_2 represents the screening of the Coulomb interaction between valence electrons by core electrons.

The two-electron wave function for the valence electrons Ψ can be expressed as an expansion over single-determinant wave functions,

$$\Psi = \sum_i c_i \Phi_i(r_1,r_2). \tag{5}$$

The functions Φ_i are constructed from the single-electron valence basis states calculated in the V^{N-2} potential,

TABLE I. Screening factors f_k for inclusion of higher-order correlations into the exchange part of Σ_1 and into Σ_2 as functions of the multipolarity k of the Coulomb interaction.

k	0	1	2	3	4	5
Σ_1^{exch}	0.72	0.62	0.83	0.89	0.94	1.00
Σ_2	0.90	0.72	0.98	1.00	1.02	1.02

$$\Phi_i(r_1,r_2) = \frac{1}{\sqrt{2}}[\psi_a(r_1)\psi_b(r_2) - \psi_b(r_1)\psi_a(r_2)]. \qquad (6)$$

The coefficients c_i and two-electron energies are found by solving the matrix eigenvalue problem

$$(H^{\text{eff}} - E)X = 0, \qquad (7)$$

where $H_{ij}^{\text{eff}}=\langle\Phi_j|H^{\text{eff}}|\Phi_i\rangle$ and $X=\{c_1,c_2,\ldots,c_n\}$.

The most complicated part of the calculations is calculation of the correlation correction operators Σ_1 and Σ_2. We use the MBPT and the Feynman diagram technique to do the calculations. The MBPT expansion for Σ starts from the second order in the Coulomb interaction. Inclusion of the second-order operators $\Sigma_1^{(2)}$ and $\Sigma_2^{(2)}$ into the effective Hamiltonian (1) accounts for most of the core-valence correlations. However, further improvement is achieved if higher-order correlations are included into Σ_1 and Σ_2.

We include higher orders into Σ_1 in the same way as for a single-valence electron atom [17]. Two dominating classes of higher-order diagrams are included by applying the Feynman diagram technique to the part of Σ_1 that corresponds to the direct Coulomb interaction. These two classes correspond to (a) screening of the Coulomb interaction between valence and core electrons by other core electrons and (b) the interaction between an electron excited from the core and the hole in the core created by this excitation [17].

The effect of screening of the Coulomb interaction by the core electrons in the exchange diagrams is approximated by introducing screening factors f_k (see Table I) into each line describing the Coulomb interaction between electrons in a Brueckner-Goldstone diagram. We assume that screening factors f_k depend only on the multipolarity of the Coulomb interaction k. The screening factors were calculated in our early works [17,18] and then used in a number of later works. It turns out that screening factors have very close values for atoms with similar electron structure. In particular, the same values can be used for all atoms of the first and second columns of the periodic table. The screening factors for Σ_1^{exch} were found by calculating the direct part of Σ_1 with and without screening.

A similar way of approximate inclusion of higher-order correlations via screening factors was used for Σ_2. The values of the factors, however, are different (see Table I). These factors were found by comparing Σ_1 in second order and in all orders with both screening and hole-particle interaction included.

One needs a complete set of single-electron states to calculate Σ and to construct the two-electron basis states (6) for the CI calculations. We use the same basis in both cases. It is constructed using the B-spline technique [19,20]. We use 40 B splines of order 9 in a cavity of radius $R_{\text{max}}=40a_B$, where a_B is Bohr's radius. The upper and lower radial components $R_a^{u,l}(r)$ of the Dirac spinors for single-electron basis orbitals ψ_a in each partial wave are constructed as linear combinations of 40 B splines,

$$R_a^{u,l}(r) = \sum_{i=1}^{40} b_{ai}^{u,l} B_i(r). \qquad (8)$$

The coefficients $b_{ai}^{u,l}$ are found from the condition that ψ_a is an eigenstate of the Hartree-Fock Hamiltonian h_0 (3).

III. RESULTS

Our results for barium, radium, and element 120 are presented in Table II. *Ab initio* results are listed in the column under the heading "Σ." Here, the all-orders correlation potential Σ_1 is used. This is the same Σ_1 used in our previous work for Ba^+, Ra^+, and the singly ionized element 120 [8]. For both barium and radium we see that all *ab initio* calculated levels lie deeper than experiment. That is, the removal energies for the two s electrons from the ground states $6s^2$ for barium and $7s^2$ for radium are larger than the experimental results, both by 0.2%. The *ab initio* excitation energies are smaller than experiment. For barium the disagreement with measured values is on the order of 1%; deviations for the $6s5d$ states are larger than for the $6s6p$ states. The results for radium are better.

As a way to empirically correct the results for radium and element 120, we use fitting factors found by fitting to measured levels for barium and radium, respectively. The empirical fitting factors f_{Ba} and f_{Ra} are different for the different partial waves s, p, and d and placed before the associated Σ_1. This is done in the same way as in our work for single-valence electron systems [8]. However, here the fitting is performed for the two-valence electron atom; it means that, as well as correcting for unaccounted core-valence correlations, information about the valence-valence correlations, incompleteness of the basis, and other higher-order corrections are also contained in this fitting.

Results for spectra calculated with the empirical fitting factors are presented in Table II under the headings "$f_{\text{Ba}}\Sigma$" and "$f_{\text{Ra}}\Sigma$." We see that by using the three fitting factors, energy levels for all states considered for both barium and radium are in excellent agreement with experiment. This includes the singlet states ${}^1P_1$ and ${}^1D_2$. In our previous works on barium and radium [12,13], where similar methods were employed, the singlet states were much worse. This improvement comes about from the different screening factors used in Σ_2 in the current work.

Now we turn to the results for radium and element 120 found with these fitting factors. It is seen from Table II that with empirical fitting factors from barium, all levels for radium move in the direction of experiment. However, the corrections are overshot. The triplet $7s7p$ levels are seen to improve, from about -1% deviation to $\sim 0.1\%$. On the other hand, the $7s6d$ levels get worse, with deviations about 1%. We note that the largest deviations from experiment for the

TABLE II. Energy for removal of two s electrons (from $^1S_0$) and excitation energies for barium, radium, and element 120 (units cm^{-1}). Results of calculations with all-orders correlation potential appear in the column Σ; those with empirical fitting factors in the columns $f_{\text{Ba}}\Sigma$ and $f_{\text{Ra}}\Sigma$. g factors for element 120 are presented in the last column.

Atom	Configuration	Term	J	Σ	$f_{\text{Ba}}\Sigma$	$f_{\text{Ra}}\Sigma$	Expt.[a]	g
Barium	$6s^2$	^1S	0	122955	122721		122721	
	$6s5d$	^3D	1	8687	9033		9034	
	$6s5d$	^3D	2	8875	9215		9216	
	$6s5d$	^3D	3	9279	9601		9597	
	$6s5d$	^1D	2	11081	11439		11395	
	$6s6p$	^3P	0	12099	12266		12266	
	$6s6p$	^3P	1	12474	12634		12637	
	$6s6p$	^3P	2	13365	13501		13515	
	$6s6p$	^1P	1	17943	18133		18060	
Radium	$7s^2$	^1S	0	124656	124402	124416	124416	
	$7s7p$	^3P	0	12916	13118	13088	13078	
	$7s6d$	^3D	1	13622	13920	13719	13716	
	$7s6d$	^3D	2	13902	14188	13993	13994	
	$7s7p$	^3P	1	13844	14030	14001	13999	
	$7s6d$	^3D	3	14645	14884	14712	14707	
	$7s7p$	^3P	2	16566	16671	16652	16689	
	$7s6d$	^1D	2	17004	17273	17094	17081	
	$7s7p$	^1P	1	20667	20775	20739	20716	
Element 120	$8s^2$	^1S	0	137502		137228		
	$8s8p$	^3P	0	15777		16061		
	$8s8p$	^3P	1	17710		17968		1.421
	$8s7d$	^3D	1	22985		23066		0.500
	$8s7d$	^3D	2	23163		23231		1.163
	$8s7d$	^3D	3	23799		23827		1.333
	$8s8p$	^3D	2	25419		25457		1.499
	$8s7d$	^1D	2	27438		27477		1.005
	$8s8p$	^1P	1	27667		27685		1.077

[a] Ionization energies from Ref. [21]; excitation energies from Ref. [22].

ab initio results for barium are for the $6s5d$ levels, with deviations $-(3-4)\%$. The fitting factor for the d wave has clearly overcompensated these corrections.

For element 120, the removal energy for the two s electrons from the ground state $8s^2$ decreases by 0.2% with fitting. This is the same difference we saw between *ab initio* and measured values for barium and radium. For the excitation energies, the differences range from 0.1% for the higher levels to over 1% for the two lowest levels, with all fitted values larger than the *ab initio* ones. We see that the differences for element 120 are smaller than for radium. This is because the *ab initio* values for radium are very good, better than those for barium. We take the fitted results as our final values for the low-lying spectra of element 120.

The differences between the *ab initio* and fitted values give an indication of the accuracy of the results. While for the higher levels these differences are about 0.1%, from a consideration of the large differences we saw for radium, we will assign a conservative uncertainty of 1% to our results for excitation energies.

We considered Breit and radiative corrections in our work on the spectra of superheavy elements 119 and 120^+ [8]. We found that by fitting the results of pure correlated calculations to the experimental values for Cs and Ba^+, the extrapolated values for Fr and Ra^+ agreed with experiment at a level better than the estimated size of Breit and radiative corrections. This method was then used for the heavier homologue elements 119 and 120^+ as a way of taking into account these corrections semiempirically.

In the present work we also fit pure correlated values of the lighter homologues to experiment for use in calculations for the heavier elements. In principle, this may be a way of taking into account Breit and radiative corrections. However, in this case our calculations are not at the same level of precision as in our work Ref. [8] dealing with one-valence electron atoms and ions. In the current work, the uncertainty in the final results stemming from correlations is larger than the expected size of Breit and radiative corrections. Therefore, we do not need to account for these corrections.

The ordering of the levels for barium, radium, and element 120 are different. Relativistic effects increase approximately as $Z^2\alpha^2$ and are larger for the heavier elements. They are responsible for pulling in s and p levels, which effectively screen d levels, pushing them out. This is the reason

TABLE III. Volume isotope shifts k for states of element 120.

State	$8s^2\ ^1S_0$	$8s8p\ ^3P_0$	$8s8p\ ^3P_1$	$8s8p\ ^3P_2$	$8s8p\ ^1P_1$
k	−0.0183	−0.0122	−0.0121	−0.0117	−0.0133

that $7s7p\ ^3P_0$ is the first excited state rather than $7s6d\ ^3D_1$ for radium. For element 120, stronger relativistic effects are responsible for pulling the $8s8p\ ^3P_1$ level below $8s7d\ ^3D_1$.

Note that we use the *LS* notation for the states. While the atoms under consideration are highly relativistic and the *jj* notation is more appropriate, the *LS* notation is used extensively in the literature (including in the tables of Moore [22]) and for this reason we adopt it here for easier comparison. In this work we calculated g factors for element 120 to help in identification of the states; these are presented in the final column in Table II.

We found in our work Ref. [8] that there is a sizable volume isotope shift for the elements 119 and 120$^+$. In this work, as in Ref. [8], calculations have been performed using a two-parameter Fermi distribution for the nuclear density with half-density radius $c=8.0$ fm and 10–90 % width $t=2.0$ fm corresponding to a root-mean-square charge radius $r_{\rm rms}\approx 6.42$ fm. We define the volume isotope shift as

$$\frac{\delta E}{E} = k\frac{\delta r_{\rm rms}}{r_{\rm rms}}, \tag{9}$$

where E is the energy required to remove the two electrons. Values of k for element 120 are listed in Table III. A table of values for $r_{\rm rms}$ calculated in the nuclear Hartree-Fock-BCS approximation yields a range from $r_{\rm rms}=6.47$ fm to $r_{\rm rms}=6.96$ fm for the light to very heavy isotopes [23]. For $r_{\rm rms}=6.90$ fm, for example, the value for the removal energy for the two s electrons in the ground state is 186 cm^{-1} less than for $r_{\rm rms}\approx 6.42$ fm. This difference amounts to 0.1%. For the level $8s8p\ ^3P_0$, the shift is 110 cm^{-1}, which is 0.7% of the value for the excitation energy.

Finally, we present the ionization energies (energy for removal of one s electron) for barium, radium, and element 120. We have obtained 42 120 cm^{-1}, 42 531 cm^{-1}, and 47 296 cm^{-1}, respectively. These were found from the difference between the two-electron removal energies in Table II and the ionization energies for singly ionized Ba, Ra, and element 120 from our work [8]. The result for Ba is *ab initio* while the values for Ra and element 120 include fitting. The results for Ba and Ra are in very good agreement with the experimental values 42 035 cm^{-1} and 42 573 cm^{-1} [21]. The higher ionization and excitation energies for neutral and singly ionized element 120 indicate that this element is more chemically inert than its lighter homologues barium and radium. For analyses of superheavy chemistry we refer the reader to the reviews [6,24].

IV. CONCLUSION

The energy levels of low states of the superheavy element $Z=120$ have been calculated with an uncertainty of about 1%. These results may be useful for experimental studies of this element and for predicting its chemical properties.

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[1] M. Bender, P.-H. Heenen, and P.-G. Reinhard, Rev. Mod. Phys. **75**, 121 (2003).
[2] S. Hofmann and G. Münzenberg, Rev. Mod. Phys. **72**, 733 (2000).
[3] Y. Oganessian, Phys. Scr., T **T125**, 57 (2006).
[4] A. Marinov *et al.*, e-print arXiv:0804.3869.
[5] M. Schädel, Angew. Chem., Int. Ed. **45**, 368 (2006).
[6] V. G. Pershina, Chem. Rev. (Washington, D.C.) **96**, 1977 (1996).
[7] E. Eliav, A. Landau, Y. Ishikawa, and U. Kaldor, J. Phys. B **35**, 1693 (2002).
[8] T. H. Dinh, V. A. Dzuba, V. V. Flambaum, and J. S. M. Ginges, Phys. Rev. A **78**, 022507 (2008).
[9] K. Rutz *et al.*, Phys. Rev. C **56**, 238 (1997).
[10] M. Morjean *et al.*, Phys. Rev. Lett. **101**, 072701 (2008).
[11] A. Landau, E. Eliav, Y. Ishikawa, and U. Kaldor, J. Chem. Phys. **113**, 9905 (2000).
[12] V. A. Dzuba and J. S. M. Ginges, Phys. Rev. A **73**, 032503 (2006).
[13] V. A. Dzuba and V. V. Flambaum, J. Phys. B **40**, 227 (2007).
[14] V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A **54**, 3948 (1996).
[15] V. A. Dzuba, Phys. Rev. A **71**, 032512 (2005).
[16] V. A. Dzuba, Phys. Rev. A **71**, 062501 (2005).
[17] V. A. Dzuba, V. V. Flambaum, and O. P. Sushkov, Phys. Lett. A **140**, 493 (1989).
[18] V. A. Dzuba, V. V. Flambaum, P. G. Silvestrov, and O. P. Sushkov, Phys. Lett. A **131**, 461 (1988).
[19] W. R. Johnson and J. Sapirstein, Phys. Rev. Lett. **57**, 1126 (1986).
[20] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 307 (1988).
[21] J. E. Sansonetti and W. C. Martin, J. Phys. Chem. Ref. Data **34**, 1559 (2005).
[22] C. E. Moore, *Atomic Energy Levels*, Natl. Bur. Stand. (U.S.) Circ. No. 467 (U.S. GPO, Washington, D.C., 1958), Vol. III.
[23] S. Goriely, F. Tondeur, and J. M. Pearson, At. Data Nucl. Data Tables **77**, 311 (2001).
[24] B. Fricke, Struct. Bonding (Berlin) **21**, 89 (1975).