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Calculation of the spectra for the superheavy element $Z=112$

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Accurate *ab initio* calculations of the energy levels of the superheavy element $Z=112$ are presented. Relativistic Hartree-Fock and configuration interaction methods are combined with the many-body perturbation theory to construct the many-electron wave function for valence electrons and to include core-valence correlations. Two different approaches in which the element is treated as a system with two or twelve external electrons above closed shells are used and compared. Similar calculations for mercury are used to control the accuracy of the calculations. The results are compared with other calculations.

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I. INTRODUCTION

The study of superheavy elements with nuclear charge $Z > 100$ is an important area of research motivated by the search for the island of stability (see, e.g., Refs. [1–3]). Synthesis and investigation of superheavy elements are conducted at leading nuclear-physics laboratories in Dubna, Berkeley, Darmstadt, and others. Elements with nuclear charge up to $Z=118$ have been synthesized [4].

The study of the element Ununbium [Uub ($Z=112$)] is an important part of this research. Since it was synthesized in Darmstadt in 1996 [5] there have been numerous works discussing its production, nuclear and chemical properties, etc. (see, e.g., Refs. [6–12], and references therein). In contrast, only very few works were devoted to the study of the electron structure and optical spectrum of the element. Eliav *et al.* [13] calculated the ionization potential of neutral Uub and few low energy levels of Uub^{+} and Uub^{2+}. A more detailed study of neutral Uub was recently reported in Refs. [14,15]. Quantum electrodynamic corrections (QEDs) for Uub were studied in Ref. [16].

In the present paper we try to address the shortage of data on the electron structure and energy spectrum of Uub by calculating its energy levels. Element 112 has an electron structure similar to that of mercury. Therefore, we use the calculations for mercury as a test of the calculations and as a guide for their accuracy. Most of the lower states of both atoms can be considered as states with two valence electrons above closed shells. We use the combined configuration interaction (CI) and many-body perturbation theory method (MBPT) [17,18] to perform calculations for such states. This method has been successfully used for many different atoms [19–23] including the superheavy element with $Z=120$ [24].

There are also states in mercury and element 112 with excitations from the $5d$ or $6d$ subshell. They cannot be considered as two-electron states and in this case we use a version of the configuration interaction technique which has been developed for atoms with open d or f shells [25,26]. Some states are covered by both methods which is another test of the accuracy of the calculations. We also compare our results with the calculations of Li *et al.* in Ref. [15].

II. METHOD OF CALCULATIONS AND RESULTS FOR MERCURY

Many states of mercury and element 112 (E112) can be considered as having two valence electrons above closed shells. The uppermost core subshell is the $5d^{10}$ subshell for mercury and the $6d^{10}$ subshell for E112. However, it is well known that mercury also has states of the discrete spectrum which have one electron excited from the $5d^{10}$ subshell [27]. The lowest such state, the $5d^{9}6s^{2}6p\,^{3}P^{o}_{2}$ state, is obviously due to the $5d_{5/2}\rightarrow 6p_{1/2}$ excitation. Its energy is 68 886.60 cm^{-1} which is roughly double the minimal excitation energy (see Table II). It is clear that the $6d_{5/2}\rightarrow 7p_{1/2}$ excitations in the E112 superheavy element must be even easier due to larger fine structure. Indeed, with fine structure increasing the $6d_{5/2}$ and $7p_{1/2}$ states move toward each other on the energy scale. The $6d_{5/2}$ state goes up while the $7p_{1/2}$ state goes down. This means that one should expect having even more states with excitations for the $6d^{10}$ subshell in the discrete spectrum of E112 than those found in mercury. And these states are expected to have lower energies.

The presence of the states with d-p excitations from the core is a serious complication for the calculations. Two-valence-electron atoms such as Ba, Ra, and E120 [18,21,22,24] can be treated very accurately by means of the configuration interaction (CI) technique combined with the many-body perturbation theory (MBPT) [17]. In this method the CI technique is used to construct the two-electron wave function and to include correlations between two valence electrons to all orders via matrix diagonalization. The MBPT is used to include the core-valence correlations. This method does include the core-valence excitations but in an approximate way, using the lowest order perturbation theory. This might be not very accurate in the case when states with the core-valence excitations are in the discrete spectrum, as in mercury and E112.

The aim of present work is to predict the spectrum of the E112 superheavy element. Since it has both types of states, with and without excitations from the $6d^{10}$ subshell, we use two different methods of calculations. One is the CI+MBPT method for two valence electrons [17,18,21,22,24] (method A) and another is the CI method for twelve electrons [25,26] (method B). We demonstrate that unless a two-electron state happens to be very close in energy to a state with the excitation of the d electron from the core the CI+MBPT method gives remarkably accurate results. The twelve-valence-electron method B is used to find positions of the states with excitations from the core.

A. CI for two electrons: Method A

Here we use the CI+MBPT method developed in our earlier works [17,18,21,22]. The calculations are done in the V^{N-2} approximation [19] which means that the initial Hartree-Fock procedure is done for a double ionized ion, with two valence electrons removed.

The effective CI Hamiltonian for a neutral two-electron atom is the sum of two single-electron Hamiltonians plus an operator representing interaction between valence electrons

$$\hat{H}^{\text{eff}} = \hat{h}_1(r_1) + \hat{h}_1(r_2) + \hat{h}_2(r_1,r_2). \tag{1}$$

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

$$\hat{h}_1 = h_0 + \hat{\Sigma}_1, \tag{2}$$

where h_0 is the relativistic Hartree-Fock Hamiltonian

$$\hat{h}_0 = c\alpha\mathbf{p} + (\beta - 1)mc^2 - \frac{Ze^2}{r} + V^{N-2}, \tag{3}$$

and $\hat{\Sigma}_1$ is the correlation potential operator which represents correlation interaction of a valence electron with the core.

The interaction between valence electrons is the sum of the Coulomb interaction and correlation correction operator $\hat{\Sigma}_2$:

$$\hat{h}_2 = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} + \hat{\Sigma}_2(r_1,r_2), \tag{4}$$

where $\hat{\Sigma}_2$ represents screening of the Coulomb interaction between valence electrons by core electrons. We use the second-order MBPT to calculate correlation operators $\hat{\Sigma}_1$ and $\hat{\Sigma}_2$. The details can be found in our earlier works [17,18,21,22,24].

The two-electron wave function for the valence electrons Ψ has a form of expansion over single-determinant wave functions

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

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

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

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

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

where $H^{\text{eff}}_{ij} = \langle \Phi_i | \hat{H}^{\text{eff}} | \Phi_j \rangle$ and $X = \{c_1, c_2, \ldots, c_n\}$. The results of calculations for Hg with method A will be discussed in Sec. II C.

B. CI for twelve electrons: Method B

The method used in this section has been developed in our earlier works [25,26]. As for the case of two valence electrons the method is based on the CI technique. The main differences between methods A and B are in the choice of the basis and in the treatment of the core-valence correlations (see below). In general, method B is less accurate than method A. However, its strong feature is the ability to deal with a large number of valence electrons.

TABLE I. Even and odd configurations of Hg and E112 and effective core polarizability α_p (a.u.) used in the calculations.

Atom	Set	Parity	Configuration	α_p
Hg	1	Even	$5d^{10}6s^2$	0.4
	2	Even	$5d^{10}6p^2$	0.4
	3	Odd	$5d^{10}6s6p$	0.386
	4	Odd	$5d^9 6s^2 6p$	0.41
E112	1	Even	$6d^{10}7s^2$	0.4
	2	Even	$6d^{10}7p^2$	0.4
	3	Odd	$6d^{10}7s7p$	0.386
	4	Odd	$6d^9 7s^2 7p$	0.41

The effective Hamiltonian for valence electrons has the form

$$\hat{H}^{\text{eff}} = \sum_{i=1}^{12} \hat{h}_{1i} + \sum_{i<j}^{12} e^2/r_{ij}, \tag{8}$$

where $\hat{h}_1(r_i)$ is the one-electron part of the Hamiltonian

$$\hat{h}_1 = c\alpha \cdot \mathbf{p} + (\beta - 1)mc^2 - \frac{Ze^2}{r} + V_{\text{core}} + \delta V. \tag{9}$$

Here α and β are Dirac matrixes, V_{core} is the Hartree-Fock potential due to core electrons, and δV is the term which simulates the effect of the correlations between core and valence electrons. It is often called polarization potential and has the form

$$\delta V = -\frac{\alpha_p}{2(r^4 + a^4)}. \tag{10}$$

Here α_p is polarization of the core and a is a cutoff parameter (we use $a = a_B$, where a_B is the Bohr radius).

The differences between the Hamiltonian (1) in the previous section and the Hamiltonian (8) are (a) the $5d$ electrons are treated as core electrons in Eq. (1) and their contribution is included into the potential V^{N-2} while the $5d$ electrons are treated as valence electrons in Eq. (8) and their contribution is not included into the potential V_{core}; (b) the $\hat{\Sigma}_2$ operator is not included in Eq. (8); the $\hat{\Sigma}_1$ operator in Eq. (1) is replaced by a less accurate polarization potential δV in Eq. (8).

To construct the many-electron wave function for twelve valence electrons we use the Hartree-Fock single-electron basis states which are found by the self-consistent procedure performed independently for each configuration of interest (see Refs. [25,26] for details). Table I lists all configurations of the valence electrons for mercury and E112 considered in the present work. The effective core polarizability parameter α_p is treated as a fitting parameter. Its values for mercury are

TABLE II. Energy levels of Hg (cm^{-1}).

					Present work			
Config.	Term	J	E_{exp} [b]	E_A [c]	Δ_A [d]	E_B [e]	Δ_B [f]	Other[a]
$5d^{10}6s^2$	^1S	0	0.000	0	0	0	0	0
$5d^{10}6s6p$	$^3P^o$	0	37 645.080	37 480	165	37 763	−699	38 248
		1	39 412.300	39 338	74	39 442	−30	38 441
		2	44 042.977	44 287	−244	42 887	1156	49 363
$5d^{10}6s6p$	$^1P^o$	1	54 068.781	54 263	−194	54 442	−373	57 402
$5d^{10}6s7s$	^2S	1	62 350.456	62 181	169			
$5d^{10}6s7s$	^1S	0	63 928.243	63 681	247			
$5d^96s^26p$	$^3P^o$	2	68 886.60			70 287	−1400	70 139
$5d^{10}6s7p$	$^3P^o$	0	69 516.66	69 223	294			
		1	69 661.89	69 397	265			
		2	71 207.51	70 106	1102			
$5d^{10}6s7p$	$^1P^o$	1	71 295.15	71 213	82			
$5d^{10}6s6d$	^1D	2	71 333.182	71 327	6			
$5d^{10}6s6d$	^3D	1	71 336.164	71 345	−9			
		2	71 396.220	71 383	13			
		3	71 431.311	71 412	19			
$5d^96s^26p$	$^3D^o$	3	73 119.2			71 825	1294	71 453
$5d^96s^26p$	$^1P^o$	1	78 813			78 174	639	79 357

[a] J. G. Li *et al.*, Ref. [15].
[b] Experiment, Ref. [27].
[c] Calculations with method A.
[d] $\Delta_A = E_{\mathrm{exp}} - E_A$.
[e] Calculations with method B.
[f] $\Delta_B = E_{\mathrm{exp}} - E_B$.

chosen to reproduce the experimental data for energy levels of the corresponding configurations. The same values are then used for the superheavy element E112. The results for mercury will be discussed in the next section.

C. Results for mercury

The results for mercury are presented in Table II. Here experimental energies are compared with the energies calculated within the frameworks of methods A and B which are described in the previous section. The energy levels of mercury were calculated by many authors before (see, e.g., Refs. [14,15,28]). A review of these calculations goes beyond the scope of the present work. In our case mercury serves only as a test of the calculations for the superheavy elements Uub. Therefore we included in Table II the results of calculations of only one other group [15] who also calculated the spectrum of Uub (see next section).

Method A gives very accurate results unless a state of interest happens to be very close to another state with the same total momentum J and parity and which has a hole in the $5d$ shell. For example, the largest deviation of the theory from experiment in method A is for the $5d^{10}6s7p\ ^3P^o_2$ state which is close to the $5d^96s^26p\ ^3P^o_2$ state. These states are strongly mixed; however, this mixing is included in a very approximate way in method A. It treats an atom as a two-valence-electron system and excitations from the core are included only in the second order of the MBPT in the $\hat{\Sigma}$ operator in the effective CI Hamiltonian. Note that this maximum deviation (1102 cm^{-1}) is only 1.5% of the energy.

Method B is less accurate; however, it gives the positions of the energy levels of the states with excitations from the $5d$ subshell which cannot be obtained by method A. The results of Ref. [15] are closer to our method B results.

III. RESULTS FOR Uub ($Z=112$)

The results of calculations for the superheavy element Uub ($Z=112$) are presented in Table III together with the results of Ref. [15]. We also present the Lande g factors in the table. This includes the calculated g factors as well as g factors obtained from analytical expressions in the *LS* and *jj* schemes. The g factors are useful for the identification of the states. The Uub is a superheavy element with large relativistic effects. Therefore the *jj* scheme works better for it than the *LS* one. However, the *LS* scheme is also useful for the comparison with mercury for which the *LS* scheme is commonly used.

The g factors in the *LS* scheme are given by (nonrelativistic notations)

TABLE III. Calculated energies (E, cm^{-1}) and g factors of ekamercury (Z=112).

	Term		g factors		Method A		Method B		Other[a]
Config.	LS	j-j	g_{NR}	g_{jj}	E	g	E	g	E
$6d^{10}7s^2$	$^1S_0$	$(7s_{1/2},7s_{1/2})_0$	0.00	0.00	0	0.00	0	0.00	0
$6d^9 7s^2 7p$	$^3P^o_2$	$(6d_{5/2},7p_{1/2})^o_2$	1.50	1.29			35 785	1.35	34 150
$6d^9 7s^2 7p$	$^3F^o_3$	$(6d_{5/2},7p_{1/2})^o_3$	1.08	1.11			38 652	1.10	37 642
$6d^9 7s^2 7p$	$^3P^o_4$	$(6d_{5/2},7p_{3/2})^o_4$	1.25	1.25			56 131	1.25	60 366
$6d^{10}7s7p$	$^3P^o_0$	$(7s_{1/2},7p_{1/2})^o_0$	0.00	0.00	51 153	0.00	51 212	0.00	48 471
	$^3P^o_1$	$(7s_{1/2},7p_{1/2})^o_1$	1.50	1.33	55 057	1.41	53 144	1.33	52 024
	$^3P^o_2$	$(7s_{1/2},7p_{3/2})^o_2$	1.50	1.50	73 736	1.50	70 416	1.49	76 641
$6d^9 7s^2 7p$	$^3D^o_2$	$(6d_{3/2},7p_{3/2})^o_2$	1.17	1.07			56 960	1.12	60 809
$6d^9 7s^2 7p$	$^3P^o_1$	$(6d_{5/2},7p_{3/2})^o_1$	1.00	1.10			58 260	1.15	64 470
$6d^9 7s^2 7p$	$^3P^o_1$	$(6d_{3/2},7p_{3/2})^o_1$	1.00	1.07			68 673	1.00	73 686
$6d^{10}7s7p$	$^1P^o_1$	$(7s_{1/2},7p_{3/2})^o_1$	1.00	1.17	79 637	1.10	78 697	1.04	85 533
$6d^9 7s^2 7p$		$(6d_{3/2},7p_{3/2})^o_0$	0.00	0.00			80 442	0.00	82 895
$6d^{10}7s8s$	$^2S_1$	$(7s_{1/2},8s_{1/2})_1$	2.00	2.00	87 785	2.00			
$6d^{10}7s8s$	$^1S_0$	$(7s_{1/2},8s_{1/2})_0$	0.00	0.00	88 861	0.00			
$6d^{10}7s8p$	$^3P^o_0$	$(7s_{1/2},8p_{1/2})^o_0$	0.00	0.00	95 903	0.00			
	$^3P^o_1$	$(7s_{1/2},8p_{1/2})^o_1$	1.50	1.33	95 084	1.39			
	$^3P^o_2$	$(7s_{1/2},8p_{3/2})^o_2$	1.50	1.50	97 342	1.50			

[a] Reference [15].

$$g_{\mathrm{NR}}(J,L,S) = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}, \quad (11)$$

where L is angular momentum of the atom, S is its spin, and J is total momentum ($\mathbf{J}=\mathbf{L}+\mathbf{S}$).

For the case of two electrons the g factor in the jj scheme is given by

$$\begin{aligned} g_{jj}(J,j_1,j_2) &= g_{\mathrm{NR}}(j_1,l_1,1/2)\frac{J(J+1) - j_2(j_2+1) + j_1(j_1+1)}{2J(J+1)} \\ &+ g_{\mathrm{NR}}(j_2,l_2,1/2)\frac{J(J+1) - j_1(j_1+1) + j_2(j_2+1)}{2J(J+1)}, \end{aligned} \quad (12)$$

where j_1 and j_2 are total momentum of each electron and J is total momentum of the atom ($\mathbf{J}=\mathbf{j_1}+\mathbf{j_2}$), and g_{NR} is given by Eq. (11). The formula (12) also works for an electron and a hole [e.g., the $(6d_{5/2}7p_{1/2})_2$ state].

The main difference in the spectra of mercury and Uub is due to the larger fine structure in the $6d$ subshell of Uub than in the $5d$ subshell of Hg. This leads to easy excitation of the $6d_{5/2}$ electron and large number of the states in the spectrum of Uub which correspond to the $6d^9 7s^2 7p$ configuration. According to calculations in Ref. [13] it also leads to the change of the ground state configuration of Uub$^+$ as compared to the Hg$^+$ ion. The ground state configuration of Uub$^+$ is shown to be the $6d^9 7s^2$ configuration compared to the $5d^{10}6s$ ground state configuration of Hg$^+$. One should also note the large negative relativistic correction for $7s$ energy in Uub which makes this state more tightly bound than the $6s$ state of Hg.

The states of the $6d^9 7s^2 7p$ configuration are calculated with method B, states of the $7s$ and $6d^{10}7s8p$ configurations are calculated with method A, and the states of the $6d^{10}7s7p$ configuration are calculated with both methods. The results of both methods are in good agreement with each other and in reasonable agreement with Ref. [15]. States of the $6d^9 7s^2 7p$ configuration are well separated in energy from the states of the same total momentum of the $6d^{10}7s7p$ and $6d^{10}7s8p$ configurations. This means that the mixing between these states is small and should not affect the accuracy of the results. Judging by comparison with mercury we expect the results for Uub to be accurate within a few percent.

Accurate calculations for superheavy elements should include the Breit interaction, quantum electrodynamic (QED) corrections, and volume isotope shift. However, as has been demonstrated in our previous works [24,29] even for atoms with Z=120 Breit and QED corrections are relatively small and extrapolation of the error from lighter analogs of the superheavy atoms is likely to produce more accurate results than the inclusion of these small corrections. The accuracy of the present calculations is lower than that for Z=120 in Refs. [24,29] due to the complex electron structure of Uub. Therefore, these small corrections can be safely neglected on the present level of accuracy. This is in agreement with the results of Ref. [16] in which QED corrections have been considered for E112 and found to contribute about 0.5% to the ionization potential.

IV. CONCLUSION

We have calculated the 17 lowest energy levels of the superheavy element Uub (Z=112). Comparison with similar calculations for mercury indicate that the accuracy of the calculations is within a few percent. The results can be used in the study of the chemical and spectroscopic properties of the superheavy element.

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