Nobelium energy levels and hyperfine-structure constants

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Advances in laser spectroscopy of superheavy ($Z > 100$) elements enabled determination of the nuclear moments of the heaviest nuclei, which required high-precision atomic calculations of the relevant hyperfine-structure (hfs) constants. Here, we calculated the hfs constants and energy levels for a number of nobelium ($Z = 102$) states using a hybrid approach combining linearized coupled-cluster and configuration interaction methods. We also carried out an extensive study of the No energies using the 16-electron configuration interaction method to determine the position of the $5f^{13}7s^26d$ and $5f^{13}7s^27p$ levels with a hole in the $5f$ shell to evaluate their potential effect on the hyperfine-structure calculations of the low-lying $5f^{14}7s6d$ and $5f^{14}7s7p$ levels. We find that unlike the case of Yb, the mixing of the low-lying levels with filled and unfilled f shells is small and does not significantly influence their properties. The resulting hfs constants for the $5f^{14}7s7p\ ^1P_1^o$ level, combined with laser-spectroscopy measurement, were used to extract nobelium nuclear properties [Raeder *et al.*, Phys. Rev. Lett. **120**, 232503 (2018)].

I. INTRODUCTION

A study of superheavy element properties is a very important and challenging task that requires a development of new experimental and theoretical methods. Only very limited experimental information about properties of the superheavy elements is available due to their low production rate of only a few atoms per second. These radioactive elements must be studied immediately following their production in nuclear fusion reactions. Experimental values of ionization potentials, transition energies, and even assignment of electron configurations are very scarce for these elements requiring theoretical calculations. The nuclear moments of the heaviest nuclei could only be inferred from nuclear spectroscopy requiring model assumptions until recent laser spectroscopy advances [1,2].

Atomic spectra of different isotopes of superheavy elements can be used to obtain information on the nuclear spin, nuclear moments, and changes in nuclear mean-charge radii between isotopes allowing direct probes of nuclear properties. Atom-at-a-time laser resonance ionization spectroscopy of nobelium was reported in [1], in which the $7s^2\ ^1S_0$-$7s7p\ ^1P_1^o$ transition was identified. Further laser spectroscopy studies of this No transition were carried out in [2] including the measurement of the hyperfine splitting of ^{253}No and the isotope shifts for ^{252,253,254}No. Combining these measurements with the state-of-the-art atomic calculations allowed one to extract the nuclear properties such as the nuclear magnetic dipole and electric quadrupole moments of No and change of the nuclear radius between 252, 253, and 254 isotopes [2]. In this work we describe these calculations in detail and present recommended

values for a number of No hyperfine-structure (hfs) constants for a future improved determination of the nuclear properties.

A problem that occurs in No calculations is the electronic structure of the low-lying levels. The configurations with two electrons above the closed $5f$ shell, such as $5f^{14}7s6d$ and $5f^{14}7s7p$, can be treated with most accurate methods of calculation, such as a combination of the configuration interaction (CI) [3] with many-body perturbation theory (the CI+MBPT method) or with a coupled-cluster approach (the CI+all-order method) (see [4–6] for more details). However, these methods cannot reproduce the energy levels of the $5f^{13}7s^26d$ and $5f^{13}7s^27p$ configurations, which have a hole in the $5f$ shell, and, hence, a mixing of these configurations with the $5f^{14}7s7p$ and $5f^{14}7s6d$ configurations. Therefore, if such states appear low in the spectra, the CI+MBPT or CI+all-order methods may not be reliable. On the other hand, if these states appear to be high in the spectra they will not affect the properties of the low-lying states with a filled $5f$ shell.

Nobelium is a chemical homologue of Yb and it is known [7] that the Yb energy levels with an unfilled $4f$ shell already appear at a level of 23 000 cm^{-1}. It leads to a significant mixing of these states with the states with a filled $4f$ shell, particularly strongly affecting the properties of the $4f^{14}6s6p\ ^1P_1^o$ level and resulting in a poor accuracy of theoretical hfs constants for this state [8,9]. To check whether this is also the case for nobelium, whose main configuration is $5f^{14}7s^2$, we consider it as a system with 16 valence electrons and perform calculations of the low-lying energy levels in the framework of (i) the conventional CI method and (ii) a recently developed method based on a CI technique, where

excitations of the valence electrons to high-energy states are treated perturbatively (the CIPT method) [10]. It allows us to determine the position of the states with filled and unfilled $5f$ shells relative to each other. Both of these methods do not take into account the core-valence correlations and, hence, are not expected to be as accurate as the CI-all-order method for the divalent states. However, the CI and CIPT methods are applicable to the calculation of properties of polyvalent atoms with reasonable accuracy.

Our analysis shows that interactions of the states with filled and unfilled $5f$ shells is practically negligible, which allows us to consider the No atom as a divalent system and apply the CI+all-order method [5] [combining CI with the linearized single-double coupled-cluster method] for calculating the hfs constants of the low-lying states. We find that the No case is very similar to Hg, where core-excited states appear much higher in the spectrum, not significantly affecting the accuracy of the $6s6p\,^1P_1^o$ hfs constants. We start with a description of these energy studies and then consider the hfs constants.

II. METHODS OF CALCULATION

Here we consider No as a system with 16 valence electrons and perform calculations in the framework of the CI method. We start from a solution of the Dirac-Fock equations and carry out the initial self-consistency procedure for the $[1s^2, \ldots, 5f^{14}7s^2]$ configuration. To optimize the calculations for a particular problem described above, we construct the orbitals for specific configurations. The $7p$ orbitals were constructed for the $5f^{14}7s7p$ configuration, i.e., freezing all orbitals and moving an electron from the $7s$ to the $7p$ shell. The $6d$ orbitals were constructed for the $5f^{13}7s^26d$ configuration. The virtual orbitals were constructed as described in [11,12]. In total, the basis set included orbitals up to $9s$, $9p$, $8d$, $8f$, and $7g$. The size of a configuration space grows very rapidly with the increased basis set. The basis used by us makes the calculation manageable while still allowing one to perform convergence tests to ensure the validity of the results. The configuration space was formed by allowing single and double excitations for the even-parity states from the $5f^{14}7s^2$ and $5f^{14}7s6d$ configurations and for the odd-parity states from the $5f^{14}7s7p$ and $5f^{13}7s^26d$ configurations.

To verify a convergence of the CI method, we calculated the low-lying energy levels for three cases: including the single and double excitations to the $7s$, $7p$, $6d$, $6f$, and $5g$ shells (we designate it as $[7sp6df5g]$) and including the single and double excitations to $[8sp7df6g]$ and $[9sp8df7g]$. In the last case the configuration space consisted of 2 460 000 determinants for the even-parity states and 3 000 000 determinants for the odd-parity states presenting already a significant computational challenge.

The results of the energy calculations using three CI spaces described above, are given in Table I. Where available, we compare our results with those obtained in Ref. [13] using the CI+all-order method, where No was treated as a divalent atom, thus only allowing one to obtain results for the $5f^{14}7snl$ configurations. We refer the reader to Ref. [13] for the description of the CI+all-order method and its application to the calculation of No energy levels.

TABLE I. The energy levels of the low-lying excited states of No counted from the ground state (in cm^{-1}). The columns $[7sp6df5g]$, $[8sp7df6g]$, and $[9sp8df7g]$ give results obtained using different sets of the configurations described in the text. The results obtained in Ref. [13] using the CI+all-order method are given in the column labeled "CI+all."

Config.	Term	$[7sp6df5g]$	$[8sp7df6g]$	$[9sp8df7g]$	CI+all
$5f^{14}7s^2$	$^1S_0$	0	0	0	0
$5f^{14}7s6d$	$^3D_1$	35287	30139	31003	28436
	$^3D_2$	35197	30354	31223	28942
	$^3D_3$	35023	30722	31608	30183
	$^1D_2$	41802	37230	37980	33504
$5f^{13}7s^27p$	$J=3$	59856	56410	56927	
	$J=4$	59959	56537	57068	
	$J=5$	68133	64396	64911	
	$J=2$	68220	64463	64984	
	$J=3$	68571	64899	65434	
$5f^{14}7s7p$	$^3P_0^o$	15321	16278	16360	19567
	$^3P_1^o$	17184	18064	18138	21042
	$^3P_2^o$	21609	22508	22536	26113
	$^1P_1^o$	30365	30173	30237	30203
$5f^{13}7s^26d$	$J=2$	44816	45492	45720	
	$J=5$	49126	49494	49731	
	$J=3$	51741	51929	52172	
	$J=6$	51614	52075	52415	
	$J=4$	53354	53426	53701	
	$J=2$	53438	53671	54016	
	$J=1$	55319	55357	55695	
	$J=4$	56120	56216	56597	
	$J=3$	56608	56577	56958	

The CI results are within 10%–20% of those obtained in Ref. [13], demonstrating sufficient accuracy of our CI approximation. We find a large energy separation between the states with filled and unfilled $5f$ shells, unlike the case of Yb. For comparison, the energy difference between the $4f^{14}6s6p\,^1P_1^o$ and $4f^{13}6s^25d$, $J=1$ states in Yb is only 3800 cm^{-1}. For No the energy difference between the similar terms $5f^{14}7s7p\,^1P_1^o$ and $5f^{13}7s^26d$, $J=1$ is found to be $\sim$25 000 cm^{-1}.

We also performed the energy level calculation employing the CIPT method to further confirm the validity of our conclusions. In contrast with the conventional CI method, a full diagonalization of the energy matrix is not needed in this approach and a much longer basis set can be used. The method is applicable to the case of 16 valence electrons including configurations with filled and unfilled $5f$ shells into the CI matrix. This method is very useful since it can deal with complicated elements, for which the CI+all-order method is not applicable and the CI method is impractical due to the extremely large size of the energy matrix. The energy interval between the $5f^{14}7s7p\,^1P_1^o$ and $5f^{13}7s^26d$, $J=1$ states, determined using the CIPT method, was several times larger than between similar terms in Yb, thus confirming the results obtained in the framework of the 16-electron CI method.

As a result, we conclude that the states with filled and unfilled $5f$ shells are located sufficiently far from each other. A mixing between them should be small and not essential in calculating the properties of the low-lying states with a filled

$5f$ shell. Thus, we use the CI+all-order method, as the most accurate, for calculation of the hfs constants.

III. HYPERFINE-STRUCTURE CONSTANTS

A. hfs couplings

The hfs coupling due to nuclear multipole moments may be represented as a scalar product of two tensors of rank k,

$$H_{\mathrm{hfs}} = \sum_{k} (\mathbf{N}^{(k)} \cdot \mathbf{T}^{(k)}),$$

where $\mathbf{N}^{(k)}$ and $\mathbf{T}^{(k)}$ act in the nuclear and electronic coordinate space, respectively. Using this expression we write the matrix element of the operator H_{hfs} as

$$\langle \gamma' I J' F M_F | H_{\mathrm{hfs}} | \gamma I J F M_F \rangle = (-1)^{I+J'+F} \sum_{k=1} \langle I || N^{(k)} || I \rangle \langle \gamma' J' || T^{(k)} || \gamma J \rangle \begin{Bmatrix} I & I & k \\ J & J' & F \end{Bmatrix}. \tag{1}$$

Here I is the nuclear spin, J is the total angular momentum of the electrons, $\mathbf{F} = \mathbf{I} + \mathbf{J}$, and γ encapsulates all other electronic quantum numbers.

In the following we restrict ourselves to the first two terms in the sum over k, considering only the interaction of magnetic dipole and electric quadrupole nuclear moments with the electrons, i.e.,

$$H_{\mathrm{hfs}} \approx \mathbf{N}^{(1)} \cdot \mathbf{T}^{(1)} + \mathbf{N}^{(2)} \cdot \mathbf{T}^{(2)}.$$

We define $\mathbf{N}^{(1)}$ and $\mathbf{N}^{(2)}$ in a dimensionless form, expressing them through the nuclear magnetic dipole moment $\boldsymbol{\mu}$ and nuclear electric quadrupole moment Q, respectively, as

$$\mathbf{N}^{(1)} = \boldsymbol{\mu}/\mu_N,$$
$$N_q^{(2)} = Q_q^{(2)}/[1 \text{ barn}],$$

where μ_N is the nuclear magneton. The reduced matrix elements $\langle I || N^{(k)} || I \rangle$ ($k = 1, 2$) are

$$\langle I || N^{(1)} || I \rangle = \sqrt{\frac{(2I+1)(I+1)}{I}} \frac{\mu}{\mu_N},$$

$$\langle I || N^{(2)} || I \rangle = \frac{1}{2} \sqrt{\frac{(2I+3)(2I+1)(I+1)}{I(2I-1)}} \left[\frac{Q}{1 \text{ barn}} \right].$$

The operator $T_q^{(k)}$ is the sum of the one-particle operators

$$T_q^{(k)} = \sum_{i=1}^{N_e} \left(T_q^{(k)} \right)_i,$$

where N_e is the number of the electrons in the atom and the expressions for one-particle electronic tensors $T_i^{(k)}$ are given (in the SI units) by

$$\left(T_q^{(1)} \right)_i = -\frac{|e|}{4\pi\varepsilon_0} \frac{i\sqrt{2} \left[\boldsymbol{\alpha}_i \cdot \mathbf{C}_{1q}^{(0)}(\hat{\mathbf{r}}_i) \right]}{c r_i^2} \mu_N,$$

$$\left(T_q^{(2)} \right)_i = -\frac{|e|}{4\pi\varepsilon_0} \frac{C_{2q}(\hat{\mathbf{r}}_i)}{r_i^3} [1 \text{ barn}],$$

where $\boldsymbol{\alpha}_i$ is the Dirac matrix, ε_0 is the dielectric constant, $\mathbf{C}_{1q}^{(0)}$ is a normalized spherical harmonic, C_{2q} is a normalized spherical function, r_i is the radial position of the ith electron, and $\hat{\mathbf{r}}_i \equiv \mathbf{r}_i/r_i$.

The formulas connecting the hfs constants A and B of an atomic state $|J\rangle$ with the matrix elements $\langle \gamma J || T^{(k)} || \gamma J \rangle$ of the electronic tensors $\mathbf{T}^{(k)}$ are

$$A = \frac{g_N}{\sqrt{J(J+1)(2J+1)}} \langle \gamma J || T^{(1)} || \gamma J \rangle,$$

$$B = -2 \left[\frac{Q}{1 \text{ barn}} \right] \sqrt{\frac{J(2J-1)}{(2J+3)(2J+1)(J+1)}} \langle \gamma J || T^{(2)} || \gamma J \rangle,$$

where $g_N = \mu/(\mu_N I)$.

TABLE II. Contributions to the magnetic-dipole and electric-quadrupole hfs constants A and B (in megahertz). The CI, CI+MBPT, and CI+all-order values, without any corrections to the hfs operators are listed in the columns labeled "CI," "CI+MBPT," and "CI+all," correspondingly. The RPA corrections to the hfs operator are listed in the column labeled "RPA." All other corrections to the hfs operator (core Brueckner, two-particle, structure radiation, and normalization) are grouped together in the column labeled "Other." The values in the column labeled "Total" are obtained as the sum of the values in the "CI+all," "RPA," and "Other" columns.

	CI	CI+MBPT	CI+all	RPA	Other	Total
$A(7s6d\,^3D_1)$	783	1054	989	184	-235	939
$A(7s6d\,^3D_2)$	-417	-728	-658	-26	47	-637
$A(7s6d\,^3D_3)$	-560	-777	-729	-53	88	-694
$A(7s6d\,^1D_2)$	112	330	277	63	-74	266
$A(7s7p\,^3P_1^o)$	-1415	-2289	-2107	-288	293	-2102
$A(7s7p\,^3P_2^o)$	-858	-1219	-1143	-156	182	-1118
$A(7s7p\,^1P_1^o)$	437	883	780	102	-144	739
$A(7s8p\,^3P_1^o)$	-1835	-2696	-2537	-336	387	-2486
$A(7s8p\,^3P_2^o)$	-1029	-1382	-1314	-174	205	-1283
$A(7s8p\,^1P_1^o)$	773	1260	1172	154	-189	1137
$B(7s6d\,^3D_1)$	572	982	928	109	624	1661
$B(7s6d\,^3D_2)$	813	1384	1316	507	557	2380
$B(7s6d\,^3D_3)$	1071	1538	1510	1136	933	3579
$B(7s6d\,^1D_2)$	2062	1721	1958	1281	679	3919
$B(7s7p\,^3P_1^o)$	-2522	-2656	-2824	-1029	-405	-4258
$B(7s7p\,^3P_2^o)$	2663	3069	3121	1777	303	5201
$B(7s7p\,^1P_1^o)$	1279	2270	2161	1342	-490	3013
$B(7s8p\,^3P_1^o)$	-303	-202	-231	-91	-50	-373
$B(7s8p\,^3P_2^o)$	546	650	648	358	53	1059
$B(7s8p\,^1P_1^o)$	546	615	621	314	-49	886

TABLE III. Contributions to the magnetic-dipole hfs constants A (in megahertz) for the two odd-parity levels of ^{259}No and ^{201}Hg ($I = 3/2$ and $\mu/\mu_N = -0.5602$). The CI, CI+MBPT, and CI+all-order values, without any corrections to the hfs operators are listed in the columns labeled "CI," "CI+MBPT," and "CI+All," correspondingly. The relative differences of the CI+MBPT and CI values and the CI+all-order and CI+MBPT values are listed in percent to illustrate the size of the second-order and higher-order corrections to the wave functions. The RPA corrections to the hfs operator are listed in the column labeled "RPA." The relative size (the ratio of the RPA correction and the total value) is listed in the next column in percent. All other corrections to the hfs operator are grouped together in the column labeled "Other." Their relative size (the ratio of the "Other" correction and the total value) is given in the next column in percent. The values in the column labeled "Total" are obtained as (CI+all) + RPA + Other. The experimental values for Hg are given in the last column.

Ion	State	CI	CI+MBPT	Diff. %	CI+all	Diff. %	RPA	RPA %	Other	Other %	Total	Experiment
No	$7s7p\,^3P_1^o$	−1415	−2289	38%	−2107	−9%	−288	14%	293	−14%	−2102	
	$7s7p\,^1P_1^o$	437	883	51%	780	−13%	102	14%	−144	−19%	739	
Hg	$6s6p\,^3P_1^o$	−3924	−5829	33%	−5499	−6%	−560	10%	408	−7%	−5651	−5454.569(3)[a]
	$6s6p\,^1P_1^o$	774	1593	51%	1422	−12%	153	11%	−113	−8%	1462	1316[b]

[a]Reference [16].
[b]Reference [17].

B. Results and estimate of uncertainties

In Ref. [2] the nuclear ground-state properties were obtained from laser spectroscopy of the ^{252,253,254}No isotopes. Using these measurements and the calculation of the hfs constants A and B for the $5f^{14}7s7p\,^1P_1^o$ state, the nuclear magnetic-dipole and electric-quadrupole moments were extracted to be $\mu/\mu_N = -0.527$ and $Q = 5.9$ b, respectively. Below, we use these values to calculate the hfs constants for the low-lying states of ^{259}No ($I = 9/2$).

This calculation was performed using the CI+all-order method, introduced in [5] and applied to calculation of nobelium energy levels in Ref. [13]. We determine the A and B hfs constants for the even- and odd-parity low-lying states of ^{259}No for the future laser spectroscopy studies of other No transitions. The results are summarized in Table II where we list the results of several computations to demonstrate the size of various contributions and to evaluate the uncertainties of the results. The first one is the two-particle CI which does not include any core corrections to the wave function. The next stage is a combination of CI and MBPT which includes core-valence correlations in the second order of the perturbation theory.

The CI+all-order results include third- and higher-order correlations of the valence electrons with the core. This calculation provides state-of-the-art wave functions, with corrections from the entire core being included, and valence-valence correlations accurately treated in the framework of the CI. We note that the CI+MBPT results include the CI values and the CI+all-order results include the CI+MBPT values, so these are listed as total values and not additive corrections. Next, we include corrections to the hfs expectation values beyond the correlation corrections to wave functions, which we refer to as the corrections to the hfs operator. The random-phase approximation (RPA) was taken into account to all orders and given separately in the table in the column labeled "RPA." The core Brueckner, two-particle, structural radiation, and normalization corrections were calculated in the second order of MBPT (see Ref. [14] for more details). They are grouped together as "Other."

Since the CI calculation for two valence electrons has a negligible uncertainty, the main source of the uncertainties is the core-valence correlations. Therefore, uncertainties in the values of the hfs constants may be estimated based on differences between the CI+all-order and CI+MBPT values. The resulting uncertainties of the magnetic-dipole constants A for the triplet ^3D_J and ^3P_J states are 5%–10%, while the uncertainties of the constants for the singlet $^1D_2$ and $^1P_1^o$ states are slightly worse, 10%–20%. The RPA and "Other" corrections tend to cancel each other for the constants A. We carried out an additional analysis demonstrating that if the core Brueckner and structural radiation corrections are accounted for in all orders of the perturbation theory, this cancellation becomes even more pronounced in most cases.

It is more complicated to estimate the uncertainties of the constants B because the relative role of different corrections is larger. The magnitude of the "RPA" and/or "Other" corrections is comparable with the "CI+all" values in some cases. In contrast with the constants A, the RPA and "Other" corrections to B have the same sign for most levels. Roughly estimating the absolute uncertainty to be equal to the magnitude of the correction "Other," we assume the fractional uncertainties of the B constants to be at the level of 20%–25%.

We also use another method to evaluate the accuracy of the hfs constants. Similar calculations of the magnetic-dipole hfs constants using the CI+all-order method were done for Hg for the lowest-lying odd-parity $^3P_1$ and $^1P_1$ states and different contributions were analyzed in Ref. [15]. Hg is a good testing case for No due to similar mixing of the core-excited states of the odd-parity configurations with $J = 1$. As illustrated by Table III, relative contributions to Hg and No hfs constants are similar, with the only exception of the "Other" contribution which is two times larger in No due to larger core and resulting larger size of the core Brueckner corrections.

In Hg, the CI+all-order value of $A(^1P_1^o)$ (with no RPA and other corrections) agrees with experiment to 8%, while the final number differs from the experimental result by 11%. This is caused by the cancellations in the values of the various corrections and some inconsistency in their accuracy. The RPA corrections are accounted for in all orders while other corrections are calculated in the second order of the perturbation theory. Assuming additional uncertainty in the No values in comparison with Hg due to larger core-Brueckner corrections, we estimate the accuracy of the $A(7s7p\,^3P_1^o)$ to be on the order of 15%.

The accuracy of $A(^3P_1^o)$ in Hg is much better, 3.5%. Therefore, we expect that in No the hfs constant $A(^3P_1^o)$ is accurate to about 5%–6% making it a good case for a benchmark comparison with experiment. Both methods give uncertainty estimates that are in reasonable agreement.

We note that the A and B hfs constants of the $7s7p\,^1P_1^o$ state were calculated also by other groups using different methods [2]. All results are in agreement within their uncertainties.

IV. CONCLUSION

We calculated the energy levels of the low-lying even- and odd-parity states in the framework of the 16-electron CI method to demonstrate significant reordering of the No energy levels in comparison with the homologue Yb. In contrast with Yb, the No states with a hole in the f shell are lying sufficiently high; a possible mixing with the states with a filled f shell is small and does not significantly influence their properties. As a result, the low-lying divalent No levels can be reliably treated with the CI+all-order method.

We predicted the values for $7s7p$, $7s6d$, and $7s8p$ magnetic-dipole and electric-quadrupole hfs constants using the CI+all-order method, also incorporating different corrections to the hfs operators. The uncertainties of the recommended values are estimated. We find that the theoretical accuracy for the $7s7p\,^3P_1^o$ hfs constant A is expected to be a factor of 3 better in comparison with the $7s7p\,^1P_1^o$ level making it particularly attractive for future more precise determination of No nuclear properties.

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