Using isotope shift for testing nuclear theory: The case of nobelium isotopes

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We calculate field isotope shifts for nobelium atoms using nuclear charge distributions which come from different nuclear models. We demonstrate that comparing calculated isotope shifts with experiment can serve as a testing ground for nuclear theories. It also provides a way of extracting parameters of nuclear charge distribution beyond nuclear root mean square (rms) radius, e.g., parameter of quadrupole deformation β. The measurements of at least two atomic transitions is needed to disentangle the contributions of the changes in deformation and nuclear rms radius into field isotopic shift. We argue that a previous interpretation of the isotope measurements in terms of $\delta\langle r^2\rangle$ between ^{252,254}No isotopes should be amended when nuclear deformation is taken into account. We calculate isotope shifts for other known isotopes and for hypothetically metastable isotope ^{286}No for which the predictions of nuclear models differ substantially.

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I. INTRODUCTION

Studying nuclear structure of superheavy elements (SHE) ($Z > 100$) is an important area of research taking nuclear physics to unexplored territory and potentially leading to the hypothetical island of stability [1–6]. The sources of experimental information are very limited since the SHE are not found in nature but produced at accelerators at a very low production rate. In addition, all produced isotopes are neutron-poor and have short lifetimes (see, e.g., reviews [1–6]). Using atomic spectroscopy to measure isotope shift and hyperfine structure (hfs) is one of the promising methods to proceed. The part of isotope shift caused by the change of nuclear volume and called "field isotope shift" (FIS) is widely used to extract the change of nuclear root-mean-square (rms) radius between two isotopes [7]. In our previous paper [8] we argue that it can also be used to study nuclear deformation. For example, using different dependence of atomic transitions on nuclear structure and having FIS measurements for at least two transitions, we could extract not only the change of rms radius but also the change in quadrupole deformation parameter β. Superheavy element E120 ($Z = 120$) was used in [8] to illustrate that if we take nuclear parameters from nuclear theory, the effect of nuclear deformation on FIS is sufficiently large to be detected by modern spectroscopic methods. The E120 element was chosen for illustration purposes because of the large value of the effect. However, real measurements for E120 are not expected any time soon. The heaviest element for which isotope shift and hfs measurements are available is nobelium ($Z = 102$) [9,10]. The isotope shift is measured for the ^{252,253,254}No isotopes and hfs is measured for the ^{253}No isotope.

In this work we study FIS of nobelium in detail. We calculate nuclear charge densities using several nuclear models based on covariant density functional theory [11]. Then we employ these densities in atomic calculations to get the FIS and compare it to experiment. We take a closer look at the interpretation of the data and argue that nuclear deformation should be taken into account in the analysis to reduce uncertainties below 10%.

We present a formula which expresses FIS via nuclear parameters. The formula is similar to what was suggested in [8]. It is an analog of the standard formula FIS $= F\delta\langle r^2\rangle$ but has more terms proportional to $\delta\langle r^2\rangle^2$, $\Delta\beta^2$, $\Delta\beta^3$. The parameters of the formula are found from the fitting of the calculated FIS. The formula is more accurate than the standard one for heavy nuclei. It can be used for predicting FIS for different isotopes if nuclear parameters are taken from nuclear theory. Since the formula contains terms related to nuclear deformation, it can be used to extract the values of the change of the parameter of nuclear quadrupole deformation $\Delta\beta$ similar to how the standard formula is used to extract the change of nuclear rms radius $\delta\langle r^2\rangle$. FIS for at least two atomic transitions is needed for this purpose. Currently the isotope shift has been measured for only one transition in nobelium. Therefore, we strongly argue in favor of new measurements and present theoretical data for three more transitions.

Finally, we make predictions for the values of the isotope shift for the hypothetically metastable isotope with neutron number $N = 184$ which has spherical shape.

II. CALCULATIONS

In this work we perform nuclear and atomic calculations. Nuclear calculations are used to provide nuclear charge densities which are connected then to observable effects, such as isotope shifts via atomic structure calculations.

A. Nuclear calculations

The nuclear properties have been calculated within the covariant density functional theory (CDFT) [11] using several state-of-the-art covariant energy density functionals (CEDFs) such as DD-ME2 [12], DD-MEδ [13], NL3* [14], PC-PK1 [15], and DD-PC1 [16]. In the CDFT, the nucleus is considered as a system of A nucleons which interact via the exchange of different mesons. The above-mentioned CEDFs represent three major classes of covariant density functional models, namely, the nonlinear meson-nucleon coupling model (NL) (represented by the NL3* functional), the density-dependent meson exchange (DD-ME) model (represented by the DD-ME2 and DD-MEδ functionals), and point coupling (PC) model (represented by the DD-PC1 and PC-PK1 functionals). The main differences between them lie in the treatment of the interaction range and density dependence. In the NL and DD-ME models, the interaction has a finite range which is determined by the mass of the mesons. For fixed density it is of Yukawa type and the range is given by the inverse of the meson masses. The third class of models (PC model) relies on the fact that for large meson masses, the meson propagator can be expanded in terms of this range, leading in zeroth order to δ forces and higher order derivative terms. Thus, in the PC model the zero-range point-coupling interaction is used instead of the meson exchange [11]. The NL, DD-ME, and PC models typically contain six to nine parameters which are fitted to experimental data on finite nuclei and nuclear matter properties, see Sec. II in Ref. [17] for details.

Pairing correlations play an important role in all open shell nuclei. In the present article, they are taken into account in the framework of relativistic Hartree-Bogoliubov (RHB) theory in which the RHB equations for the fermions are given by [11]

$$\begin{pmatrix} \hat{h}_D - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}_D^* + \lambda \end{pmatrix} \begin{pmatrix} U(\boldsymbol{r}) \\ V(\boldsymbol{r}) \end{pmatrix}_k = E_k \begin{pmatrix} U(\boldsymbol{r}) \\ V(\boldsymbol{r}) \end{pmatrix}_k. \quad (1)$$

Here, $\hat{h}_D$ is the Dirac Hamiltonian for the nucleons with mass m; λ is the chemical potential defined by the constraints on the average particle number for protons and neutrons; $U_k(\boldsymbol{r})$ and $V_k(\boldsymbol{r})$ are quasiparticle Dirac spinors [11,17]; and E_k denotes the quasiparticle energies. The Dirac Hamiltonian

$$\hat{h}_D = \boldsymbol{\alpha p} + V_0 + \beta(m + S) \quad (2)$$

contains an attractive scalar potential

$$S(\boldsymbol{r}) = g_\sigma \sigma(\boldsymbol{r}) \quad (3)$$

and a repulsive vector potential

$$V_0(\boldsymbol{r}) = g_\omega \omega_0(\boldsymbol{r}) + g_\rho \tau_3 \rho_0(\boldsymbol{r}) + eA_0(\boldsymbol{r}). \quad (4)$$

Since the absolute majority of nuclei are known to be axially and reflection symmetric in their ground states, we consider only axial and parity-conserving intrinsic states and solve the RHB equations in an axially deformed harmonic oscillator basis [17]. Separable pairing of the finite range of Ref. [18] is used in the particle-particle channel of the RHB calculations.

The accuracy of the description of the ground state properties (such as binding energies, charge radii, etc.) of even-even nuclei has been investigated globally in Refs. [17,19]. The best global description of experimental data on charge radii has been achieved by the DD-ME2 functional (characterized by a rms deviation of $\Delta r_{ch}^{\rm rms} = 0.0230$ fm), followed by DD-PC1 (which also provides best global description of binding energies), NL3*, and finally by DD-MEδ (characterized by a rms deviation of $\Delta r_{ch}^{\rm rms} = 0.0329$ fm) (see Table VI in Ref. [17] and Fig. 7 in Ref. [19]). However, the spread of rms deviations for charge radii between the above-mentioned functionals is rather small [$\Delta(\Delta r_{ch}^{\rm rms}) = 0.0099$ fm]. On the other hand, the charge radii of some isotopic chains (especially, those with high proton number Z) are not very accurately measured. Thus, strictly speaking we have to consider the accuracy of the description of charge radii by these functionals as comparable. Note that the nobelium nuclei under study have well-pronounced prolate or spherical minima in potential energy surfaces. Thus, the equilibrium quadrupole deformations obtained in static (CDFT) and dynamic (five-dimensional collective Hamiltonian based on CDFT) calculations are expected to be very similar (see Ref. [20] for examples in higher Z superheavy nuclei).

In the context of the study of isotopic shifts in superheavy elements it is necessary to mention substantial differences in model predictions for the nuclei located beyond currently measured. This is contrary to the fact that nuclear theories in general agree on the properties of SHE which have already been measured in experiment (see, for example, Figs. 7 and 8 in Ref. [21]). For example, some CEDFs (such as NL3*, DD-ME2, and PC-PK1) predict a band of spherical nuclei along and near the proton number $Z = 120$ and neutron number $N = 184$ (see Figs. 6(a), (b), and (e) in Ref. [21]). However, for other functionals (DD-PC1 and DD-MEδ) oblate deformed shapes dominate at and in the vicinity of these lines (see Figs. 6(c) and (d) in Ref. [21]). Nuclear measurements of the energies of the excited 2^+ states are needed to discriminate experimentally between spherical and oblate deformed ground states. Such experiments are not possible nowadays. It would be interesting to see whether atomic measurements would be able to help with such a discrimination.

B. Atomic calculations

We start from an estimation of mass shift to demonstrate that it can be neglected. Mass shift is the sum of normal mass shift and specific mass shift which has the same order of magnitude (see, e.g., [22]). In the nonrelativistic limit the normal mass shift (NMS) between isotopes with mass numbers A_1 and A_2 is given by

$$\delta\nu_{\rm NMS} = \left(\frac{1}{A_1} - \frac{1}{A_2}\right) \frac{\nu_{\rm exp}}{1822.888}. \quad (5)$$

Substituting numbers for the $^1{\rm S}_0 - {}^1{\rm P}_1$ transition in ^{254}No and ^{252}No we get $\delta\nu_{\rm NMS} = 5 \times 10^{-4}$ cm^{-1}. Total mass shift can be several times larger than the normal mass shift, therefore a reasonable estimation for the mass shift in nobelium stands at $\approx 10^{-3}$ cm^{-1}. If the uncertainty of the isotope shift measurements is smaller than this value, then taking into account mass shift and using the King plot to separate mass shift and field shift might be important for an accurate interpretation of the

measurements. We leave this for future work. In this work we focus on FIS.

Nuclear calculations produce nuclear charge density as a two-dimensional function $\rho(z, r_\perp)$, where z is the coordinate along the axis of symmetry and $r_\perp$ is the radial coordinate in the direction perpendicular to the axis of symmetry. Atomic electrons feel the nucleus as a spherically symmetric system, averaged over nuclear rotations. This is because atomic transition frequencies are three orders of magnitude smaller than nuclear rotational transition frequencies (see, e.g., [23]). Note that a correction to this picture has been calculated for hydrogen-like ions where electron frequencies are much bigger. Even in this case the correction is small [24]. Therefore, we transform $\rho(z, r_\perp)$ into spherical coordinates $\rho(r, \theta)$ and average it over θ, $\rho(r) = \int \rho(r, \theta) d\theta$. The density ρ is normalized by the condition $\int \rho dV = Z$. In the end we have nuclear charge density in numerical form rather than a set of parameters as in the case of using standard Fermi distribution. However, it is often useful to have such parameters as nuclear rms radius R_p, parameter of quadrupole deformation β, etc. Having them allows to study the sensitivity of observable effects (isotope shift in our case) to the change in the values of these parameters.

In our previous work [8] we studied various types of nuclear charge distribution variations including quadrupole deformation, change of nuclear skin thickness, and density suppression in the nuclear center. The effect of the density suppression is significantly smaller than the effect of the deformation and hardly can be separated using experimental FIS data. It is known from the nuclear models that the skin thickness is approximately the same in different nuclei and it hardly produces a significant effect on FIS. Moreover, the effect of the skin thickness on FIS cannot be separated from the effect of the deformation [25], numerically they are equivalent. Therefore, we concentrate on the effect of the quadrupole deformation β. In the end, the answer to the question which type of shape variation really takes place would come from nuclear theory. We use different nuclear models to calculate FIS and compare the results with experiment. A particular nuclear model and its predictions would be endorsed by the result.

It was also demonstrated in Ref. [8] that the three types of shape variation could be distinguished from the change of nuclear rms radius because of the different behavior of the $p_{1/2}$ and $p_{3/2}$ states (see Ref. [8] for more details). Therefore in this work we restrict our discussion to just two parameters, R_p and β. Their values are found by integrating nuclear charge density.

An alternative approach is possible in which the calculations start from the standard Fermi distribution for nuclear density and the effect of nuclear deformation is modeled by increasing the nuclear skin sickness. In this approach the discrimination between nuclear models would be done on the final stage of the study when the calculated isotope shift is compared to experiment.

The results of the calculations are presented in a form in which electron and nuclear variables are factorized, so that the electron structure factors do not depend on the nuclear isotope and therefore are not affected by the nuclear calculation uncertainty. The aim of atomic calculations is to find these electron structure factors. To do this we use nuclear charge densities in a particular nuclear model for two different isotopes and integrate them to get nuclear potentials V_1 and V_2. It is assumed on this stage that nuclear density is known exactly. All nuclear uncertainties are accounted for in the actual values of the nuclear factors. FIS can be found by direct comparison of the calculations for two different isotopes. This works well for isotopes which differ by a large number of neutrons, $\Delta N \gg 1$. For neighboring isotopes, where $\Delta N \approx 1$, the FIS is small and its calculated value is affected by numerical uncertainties. To suppress numerical noise we use the so-called finite field method [27]. We construct the nuclear potential according to the formula $V_N = V_1 + \lambda(V_2 - V_1)$, where V_1 and V_2 are nuclear potentials for two isotopes and λ is a numerical factor which can be large to enhance the difference between two isotopes and thus suppress numerical noise. First, the calculations are done for $\lambda = 0$ to obtain reference transition frequencies. Then, they are performed for several values of $\lambda > 1$ and the frequencies are extrapolated to $\lambda = 1$. In practice, we use $\lambda = 2$ and $\lambda = 4$.

To perform electron structure calculations we start from the so-called CIPT method (configuration interaction with perturbation theory) [28]. It treats nobelium as a system with 16 external electrons allowing excitations from the $5f$ subshell into the CI space. The aim of this study is to check whether the mixing of the $4f^{14}7snp$ ($n = 7, 8$) and $4f^{13}7^2s6d$ configurations has any significance for our states of interest. Such study was performed before [10,29] for the lowest odd states of No, $7s7p\ ^3\mathrm{P}^\mathrm{o}_1$ and $^1\mathrm{P}^\mathrm{o}_1$. The answer was negative. Now we want to extend our study to two more states $7s8p\ ^3\mathrm{P}^\mathrm{o}_1$ and $^1\mathrm{P}^\mathrm{o}_1$. Therefore, we performed the CIPT calculations again and found that there is no strong mixing of our states of interest with the state involving excitations from the $5f$ shell. This means that nobelium can be treated as an atom with two valence electrons above closed shells. We use the well-established CI + MBPT method [30,31] to perform the calculations.

The effective CI hamiltonian has a form

$$H^{\mathrm{CI}}(r_1, r_2) = \hat{h}_1(r_1) + \hat{h}_1(r_2) + \frac{e^2}{r_{12}} + \Sigma_2(r_1, r_2), \qquad (6)$$

where $\hat{h}_1$ is the single-electron part of the Hamiltonian, which is the sum of the Hartree-Fock operator $\hat{H}^{\mathrm{HF}}$ and correlation potential Σ_1, $\hat{h}_1 = \hat{H}^{\mathrm{HF}} + \Sigma_1$. Correlation potential Σ_1 is an operator which includes correlations between a particular valence electron and the electrons in the core. The operator Σ_2 can be understood as a screening of the Coulomb interaction between valence electrons by core electrons. We calculate Σ_1 and Σ_2 in second order of the many-body perturbation theory. The contribution of higher orders is relatively small but not totally negligible [29,32,33]. To simulate them, we rescale the Σ_1 operator in the s and p waves to fit the known energy of the $^1\mathrm{S}_0 - {}^1\mathrm{P}^\mathrm{o}_1$ transition, $\Sigma_1(s) \to 0.8\Sigma_1(s)$, $\Sigma_1(p) \to 0.94\Sigma_1(p)$. The rescaling helps to make more accurate predictions for the positions of other odd levels. It also improves the wave functions used to calculate transition amplitudes.

TABLE I. Excitation energies, electric dipole transition amplitudes and rates of spontaneous decay via electric dipole transitions to the ground state for four odd states of nobelium.

Upper	Excitation energies (cm^{-1})			A_{ab}	Transition
state	Present	Exp. [9]	CI+all [29]	(a.u.)	rate (s^{-1})
$7s7p\ ^3P^o_1$	21213		21042	1.37	1.2×10^7
$7s7p\ ^1P^o_1$	29963	29961	30203	4.24	3.3×10^8
$7s8p\ ^3P^o_1$	41482			0.097	3.6×10^5
$7s8p\ ^1P^o_1$	42926			0.86	4.0×10^7

We perform the calculations of the electric dipole transition rates between the ground and four lowest in energy odd states to see whether the rates are sufficiently large for the measurements. We use random-phase approximation (RPA) for the calculations. The RPA equations for the core states have a form

$$(\hat{H}^{\rm HF} + \epsilon_c)\delta\psi_c = -(d + \delta V)\psi_c, \tag{7}$$

where d is electric dipole operator, the index c numerates the states in the core, $\delta\psi_c$ is the correction to the core orbital caused by external electric field, and δV is the correction to the self-consistent Hartree-Fock potential caused by the change of all core states. The RPA equations are solved self-consistently for all states in the core. As a result, we have δV which is used to calculate transition amplitudes between valence states

$$A_{ab} = \langle a|d + \delta V|b\rangle. \tag{8}$$

Here, a and b are two-electron wave functions found in the CI + MBPT calculations. The rate of spontaneous decay of the state b into the state a via an electric dipole transition is given by (in atomic units)

$$T_{ab} = \frac{4}{3}(\omega_{ab}\alpha)^3 \frac{A^2_{ab}}{2J_b + 1}. \tag{9}$$

III. RESULTS

A. Energies and transition rates

The results of calculations for the energies and transition rates are presented in Table I. Good agreement with experiment is the result of fitting. The *ab initio* CI + MBPT result for the energy of the $7s7p\ ^1P^o_1$ state is 31652 cm^{-1}. This value differs from the experimental one by 5.6%. Comparing it with the CI+all-order result of Ref. [29] shows that most of this difference is due to higher-order correlations.

The $7s7p\ ^1P^o_1$ state has the largest electric dipole transition amplitude and largest transition rate to the ground state. There are at least two more transitions (first and last lines of Table I) which are probably strong enough to be experimentally studied. Note, that at least two transitions are needed to use isotope shift to extract nuclear deformation (see below).

B. Comparing nuclear models

Figures 1 and 2 show symmetrized nuclear densities [$\rho(r) = \int \rho(r,\theta)d\theta$] for nuclear models used in this work.

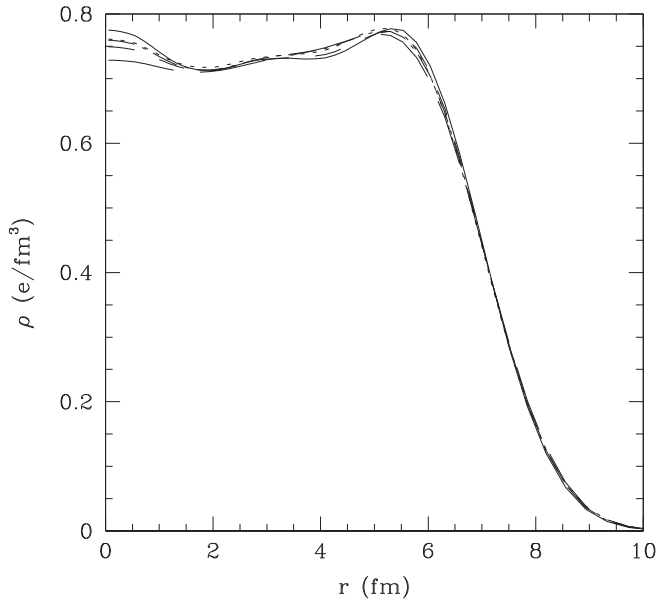

FIG. 1. Symmetrized nuclear densities in five nuclear models considered in this work. See Fig. 2 for details.

Table II shows the parameters of nuclear charge distribution for these models (CEDFs) and corresponding calculated isotope shifts for the $7s^2\ ^1S_0$ - $7s7p\ ^1P^o_1$ line of ^{252}No and ^{254}No. Experimental value for the isotope shift is 0.336(23) cm^{-1} [10]. The DD-MEδ model leads to the best agreement of the calculated and experimental IS; the calculated value is only about 10% larger then the experimental one. Note

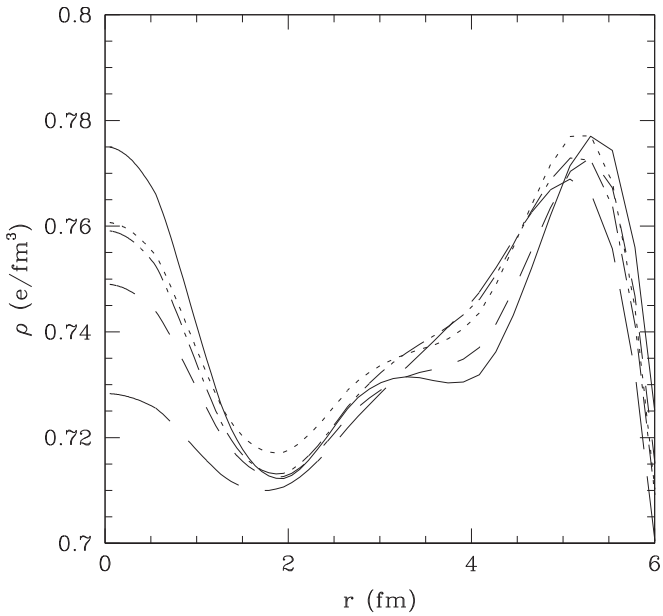

FIG. 2. Upper left part of Fig. 1 showing the details of nuclear density in five nuclear models. Solid line—DD-MEδ, dotted line—DD-ME2, short dashed line—NL3*, long dashed line—PC-PK1, dot-short dashed line—DD-PC1.

TABLE II. Parameters of nuclear model and corresponding calculated isotope shift for the $7s^2\ ^1S_0$ - $7s7p\ ^1P^o_1$ transition in ^{252,254}No. R_p is nuclear rms charge radius ($R_p = \sqrt{\langle r^2 \rangle}$), β is a parameter of nuclear quadrupole deformation, IS is calculated isotope shift, F is field shift constant ($F = \mathrm{IS}/\delta\langle r^2 \rangle$). Here, $\Delta\beta = \beta_1 - \beta_2$; the subscripts 1/2 correspond to the isotope with higher/lower value of neutron number.

Nuclear	^{252}No		^{254}No		$\delta\langle r^2 \rangle$		IS	F
model	R_p (fm)	β	R_p (fm)	β	fm^2	$\Delta\beta$	cm^{-1}	cm^{-1}/fm^2
DD-ME2	5.97171	0.298	5.98349	0.298	0.1408	0.000	−0.482	−3.42
DD-MEδ	5.96390	0.284	5.97259	0.278	0.1037	0.006	−0.374	−3.61
NL3s	5.97447	0.300	5.98772	0.298	0.1585	0.002	−0.503	−3.17
PC-PK1	5.98639	0.306	5.99967	0.305	0.1592	0.001	−0.538	−3.38
DD-PC1	5.97208	0.297	5.98225	0.295	0.1216	0.001	−0.431	−3.54

also that this model predicts the largest value of $\Delta\beta$ between two isotopes. The last column of Table II presents the ratios of calculated isotope shift to $\delta\langle r^2 \rangle$, which is the field shift constant F. In the absence of nuclear deformation FIS could be approximated by the standard formula $\delta\nu = F\delta\langle r^2 \rangle$, where F does not depend on nuclear isotope, i.e., it should be the same for any nuclear model since FIS is dominated by one nuclear parameter $\delta\langle r^2 \rangle$. However, we see that F varies significantly, i.e., there is another parameter which may affect $\delta\nu$. This is an indication that nuclear deformation may be important.

In Ref. [10] the nuclear field constant F was calculated without taking into account nuclear deformations. The CI + MBPT value of Ref. [10] is -3.47 cm^{-1}/fm^2. It is in excellent agreement with our value -3.42 cm^{-1}/fm^2 obtained with the same method and with the use of the DD-ME2 nuclear model in which $\Delta\beta = 0$ for the two isotopes (see Table II). However, the calculations of FIS based on this model overestimate FIS by about 40%. If we assume that the overestimation of the FIS mostly comes from the overestimation of $\delta\langle r^2 \rangle$, then the DD-ME$\delta$ results provide a more consistent picture. Indeed, the transition from the DD-ME2 to DD-MEδ model leads to the reduction of $\delta\langle r^2 \rangle$ from 0.1408 fm^2 down to 0.1037 fm^2 (see Table II). The latter value is very close to $\delta\langle r^2 \rangle = 0.105(7)(7)$ fm^2 found in Ref. [10]. In addition, the calculated FIS of the DD-MEδ model of -0.374 cm^{-1} (see Table II) is very close to the experimental value of $-0.336(23)$ cm^{-1} (see Ref. [10]). Note that the best agreement with experiment is achieved with the nuclear model which gives the largest change in nuclear deformation parameter between two isotopes. This indicates that nuclear deformation may give a noticeable contribution to the FIS. However, it is not possible to include it into analysis in the current situation when isotope shift is known for only one atomic transition. At least two transitions are needed to distinguish between $\delta\langle r^2 \rangle$ and $\Delta\beta$ (see next section).

C. Using isotope shift measurements to find parameters of nuclear charge distribution

It was suggested in our previous work [8] to fit the field isotope shift between two isotopes with the formula which depends on the change of two nuclear parameters, nuclear rms radius, and quadrupole deformation parameter β. Here, we present the formula in a slightly different form

$$\delta\nu = F\delta\langle r^2 \rangle + G(\delta\langle r^2 \rangle)^2 + a\Delta(\beta^2) + b\Delta(\beta^3) + c\delta\langle r^2 \rangle\Delta(\beta^2). \quad (10)$$

Here, $\delta\langle r^2 \rangle = \langle r^2 \rangle_1 - \langle r^2 \rangle_2$ is the change of square of nuclear rms radius, $\Delta(\beta^2) = \beta_1^2 - \beta_2^2$, $\Delta(\beta^3) = \beta_1^3 - \beta_2^3$, and the indexes 1 and 2 numerate isotopes, index 1 corresponds to an isotope with higher value of the neutron number. The coefficients F, G, a, b, c in this formula are found by a least squares fitting of calculated FIS for a wide range of nuclear parameters. The values of these parameters for four electric dipole transitions in nobelium are presented in Table III. Note that the value of F for the second transition is in excellent agreement with the CI + MBPT calculations of Ref. [10].

The first term in Eq. (10) represents a standard formula for field IS. It ignores nuclear deformation and relativistic corrections. It was shown in Ref. [34] that relativistic effects make the field constant F isotope-dependent. It was suggested to use a modified formula $\delta\nu_i = F'\delta\langle r^{2\gamma} \rangle$, where $\gamma = \sqrt{1-(z\alpha)^2}$. Modified field shift constant F' does not depend on isotopes. However, this formula works well only for spherical nuclei [8]. In contrast, formula (10) can be used for a wide range of nuclei. Relativistic corrections in it are fitted with quadratic in the $\delta\langle r^2 \rangle$ term [second term in Eq. (10)]. This formula can be used to predict FIS for different isotopes and atomic transitions if nuclear parameters are taken from nuclear theory.

TABLE III. The parameters of formula (10) for isotope shifts from the ground state ($7s^2\ ^1S_0$) to excited odd states of nobelium.

Odd states	F cm^{-1}/fm^2	G cm^{-2}/fm^4	a cm^{-1}	b cm^{-1}	c cm^{-1}/fm^2
$7s7p\ ^3P^o_1$	−3.7828	0.0288	−1.4013	1.3708	−0.0215
$7s7p\ ^1P^o_1$	−3.5042	0.0254	−1.2247	1.2234	−0.0152
$7s8p\ ^3P^o_1$	−3.2063	0.0265	−1.0941	1.1304	−0.0071
$7s8p\ ^1P^o_1$	−3.3112	0.0245	−1.1592	1.1919	−0.0090

TABLE IV. Isotope shifts between ^{254}No and ^{286}No in different nuclear models for four electric dipole transitions from the ground state (cm^{-1}).

Nuclear	R_p for ^{286}No	$\delta\langle r^2\rangle$	Upper state			
model	(fm)	(fm^2)	$7s7p\ ^3P^o_1$	$7s7p\ ^1P^o_1$	$7s8p\ ^3P^o_1$	$7s8p\ ^1P^o_1$
DD-ME2	6.084420	1.1872	−4.52	−4.18	−3.84	−3.97
DD-MEδ	6.075497	1.2111	−4.61	−4.27	−3.90	−4.03
NL3*	6.097316	1.3029	−4.94	−4.57	−4.20	−4.34
PC-PK1	6.114652	1.3655	−5.17	−4.78	−4.39	−4.54
DD-PC1	6.085116	1.2212	−4.64	−4.29	−3.95	−4.08
Average		1.2576	−4.78(40)	−4.42(36)	−4.06(33)	−4.19(35)

The formula can also be used in an opposite way: the change of nuclear parameters can be found from the isotope shift measurements. Since formula (10) depends on two nuclear parameters, the measurements of isotope shift for at least two atomic transitions are needed. Then standard mathematical procedures can be used to solve the system of two quadratic equations to find the change of nuclear parameters.

For neighboring isotopes the second and last terms in Eq. (10) can be neglected (see Table III) and the remaining terms reduced to

$$\delta\nu = F\delta\langle r^2\rangle + d\Delta\beta. \tag{11}$$

The parameters F and d in this formula are isotope-dependent and should be calculated for one of the considered isotope. The parameter d is related to a and b in Eq. (10) by $d = a(\beta_1+\beta_2) + b(\beta_1^2+\beta_1\beta_2+\beta_2^2)$ and $\Delta\beta = \beta_1 - \beta_2$.

So far the IS has been measured for one transition (second transition in Table III) between isotopes ^{252,253,254}No. According to nuclear theory [21], all these isotopes have deformed shapes, e.g., for $^{252,254}\Delta\beta = 0.006$ for DD-MEδ CEDF (see Table II). Using the formula (11) and the numbers from Table III we find that the contribution of the second term in Eq. (11) into IS is 0.003 cm^{-1}. This is 8 times smaller than the uncertainty of the measurements (measured value for IS is 0.336(23) cm^{-1} [10]). Therefore, to see the effect of nuclear deformation one has to either increase the accuracy of the measurements or use different isotopes. Note also that the measurements need to be done for at least two atomic transitions. Currently, IS is measured only for one transition in No [10].

Finally, we calculated isotope shifts between the ^{254}No and ^{286}No isotopes in different nuclear models; the results are presented in Table IV. Note that the ^{286}No nucleus has neutron number $N = 184$ which is a magic number in this mass region [6,21] corresponding to a large shell closure. Thus, according to nuclear theory this nucleus has spherical shape. It is expected to be a long-living isotope [6]. One transition frequency has been already measured in the ^{254}No isotope [9]. One can use the isotope shift from Table IV to correct measured frequencies of atomic transitions from ^{254}No to ^{286}No isotopes and use the data for a search of long-living nobelium isotopes in astrophysical data [35]. Note that all nuclear models give very close predictions for the IS (see Table IV). We use the spread of calculated results for an estimation of the uncertainties in the predictions and an average calculated value as the central point of these predictions.

We should note that there are other corrections affecting isotopic shift including the nuclear polarization effect and QED corrections. For example, they are seen in a detailed comparison of different contributions to the isotope shift for the $2p_{1/2} - 2s$ transition in Li-like ions $^{150,142}Nd^{57+}$ in Ref. [37]. However, the effect of the quadrupole deformation increases with the nuclear charge significantly faster than other effects due to the singularity of the Dirac wave function at the origin—see, for example, Ref. [37]. This is why we concentrate on the effect of the quadrupole deformation when considering superheavy elements like nobelium.

D. Nuclear deformation and nonlinearity of King plot

It was suggested in Ref. [36] to use a possible nonlinearity of the King plot to search for new particles. If some presently unknown bosons mediate interaction between atomic electrons and neutrons in the nucleus, then field shift constant F would depend on the number of neutrons. This would manifest itself in the nonlinearity of the King plot. Let us consider how this consideration is affected by nuclear deformation. The only condition for the King plot to be linear is the separation of nuclear and electron variables. Let us consider standard formula for isotope shift, namely, $\delta\nu = F\delta\langle r^2\rangle + MN$. Here, F is field shift constant, $\delta\langle r^2\rangle$ is a nuclear factor describing change in nuclear structure between two isotopes, M is the mass factor $M = (M_b - M_a)/M_bM_a$, N is electron structure factor related to mass shift, and the indexes a and b numerate isotopes. If F does not depend on the nucleus and $\delta\langle r^2\rangle$ does not depend on electrons then one can write for two atomic transitions

$$(\delta\nu_1/M) = \frac{F_1}{F_2}(\delta\nu_2/M) + \frac{F_1}{F_2}N_2 + N_1. \tag{12}$$

One can see that on the $\delta\nu_1/M, \delta\nu_2/M$ plane the points corresponding to different isotopes are all on the same line. If formula (11) is used for the field shift then an extra term

appears in Eq. (12):

$$(\delta\nu_1/M) = \frac{F_1}{F_2}(\delta\nu_2/M) + \frac{F_1}{F_2}N_2 + N_1 + \frac{\Delta\beta}{M}\left(d_1 - \frac{F_1}{F_2}d_2\right). \quad (13)$$

This last term does depend on isotopes and thus breaks the linearity of the King plot. It is instructive to see when this term is zero. The most obvious case is $\Delta\beta = 0$, i.e., all considered isotopes have the same nuclear deformation. This is an unlikely scenario for heavy nuclei. However, the terms can be small if deformations are similar. The less obvious case is $d_1 - d_2F_1/F_2 = 0$. Note that the expression $d_1F_2 - d_2F_1$ is the determinant of the system of two linear equations for $\delta\langle r^2\rangle$ and $\Delta\beta$ if IS for two transitions is given by Eq. (11). The determinant is zero means that the equations are proportional to each other and cannot be resolved. This might be the case of the transitions between similar states, e.g., $7s - 7p_{3/2}$ and $7s - 8p_{3/2}$ transitions in No^+. Exact proportionality is unlikely but strong suppression is possible (i.e., $d_1F_2 \approx d_2F_1$). The suppression is less likely in many-electron atoms since the states are affected by configuration mixing and it is different for low and high energy states so that similar transitions can hardly be found.

IV. CONCLUSION

We considered five nuclear models of nuclear charge distribution in two isotopes of nobelium, ^{252}No and ^{254}No, and calculated the field isotope shift for four electric dipole atomic transitions. It was demonstrated that comparing the calculated isotope shift with experiment helps to discriminate between nuclear models endorsing the predictions of the best-fit model. It was also shown that having isotope shift measurements for at least two atomic transitions can be used to extract from the measurements not only the change of nuclear rms radius but also the change in nuclear shape. Referring to the best-fit model endorses a particular type of shape change, e.g., change in nuclear quadrupole deformation, nuclear skin thickness, or nuclear density suppression in the origin. It was demonstrated that a change in nuclear shape between isotopes leads to nonlinearity of the King plot complicating its use for the search of new physics.

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[25] At first glance, the deformation of nuclei can be integrated out by introducing effective skin thickness for spherical Fermi density distribution and using it in atomic calculations. However, in this way the connection to nuclear physics will be lost. This is because the deformation in the nuclei has a clear physical meaning and manifests itself, for example, via the rotational bands and such bands are present in the ^{252,254}No nuclei. The deformation parameter β of the nucleus can be experimentally extracted either from Coulomb measurements or from rotational

spectra of ground state bands. The rotational properties and deformation parameters β of the nuclei under study are well described in the CDFT (see Ref. [26] and references quoted therein).

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