Measurement of QED and Hyperfine Splitting in the $2s_{1/2}$ - $2p_{3/2}$ X-Ray Transition in Li-like ²⁰⁹Bi⁸⁰⁺

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A measurement of the $2s_{1/2}-2p_{3/2}$ x-ray transition in trapped Li-like Bi⁸⁰⁺ ions was made that resolved the 0.820 \pm 0.026 eV hyperfine splitting of the $(1s^22s)_{F=4,5}$ ground configuration, providing the first such measurement in a multielectron highly charged ion. The intensity ratio of the two components is shown to be a new electron density diagnostic. The statistically averaged 2788.139 \pm 0.039 eV energy of the $2s_{1/2}-2p_{3/2}$ transition provides the most accurate test of QED in a high-*Z* ion to date, demonstrating the need for including higher-order terms in the Lamb shift calculations. [S0031-9007(98)05714-7]

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The hyperfine interaction between the nucleus and bound electrons is among the most important manifestations of nuclear properties affecting atomic transitions. The interaction couples the total angular momentum of the bound electron to the nuclear momentum, requiring the introduction of a larger set of quantum numbers, resulting in new physical properties and greatly increasing the number of possible transitions. The hyperfine interaction has been studied in the components of optical lines terminating on a split ground state, where extensive investigations on neutral atoms have resulted in the identification of the so-called hyperfine anomaly attributed to nuclear structure effects [1]. A hyperfine structure was also noted in the investigation of K-shell and nuclear γ -ray transitions in several electronic and muonic atoms [2]. However, no extension of such studies to x-ray lines in highly charged ions has yet been made. One reason is the difficulty of producing highly charged ions suitable for measurements with the required precision. The energy splitting due to the hyperfine interaction represents a very small fraction of the total x-ray energy and is readily masked by line broadening mechanisms associated with the production and excitation of the highly charged ions. Because of the simplified atomic structure of highly charged ions and the increased overlap of electronic wave functions with the nucleus, such measurements promise to be a fertile test bed for theories of the nuclear structure, in particular, the Breit-Rosenthal effect due to the finite distribution of the nuclear charge [3] and the Bohr-Weisskopf effect due to the finite distribution of the nuclear magnetization [4], and for testing quantum electrodynamical (QED) effects in ultrahigh nuclear fields [5].

In this Letter, we report the first observation of the hyperfine splitting of an x-ray transition in a highly charged heavy ion. Our measurement focused on the $2p_{3/2} \rightarrow 2s_{1/2} F = 4$ and F = 5 transitions in Li-like ²⁰⁹Bi⁸⁰⁺. The measurement yields several novel physics results. (1) The measurement provides the first experimental determination of the value of the hyperfine splitting of a

highly charged *multi*electron ion, demonstrating the importance of the nuclear size corrections and electron correlations in the theoretical treatment of hyperfine splitting, complementing the measurements of hyperfine transitions within the ground state of H-like ¹⁶⁵Ho⁶⁶⁺ and ²⁰⁹Bi⁸²⁺ [6] performed in the visible and UV. (2) We show that the ratio of the intensity of the hyperfine components depends on the electron density and represents a novel diagnostic tool for low-density plasmas. (3) The high resolution of our measurement allowed us to determine the total transition energy of the $2s_{1/2}$ - $2p_{3/2}$ transition with a statistical precision of 6 ppm and an overall accuracy of 14 ppm, testing the predicted QED contribution to the transition energy within 1.5×10^{-3} . This is better than the accuracy achieved in any test of the QED terms in any highly charged ion [7,8], and 40 times better than the accuracy achieved in the best test of the 1s QED contribution in H-like uranium [9]. Our measurement distinguishes between the most advanced calculations of the OED terms and finds disagreement up to 6 times the experimental 1- σ confidence limit demonstrating the incompleteness of present calculations. A critical test of the QED calculations is especially warranted in light of two significant changes to the non-OED values commonly used for isolating the OED terms from the experimental data. First, the non-QED energies computed with relativistic many-body perturbation theory [10,11] were revised in a large configuration interaction (CI) calculation [12] that included higher-order Breit-Breit interaction terms not considered before, shifting the non-QED energies of Li-like uranium, for example, by almost 0.4 eV. Second, it was shown that the nuclear polarization contributions [13] had been systematically overestimated by a factor of 2π [14], incorrectly improving agreement between theory and measurement in many cases.

Coupling with the I = 9/2 nuclear magnetic moment splits the $1s^22s$ (J = 1/2) ground level of $^{209}\text{Bi}^{80+}$ into two hyperfine structure components with angular momentum F = 4 and F = 5. The predicted separation of the

TABLE I. Contributions to the ground state hyperfine splitting of Bi^{80+} and comparison with measurement (in eV).

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Point nucleus ^a	+0.958
Finite charge distribution ^a	-0.111(2)
Finite magnetization distribution ^a	-0.014(6)
QED ^b	-0.003
Electron correlations (Coulomb) ^a	-0.036
Electron correlations (Breit) ^a	+0.002
Electron correlations (finite size) ^a	+0.004(2)
Total theory	0.800(7)
Experiment	0.820(26)
aD-f	

^aReference [15].

^bScaled value from Ref. [5].

two components is 0.8 eV [15] (cf. Table I), and the energy of each component is such that the average weighted by the respective statistical weights equals the unshifted $1s^22s_{1/2}$ ground level energy. The hyperfine interaction also splits the $1s^22p_{3/2}$ upper level into the four levels F = 3, 4, 5, 6. Because the interaction of the $2p_{3/2}$ electron with the nucleus is small, the $1s^22p_{3/2}$ hyperfine components separate about 40 times less than the ground state components. This separation is comparable to the natural width of the levels based on a total radiative transition rate of $2.69 \times 10^{13} \text{ s}^{-1}$ and is neglected in the following.

The measurement of the ground state splitting of 209Bi⁸⁰⁺ was enabled by recently developed techniques to produce cold ions in a high-energy electron beam ion trap and to observe their emission with very highresolution spectrometers [16]. The measurement utilized a von Hámos-type spectrometer [17] employing a 80 \times $50 \times 0.25 \text{ mm}^3$ quartz(1120) crystal bent to a 75-cm cylindrical radius and a $100 \times 30 \text{ mm}^2$ position-sensitive proportional counter with a 250- μ m spatial resolving power. The spectrometer was set to a Bragg angle of 65.5° providing a nominal resolving power of 10 500, i.e., a 0.26-eV instrumental linewidth. Employing a 100-keV, 170-mA electron beam, one Bi spectrum was collected over an 8-10 h, period. During three run periods, a total of 12 Bi spectra were recorded and separately analyzed (cf. Table II). The sum of the spectra collected in run period C is shown in Fig. 1(a), which illustrates that the two hyperfine components are clearly resolved from another in our measurements. The observed linewidth is $\leq 0.5 \text{ eV}$, indicating an ion temperature below 800 eV.

In statistical equilibrium, the relative intensity $I_{F=4}/I_{F=5}$ of the two hyperfine components is proportional to their statistical weights, i.e., 9:11 or $I_{F=4}/I_{F=5} = 0.82$. The observed ratio differed significantly from this value (cf. Fig. 1). The average observed ratio was 1.40 ± 0.07 . We constructed a collisional-radiative model, which showed that the line ratio depended on electron density and that the statistical ratio was not reached unless the electron density approached 10^{14} cm⁻³ (cf. Fig. 2). The calculation considered collisional excitations and radia-

TABLE II. Values of the ground state hyperfine splitting determined from sequentially recorded spectra in run periods A-C. Systematic errors are estimated to contribute less than 0.003 eV and are included in the average.

Spectrum (period)	Time (h)	ΔE (eV)	Uncertainty (eV)
(period)	(11)	(01)	(01)
1(A)	10.0	0.606	0.115
2(A)	26.5	0.755	0.130
3(A)	36.0	0.836	0.098
4(A)	59.0	0.883	0.078
5(B)	8.0	0.878	0.150
6(B)	19.0	0.831	0.110
7(B)	39.0	0.982	0.112
8(C)	8.0	0.683	0.106
9(C)	22.5	0.868	0.069
10(C)	31.5	0.677	0.101
11(C)	47.5	0.833	0.049
12(C)	56.0	0.851	0.130
Average		0.820	0.026

tive transitions between all hyperfine levels of the $1s^22s$ and $1s^22p$ configurations. Using the distorted-wave formalism [18], we calculated 4.37×10^{12} cm⁻³ s⁻¹ for the $2s_{1/2} \rightarrow 2p_{1/2}$ and 5.63×10^{12} cm⁻³ s⁻¹ for the $2s_{1/2} \rightarrow$



FIG. 1. Crystal spectrometer spectra obtained with a 100-keV, 170-mA electron beam: (a) $2s_{1/2}-2p_{3/2}$ transition in Li-like ²⁰⁹Bi⁸⁰⁺ showing the two components due to the F = 4 and F = 5 splitting of the ground state; (b) He-like Cl¹⁵⁺ K-shell calibration spectrum. Lines w, x, y, and z denote the transitions from upper levels 1s2p ¹ P_1 , 1s2p ³ P_2 , 1s2p ³ P_1 , and 1s2s ³ S_1 , respectively, to the $1s^2$ ¹ S_0 He-like ground level; lines q and r denote the transitions 1s2s2p ² $P_{3/2}$ and 1s2s2p ² $P_{1/2}$ to the $1s^22s$ ² $S_{1/2}$ Li-like ground level.



FIG. 2. Electron density dependence of the intensity ratio of the F = 4 and F = 5 components (solid line). Results for 10 times smaller and larger $F = 4 \rightarrow 5$ radiative rates A_r are shown as dashed lines. The measured ratio is shown for comparison.

 $2p_{3/2}$ excitation rate coefficient for 100-keV electrons. The $F = 5 \rightarrow 4$ magnetic dipole radiative transition rate was calculated to be 12.3 s⁻¹. The results of this prediction can be compared with the measured $I_{F=4}/I_{F=5}$ ratio (cf. Fig. 2) because the electron density in the measurement is known from the energy, current, and 70- μ m diameter of the electron beam [19]. Predictions for a tenfold higher or lower 5 \rightarrow 4 transition rate are also shown. The measured value lies below the predictions using the calculated value of 12.3 s⁻¹, but is in reasonable agreement considering the uncertainty limits and markedly differs from the other two curves.

The Bi spectrum was calibrated by observing the *K*-shell spectrum of He-like C1¹⁵⁺ at identical trap and beam conditions, as illustrated in Fig. 1(b). Fifteen spectra of Cl were recorded in an alternating fashion with the 12 Bi spectra to check for electronic drifts as well as the stability of the source. No shifts were found. The energy of the C1¹⁵⁺ lines is accurately described by experimentally tested two-electron energy calculations [20]. Recent refinements in these calculations [21] indicate that the uncertainty in these calculations is about 0.034 eV for chlorine, i.e., about the level of accuracy to which they were tested in neighboring Ar¹⁶⁺ [22]. For calibration, we use the $1s2p \ ^1P_1 \rightarrow 1s^2 \ ^1S_0$ and the $1s2s \ ^3S_1 \rightarrow 1s^2 \ ^1S_0$ line and set their energies to 2789.689 ± 0.034 and 2756.895 ± 0.034 eV, respectively [21].

The analysis of the 12 Bi spectra (cf. Table II) yielded an average value of 0.820 ± 0.026 eV for the separation of the F = 4 and F = 5 hyperfine levels. The separation has been calculated recently by Shabaeva and Shabaev [15]. Their result for a point nucleus (cf. Table I) differs markedly from the measured value. Adding corrections for QED and the finite size of the nuclear charge and magnetization brings the theoretical value in agreement with our measurement. Corrections must also be made for electron correlations. These are larger than the experimental uncertainty and, when included, produce a theoretical value that is smaller than measured, but still within the experimental uncertainty.

The energy *E* of the $1s^22s_{1/2}-1s^22p_{3/2}$ transition was determined from a statistical average of the individual components, $E = \frac{11}{20} \times (2787.770) + \frac{9}{20} \times (2788.591) = 2788.139 \text{ eV}$, with a standard error of 0.018 eV. The overall uncertainty is increased to 0.039 eV because of the uncertainty in the energies of the C1¹⁵⁺ calibration lines. In standard procedure, the QED contribution to the transition energy was obtained by subtracting the non-QED part from the measured energy. Based on the non-QED energies computed in [12], we subtracted 2814.456 eV and obtained a value of -26.317 ± 0.039 eV for the QED contribution to the Bi⁸⁰⁺ $2s_{1/2}-2p_{3/2}$ transition. No adjustment for nuclear polarization is made, which is estimated to contribute considerably less than the experimental uncertainty limits [14].

A comparison of the measured value with *ab initio* calculations of the screened QED terms performed by Blundell [11] and Chen *et al.* [12] is shown in Fig. 3. Also shown are the QED values calculated by Indelicato and Desclaux [23] using screened hydrogenic values. Unlike the earlier measurements of Li-like Th⁸⁷⁺ and U⁸⁹⁺ [8], the present measurement clearly distinguishes between calculations.

In summary, we have made the first spectrally resolved measurement of the hyperfine components of an x-ray transition from a highly charged ion. By studying the $2s_{1/2}$ - $2p_{3/2}$ transition in Bi⁸⁰⁺, we made the first determination of the hyperfine splitting of the 2*s* ground state in a highly charged multielectron ion. While the present measurement is not as accurate as measurements of the 1*s* ground state splitting [6], longer ex-



FIG. 3. Comparison of the measured and calculated QED contribution to the $2s_{1/2}$ - $2p_{3/2}$ transition in highly charged Li-like ions. Solid circle: present measurement; open diamonds: data from Ref. [8]. The theoretical values are from Refs. [11,12,23].

posure times and the use of higher beam currents may double the present accuracy. An order-of-magnitude improvement may be achieved by applying the present technique to the $2s_{1/2}$ - $2p_{1/2}$ transition, which is split by the same amount as the $2s_{1/2}-2p_{3/2}$ transition but has about 12 times less energy, provided it is measured with the same relative accuracy. The intensity ratio of the two hyperfine components was shown to be density sensitive. This sensitivity must be taken into account in transition energy determinations where individual components are not resolved, as the lowdensity intensity-averaged line position differs systematically from the high-density value. The close vicinity to a reference line enabled a very accurate determination of the $2s_{1/2}$ - $2p_{3/2}$ transition energy and the most precise determination of the QED term in a highly charged ion to date. Marked discrepancies with existing QED calculations were found. The present calculations consider only the lowest-order correction terms. The discrepancies demonstrate the need to include higher-order terms to increase the level of accuracy to that of the measurement. Important additional terms are higher-order electron correlations to eliminate the current dependence of the self-energy on the choice of potentials [24], two-loop corrections [25] shown to be important in atomic hydrogen [26], relativistic nuclear recoil contributions [11], or the effects of a large perturbing magnetic field on the radiative corrections [27]. Further improvements in the measurement accuracy of cold, stored ions are within reach. Indeed, a doubling of the current accuracy would already be possible, if the reference lines were known to a higher degree of certainty. Inclusion of these terms in an *ab initio* fashion will, thus, be mandatory for a meaningful comparison with future measurements and for advancing our understanding of QED in highly charged ions.

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