Measurement of the self-energy contribution to the 2s-3p resonance transition in neonlike ytterbium

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The self-energy contribution to the transition $(2s_{1/2}2p^6 3p_{3/2})_{J=1} \rightarrow 2s^2 2p^6$ in neonlike Yb^{60+} has been measured in an electron-beam ion trap to be 18.4±0.8 eV. This value is 10% larger than the value obtained from multiconfiguration Dirac-Fock calculations in the commonly used effective-charge approach. The measurement supports earlier suggestions that the effective-charge approach may overcorrect the screening effect on the self-energy corrections for transitions in neonlike ions.

I. INTRODUCTION

While the self-energy contribution to levels in hydrogenic ions has been calculated with high precision from first principles,[1,2] this is not the case for the self-energy contribution to levels in multielectron ions. Instead, atomic structure calculations of multielectron ions commonly make use of the so-called effective-charge approach[3,4] to estimate the self-energy contributions. This approach determines a phenomenological screening parameter of the nuclear potential which can be used to adjust the hydrogenic calculations.

As a first step in the effective-charge approach accurate relativistic orbitals are computed with multiconfigurational Dirac-Fock (MCDF) codes. Next, an effective nuclear charge, $Z_{\rm eff}$, for each orbital is found which would result in a hydrogenic orbital of similar character (the same expectation value $\langle r \rangle$, for example) as the corresponding MCDF orbital. An interpolation among the hydrogenic self-energies tabulated by Mohr[1] for $n=1,2$ levels is then used to provide the self-energy contribution to a given level in the field of charge $Z_{\rm eff}$. The tabulation is extended to higher-n orbitals with the n^{-3} scaling of the self-energy. The self-energy correction to the total energy for a given ion in a certain state is then calculated as a sum of products of self-energy corrections for each level and generalized occupation number. The self-energy contribution to a given transition between atomic states is then obtained as the difference between the total self-energies for the initial and final ionic states.

Because no calculations of the self-energy contributions to transitions in multielectron ions with more than two electrons exist which are based on first principles, it is of interest to determine the self-energy contribution experimentally and thus to test the accuracy of the effective-charge approach. Such a test is best done for high-Z ions, since quantum electrodynamical (QED) effects increase with Z^4.

Previous experiments have measured the 2s-3p transition energy in neonlike silver ($Z=47$), xenon ($Z=54$), and lanthanum ($Z=57$) from tokamak plasmas[5,6] and in neonlike gold ($Z=79$) and bismuth ($Z=83$) from beam-foil interactions.[7,8] The experimental uncertainty of the tokamak measurements varies between 30 and 70 ppm; that of the beam-foil measurements is about 500 ppm, although recent experiments have reduced this uncertainty to 170 ppm.[9] Here we report on a measurement of the 2s-3p resonance transition in neonlike ytterbium ($Z=70$) performed in an electron-beam ion trap[10-12] (EBIT). The uncertainty of the present measurement is 85 ppm. This allowed us to infer the value of the self-energy contribution to within 4%.

II. EXPERIMENT

A spectrum of the $n=3$ to $n=2$ transitions in Yb^{60+} is shown in Fig. 1. The spectrum has been obtained with a flat-crystal, survey spectrometer in first order using a Si(220) crystal with a 2d spacing of 3.840 Å. This spectrometer was used earlier to obtain spectra of neonlike barium.[11] The dominant features are due to 2p-3d electric dipole transitions in neonlike ytterbium. The lines are labeled 3C and 3D in the notation of Loulergue and Nussbaumer[13] and correspond to the transitions $(2p^5_{1/2}3d_{3/2})_{J=1} \rightarrow (2p^6)_{J=0}$ and $(2p^5_{3/2}3d_{5/2})_{J=1} \rightarrow (2p^6)_{J=0}$, respectively. The spectrum also shows the transition $(2p^5_{1/2}3s_{1/2})_{J=1} \rightarrow (2p^6)_{J=0}$, labeled 3F, as well as various unmarked satellite lines due to transitions in lower charge states. The 2s-3p resonance transition we are interested in is situated on the high-energy side of line 3C and corresponds to the transition from upper level $(2s_{1/2}2p^6 3p_{3/2})_{J=1}$ to the ground state. The line is labeled 3A and is found to be about 20 times less intense than line 3D. Its energy is strongly affected by QED effects because, unlike other transitions, it involves a 2s core level. Finally, the spectrum also shows an electric quadrupole transition, labeled E2S, from the upper level $(2s_{1/2}2p^6 3d_{3/2})_{J=2}$. The line has been of interest in high-density plasma research because of its density sensitivity.[14] Similar to line 3A, line E2S is also strongly

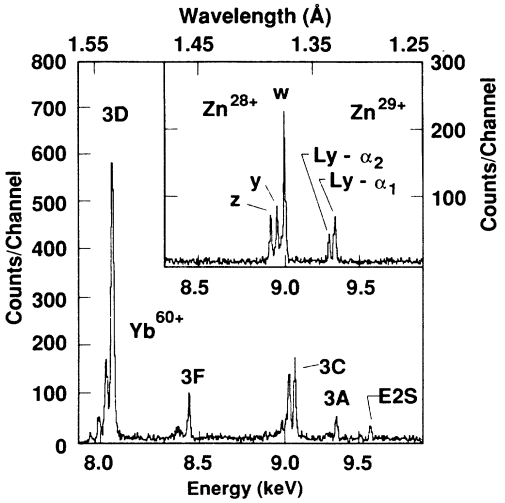

FIG. 1. Spectrum of $n=2-3$ transition in neonlike ytterbium in the wavelength region 1.25–1.55 Å. The spectrum has been obtained with a flat-crystal spectrometer. Unmarked features are transitions in lower charge states. The spectrum of hydrogenlike and heliumlike zinc used for calibration is shown in the inset.

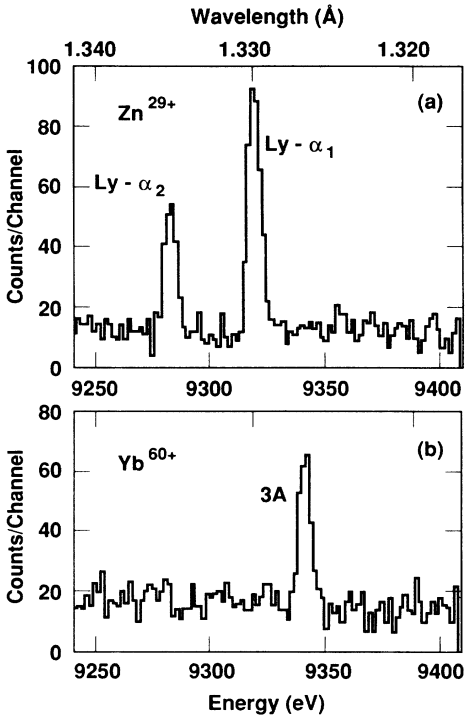

FIG. 2. Spectra in the wavelength region 1.32–1.34 Å obtained with a von Hámos–type spectrometer. (a) Lyman-α lines $2p_{3/2}\rightarrow 1s_{1/2}$ and $2p_{1/2}\rightarrow 1s_{1/2}$, labeled Ly-$\alpha_1$ and Ly-α_2, respectively, in hydrogenlike zinc used for calibration. (b) Transition $(2s_{1/2}2p^6 3p_{3/2})_{J=1}\rightarrow(2s^2 2p^6)_{J=0}$, labeled $3A$, in neonlike ytterbium. The background is due to detector noise and cosmic rays.

affected by QED effects. However, its intensity is weaker than that of line $3A$.

To determine the wavelength of line $3A$ with better precision than possible with the survey spectrometer, the line has been measured with a von Hámos–type[15] crystal spectrometer. The spectrometer uses a quartz $(20\bar{2}3)$ crystal ($2d=2.750$ Å) bent to a radius of curvature of 30 cm and a multiwire proportional counter of the type described in Ref. 16. The resolving power of the spectrometer is $\lambda/\Delta\lambda=1500$. A detailed description of the instrument can be found in Ref. 17. A spectrum of line $3A$ observed with the von Hámos spectrometer is presented in Fig. 2(b). The spectrum represents data collected during an 18-h time interval.

The wavelength of line $3A$ was determined with respect to the theoretical wavelengths of the Ly-α_1 and Ly-α_2 lines of hydrogenic zinc. The location of the Ly-α lines with respect to the position of line $3A$ is shown in Fig. 2(a). The figure shows that the wavelengths of the hydrogenic lines are very close to that of the neonlike line. Hence errors due to uncertainties in the dispersion of the spectrometer are small.

The use of hydrogenlike lines as reference lines is possible, because their wavelengths can be calculated with high precision.[1,2] Moreover, this precision is higher than the experimental precision with which we can determine the transition energy of line $3A$.

Zinc and ytterbium were introduced into EBIT with a metal vapor vacuum arc source.[10,18] Unfortunately, both metals could not simultaneously be injected. To estimate systemic errors arising, for example, from changes in the dispersion due to thermal expansion or electronic drift, we recorded a spectrum of zinc before and after measuring a spectrum of ytterbium. The center positions of the Ly-α lines measured in the two spectra of Zn^{29+} agree within 0.35 channels (corresponding to 0.5 eV). This variation represents the largest contribution to the overall uncertainty of the measurement, which is estimated to be ± 0.8 eV.

Using calculations by Johnson and Soff[2] we have set the wavelengths of the Ly-α lines equal to 1.330 52 and 1.335 85 Å. As a result, the wavelength of line $3A$ is determined to be 1.327 19 $\pm$0.000 11 Å. Using the conversion constant[19] $hc/e=12\,398.42$ eV Å we find the energy of the neonlike transition to be 9341.86 ± 0.80 eV.

In Table I the measured value of the transition energy of line $3A$ is compared to the value calculated with the MCDF code of Ref. 20. The code includes QED corrections and computes the self-energy contribution using the effective-charge approach of Ref. 3 (cf. Table I). The experimental value is 2.97 eV smaller than the calculated energy. Previous measurements of line $3A$ in neonlike silver,[5] xenon, and lanthanum[6] have also indicated that the calculated transition energies are too large. As shown in Fig. 3, the differences between experimental and theoretical transition energies clearly increase as a function of Z.

For completeness we have also determined the wavelength of lines $3A$, $3C$, and $E2S$ from the spectra recorded with the flat-crystal spectrometer. The technique is similar to the one used above. As reference lines we have

TABLE I. Comparison of measured and calculated energies of transitions in Yb^{60+}. The theoretical values are calculated with the MCDF code of Ref. 20 in the extended average level method. QED contributions are calculated in the effective-charge approach of Ref. 3. No correction for residual correlation energies have been made. All energies are in eV.

Transition	Key	E_{expt}	E_{MCDF}	ΔE
von Hámos spectrometer				
$2s_{1/2}2p^6 3p_{3/2} \rightarrow 2s^2 2p^6$	$3A$	9341.36±0.80	9344.83	−2.97
Flat-crystal spectrometer				
$2s_{1/2}2p^6 3p_{3/2} \rightarrow 2s^2 2p^6$	$3A$	9341.4±2.5	9344.8	−3.4
$2s^2 2p_{1/2}^5 3d_{3/2} \rightarrow 2s^2 2p^6$	$3C$	9075.7±2.5	9077.4	−1.7
$2s_{1/2}2p^6 3d_{5/2} \rightarrow 2s^2 2p^6$	$E2S$	9571.2±3.0	9575.5	−4.3

chosen the hydrogenic line Ly-α_1 and the resonance transition $1s2p\,^1P_1 \rightarrow 1s^2\,^1S_0$, line w in the notation of Gabriel,[21] of heliumlike zinc (cf. Fig. 1). The wavelength of line w was taken as 1.377 76 Å. This value of 0.000 08 Å lower than the theoretical value given by Drake[22] and 0.000 16 Å lower than the value calculated by Vainshtein and Safronova.[23] The lower value was chosen following the discussion in Ref. 24 where an analysis of measured wavelengths of heliumlike resonance lines has indicated that theoretical values for medium-Z elements such as zinc are usually too large. In particular, the analysis in Ref. 24 suggested that the wavelength of the heliumlike resonance line calculated by Drake[22] is too large by about 60 ppm while that of Vainshtein and Safronova[23] is too large by about 125 ppm.

The transition energies of lines $3A$, $3D$, and $E2S$ are listed in Table I. Due to the lower resolution of the flat-crystal spectrometer the uncertainty in the measurements is higher than for line $3A$ measured with the von Hámos spectrometer. The experimental uncertainties are between 2.5 and 3.0 eV and are mainly due to uncertainties in the dispersion and in the center position of a given line. The wavelengths of lines $3D$ and $3F$ are not given in the table, because the lines are situated far from the reference lines so that their wavelengths could not be reliably determined.

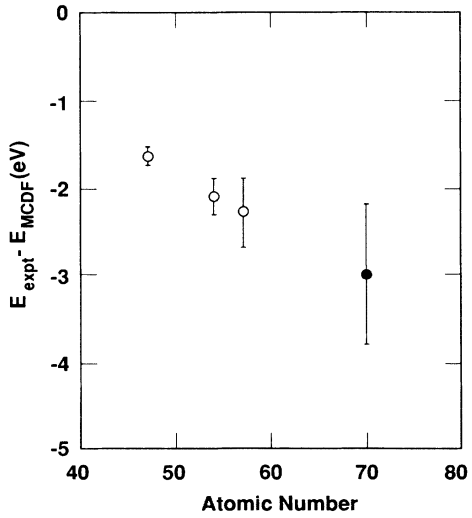

FIG. 3. Comparison of measured and theoretical transition energies of line $3A$. The solid circle represents the present result for ytterbium. The open circles are data from Ref. 6. Error bars reflect experimental uncertainties.

III. DETERMINATIONS OF THE SELF-ENERGY CONTRIBUTION

In order to obtain the self-energy contribution, we subtract the relativistic Coulomb energy E_{Coul} and the contributions from the Breit interaction E_{Breit}, vacuum polarization E_{VP} and residual correlation energy E_{corr} from the transition energy of line $3A$ measured with the von Hámos spectrometer. The value of each term is listed in Table II. All terms except E_{corr} have been calculated in the extended average level method using the MCDF code of Grant *et al.*[20] E_{corr} is comprised of the (super) Coster-Kronig fluctuation energy (−2.09 eV), which has been calculated with the Grant code in the optimal level method, and the ground-state correlation energy (+1.0 eV), which has been estimated from nonrelativistic calculations according to the procedure described in Ref. 25. The resulting value of the self-energy contribution to the transition energy of line $3A$ is −18.37±0.80 eV. (The error is solely due to experimental uncertainties and does not take into account uncertainties in the calculated energies.)

Table II lists the self-energy contribution Se_{MCDF}, calculated using the effective-charge approach as well as the self-energy contribution Se_{hydro} to the energy of a $2s$-$3p$ transition in the field of a bare ytterbium nucleus. Neither agrees with the experimental value, although they appear to provide an upper and lower bound on the size of the actual self-energy contribution. In particular, the value calculated in the effective-charge approach differs from the measured value by −1.9 eV; the hydrogenic value differs by +1.5 eV.

The transition energy of line $3A$ measured with the flat-crystal spectrometer agrees closely with that from the von Hámos spectrometer.

IV. DISCUSSION AND CONCLUSION

We have presented a measurement of the self-energy contribution to the $2s$-$3p$ resonance transition in neonlike

TABLE II. Self-energy contribution to the transition $(2s_{1/2}2p^6 3p_{3/2})_{J=1} \rightarrow (2s^2 2p^6)_{J=0}$ in Yb^{60+}. The experimental self-energy Se_{expt} is obtained by subtracting the calculated values for the relativistic Coulomb energy E_{Coul}, the transverse Breit energy E_{Breit}, the vacuum polarization energy E_{VP}, and the residual correlation energy E_{corr}, from the measured transition energy E_{expt}. Se_{MCDF} is the self-energy computed using the effective-charge approach, and Se_{hydro} is the self-energy computed assuming hydrogenic wave functions and a bare ytterbium nucleus. All values are in eV.

E_{expt}	E_{Coul}	E_{Breit}	E_{VP}	E_{corr}	Se_{expt}	Se_{MCDF}	Se_{hydro}
+9341.86	+9373.63	−15.40	+3.09	−1.09	−18.37	−16.49	−19.91

ytterbium. The measured value is 18.37±0.80 eV and is larger than the value calculated in the effective-charge approach commonly used to estimate the self-energy contributions to transition in high-Z multielectron ions. On the other hand, it is smaller than the value obtained from hydrogenic wave functions, indicating that the nuclear potential is indeed screened by a non-negligible amount.

Uncertainties in the measured value of the self-energy contribution may not only arise from experimental errors but also from uncertainties in the calculations, in particular from uncertainties in the estimation of the ground-state correlation energy. Our estimate of the ground-state correlation energy (+1.0 eV) relies on a nonrelativistic calculation for neutral zinc,[26] because no suitable relativistic (or even nonrelativistic) calculation exists for Yb^{60+}. Relativistic effects could possibly reduce the size of the ground-state correlation energy. If the ground-state correlation energy were to vanish, the difference between measured and calculated self-energy would shrink to 0.9 eV and therefore would be close to the experimental error limits. *Ab initio* calculations of the residual correlation energies are needed to address this possibility.

The effective-charge approach has yielded satisfactory results for estimating the self-energy contribution to transitions in the case of $2s$-$2p$ transitions in lithiumlike ions[27] as well as in the case of $4s$-$4p$ transitions in copperlike and zinclike ions.[28] For these cases correlation effects are either small or are fully accounted for in the calculations. On the other hand, it was shown that the effective-charge approach overcorrects the screening effect on the self-energy corrections for the $3p$-$3s$ transitions in sodiumlike ions.[29] Similarly, measurements of $2s$-$3p$ transitions in fluorinelike and neonlike ions[7,8,30] have provided a first indication that the method may not yield accurate answers for transitions involving $2s$ vacancy states. The present measurement appears to support the suggestions that the effective-charge approach underestimates self-energy contributions to transitions involving a $2s$ vacancy in neonlike ions.

Finally, we note that this is the first precision wavelength measurement for highly charged ions performed by looking into an ion source. The results demonstrate the utility of the EBIT technique for wavelength measurements.

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