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Observability of Hyperfine Structure and Lamb, Nuclear-Volume Shifts in $1snl$-$1snl'$ Transitions of Heliumlike Ions

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The hyperfine-structure widths of $1snl$–$1snl'$ transitions in heliumlike ions are estimated for $n=2,3$ and Z up to 30. Relevant parameters such as spin-orbit and electrostatic parameters are also calculated on the basis of screened hydrogenic functions. It is found that the hyperfine-structure widths are greater than 10 Å at accessible visible wavelengths in some cases. Also, absolute wavelength shifts due to Lamb and nuclear-volume effects are of the order of several angstroms.

Herzberg and Moore,[1] in studying magnetic hyperfine structure in the $1s2s$-$1s2p$ transitions of Li II, noted that it was comparable with the fine structure in some cases and could even be larger than the singlet-triplet intervals for large n and l. Such conditions present interesting varieties of coupling schemes. The observed wavelengths of these transitions are also of interest in ascertaining values of Lamb shift and volume-isotope (nuclear electric monopole) shift. The purpose of this article is to explore the importance of nuclear effects in the spectra of the most abundant isotopes of heliumlike ions up to Zn XXIX ($Z\approx30$). As Z increases, the electrons are pulled closer to the nucleus so that nucleus-electron interactions become larger, increasing as Z^3. In this respect the high-Z ions can act as nuclear probes in the same way that mesic atoms are currently used. The production of such ions is now feasible,[2,3] and we wish to note that the observability of hyperfine structure in their spectra is maximized if low-energy transitions of the type $1s2s$-$1s2p$ or $1s3l$-$1s3l'$ are studied, both because the wavelengths can fall in the visible or near-ultraviolet range and because the width of the hyperfine structure can be very large. This will apply to the odd-even or even-odd isotopes. The same transitions for isotopes which are not affected by hyperfine interaction can be useful for studies of Lamb shift and volume-isotope shift. This has also been pointed out by Accad, Pekeris, and Schiff.[4]

The $1snl$-$1snl'$ transitions have not yet been observed except in the lowest-Z atoms. Edlen and Lofstrand[5] have discussed the situation in their work on C V. Calculations of S-, P-, D-term energies have however been carried out by Weiss,[6] Sanders and Scherr,[7] Accad, Pekeris, and Schiff,[4] and Brown.[8] From the results of these workers one can obtain wavelengths accurate, in general, to within a few angstroms, which then allows us to make estimates of the nuclear effects and their observability. Well-known formulas are used here to compute the magnetic hyperfine parameter a_{1s}, spin-orbit parameters ζ_{nl}, first-order Lamb shifts $E_L(n,j)$, and the volume-isotope shifts $E_N(n,0)$, on the assumption of screened hydrogenic wave functions. The exchange electrostatic integrals $G_l(1s,nl)$ have also been computed using

TABLE I. Predicted $1snl$-$1snl'$ wavelengths and hyperfine-structure widths in heliumlike ions.

					Approximate wavelengths (Å)					Hyperfine-structure widths (Å)		
	Z	I	μ_I	a_{1s}(cm^{-1})	λ_A	λ_B	λ_C	λ_D	λ_E	$\delta\lambda_A$	$\delta\lambda_C$	$\delta\lambda_E$
B^{11} IV	5	$\frac{3}{2}$	2.688	1.90	2815	15 470	10 520	71 200	22 500	0.15	2.1	9.6
N^{14} VI	7	$\frac{1}{2}$	−0.283	1.18	1890	9 870	6 960	42 800	13 800	0.043	0.57	2.2
F^{19} VIII	9	$\frac{1}{2}$	+2.629	32.5	1410	7 080	5 120	30 400	9 920	0.67	8.5	32
Na^{23} X	11	$\frac{3}{2}$	+2.218	16.7	1170	5 380	3 960	23 800	7 750	0.22	2.6	10
Al^{27} XII	13	$\frac{5}{2}$	3.639	27.1	982	4 230	3 150	19 500	6 350	0.26	2.7	11
P^{31} XIV	15	$\frac{1}{2}$	+1.132	64.9	844	3 390	2 550	16 500	5 380	0.46	4.2	19
Cl^{36} XVI	17	$\frac{3}{2}$	+0.822	22.9	740	2 750	2 090	14 300	4 670	0.13	1.0	5.0
K^{39} XVIII	19	$\frac{3}{2}$	+0.391	15.2	659	2 250	1 730	12 700	4 120	0.066	0.45	2.6
Sc^{45} XX	21	$\frac{7}{2}$	+4.756	107	594	1 860	1 440	11 300	3 690	0.38	2.2	15
V^{51} XXII	23	$\frac{7}{2}$	+5.148	152	541	1 550	1 210	10 300	3 340	0.44	2.2	17

screened hydrogenic functions, with the help of a computer program developed previously.[9] Knowledge of the relative values of these various parameters is important for evaluation of the probable coupling scheme in a given case.

Table I, assembled for the abundant isotopes, lists wavelengths and parameters for the following transitions:

A: $1s2s(^3S)$-$1s2p(^3P)$,

B: $1s3s(^1S)$-$1s3p(^1P)$,

C: $1s3s(^3S)$-$1s3p(^3P)$,

D: $1s3p(^1P)$-$1s3d(^1D)$,

E: $1s3p(^3P)$-$1s3d(^3D)$.

The wavelengths of transitions A are obtained with the use of the Z-expansion coefficients of Ref. 7; the wavelengths of transitions D and E are obtained by using the results of Refs. 7 and 8; and the wavelengths of transitions B and C were obtained by using the results of Ref. 4, together with a polynomial extrapolation. These wavelengths are approximate inasmuch as relativistic and radiative corrections are not included, but are adequate to specify the spectral range of interest. Table I also lists the magnetic hyperfine parameter a_{1s}, computed from Kopfermann's[10] expressions (25)–(28), and the resulting hyperfine-structure widths $\delta\lambda$ expected in transitions A, C, and E. The singlet transitions B and D have no hyperfine splitting if LS coupling holds. It is seen that $\delta\lambda$ reaches striking values of about 8 Å for transition C of F VIII at ≈5120 Å, and even 19 Å for transition E of P XIV at ≈5380 Å, lying in the accessible visible region. Observation of these very wide hyperfine structures should prove extremely interesting for the study of nuclear-electronic interactions. The calculated strengths of transitions B, C, D, and E are greater than that of (observed) transition A (Weiss,[6] Schiff *et al.*[11]) so that they should be readily observable. In more detail, predicted hyperfine patterns for F VIII and Al XII are illustrated in Fig. 1.

Table II lists, for the same ions, hydrogenically calculated spin-orbit interaction parameters ζ_{nl}

TABLE II. Hyperfine parameter, spin-orbit parameters, and Coulomb exchange integrals (cm^{-1}).

	a_{1s}	ζ_{2p}	ζ_{3p}	ζ_{3d}	$G_0(1s,2s)$	$G_1(1s,2p)$	$G_0(1s,3s)$	$G_1(1s,3p)$	$G_2(1s,3d)$
Li^7 II	0.498	5.3	1.6	0.24	4 000	3 400	980	1 000	21
Be^9 III	0.426	24	7.5	1.2	8 400	6 900	2 150	2 000	52
B^{11} IV	1.90	73	23	3.7	13 000	10 500	3 400	3 000	90
N^{14} VI	1.18	350	110	19	22 500	18 000	5 900	4 900	180
F^{19} VIII	32.5	1 100	350	59	32 000	25 500	8 500	6 900	280
Na^{23} X	16.7	2 600	850	145	42 000	33 000	11 000	8 900	380
Al^{27} XII	27.1	5 300	1 800	300	51 000	40 500	13 500	11 000	480
P^{31} XIV	64.9	9 800	3 200	560	61 000	48 000	16 000	13 000	580
Cl^{35} XVI	22.9	17 000	5 500	950	70 500	55 500	19 000	15 000	690
K^{39} XVIII	15.2	26 000	8 800	1500	75 000	59 000	20 000	16 000	740
Sc^{45} XX	107	40 000	13 000	2300	90 000	70 500	24 000	19 000	900
V^{51} XXII	152	59 000	20 000	3400	99 500	78 000	26 000	21 000	1000
Mn^{55} XXIV	184	83 000	28 000	4800	110 000	85 500	29 000	23 000	1100
Co^{59} XXVI	219	110 000	38 000	6600	120 000	93 000	31 000	25 000	1200
Cu^{63} XXVIII	308	150 000	51 000	8900	130 000	100 000	34 000	27 000	1300

TABLE III. ^3L-^1L intervals (cm^{-1}) in C v.

	$1s2s$	$1s2p$	$1s3s$	$1s3p$	$1s3d$
$2G_l(1s,nl)$	35 500	28 400	9 300	7910	266
Observed	43 760	28 150	11 600	7960	219

and the electrostatic exchange integrals $G_l(1s, nl)$. Fine structure has been calculated very accurately by Accad *et al.*[4] for the $1snp$ configurations, for Z up to 10. The present values of ζ_{nl}, though approximate, give an idea of the order of magnitude of the $1s2p$, $1s3p$, and $1s3d$ fine-structure splitting through higher Z. Their accuracy improves for higher Z. We can compare the value of 1853 cm^{-1} predicted by Accad *et al.* for the interval $1s2p(^3P_2$-$^3P_0)$ of F VIII, which should approach $\frac{3}{2}\zeta_{nl}$ as Z increases, with the entry in Table I which yields 1650 cm^{-1}.

One can say, for example, that the hyperfine interaction is of the same order of magnitude as the fine structure of the $1s3d(^3D)$ term in F VIII, as Herzberg and Moore observed for higher terms in Li II. On the other hand, for still larger Z, the $1snl$ configurations begin to approach jj coupling, with a_{1s} being smaller than either ζ_{nl} or $G_l(1s, nl)$, so that the theoretical interpretation will be simplified.

The values of $G_l(1s, nl)$ are useful for predicting the singlet-triplet separations which are just $2G_l(1s, nl)$ in LS coupling. The values given here are compared with observation[5] in the case of C v, in Table III.

The binding energies of $1s$ and $2s$ electrons are decreased by the Lamb shift and also by the effect of the finite nuclear size (volume-isotope shift). Relativistic p wave functions also possess nonzero Lamb shifts because of their finite probability at the nucleus. Since the electron wave functions become more hydrogenic with increasing Z it is a reasonable approximation to add together the separately calculated shifts of the two electrons in heliumlike ions. Table IV, listing the abundant odd-odd and even-even isotopes that do not possess magnetic hyperfine structure, gives values of first-order Lamb shifts $E_L(n, j)$ and volume-isotope shifts $E_N(n, 0)$ as calculated from the expressions given by Garcia and Mack[12] or Bethe and Salpeter.[13] The net shift in the energy of the transition $1s2s(^3S_1)$-$1s2p(^3P_1)$ for example, with respect to uncorrected relativistic values, is $\Delta E = E_L(2s) - E_L(2p_{1/2}) + E_N(2s)$. This quantity is given in Table IV as a wavelength shift to show how sizable it is. The given shifts for C v and O VII agree reasonably with the Lamb shifts ($\lambda_{theor} - \lambda_{tot}$) in Table XXIX of Ref. 4. The shifts will be still larger for some of the $1s3l$-$1s3l'$ transitions. It may be noted here that the singlet transitions, which as mentioned above, have little or no hyperfine splitting depending on the coupling, will be most useful for studies of these shifts in the odd isotopes.

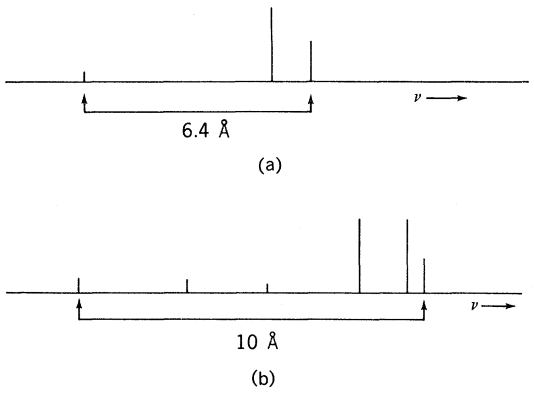

FIG. 1. Predicted hyperfine patterns: (a) transition C, $1s3s(^3S_1)$-$1s3p(^3P_2)$ in F VIII; (b) transition E, $1s3p(^3P_2)$-$1s3d(^3D_3)$ in Al XII.

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TABLE IV. Lamb and volume-isotope shifts (cm^{-1}); wavelength shift in $1s2s\,(^3S)$-$1s2p\,(^3P)$ transition.

	Z	$E_L(2,0)$	$E_L(2,\frac{1}{2})$	$E_L(2,\frac{3}{2})$	$E_N(2,0)$	λ_A(Å)	$\Delta\lambda_A$(Å)
C v	6	24	−0.56	0.54	0.05	2279	1.21
O VII	8	65	−1.76	1.71	0.20	1638	1.70
Ne IX	10	138	−4.30	4.19	0.53	1272	2.17
Mg XI	12	252	−8.91	8.68	1.20	1031	2.61
Si XIII	14	414	−16.5	16.1	2.32	858	2.95
S XV	16	628	−28.2	27.4	4.38	726	3.19
A XVII	18	893	−45.1	43.9	7.47	620	3.30
Ca XIX	20	1210	−68.8	66.9	13.0	533	3.27
Ti XXI	22	1630	−101	98.1	19.5	460	3.15
Cr XXIII	24	1960	−143	139	29.0	397	2.92
Fe XXV	26	2370	−196	191	42.0	344	2.62
Ni XXVII	28	2770	−264	257	58.3	297	2.17
Zn XXIX	30	3150	−348	339	80.5	257	1.91

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Algebraic 1 Matrices and Radial Momentum Distributions from Hylleraas-Type Wave Functions. ^1S Ground States of He and He-Like Ions*

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Spin-free 1 matrices $\gamma(\vec{r}\,|\,\vec{r}\,')$'s are obtained in algebraic form from simple Hylleraas-type (HY) wave functions for the ^1S ground states of He and several He-like ions. The algebraic $\gamma(\vec{r}\,|\,\vec{r}\,')$'s are then Fourier transformed to momentum space in order to obtain radial momentum distributions $I_0(p)$'s. The analytical method developed here allows $I_0(p)$'s to be calculated in a direct manner from HY wave functions. Although the present emphasis is on the method rather than on the "goodness" of individual $I_0(p)$'s, results for the ^1S He and Li^+ ground states are obtained from six-term HY functions which incorporate 99.1 and 98.0%, respectively, of the correlation energy.

I. INTRODUCTION

The purpose of this paper is to develop an analytical method for evaluating radial momentum distributions from two-electron Hylleraas-type (HY) wave functions $\Psi(r_1, r_2, r_{12})$'s. This is accomplished by obtaining the corresponding (spin-free) first-order density matrix[1] $\gamma(\vec{r}\,|\,\vec{r}\,')$ in algebraic form. Then, $\gamma(\vec{r}\,|\,\vec{r}\,')$ is Fourier transformed to momentum space, as described by Benesch and Smith,[2] in order to obtain the radial momentum distribution $I_0(p)$. A secondary purpose of this paper is to apply the analysis to relatively simple (two-, three-, and six-term) HY functions for the ^1S ground states of He and He-like ions.

The extension of the algebraic density matrix method to N-electron HY and configuration interaction (CI) wave functions is pointed out in Sec. II. The problem of Fourier transforming a $\gamma(\vec{r}\,|\,\vec{r}\,')$ which explicitly contains angular functions is briefly discussed in Sec. III.

We stress here that the Fourier transformation of the algebraic 1 matrix will yield $I_0(p)$ to exactly the same accuracy with which the original HY function was determined.[3] This is to be contrasted with the Fourier transformation of the natural orbital (NO) expansion of $\gamma(\vec{r}\,|\,\vec{r}\,')$. Although the Fourier transformation of the NO's is accomplished exactly,[3] the NO expansion of a $\gamma(\vec{r}\,|\,\vec{r}\,')$ obtained from a HY function is necessarily truncated due to the problem of choosing a suitable *finite* basis set for expanding the NO's. In practice, this truncation error is very small. However, the determination of $\gamma(\vec{r}\,|\,\vec{r}\,')$ in algebraic form from a HY function eliminates the need for the NO expansion. The resulting $I_0(p)$ therefore does not incorporate *any* truncation error.

II. ALGEBRAIC EVALUATION OF $\gamma(\vec{r}\,|\,\vec{r}\,')$ FROM TWO-ELECTRON HY FUNCTIONS

As previously shown,[2] the radial momentum distribution $I_0(p)$ is obtained by Fourier transformation of the spin-free 1 matrix $\gamma(\vec{r}\,|\,\vec{r}\,')$ derived from a normalized N-electron wave function Ψ, namely,

$$I_0(p) = p^2 \int_0^{2\pi} \int_0^{\pi} \hat{\gamma}(\vec{p}\,|\,\vec{p}) \sin\alpha \, d\alpha \, d\beta$$

$$= p^2 \, \hat{\gamma}_0(p\,|\,p) \, . \qquad (1)$$

The *diagonal* momentum-space 1 matrix is given[2] by