QED Corrections of $O(mc^2\alpha^7 \ln \alpha)$ to the Fine Structure Splittings of Helium and He-like Ions

Tao Zhang,[1] Zong-Chao Yan,[2] and G. W. F. Drake[1]
[1]*Department of Physics, University of Windsor, Windsor, Ontario, Canada N9B 3P4*
[2]*ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138*
(Received 1 February 1995; revised manuscript received 12 June 1996)

A reformulation of the external potential Bethe-Salpeter formalism is developed for two-electron atoms. QED and relativistic corrections to energy levels of order $\alpha^7 mc^2 \ln \alpha$ are derived and expressed in terms of expectation values of nonrelativistic operators. Corrections of order $\alpha^7 mc^2$ from exchange diagrams are also found. The total contributions of order $\alpha^7 mc^2 \ln \alpha$ to the $1s2p\,^3P_J$ fine structure intervals of helium are $\Delta\nu_{01} = 82.6$ kHz and $\Delta\nu_{12} = -10.0$ kHz. Results are given for He-like ions up to $Z = 12$ and compared with experiment. [S0031-9007(96)00908-8]

PACS numbers: 31.15.Ar, 31.30.Jv

Over the past two decades, much theoretical progress has been made in understanding higher-order QED effects in one- or two-body bound systems such as hydrogen, positronium, and muonium. In contrast, since Douglas and Kroll [1] derived the $O(\alpha^6 mc^2)$ QED and relativistic corrections to fine structure in helium, little theoretical progress in higher-order analysis has been made. This is partially because the nonrelativistic wave function of helium is not known analytically. However, the development of highly accurate nonrelativistic wave functions [2,3] makes possible high-precision tests of higher-order QED and relativistic effects in helium. On the other hand, past and recent experiments for helium [4,5] have achieved very high precision sensitive to higher-order QED and relativistic effects beyond the Douglas and Kroll terms, provided that all lower-order corrections are known sufficiently accurately. A recent measurement in N^{5+} [6] is particularly interesting because in this case the lowest-order contributions nearly cancel. A previous Letter [7] presented high-precision calculations for the fine structure splittings of the $1s2p\,^3P_J$ states in helium and helium-like ions, including all terms up to $O(\alpha^6 mc^2)$ (or α^4 a.u.). However, the results differ by up to 96 kHz from a recent measurement of the splittings, accurate to ± 3 kHz [5].

In this Letter, we present calculations of corrections beyond the Douglas and Kroll terms. We reformulate the external potential Bethe-Salpeter theory for two-electron atoms in an initially covariant form. A time-ordered formulation obtained by expressing the electron propagators in terms of positive- and negative-energy projection operators is used for the $O(\alpha^7 mc^2)$ fine structure calculation. Our time-ordered formalism is different from that of Sucher [8] and is more suitable for calculation of corrections arising from the relativistic momentum region. The main difference is in the calculation of the relativisitic contributions. Using our formulas, we derive QED and relativistic corrections expressed in terms of expectation values of nonrelativistic operators. A higher-order cancellation of infrared logarithmic terms takes place in the corrections of the electron-electron type. This infrared cancellation is unique in multielectron atoms and leads to a simple one-electron term which reproduces the spin-dependent part of the one-electron Lamb shift of $O(\alpha^7 \ln(Z\alpha)^{-2} mc^2)$ [9]. All electron-electron logarithmic corrections are of ultraviolet origin, arising from both the relativistic and nonrelativistic momentum regions. A test of the off-leading-order contributions from the relativistic momentum region has never been carried out in any one- or two-body bound system due to insufficient experimental accuracy.

The time-ordered diagrams contributing to the fine structure splittings of helium up to order $\alpha^7 mc^2 \ln \alpha$ are shown in Fig. 1. They represent the no-pair single transverse photon diagrams 1a and 1b, and the one-pair single (2a–2d)

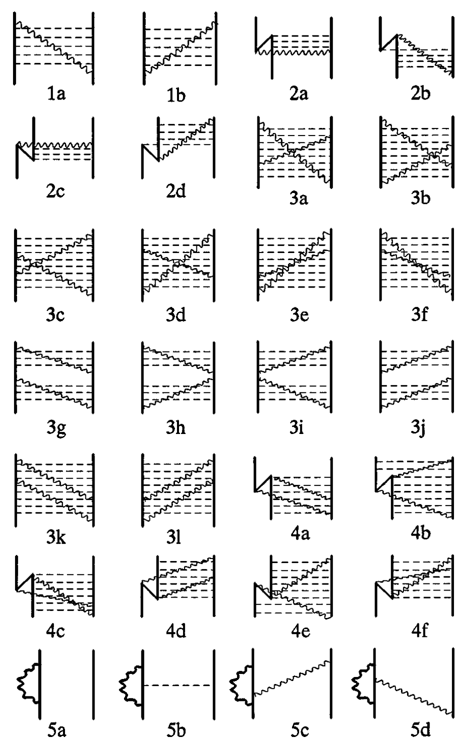

FIG. 1. Time-ordered diagrams contributing to the fine structure splittings of helium to order $\alpha^7 mc^2$. The curved wavy lines denote covariant photons, the straight wavy lines transverse photons, and the dashed lines instantaneous Coulomb photons.

0031-9007/96/77(9)/1715(4)$10.00

and double (4a–4f) transverse photon diagrams, as well as the no-pair double transverse photon diagrams (3a–3l). In addition, two-pair single and double transverse photon diagrams contribute. The derivation of corrections from exchange diagrams in a nonrelativistic approximation is given in Ref. [10]. The contributions of $O(\alpha^7 mc^2 \ln\alpha)$ from the radiative diagrams are derived and expressed in terms of expectation values of nonrelativistic operators, and presented in Ref. [11]. The results are expressed here in atomic units, with $\alpha^7 mc^2 = \alpha^5$ a.u.

The total logarithmic contributions are found to be [10]

$$\Delta E_{\mathrm{so},Z} = -2Z\alpha^5 \ln(Z\alpha)^{-2} \times \langle\phi_0|\delta(\mathbf{r}_1)\frac{1}{r_1^2}\boldsymbol{\sigma}_1\cdot(\mathbf{r}_1\times\mathbf{p}_1)|\phi_0\rangle, \tag{1}$$

$$\Delta E_{\mathrm{so},e} = -9\alpha^5 \ln\alpha\langle\phi_0|\delta(\mathbf{r})\frac{1}{r^2}\boldsymbol{\sigma}_1\cdot(\mathbf{r}\times\mathbf{p}_1)|\phi_0\rangle, \tag{2}$$

$$\Delta E_{\mathrm{ss}} = \frac{15}{2}\alpha^5 \ln\alpha\langle\phi_0|\delta(\mathbf{r})\frac{1}{r^2}\boldsymbol{\sigma}_1\cdot\hat{\mathbf{r}}\boldsymbol{\sigma}_2\cdot\hat{\mathbf{r}}|\phi_0\rangle. \tag{3}$$

These terms are obtained as follows. The nonrelativistic contribution of order α^5 a.u. from exchange diagrams plus the logarithmic correction from radiative diagrams is found to be [10]

$$\Delta E = \alpha^5\left[9\left(\frac{R_{\mathrm{so}}}{4\pi} + L_{\mathrm{so}}\right) - \frac{15}{2}\left(\frac{R_{\mathrm{ss}}}{4\pi} + L_{\mathrm{ss}}\right)\right] + \alpha^5\langle\phi_0|O_{\mathrm{so}} + O_{\mathrm{ss}}|\phi_0\rangle, \tag{4}$$

where

$$O_{\mathrm{so}} = -2Z\ln(Z\alpha)^{-2}\frac{\delta(\mathbf{r}_1)}{r_1^2}\boldsymbol{\sigma}_1\cdot\mathbf{r}_1\times\mathbf{p}_1 - (9\ln\alpha + 3\ln B - 9\ln 2 + \tfrac{221}{12})\frac{\delta(\mathbf{r})}{r^2}\boldsymbol{\sigma}_1\cdot\mathbf{r}\times\mathbf{p}_1 + \frac{8i}{9}\delta(\mathbf{r})\boldsymbol{\sigma}_1\cdot[\hat{\mathbf{r}}\times(\hat{\mathbf{r}}\cdot\mathbf{p}_1)\mathbf{p}_2], \tag{5}$$

$$O_{\mathrm{ss}} = (\tfrac{15}{2}\ln\alpha - \tfrac{35}{2}\ln B - \tfrac{9}{2}\ln 2 - \tfrac{1555}{96})\frac{\delta(\mathbf{r})}{r^2}\boldsymbol{\sigma}_1\cdot\hat{\mathbf{r}}\boldsymbol{\sigma}_2\cdot\hat{\mathbf{r}} + \frac{2i}{9}\frac{\partial(\mathbf{r})}{r^2}\boldsymbol{\sigma}_1\cdot\hat{\mathbf{r}}(\boldsymbol{\sigma}_2 - 3\boldsymbol{\sigma}_2\cdot\hat{\mathbf{r}}\hat{\mathbf{r}})\cdot\mathbf{p}_1. \tag{6}$$

Here, B is an ultraviolet cutoff which cancels from the final result, and the nonlogarithmic terms R_{so}, L_{so}, etc. are analagous to the Feinberg-Sucher terms of $O(\alpha^3)$ a.u. [8,12], as defined in Ref. [10]. They are included for completeness, but they do not contribute to terms proportional to $\ln\alpha$. The relativistic contribution is

$$\Delta E = \alpha^5\langle\phi_0|I_{\mathrm{so}}\frac{\delta(\mathbf{r})}{r^2}\boldsymbol{\sigma}_1\cdot(\mathbf{r}\times\mathbf{p}_1) + I_{\mathrm{ss}}\frac{\delta(\mathbf{r})}{r^2}\boldsymbol{\sigma}_1\cdot\hat{\mathbf{r}}\boldsymbol{\sigma}_2\cdot\hat{\mathbf{r}}|\phi_0\rangle, \tag{7}$$

where

$$I_{\mathrm{so}} = -\frac{3}{4}\pi - \frac{11}{3} + 3\ln B + 3\ln 2, \tag{8}$$

$$I_{\mathrm{ss}} = -\frac{5}{2}\pi - \frac{80}{3} + \frac{27}{2}\ln 2 + \frac{35}{2}\ln B. \tag{9}$$

The correctness of the ultraviolet logarithmic contributions is checked by fourteen individual cancellations and two overall cancellations of spin-orbit and spin-spin logarithmic cutoff terms between contributions arising from the nonrelativistic momentum region and contributions from the relativistic momentum region. The total exchange correction plus the logarithmic QED contribution becomes

$$\Delta E = \alpha^5\left[9\left(\frac{R_{\mathrm{so}}}{4\pi} + L_{\mathrm{so}}\right) - \frac{15}{2}\left(\frac{R_{\mathrm{ss}}}{4\pi} + L_{\mathrm{ss}}\right)\right] + \alpha^5\langle\phi_0|O_{\mathrm{so}} + O_{\mathrm{ss}}|\phi_0\rangle, \tag{10}$$

where

$$O_{\mathrm{so}} = -2Z\ln(Z\alpha)^{-2}\frac{\delta(\mathbf{r}_1)}{r_1^2}\boldsymbol{\sigma}_1\cdot(\mathbf{r}_1\times\mathbf{p}_1) + (12\ln 2 - 9\ln\alpha - \tfrac{265}{12} - \tfrac{3}{4}\pi)\frac{\delta(\mathbf{r})}{r^2}\boldsymbol{\sigma}_1\cdot(\mathbf{r}\times\mathbf{p}_1) + \frac{8i}{9}\delta(\mathbf{r})\boldsymbol{\sigma}_1\cdot[\hat{\mathbf{r}}\times(\hat{\mathbf{r}}\cdot\mathbf{p}_1)\mathbf{p}_2], \tag{11}$$

$$O_{\mathrm{ss}} = (\tfrac{15}{2}\ln\alpha - \tfrac{5}{2}\pi + 9\ln 2 - \tfrac{4115}{96})\frac{\delta(\mathbf{r})}{r^2}\boldsymbol{\sigma}_1\cdot\hat{\mathbf{r}}\boldsymbol{\sigma}_2\cdot\hat{\mathbf{r}} + \frac{2i}{9}\frac{\delta(\mathbf{r})}{r^2}\boldsymbol{\sigma}_1\cdot\hat{\mathbf{r}}(\boldsymbol{\sigma}_2 - 3\boldsymbol{\sigma}_2\cdot\hat{\mathbf{r}}\hat{\mathbf{r}})\cdot\mathbf{p}_1. \tag{12}$$

Collecting the logarithmic terms in Eqs. (4)–(12) then gives Eqs. (1)–(3).

In addition to the above, there is also a second-order perturbation correction from diagrams 5b–5d which can be interpreted as a spin-dependent Breit correction to the electron charge density at the nucleus in the standard expression for the Lamb shift. The logarithmic part is thus

$$\Delta E^{(2)} = \frac{4Z\alpha^5 mc^2}{3}\ln(Z\alpha)^{-2}[\langle\phi_0|\delta(\mathbf{r}_1) + \delta(\mathbf{r}_2)|\phi_1\rangle + \langle\phi_1|\delta(\mathbf{r}_1) + \delta(\mathbf{r}_2)|\phi_0\rangle], \tag{13}$$

where ϕ_1 is the perturbed wave function induced by electron-electron spin-orbit and spin-spin terms $H_{\mathrm{so},e}$ and H_{ss}, and electron-nucleus spin-orbit term $H_{\mathrm{so},Z}$ in the nonrelativistic Breit interaction. It therefore satisfies the perturbation equation

$$(H_0 - E_0)\phi_1 + (H_{\text{so},e} + H_{\text{so},Z} + H_{\text{ss}})\phi_0 = E_1\phi_0 . \tag{14}$$

The calculation of a corresponding second-order Breit term was described in Ref. [7]. Although $\Delta E^{(2)}$ nominally scales as $Z^6 \ln(Z\alpha)^{-2}$, it vanishes in a one-electron approximation, and so the leading Z dependence is $Z^5 \ln(Z\alpha)^{-2}$. Numerical values of $\Delta E^{(2)}$, ΔE_{so}, and ΔE_{ss} were calculated using correlated variational basis sets [2,7].

The various contributions for ions up to $Z = 12$ are listed in Table I. It is significant that there is a strong cancellation between the electron-nucleus term $\Delta E_{\text{so},Z}$ in column 5 and the remaining $\Delta E_{\text{so},e} + \Delta E_{\text{ss}} + \Delta E^{(2)}$ terms in column 6, even though the former nominally increases more rapidly with Z, and eventually becomes dominant. Because of this cancellation, the net change due to the $\alpha^5 \ln(Z\alpha)^{-2}$ a.u. and $\alpha^5 \ln\alpha$ a.u. terms is relatively small for Z in the range $5 \le Z \le 10$ from those given previously [7]. However, these terms combine with the same sign in the case of the helium ν_{01} interval to produce a net shift of 82.6 kHz, and bring the predicted splitting into much better agreement with the measurement of Shiner *et al.* [5]. Table II gives a more detailed listing for this case. For $5 \le Z \le 9$, the predicted splittings agree with the relativistic configuration interaction (CI) calculations of Chen *et al.* [17] to within the ± 0.02 cm^{-1} accuracy of their tabulation. Their results include only the asymptotically dominant $\Delta E_{\text{so},Z}$ part of the $O(\alpha^5 \ln(Z\alpha)^{-2})$ a.u. terms, calculated in a hydrogenic approximation, through their use of QED shifts from Ref. [18].

The comparison with experiment is summarized in Table III. The results are numerically accurate to the figures quoted, with uncertainties estimated from the known terms of pure order α^5 a.u. and $\alpha^4 m/M$ a.u. not included in the calculation. The total additional contributions for helium of 82.6 kHz for ν_{01} and -10.0 kHz for ν_{12} leave residual discrepancies with experiment of -13.2 and 6.4 kHz, respectively, which is less than the estimated uncertainty. The only significant discrepancy is for the case of Be^{2+}, where the difference between theory and experiment for ν_{12} is 0.0026(4) cm^{-1}. In the case of N^{5+}, 30% of the total for ν_{01} comes from the Douglas-Kroll and second-order terms of order α^4 a.u., and 0.12% from the electron-electron terms of order $\alpha^5 \ln\alpha$ a.u. (column 6 of Table I).

In summary, we have obtained the QED and relativistic corrections of order $\alpha^5 \ln\alpha$ a.u. contributing to the fine

TABLE I. Contributions to the ν_{01} and ν_{12} fine structure intervals for the $1s2p\,^3P_J$ states of He-like ions (in units of Z^4 MHz). The leading Z dependence of the terms in each column is as indicated, and $\alpha^{-1} = 137.035\,9895$.

Z	$Z^4\alpha^2$	$Z^4\alpha^3$	$Z^6\alpha^4$	$Z^6\alpha^5 \ln(Z\alpha)^{-2}$ [a]	$Z^5\alpha^5 \ln\alpha$ [b]	Total
			ν_{01}			
2	1847.735 62	3.419 00	−0.100 48	0.001 99	0.003 18	1851.059 30
3	1917.794 25	3.249 78	1.230 25	0.010 17	−0.020 44	1922.264 01
4	1346.965 54	1.943 84	4.566 97	0.023 56	−0.050 75	1353.449 17
5	765.885 68	0.685 51	10.374 54	0.041 31	−0.080 46	776.906 58
6	270.387 76	−0.367 57	19.266 64	0.062 87	−0.108 31	289.241 40
7	−139.085 60	−1.229 55	31.908 82	0.087 80	−0.134 13	−108.452 67
8	−477.534 53	−1.937 91	48.988 58	0.115 75	−0.158 05	−430.526 17
9	−759.770 50	−2.526 32	71.204 02	0.146 44	−0.180 27	−691.126 63
10	−997.723 40	−3.021 03	99.257 05	0.179 62	−0.200 91	−901.508 67
11	−1200.570 21	−3.441 85	133.854 60	0.215 06	−0.220 16	−1070.162 55
12	−1375.269 14	−3.803 69	175.702 84	0.252 58	−0.238 06	−1203.355 48
			ν_{12}			
2	145.015 11	−1.409 06	−0.406 65	0.003 98	−0.004 61	143.198 77
3	−767.519 17	−4.192 63	−2.094 85	0.020 35	−0.033 56	−773.819 85
4	−1731.624 75	−6.392 08	−5.956 57	0.047 12	−0.068 66	−1743.994 93
5	−2505.214 48	−8.006 17	−12.768 28	0.082 63	−0.103 97	−2526.010 27
6	−3108.938 46	−9.212 76	−23.278 40	0.125 73	−0.138 22	−3141.442 10
7	−3585.336 88	−10.141 05	−38.172 46	0.175 59	−0.171 16	−3633.645 95
8	−3968.098 87	−10.874 55	−58.182 60	0.231 50	−0.202 74	−4037.127 26
9	−4281.239 48	−11.467 57	−84.021 01	0.292 88	−0.233 11	−4376.668 28
10	−4541.615 69	−11.956 35	−116.402 21	0.359 24	−0.262 28	−4669.877 29
11	−4761.286 41	−12.365 90	−156.036 40	0.430 13	−0.290 45	−4929.549 02
12	−4948.930 90	−12.713 85	−203.638 96	0.505 16	−0.317 54	−5165.096 09

[a] $\Delta E_{\text{so},Z}$.
[b] $\Delta E_{\text{so},e} + \Delta E_{\text{ss}} + \Delta E^{(2)}$.

TABLE II. Detailed listing of contributions to the fine structure intervals of helium. Units are MHz.

Term	ν_{01}	ν_{12}
α^2	29 564.600 02	2317.232 22
$\alpha^2\mu/M$	$-0.830\,97$	3.009 64
$\alpha^2(\mu/M)^2$	0.000 80	$-0.000\,08$
α^3	54.707 87	$-22.548\,22$
$\alpha^3\mu/M$	$-0.003\,82$	0.003 21
α^4 Douglas-Kroll	$-3.335\,19(3)$	1.533 93(5)
α^4 2nd order	1.727 52(15)	$-8.040\,29(29)$
$\alpha^5\ln(Z\alpha)^{-2}$ and $\alpha^5\ln\alpha$		
$\Delta E_{\mathrm{so},Z}$	0.031 82	0.063 64
$\Delta E_{\mathrm{so},e}$	$-0.011\,09$	$-0.022\,19$
ΔE_{ss}	0.019 36	$-0.007\,74$
$\Delta E^{(2)}$	0.042 50	$-0.043\,80$
Total	29 616.948 83(15)	2291.180 33(30)

structure splittings of helium and He-like ions. The results are valid in the low to intermediate range of nuclear charge where an expansion in powers of $Z\alpha$ converges sufficiently rapidly. The comparison with experiment for helium now shows better agreement with the recent measurement of Shiner *et al.* [5] than with the older measurement of Hughes *et al.* [4], especially for the ν_{01} interval. The terms remaining to be calculated are those of order α^5 a.u. and $\alpha^4(m/M)$ a.u. A complete evaluation of these will reduce the theoretical uncertainty for helium to less than 1 kHz, and allow a determination of the fine structure constant to an accuracy of 1.6 parts in 10^8 from a comparison with experiment.

The Natural Sciences and Engineering Research Council of Canada is acknowledged for financial support.

TABLE III. Comparison of theoretical and experimental fine structure intervals for the $1s2p\,^3P_J$ states. Units are MHz for He and Li^+, and cm^{-1} for the others. Theoretical uncertainties are due entirely to terms of $O(\alpha^5)$ a.u. not yet calculated.

Interval		Present work	Experiment	Ref.
He	ν_{01}	29 616.949(15)	29 616.962(3)	[5]
			29 616.844(21)	[4]
	ν_{12}	2291.180(12)	2291.174(3)	[5]
			2291.196(5)	[4]
Li^+	ν_{01}	155 703.4(1.5)	155 704.27(66)	[13]
	ν_{12}	$-62\,679.4(0.5)$	$-62\,678.41(66)$	[13]
Be^{2+}	ν_{01}	11.557 43(60)	11.5586(5)	[14]
	ν_{12}	$-14.892\,39(20)$	$-14.8950(4)$	[14]
B^{3+}	ν_{01}	16.1968(20)	16.203(18)	[15]
	ν_{12}	$-52.6617(10)$	$-52.660(16)$	[15]
N^{5+}	ν_{01}	$-8.686(20)$	$-8.6709(10)$	[6]
	ν_{12}	$-291.014(15)$		
F^{7+}	ν_{01}	$-151.254(90)$		
	ν_{12}	$-957.840(80)$	$-957.883(19)$	[16]

[1] M. Douglas and N.M. Kroll, Ann. Phys. (N.Y.) **82**, 89 (1974); M. Douglas, Ph.D. thesis, University of California, 1971 (unpublished).
[2] G.W.F. Drake and Z.-C. Yan, Phys. Rev. A **46**, 2378 (1992).
[3] J. Baker, D.E. Freund, R.N. Hill, and J.D. Morgan, III, Phys. Rev. A **41**, 1247 (1990).
[4] S.A. Lewis, F.M.J. Pichanick, and V.M. Hughes, Phys. Rev. A **2**, 86 (1970); W. Frieze, E.A. Hinds, V.W. Hughes, and F.M.J. Pichanick, Phys. Rev. A **24**, 279 (1981).
[5] D. Shiner, R. Dixson, and P. Zhao, Phys. Rev. Lett. **72**, 1802 (1994); R. Dixson and D. Shiner, Bull. Am. Phys. Soc. **39**, 2, 1059, (1994).
[6] E.G. Myers, D.J.H. Howie, J.K. Thompson, and J.D. Silver, Phys. Rev. Lett. **76**, 4899 (1996).
[7] Z.-C. Yan and G.W.F. Drake, Phys. Rev. Lett. **74**, 4791 (1995).
[8] J. Sucher, Phys. Rev. **109**, 1010 (1957); Ph.D. thesis, Colombia University, 1958 (unpublished).
[9] G.W. Erickson and D.R. Yennie, Ann. Phys. (N.Y.) **35**, 271, 447 (1965); G.W.F. Drake, Adv. At. Mol. Phys. **18**, 399 (1982).
[10] T. Zhang, Phys. Rev. A **54**, 1252 (1996).
[11] T. Zhang, Phys. Rev. A **53**, 3896 (1996).
[12] H. Araki, Prog. Theor. Phys. **17**, 619 (1957).
[13] E. Riis, A.G. Sinclair, O. Poulsen, G.W.F. Drake, W.R.C. Rowley, and A.P. Levick, Phys. Rev. A **49**, 207 (1994).
[14] T.J. Scholl, R. Cameron, S.D. Rosner, L. Zhang, and R.A. Holt, Phys. Rev. Lett. **71**, 2188 (1993).
[15] T.P. Dinneen, N. Berrah-Mansour, H.G. Berry, L. Young, and R.C. Pardo, Phys. Rev. Lett. **66**, 2859 (1991).
[16] E.G. Myers, P. Kuske, H.J. Andrä, I.A. Armour, N.A. Jelley, H.A. Klein, J.D. Silver, and E. Träbert, Phys. Rev. Lett. **47**, 87 (1981); E.G. Myers, Nucl. Instrum. Methods Phys. Res., Sect. B **9**, 662 (1985).
[17] M.H. Chen, K.T. Cheng, and W.R. Johnson, Phys. Rev. A **47**, 3692 (1993); D.R. Plante, W.R. Johnson, and J. Sapirstein, Phys. Rev. A **49**, 3519 (1994).
[18] G.W.F. Drake, Can. J. Phys. **66**, 586 (1988).