Electron-impact excitation of the resonance transition in Be^+: An *ab initio* treatment of core-correlation and -polarization effects

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We present theoretical electron-impact-excitation cross sections for several transitions in Be^+, and fluorescence radiation polarizations for the Be^+ resonance doublet. The projectile-electron energy varies from 0.3—2.0 Ry. A five-state close-coupling approximation is used. The target model is the most sophisticated employed in any scattering calculation to date, and yields oscillator strengths for several transitions in Be^+ that are the most accurate available. Our results do *not*, however, improve upon previous work as regards the notable discrepancies between calculations and experimental measurements for excitation of the resonance transition. This indicates that high rigor in the treatment of short-range core-correlation effects is not required for an accurate description of these processes, and therefore either that other, heretofore ignored, effects must be taken into account in the theory or that other measurements are necessary. An accurate measurement of the hyperfine structure of the $j=\frac{3}{2}$ fine-structure level of the doublet would be of particular and decisive importance.

I. INTRODUCTION

This paper is a contribution to the clarification of the physical effects that are important in the response of the Be^+ system to electron impact. A notable discrepancy between theoretical predictions[1,2] and experimental data[3] exists for the excitation cross section of the $1s^2 2s\ ^2S^e_{1/2}-1s^2 2p\ ^2P^o_{1/2,3/2}$ transition (the resonance doublet) of Be^+. At threshold, calculations exceed measurements by $\sim 20\%$, which is more than twice the quoted high-confidence-level (98%) uncertainty attributed to the latter data. The calculated linear polarization of the fluorescence radiation for this doublet also exhibits appreciable departure from measurements, especially close to threshold, where it exceeds experiment by $\sim 50\%$.[1] This is particularly disturbing as the latter measurement is relatively simple, and does not require any absolute calibration, in contrast to the measurement of the absolute excitation cross section.

The Be^+ system consists of a relatively inert heliumlike core surrounded by a single valence electron. One would therefore expect that processes inducing the resonance transition in the valence electron would be negligibly influenced by core-correlation effects. Yet increasingly sophisticated treatments (see Refs. 1 and 2) of the $Be^+ + e^-$ system have failed to explain the experimental results.

The most elaborate of these were two five-state $[1s^2(2s+2p+3s+3p+3d)]$ close-coupling calculations, both of which included all effects of exchange between the projectile and target electrons. One of these[1] also included the effects of core polarization on the scattered electron using a semiempirical model, the parameters of which were chosen with reference to the energy levels of Be^+. The other[2] treated the $n=3$ levels in the close-coupling expansion as pseudostates, and here the parameters were chosen to minimize the dominant partial-wave collision strengths.

Although these calculations resulted in noticeable improvements over two-state calculations,[1] agreement with the measurements remained poor. Comparison between the two five-state calculations suggested[2] that the inclusion of higher terms in the close-coupling expansion would likely not be productive. The two-state calculations with and without the inclusion of the long-range core-polarization effect were little different. The major weaknesses in previous calculations were thus identified as being the reliance on semiempirical methods and the somewhat crude treatment of short-range (mainly core) correlation.

Our primary goal was to determine whether a more accurate treatment of this effect in the Be^+ target model and in the collision process would have a significant effect on the calculated cross section and perhaps also bring the theory and experiment for the fluorescence radiation polarization into better agreement. The results of our work indicate decisively that the explanation of the disagree-

TABLE I. Orbitals used in the description of the Be^+ ion target. HO means the orbital is hydrogenic, HP that it is a hydrogenic pseudostate, and PCO that it is a polarized core orbital. The core appropriate to each orbital is given in column 3.

Label	Type	Core
$1s$	HO	Be^{4+}
$1s'$	PCO	Be^{3+}
$\overline{2p}$	HP	Be^{4+}
$\overline{2p}'$	PCO	Be^{3+}
$2s$	PCO	Be^{2+}
$2p$	PCO	Be^{2+}
$3s$	PCO	Be^{2+}
$3p$	PCO	Be^{2+}
$3d$	PCO	Be^{2+}

TABLE II. Total energies, in Ry, of the lowest five levels of Be^+ in various models. "Present" in columns 2 and 5 refers to the 44-configuration calculation described in the text. The exact and SCHF (single configuration Hartree-Fock) calculations are due to Weiss (Refs. 11 and 12).

State	Total Energy (Ry) Calculation Present	Exact	SCHF	Correlation included in Present
$2s\,^2S^e$	−28.605 75	−28.649 58	−28.554 78	54%
$2p\,^2P^o$	−28.311 62	−28.358 64	−28.261 70	51%
$3s\,^2S^e$	−27.800 60		−27.755 54	
$3p\,^2P^o$	−27.724 50		−27.679 40	
$3d\,^2D^e$	−27.710 81		−27.667 14	

ment between calculation and measurement lies elsewhere.

We begin our presentation with a detailed description of the model used for the Be^+ target. The calculated properties of the 44-configuration approximation we employ for the Be^+ target are compared with measurements and other calculations for Be^+ in Sec. II. In Sec. III, the results of our calculation for the $Be^+ + e^-$ collision problem are presented. The linear polarization of the fluorescence radiation is treated in Sec. IV. Finally, in Sec. V, we discuss the significance of the present work and suggest directions for future study.

II. THE TARGET

We have made use of a 44-configuration approximation for the Be^+ target ion. Nine orbitals, including a hydrogenic pseudostate, are incorporated into our model. To obtain an idea of the quality of this ion model, its structure and radiative properties are compared with other calculations and/or with experimental data as appropriate. All major computations were carried out using the University College London codes SUPERSTRUCTURE,[4] COLALG,[5] IMPACT,[6] and DSTWAV.[5] As checks on versions of these programs adapted to our purposes, we successfully reproduced selected two- and five-state results of Hayes *et al.*[1]

The orbitals involved are presented in Table I. In column 1 of this table we list the labels given these orbitals. The $1s$, $1s'$, $\overline{2p}$, and $\overline{2p}\,'$ orbitals contribute mainly to the Be^{2+} core; the remaining five orbitals describe essentially the valence electron. In the entries in column 2 we list the type of each orbital. The radial part of the $\overline{2p}$ hydrogenic pseudostate may be given by the formula[7]

$$(32Z/129)^{1/2}e^{-Zr}(Zr)^2(1+Zr/2)\,, \tag{1}$$

where $Z=4$ and r is measured in Bohr radii a_0. The eigenenergy of such a pseudostate may be shown to be $-7Z^2/86$ a.u. (hartrees). The $1s'$, $2s$, $2p$, $\overline{2p}\,'$, $3s$, $3p$, and $3d$ orbitals are polarized-core orbitals, generated by the method of Seaton and Wilson.[8] The core appropriate to each orbital is indicated in column 3 of Table I. The core configuration for the $1s'$ and $\overline{2p}\,'$ orbitals is $1s+\overline{2p}$. That used to generate the valence orbitals is $1s^2+1s\,1s'+1s'^2+\overline{2p}^{\,2}+\overline{2p}\,\overline{2p}\,'+\overline{2p}\,'^2+1s\,\overline{2p}+1s\,\overline{2p}\,'+1s'\overline{2p}+1s'\overline{2p}\,'$. This latter ten-configuration Be^{2+} core has the dipole polarizability $0.051\,40a_0^3$, as compared with two previous determinations: $0.051\,23a_0^3$ (Ref. 9), $0.052\,24a_0^3$ (Ref. 10).

The Be^+ target is approximated by the 44 configurations

$$\begin{aligned}&1s^2(2s+2p+3s+3p+3d)\\&+1s^2(1s'+\overline{2p}+\overline{2p}\,')+1s\,1s'(1s'+\overline{2p}+\overline{2p}\,'+2s+2p+3s+3p+3d)\\&+(1s\overline{2p}+1s'^2+1s'\overline{2p}+\overline{2p}^{\,2})(\overline{2p}+\overline{2p}\,'+2s+2p+3s+3p+3d)\,.\end{aligned} \tag{2}$$

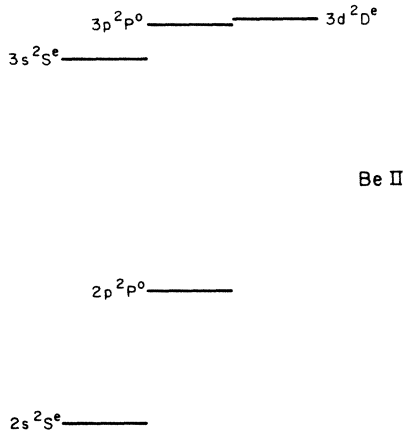

FIG. 1. Partial level scheme of Be^+.

The configurations listed in the last two lines in (2) are "correlation configurations," and we retain only their contributions to terms contained in the configurations in the first line of (2).

In Table II we present total energies of the five lowest states of the Be^+ system as calculated using the present model, together with two other determinations.[11,12] The level notation of the Be^+ ion is that illustrated in Fig. 1. In column 2 we present the results of our 44-configuration calculation. The "exact" energies given in column 3 are the estimates of Weiss (Refs. 11 and 12). In column 4 we list Hartree-Fock energies[12] for these levels. Defining the correlation energy as the difference between the exact and Hartree-Fock energies, the present model is seen to include 54% of the correlation energy of the ground state, and 51% of the correlation energy of the first excited state. The dominant contribution ($\sim$90%) of the calcu-

TABLE III. Excitation energies for Be^+ in Ry. The experimental values are those of Johansson (Ref. 13). Weighted averages are used for the doublets.

Transition	Excitation energy (Ry) Present calculation	Experiment	Error in calculation
$2s\,^2S^e$-$2p\,^2P^o$	0.294 13	0.290 99	1.1%
$3s\,^2S^e$	0.805 15	0.804 03	0.1%
$3p\,^2P^o$	0.881 25	0.879 35	0.2%
$3d\,^2D^e$	0.894 93	0.893 54	0.2%

lated correlation energy arises from the Be^{2+} ion core. Previous five-state calculations have included much smaller fractions of the correlation energy, typically less than 10%.

Excitation energies for the first four excited states are given in Table III. For the doublets we use statistically weighted averages over the experimental data.[13] The exact values from Table II yield an excitation energy of 0.290 94 Ry for the $2p\,^2P^o$ level. Our results, though cruder, agree with this and with the measurements to within 1.1%.

The oscillator strengths, or f values, for electric dipole transitions among the five lowest levels of the Be^+ system are given in Table IV. Agreement between f values calculated in the length (f_L) and velocity (f_V) gauges is a necessary, though not a sufficient, condition that the exact wave function must satisfy. Hartree-Fock calculations are gauge dependent[14] in general, and one must include some of the contribution of correlation effects in order to obtain less variation among transition matrix elements computed in different gauges. In columns 4 and 5 of Table IV we quote the results of calculations by Beck and Nicolaides.[15] These authors have used 139 configurations (incorporating 24 radial functions) to approximate the $2s\,^2S^e$ state, and 183 configurations (incorporating 29 radial functions) to describe the $2p\,^2P^o$ state. A computational effort of this magnitude reduces the disagreement between oscillator strengths calculated in the length and velocity gauges to be $\frac{1}{7}$ that in the Hartree-Fock case for the resonance transition. Our model, based upon a much more modest choice of configurations (44 configurations incorporating nine radial functions describe all five lowest levels) due to computational limitations on the size of the collision problem, reduces the discrepancy by $\frac{1}{2}$ for this same transition (line 1, columns 6 and 7). Experimental determinations[16–18] of f for this case (lines 1–3, column 8) are not sufficiently decisive to guide calculations. For transitions other than the resonance one, our model for Be^+ predicts $f_L - f_V$ to be, in most cases, about an order of magnitude smaller than $f_L - f_V$ for the corresponding Hartree-Fock calculations. Accurate ionic oscillator strengths are crucially important at all energies in collision calculations.[14]

The "experimental" f value quoted in Table IV are obtained from measurements[16–19] of transition lifetimes. Neglecting all but the dominant transition contributing to the decay rate of level a (a reasonable approximation in the present instances), the f values are given by the formula

$$f_{ab} = 1.245 \times 10^{-10} (g_a / g_b) / (T_a \Delta E_{ab}^2) , \quad (3)$$

where g_i is the statistical weight of the state i, T_a is the lifetime of the level in seconds, and ΔE_{ab} is the energy separation, in rydbergs, between the level a and the lower level b.

To further test the quality of the present approximation for the Be^+ target, we carried out extensive calculations of the bound states of Be for several symmetries using our Be^+ target as the appropriate "core." (The collision problem is solved for negative energies.[8]) The accuracy of ionization energies and quantum defects obtained by this

TABLE IV. Oscillator strengths for various transitions for the Be^+ ion. The Hartree-Fock calculations are those of Weiss (Ref. 12). BN refers to the 139 ($2s\,^2S^e$)+183 ($2p\,^2P^o$)-configuration calculations of Beck and Nicolaides (Ref. 15). "Present" refers to the present calculation.

Transition	Hartree-Fock f_L	Hartree-Fock f_V	BN f_L	BN f_V	Present f_L	Present f_V	Experiment
$2s\,^2S^e$-$2p\,^2P^o$	0.5112	0.5491	0.5011	0.4960	0.5051	0.4938	0.54 ±0.03[a] 0.46 ±0.01[b] 0.52[c]
$3p\,^2P^o$	0.0804	0.0731			0.0793	0.0812	0.072±0.010[d]
$2p\,^2P^o$-$3s\,^2S^e$	0.0665	0.0671			0.0649	0.0644	0.048±0.004[a] 0.069±0.010[b]
$3d\,^2D^e$	0.6520	0.6325			0.6327	0.6320	0.62 ±0.04[b] 0.57 ±0.06[d]
$3s\,^2S^e$-$3p\,^2P^o$	0.8386	0.8798			0.8422	0.8346	
$3p\,^2P^o$-$3d\,^2D^e$	0.0808	0.0612			0.0784	0.0803	

[a]Reference 16.
[b]Reference 17.
[c]Reference 18.
[d]Reference 19.

TABLE V. Energies, in Ry, of states of Be relative to the series limit (the $2s\,^2S^e$ state of Be^+) at 0.685 246 Ry (Ref. 21). The other experimental values are those of Johansson (Ref. 13) with this series limits. Results labeled NS are from Ref. 20.

State	ϵ (expt) (Ry)	$[\epsilon(\text{expt})-\epsilon(\text{calc})]\times 10^4$ (Ry) NS	Present
$2s^2\,^1S^e$	−0.6852	−15	−11
$2s2p\,^3P^o$	−0.4849	−10	−22
$2s2p\,^1P^o$	−0.2973	−50	−47
$2p^2\,^1D^e$	−0.1669	−15	−36
$2p^2\,^3P^e$	−0.1412	−32	−39

method, when compared with experimental data, is in good agreement with that obtained using a model[20] that also includes both the effects of long-range core and dielectronic polarization, and short-range correlation. In this earlier work,[20] terms representing long-range polarization of the core were explicitly incorporated into the Hamiltonian, and short-range correlation effects were modeled by semiempirically adjusting the polarization cutoff function. In the present work the inclusion of all of these effects is approached via the elaborate multiconfiguration Be^+ target wave function. Illustrative results are presented in Table V.

III. CROSS SECTION

We make use of the linear-algebraic method[6,22] in a five-state close-coupling approximation to determine the impact-excitation cross section for the $2s\,^2S^e-2p\,^2P^o$ transition. Partial-wave summations are carried to convergence by augmenting the close-coupling calculations ($L=0$–9) with distorted-wave results ($L=10$ and up). The total cross section from the present calculation is plotted together with two previous theoretical calculations[1,2] and the experimental data[3] in Fig. 2. The data generated in the present calculation are given in Table VI. Total cross sections reflect convergence to better than 0.5% at all energies.

The curve representing the experimental data is the parametrization[3]

$$\begin{aligned}\sigma &= -5.80\ln E + 11.01 \quad \text{for } 0.32 < E < 1.54\ , \\ \sigma &= (8.44\ln E + 9.41)/E \quad \text{for } 1.54 < E < 54.39\ ,\end{aligned} \tag{4}$$

where σ is in units of πa_0^2 and E is in rydbergs. The experimental uncertainty is typically about 10%, varying from 8% to 15%.[3]

As stated earlier, the present calculation indicates that the inclusion of core correlation has no appreciable effect on the agreement between the cross sections from theory and experiment. Indeed, the total cross section from the present calculation is seen to be slightly (less than 1%) *higher* than that from a previous five-state calculation[1] at threshold. In Table VII we compare the near-threshold partial-wave cross-section contributions for $L=0$–8 from the present work with the results from previous calcula-

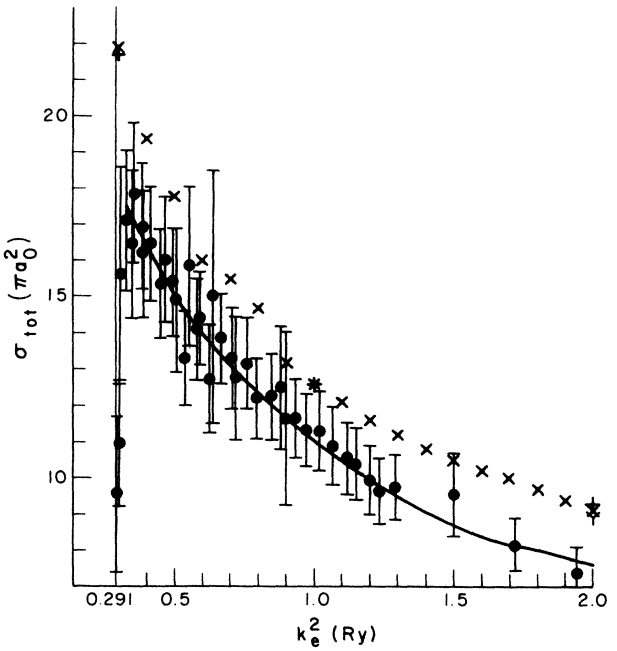

FIG. 2. Total impact-excitation cross section for the resonance multiplet of Be^+. The results of three five-state close-coupling calculations are shown: ×, present calculation, includes core correlation and polarization *ab initio;* +, Hayes *et al.* (*CCII* five-states, Ref. 1), includes core-polarization semiempirically; Y Henry *et al.* (Ref. 2), includes three pseudostates. The measurements of Taylor *et al.* (Ref. 3) are shown as solid circles with error bars (representing total uncertainties at 98% confidence level); a parametrized fit [Eq. (4)] to the data is shown as the solid line.

TABLE VI. Q_0 and Q_1 are, respectively, the cross sections for excitation from the $2s\,^2S^e$ level into the $2p\,^2P^o_{(M=0)}$ and $2p\,^2P^o_{(M=1)}$ sublevels. The total cross section for excitation into the $2p\,^2P^o$ levels, Q_{tot}, is Q_0+2Q_1. All cross sections are in units of Bohr area, πa_0^2.

Projectile electron energy (Ry)	Q_0	Q_1	Q_{tot}
0.3	16.43	2.74	21.9
0.4	13.43	2.97	19.4
0.5	11.45	3.15	17.8
0.6	9.21	3.38	16.0
0.7	8.51	3.47	15.5
0.8	8.18	3.25	14.7
0.9	6.79	3.19	13.2
1.0	6.22	3.16	12.6
1.1	5.77	3.14	12.1
1.2	5.34	3.08	11.6
1.3	5.03	3.07	11.2
1.4	4.72	3.03	10.8
1.5	4.46	3.00	10.5
1.6	4.22	2.97	10.2
1.7	4.04	2.96	10.0
1.8	3.84	2.92	9.7
1.9	3.63	2.86	9.4
2.0	3.45	2.81	9.1

TABLE VII. Partial-wave contributions to the total $2s\,^2S^e$–$2p\,^2P^o$ impact-excitation cross section for Be^+ at 0.3 Ry. The results of two five-state calculations [the present and those of Hayes *et al.* (Ref. 1)] and one two-state calculation (Ref. 1) are presented. All cross sections are in units of the Bohr area, πa_0^2.

		Hayes *et al.*	
L	Present	Five-state	Two-state
0	0.258	0.254	0.252
1	2.878	2.785	2.877
2	1.535	1.455	1.777
3	10.895	10.603	11.775
4	5.079	5.232	5.197
5	1.089	1.174	1.171
6	0.158	0.182 [b]	0.182
7	0.017	0.021 [b]	0.021
8	0.001	0.002 [b]	0.002
9 and up	$<2\times10^{-4}$ [a]	$<2\times10^{-4}$ [c]	$<2\times10^{-4}$ [c]
Total	21.9	21.7	23.3

[a]Five-state results for $L=9$, distorted wave results for $L\geq 10$.
[b]Two-state results.
[c]Coulomb-Bethe results.

tions. It is apparent that the contribution of the $L\geq 4$ symmetries to the total cross section is less in our model than in the results of Hayes *et al.*[1] However, this deficit is made up by larger contributions from the $L\leq 3$ partial waves in the present calculation.

The experimental data include cascade effects, whereas the theoretical treatment does not. Cascade is not present for projectile-electron energies less than 0.8 Ry, however, and it is in this region that the disagreement is most notable. It is obvious that the disagreement between theory and experiment persists.

The $^1S^e$ elastic partial cross section exhibits a resonance just above the $2s\,^2S^e$ level. This is identified with the $2p^2\,^1S^e$ autoionizing resonance. Comparison between a recent experimental measurement and various theoretical determinations of the parameters of this resonance (Ref. 23 and citations therein) shows strong sensitivity of these parameters to the treatment of correlation effects. This is again apparent from a perusal of Table VIII, where we present the location of the resonance maximum and full width at half maximum as obtained from increasingly sophisticated close-coupling calculations for the $Be^+ + e^-$ system. In all instances, the inclusion of another state in the close-coupling expansion, reflecting mostly a more complete treatment of long-range correlations, is seen to have an appreciable effect on either the location or the width of the resonance, or both. That long-range correlations are the important variety in this instance can also be seen by comparing the present five-state calculation with the results from a previously described semiempirical model[20] where short-range correlations are not treated nearly as comprehensively.

Other cross sections that can be calculated with the same collision symmetries as those required for the resonance transition are given in Tables IX–XI. We do not expect all of these results to be of quite the quality of the results of Table VI due to the neglect of couplings to important higher-lying levels in several cases. They do suggest, however, that the cascade contribution to the excitation function would be as much as 10% at the highest energies considered here, further aggravating the disagreement.

IV. POLARIZATION OF THE FLUORESCENCE RADIATION

In Fig. 3 we compare theory and experiment for the linear polarization of the fluorescence radiation from the $2p\,^2P^o$ level. The experimental data are given by the parametrization[3]

$$P=-7.08\ln E+28.4\ , \tag{5}$$

where E is in eV. The uncertainty in P is about 3%. P is measured at a right angle to the incident electron beam.[3,24]

Theoretically, the percentage polarization is given by the expression[24,25]

TABLE VIII. Parameters for the $2p\,^2\,^1S^e$ resonance. The states included in the close-coupling expansion in each calculation are listed in the first column. The column labeled ϵ gives the location of the resonance above the Be series limit (the $2s\,^2S^e$ state of Be^+), and that labeled Γ the full width at half maximum. The results labeled NS are from Ref. 20. The experimental data are those of Clark *et al.* (Ref. 23).

Coupled states	Determination	ϵ (Ry)	Γ (Ry)
$2s\,^2S^e$, $2p\,^2P^o$	Present calculation	0.0589	3.5×10^{-5}
$2s\,^2S^e$, $2p\,^2P^o$, $3s\,^2S^e$	Present calculation	0.0577	1.4×10^{-7}
$2s\,^2S^e$, $2p\,^2P^o$, $3s\,^2S^e$, $3p\,^2P^o$	Present calculation	0.0564	2.1×10^{-5}
$2s\,^2S^e$, $2p\,^2P^o$ $3s\,^2S^e$, $3p\,^2P^o$, $3d\,^2D^e$	Present calculation	0.0252	9.57×10^{-4}
$2s\,^2S^e$, $2p\,^2P^o$, $3d\,^2D^e$	NS calculation	0.0241	7.72×10^{-4}
	Experiment	0.0091	6.83×10^{-4}

TABLE IX. Q is the cross section in units of the Bohr area, πa_0^2, for excitation from the $2s\,^2S^e$ level to the $3s\,^2S^e$ level for Be^+.

Projectile electron energy (Ry)	Q
0.9	0.59
1.0	0.57
1.1	0.55
1.2	0.51
1.3	0.48
1.4	0.45
1.5	0.43
1.6	0.41
1.7	0.39
1.8	0.37
1.9	0.35
2.0	0.34

$$P=300(9\alpha-2)(Q_0-Q_1)/[12Q_0+24Q_1+(9\alpha-2)(Q_0-Q_1)]\,, \quad (6)$$

where Q_0 and Q_1 are the cross sections for excitation of the $M=0$ and $M=1$ sublevels of the $2p\,^2P^o$ level, and

$$\alpha=(254+25f_{02}+30f_{12}+21f_{13}+70f_{23})/900 \quad (7)$$

for $^9Be^+$.

The factors

$$f_{FF'}=[1+(2\pi\Delta\nu_{FF'}/A)^2]^{-1} \quad (8)$$

take into account precessional motions due to hyperfine structure. Here $\Delta\nu_{FF'}$ is the frequency separation of the hyperfine levels F and F' of the $2p\,^2P^o_{3/2}$ state, and A ($=1.170\times10^8\ \mathrm{sec}^{-1}$, using f_L from Table IV) is the decay rate of the $2p\,^2P^o_{3/2}$ level. The hyperfine structure splittings $\Delta\nu_{FF'}$ for $^9Be^+$ $2p\,^2P^o_{3/2}$ are related to the electric dipole and magnetic quadrupole interaction constants A_{E1} and B_{M2}, respectively, by[26]

$$\Delta\nu_{32}=3A_{E1}+B_{M2}\,,$$
$$\Delta\nu_{21}=2A_{E1}-B_{M2}\,, \quad (9)$$
$$\Delta\nu_{10}=A_{E1}-B_{M2}\,.$$

TABLE X. Q_0 and Q_1 are, respectively, the cross sections for excitation from the $2s\,^2S^e$ level into the $3p\,^2P^o_{(M=0)}$ and $3p\,^2P^o_{(M=1)}$ sublevels for Be^+. The total cross section for excitation into the $3p\,^2P^o$ levels, Q_{tot}, is Q_0+2Q_1. All cross sections are in units of Bohr area, πa_0^2.

Projectile electron energy (Ry)	Q_0	Q_1	Q_{tot}
0.9	0.327	0.044	0.41
1.0	0.308	0.036	0.38
1.1	0.288	0.031	0.35
1.2	0.264	0.027	0.32
1.3	0.239	0.024	0.29
1.4	0.218	0.022	0.26
1.5	0.199	0.020	0.24
1.6	0.182	0.019	0.22
1.7	0.168	0.018	0.20
1.8	0.155	0.017	0.19
1.9	0.143	0.016	0.18
2.0	0.133	0.016	0.16

TABLE XI. Q_0, Q_1, and Q_2 are, respectively, the cross sections for excitation from the $2s\,^2S^e$ level into the $3d\,^2D^e_{(M=0)}$, $3d\,^2D^e_{(M=1)}$, and $3d\,^2D^e_{(M=2)}$ sublevels for Be^+. The total cross section for excitation into the $3d\,^2D^e$ levels, Q_{tot}, is $Q_0+2Q_1+2Q_2$. All cross sections are in units of the Bohr area, πa_0^2.

Projectile electron energy (Ry)	Q_0	Q_1	Q_2	Q_{tot}
0.9	0.387	0.050	0.024	0.54
1.0	0.443	0.068	0.040	0.66
1.1	0.444	0.085	0.050	0.71
1.2	0.419	0.099	0.057	0.73
1.3	0.383	0.110	0.062	0.73
1.4	0.344	0.118	0.065	0.71
1.5	0.307	0.124	0.067	0.69
1.6	0.274	0.127	0.069	0.67
1.7	0.246	0.129	0.070	0.65
1.8	0.221	0.130	0.071	0.62
1.9	0.201	0.129	0.071	0.60
2.0	0.183	0.128	0.072	0.58

The equations for P and α are the appropriate forms of more general results.[24,25] The approximations that cascade is negligible, that algebraic recoupling is sufficient, and that the fine-structure separation is large compared with the line width, are made throughout in their derivation. The first of these assumptions is clearly incorrect at higher energies, and we must therefore limit our use of these results to the near-threshold region.

The quantity α varies from $\frac{4}{9}=0.444$ (assuming negligible hyperfine splittings) down to $\frac{127}{450}=0.282$ (assuming large hyperfine splittings). At threshold, $Q_1/Q_0=0$ must hold,[24] whence

$$P_{th}=300(9\alpha-2)/[12+(9\alpha-2)] \quad (10)$$

varies, respectively, from 42.9% to 12.9% for these extreme values of α. Clearly an accurate determination of the hyperfine structure is necessary for a meaningful comparison of theory and experiment for P.

Calculations of the hyperfine structure of the $^9Be^+$ $2p\,^2P^o_{3/2}$ level are *very* sensitive to estimates of correlation and relativistic effects.[26] The electric dipole and magnetic quadrupole interaction constants from a nonrelativistic perturbation-theoretic treatment by Garpman *et al.*[27] are

$$A_{E1}/g_I=1.87\pm1.50\ \mathrm{MHz}\,\mu_N^{-1}$$

and (11)

$$B_{M2}/Q=43.03\pm45\ \mathrm{MHz\,barn}^{-1}\,.$$

(Another calculation by Heully and Martensson-Pendrill[28] using relativistic perturbation theory is in excellent agreement with the cited nonrelativistic work. The latter au-

thors do not, however, estimate the errors in their computation.) Here g_I is the nuclear g factor in nuclear magnetons (μ_N) and $\mathcal{Q}$ is the nuclear quadrupole moment in barns (10^{-28} m^2). Using for g_I the value[29] ($-0.784\,955\pm0.000\,001\,5$) μ_N for the bare nucleus, and for $\mathcal{Q}$ the value[30] 0.053 ± 0.003 barn, the values in (11) are

$$A_{E1}=-(1.47\pm1.18)\text{ MHz}$$

and (12)

$$B_{M2}=(2.28\pm2.4)\text{ MHz}\ .$$

Within this range of values for A_{E1} and B_{M2} it is possible to obtain $\alpha=0.41$, bringing our calculations into better agreement with the near-threshold measurements of P. As indicated in Fig. 3, the yet lower value $\alpha=0.375$ further improves the agreement between theory and experiment. However, an experimental estimate[31] of $|A_{E1}|$ (≤ 0.6 MHz) favors the larger value of $\alpha=0.444$, but this was based on a theoretical value of 2.00 MHz for B_{M2}. A recent calculation by Beck[32] which includes relativistic (mass and quantum-electrodynamical) corrections, and the effects of finite nuclear size and mass, predicts B_{M2} to be roughly twice as large; these new results do not, however, appreciably reduce α [now 0.431 using the hyperfine-level intervals of Ref. 32 in Eq. (8)].

The partial waves ($L=3,4$) which dominate the total cross section Q_{tot} for excitation from the $2s\,^2S^e$ level to the $2p\,^2P^o$ level also dominate the partial cross sections Q_0 and Q_1 for excitation into the magnetic sublevels (with $M=0$ and 1, respectively) of the $2p\,^2P^o$ level. An instance of this is illustrated in Table XII, where we give the partial wave contributions to Q_0 and Q_1 at 0.3 Ry. This is a significant observation; its implication is that the line-radiation polarization P is also strongly dependent on the dominant partial waves.

High-precision measurements of the hyperfine structure have been carried out for the $2p\,^2P^o_{1/2}$ fine-structure level only.[33] A measurement of similar quality for the splittings between the $F=0,1,2,3$ hyperfine levels corresponding to the $2p\,^2P^o_{3/2}$ fine-structure level of Be^+ would be very useful in deciding the issue at hand.

V. CONCLUSION

It has been demonstrated that the rigorous inclusion of short-range core correlations does not appreciably modify the theoretical impact-excitation cross section for the resonance transitions, and fails to resolve serious discrepancies between calculated and measured cross sections and fluorescence radiation polarizations in Be^+.

By the same token, it has also been demonstrated that the semiempirical treatment of valence electron states is appropriate to the Be^+ ion. This result has been taken into account in work presently in progress; using semiempirical methods we are studying the convergence properties of increasingly larger close-coupling expansions. From this work we hope to obtain a clearer picture of the role played by long-range correlations at near-threshold energies, and also get some idea of the efficacy of the close-coupling approximation in the treatment of such "hydrogenlike" cases. The influence of resonances will be

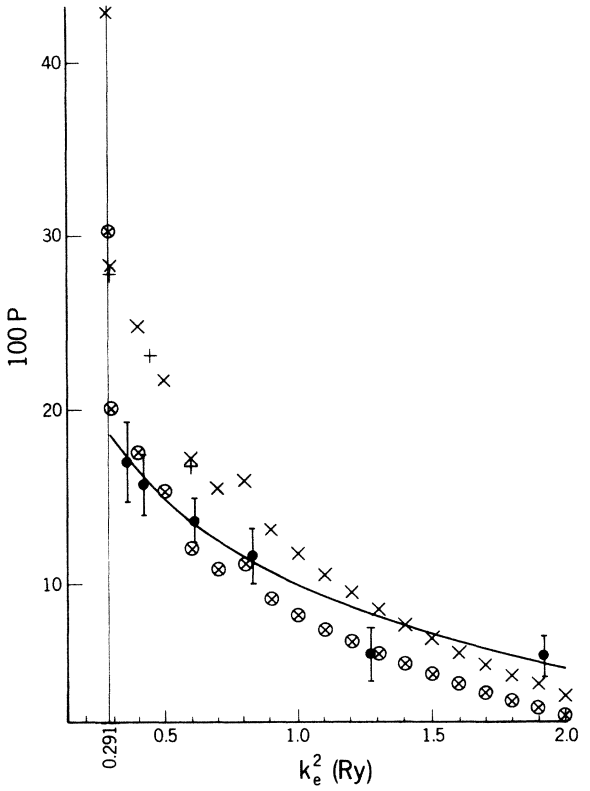

FIG. 3. Percentage linear polarization, of the Be^+ $2p\,^2P^o_{3/2,1/2}-2s\,^2S^e_{1/2}$ doublet fluorescence radiation following collisional excitation, at right angles to the projectile electron. The results of the present five-state close-coupling calculation and those of Hayes *et al.* (Ref. 1) for assumed negligible hyperfine structure [$\alpha=0.444$ in Eq. (6)] of the $2p\,^2P^o_{3/2}$ level are shown as $\times$ and $+$, respectively. Also shown, as $\otimes$, are the results of the present calculation with an assumed appreciable hyperfine structure [$\alpha=0.375$ in Eq. (6)]. The values at threshold are independent of collisional effects, and are 42.9% for $\alpha=0.444$, and 30.3% for $\alpha=0.375$. The experimental data of Taylor *et al.* (Ref. 3) are shown along with their parametric fit [Eq. (5)] as the solid circles with error bars (representing standard deviations combined in quadrature with systematic uncertainties), and the solid line, respectively.

TABLE XII. Q_0 and Q_1 are, respectively, the partial cross sections for excitation from the $2s\,^2S^e$ level into the $2p\,^2P^o_{(M=0)}$ and $2p\,^2P^o_{(M=1)}$ sublevels. The incident electron energy is 0.3 Ry. All cross sections are in units of the Bohr area, πa_0^2.

L	Q_0	Q_1
0	0.086	0.086
1	2.267	0.306
2	1.120	0.207
3	9.499	0.697
4	2.910	1.085
5	0.473	0.308
6	0.067	0.045
7	0.007	0.005
8	0.001	$<10^{-3}$
9	$<10^{-4}$	$<10^{-4}$

examined in detail.

In search of other physical effects that might explain the discrepancy between theory and experiment, in the context of impact excitation of Be^+, we have also examined the influence of relativistic effects. The inclusion of fine structure in the algebraic-recoupling approximation[34] does not affect the quoted cross sections to more than 5 parts in 10000 at threshold.

The theoretical determination of the polarization of the fluorescence radiation is strongly influenced by estimates of the hyperfine structure of the $2p\ ^2P^o_{3/2}$ level. Calculations of this hyperfine structure are difficult and of unknown reliability, mainly because of severe cancellations arising from correlation effects. A high-precision measurement would serve to clarify the role of correlation in both the static and dynamic properties of the Be^+ ion.

Incidental to the present calculation are oscillator strengths for several transitions in Be^+ that are more accurate than heretofore available, and cross sections for electron-impact excitation of the $2s\ ^2S^e$–$3s\ ^2S^e$, $3p\ ^2P^o$, and $3d\ ^2D^e$ transitions.

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