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Generalized oscillator strengths for the $(1s^2 2s^2)\,^1S \rightarrow (1s^2 2s2p)\,^1P$ transition in some Be-like ions

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Generalized oscillator strengths $f(K)$ have been calculated for the $(1s^2 2s^2)\,^1S \rightarrow (1s^2 2s2p)\,^1P$ transition of the Be-like ions when $Z=4-8$. A "length" formula and two versions of a "velocity" formula for $f(K)$ were used in each instance. For each ion, K- and L-intrashell pair correlation functions were included in the description of the ground-state wave function, and the K-shell pair function was also introduced into the excited state. The pair functions were determined after the general manner proposed by Sinanoğlu. For $K=0$, $f(K)$ is equivalent to the optical oscillator strength and our results can therefore be compared with several other theoretical values and with experiment. The excellent agreement of our $f(0)$ values when compared with experiment, coupled with the high degree of consistency amongst the $f(K)$ values when evaluated, in turn, from the three formulations mentioned above, suggests that our correlated results should possess considerable reliability, particularly at the lower end of the Z range. The sensitivity of the $f(K)$ values to the presence of electron correlation effects has been examined by repeating the calculations using Hartree-Fock descriptions for both the ground and excited states. Comparison between our correlated and noncorrelated results revealed that the presence of the pair functions was indispensable in order to achieve agreement between $f(K)$ values derived from the "length" and "velocity" formulations. For Be, the $f(K)$ values were used to obtain total inelastic scattering cross sections, within the first Born approximation, for both proton and electron impact. Although our allowance for electron correlation produced significant changes in the "length"-based cross sections, "velocity" values proved to be considerably less sensitive over a large energy range for both types of projectile.

I. INTRODUCTION

The generalized oscillator strength $f(K)$ of an atom or molecule is an important property of the system representing its response to a sudden change K in the momentum of its electrons. Further, in the limit $K \rightarrow 0$, the expression for $f(K)$ becomes equal to that used for calculating optical oscillator strengths. The concept of the generalized oscillator strength arises in the study of inelastic scattering cross sections and, since $f(K)$ is independent of the exciting projectile and of its velocity, there is an increasing tendency to present the results of inelastic scattering experiments in this form. A knowledge of $f(K)$ and, in particular, the *absolute* values for the related inelastic scattering cross sections is required in research fields as diverse as plasma physics, atmospheric physics, astrophysics, and radiation physics. Consequently, reliable theoretical determinations of such quantities can be of special interest. An excellent discussion of generalized oscillator strengths and their applicability has been given recently by Inokuti.[1]

Although several theoretical studies of $f(K)$ have been carried out for He for a number of excitations,[2-6] calculations for other systems are somewhat scarce, and notably, no previous predictions would appear to be available for Be and its isoelectronic series of ions. In the present article, therefore, we have evaluated $f(K)$ for the $(1s^2 2s^2)\,^1S \rightarrow (1s^2 2s2p)\,^1P$ transition for the Be-like ions when $Z=4-8$. The results for Be have been used within the first Born approximation to determine the total inelastic scattering cross sections for both electron and proton impact.

It is clear from the results of other workers[2-6] that, for He, calculations of the generalized oscillator strengths are sensitive to the presence of electron correlation—particularly when describing the wave function for the ground state. To examine the influence of correlation effects on $f(K)$ for the Be-like ions we have used both a correlated and an uncorrelated description of the wave functions. In each instance, three sets of results were determined by employing different formulations for $f(K)$ since their relative agreement will provide us with some measure of their reliability.

For $K=0$, our results are compared with the optical oscillator strengths determined by several other workers from both theory and experiment.

II. CALCULATIONS

The generalized oscillator strength associated with the transition of an N-electron system from state m to the state n is defined by

$$f(K)=\frac{2\Delta E}{K^2}\,|\mathcal{E}(K)|^2, \tag{1}$$

where

$$\mathcal{E}(K)=\left\langle \Psi_n,\ \sum_{j=1}^{N} e^{iKz_j}\,\Psi_m\right\rangle \tag{2}$$

and ΔE is the energy difference[7] between the states m and n. For exact wave functions $\mathcal{E}(K)$ can also be written in either of the following forms:

$$\mathcal{E}(K)=\frac{1}{2(E_n-E_m)}\left[K^2\left\langle \Psi_n,\ \sum_{j=1}^{N} e^{iKz_j}\,\Psi_m\right\rangle-2iK\left\langle \Psi_n,\ \sum_{j=1}^{N}\left(e^{iKz_j}\,\frac{\partial}{\partial z_j}\right)\Psi_m\right\rangle\right] \tag{3}$$

or

$$\mathcal{E}(K)=\frac{2iK}{2(E_n-E_m)+K^2}\left\langle \sum_{j=1}^{N}\left(e^{-iKz_j}\,\frac{\partial}{\partial z_j}\right)\Psi_n,\ \Psi_m\right\rangle . \tag{4}$$

The equivalence of relations (2), (3), and (4) does not hold, however, when approximate wave functions are used. Expression (2) is customarily termed the "length" formula while expressions (3) and (4) are referred to as "velocity" formulas.[1] Values for $f(K)$ obtained using relations (2)–(4) are symbolized here by L, $V1$ and $V2$, respectively.

Within the first Born approximation, the differential inelastic scattering cross section of a target for incoming projectiles of kinetic energy T and mass m_p is related to $f(K)$ by

$$I(K)=\frac{2\pi m_p}{T\Delta E}\,\frac{f(K)}{K}, \tag{5}$$

where K represents the momentum transfer which occurs during the scattering process. The total inelastic scattering cross section expressed as a function of T is then written as

$$Q(T)=\int_{K_{\min}}^{K_{\max}} I(K)\,dK, \tag{6}$$

where, from the kinematics of the reaction,

$$K_{\max}=m_r\left(\frac{2T}{m_p}\right)^{1/2}+\left[2m_r\left(\frac{Tm_r}{m_p}-\Delta E\right)\right]^{1/2}, \tag{7a}$$

$$K_{\min}=m_r\left(\frac{2T}{m_p}\right)^{1/2}-\left[2m_r\left(\frac{Tm_r}{m_p}-\Delta E\right)\right]^{1/2}, \tag{7b}$$

and m_r is the reduced mass of the projectile.

For the $(1s^2 2s^2)\,{}^1S \rightarrow (1s^2 2s2p)\,{}^1P$ transition of the Be-like ions, the correlated ground-state wave functions Ψ_g were written, following Sinanoğlu,[8] in the form

$$\Psi_g=\mathcal{A}\left[(1s\alpha)(1s\beta)(2s\alpha)(2s\beta)\left(1+\frac{1}{\sqrt{2!}}\,\frac{U_{1s1s}}{(1s\alpha)(1s\beta)}+\frac{1}{\sqrt{2!}}\,\frac{U_{2s2s}}{(2s\alpha)(2s\beta)}\right)\right], \tag{8}$$

where $\mathcal{A}$ is the antisymmetrizer and $\mathcal{A}[(1s\alpha)(1s\beta)(2s\alpha)(2s\beta)]$ represents the Hartree-Fock (HF) determinantal wave function. The terms U_{1s1s} and U_{2s2s} are K- and L-shell pair correlation functions, respectively. The HF orbitals were determined in the usual manner as a linear combination of functions within a basis set of Slater-type orbitals (STO's). The complete set of virtual orbitals arising from such a calculation were then used as expansion functions for the representation of each of the pair functions U_{1s1s} and U_{2s2s}. Further details concerning the construction of the wave function and the scheme of calculation will be reported at length in a forthcoming paper.[9] For our uncorrelated calculations of $f(K)$, Ψ_g was represented by the HF wave function alone. Turning now to the description of the $(1s^2 2s2p)\,{}^1P$ state for each ion, the correlated calculations used the excited-state wave function

$$\Psi_e = \mathcal{A}\left[[(1s\alpha)(1s\beta)(2s\alpha)(2p\beta) + (1s\alpha)(1s\beta)(2p\alpha)(2s\beta)] \left(1 + \frac{1}{\sqrt{2!}} \, \frac{U_{1s1s}}{(1s\alpha)(1s\beta)} \right) \right] \tag{9}$$

whereas the uncorrelated wave function for Ψ_e was written as

$$\mathcal{A}[(1s\alpha)(1s\beta)(2s\alpha)(2p\beta) + (1s\alpha)(1s\beta)(2p\alpha)(2s\beta)].$$

The $1s$ and $2s$ orbitals and the pair function U_{1s1s} were the same as those used in the construction of the ground-state wave functions; the $2p$ orbitals were taken from Tatewaki, Taketa, and Sasaki.[10] Such a choice of s functions for Ψ_e has the advantage of retaining orbital orthogonality with the ground state.

With an STO basis set, the use of the spherical wave expansion

$$e^{i\vec{K}\cdot\vec{r}} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(Kr) P_l(\theta) \tag{10}$$

reduces the evaluation of the matrix elements in $\mathcal{E}(K)$ to the determination of radial integrals of the type

$$A(\alpha, n, l, \beta) = \int_0^\infty e^{-\alpha r} r^n j_l(\beta r)\, dr .$$

Manipulation of this integral leads, after some detailed analysis, to the following result[11]

$$A(\alpha, n, l, \beta) = \left(\frac{\beta^l \Gamma(\frac{1}{2}) \Gamma(l+n+1)}{2^{l+1} \Gamma(l+\frac{3}{2})(\alpha^2+\beta^2)^{(l+n+1)/2}} \right) \times F\left(\frac{l+n+1}{2} ;\ \frac{1+l-n}{2} \,\middle|\, \frac{2l+3}{2} \,\middle|\, \frac{\beta^2}{\alpha^2+\beta^2} \right), \tag{11}$$

where $F(a; b\,|\,c\,|\,d)$ is the hypergeometric function. By use of the series expansion for F it is easy to show that, for $n > 1$, Eq. (11) reduces to the expression given by Geller.[12] For each ion, the L, $V1$ and $V2$ formulas for $\mathcal{E}(K)$ were used, in turn, to evaluate $f(K)$, first, using our correlated descriptions for Ψ_g and Ψ_e and, second, using the uncorrelated wave functions. In each instance, we used the experimental values for ΔE—a procedure which follows that adopted by Weiss.[13]

In Table I we present values for $f(K)$ which are the average of our correlated L, $V1$ and $V2$ calculations; these averaged results for each ion are also displayed in Fig. 1. For reasons of space, individual results arising from the uncorrelated and correlated "length" and "velocity" calculations are listed in Table II only for Be; $f_L(K)$, $f_{V1}(K)$ and $f_{V2}(K)$ are shown graphically, however, in Fig. 2 for selected ions. Our values for the optical oscillator strengths for each ion are compared with the results of other workers[14-22] in Table III. The electron and proton inelastic scattering cross sections for Be are given in Tables IV and V, respectively; for ease of discussion the results for $Q(T)$ are also presented in Figs. 3 and 4.

III. DISCUSSION

For the Be-like series, allowance for ground-state correlation effects is likely to be of even greater importance than that found by Kennedy and Kingston[3] for He. This will be especially true for the L shell since it is within this shell that excitation occurs. In addition, it is known[23, 24]

TABLE I. Average of the L, $V1$, and $V2$ values for the generalized oscillator strengths $f(K)$ for the ^1S-^1P transition of the Be-like ions, when $Z = 4$–8, derived from correlated wave functions.

K	Be	B^+	C^{++}	N^{3+}	O^{4+}
0.0	1.1252	0.9335	0.6974	0.5605	0.4697
0.1	1.0754	0.9222	0.6932	0.5585	0.4685
0.2	0.9402	0.8892	0.6808	0.5526	0.4652
0.3	0.7555	0.8370	0.6607	0.5427	0.4597
0.4	0.5618	0.7695	0.6335	0.5291	0.4520
0.5	0.3899	0.6914	0.6002	0.5120	0.4422
0.6	0.2548	0.6077	0.5619	0.4919	0.4305
0.7	0.1583	0.5232	0.5199	0.4690	0.4169
0.8	0.0945	0.4417	0.4757	0.4439	0.4018
0.9	0.0547	0.3661	0.4304	0.4171	0.3851
1.0	0.0310	0.2985	0.3852	0.3891	0.3673
1.1	0.0173	0.2397	0.3413	0.3604	0.3486
1.2	0.0096	0.1898	0.2995	0.3316	0.3291
1.3	0.0054	0.1486	0.2604	0.3030	0.3092
1.4	0.0030	0.1150	0.2244	0.2752	0.2892
1.5	0.0017	0.0882	0.1917	0.2483	0.2692
1.6	0.0010	0.0671	0.1626	0.2227	0.2494
1.7	0.0006	0.0507	0.1368	0.1987	0.2300
1.8	0.0003	0.0380	0.1144	0.1762	0.2113
1.9	0.0002	0.0284	0.0950	0.1554	0.1932
2.0	0.0001	0.0211	0.0785	0.1364	0.1760
2.1	0.0001	0.0156	0.0644	0.1192	0.1597
2.2	0.0000	0.0115	0.0526	0.1036	0.1443
2.3	0.0000	0.0085	0.0427	0.0897	0.1299
2.4	0.0000	0.0062	0.0346	0.0773	0.1166
2.5	0.0000	0.0045	0.0278	0.0663	0.1042
2.6	0.0000	0.0033	0.0223	0.0567	0.0929
2.7	0.0000	0.0024	0.0178	0.0483	0.0825
2.8	0.0000	0.0018	0.0142	0.0410	0.0730
2.9	0.0000	0.0013	0.0112	0.0346	0.0644
3.0	0.0000	0.0009	0.0089	0.0292	0.0567
3.1	0.0000	0.0007	0.0070	0.0245	0.0497
3.2	0.0000	0.0005	0.0055	0.0205	0.0435
3.3	0.0000	0.0003	0.0043	0.0171	0.0380
3.4	0.0000	0.0003	0.0034	0.0142	0.0330
3.5	0.0000	0.0002	0.0026	0.0118	0.0286

that, for the ground state of these ions, correlation produces shifts in the density for the 2s orbital of considerably greater magnitude than those which occur for the 1s orbital. Consequently, it is pleasing to note that, while we achieved about 90% of the generally accepted K-shell pair correlation energy for each ion, comparisons[9] with the results of other workers[25-27] for Be and B$^+$ suggest that our L-shell correlation energies are unlikely to differ from the exact values by more than about 1%. That K-shell correlation should also be included in our construction of Ψ_g and Ψ_e did seem desirable, however, in the light of comments by Burke, Hibbert, and Robb.[14] They suggested that the lack of core correlation will affect oscillator strengths determined by velocity formulas because the gradient operator is sensitive to changes in the wave functions close to the origin. Therefore, K-shell correlation was introduced into Ψ_g and Ψ_e and, since the HF density for this shell is almost completely independent of the state of the ion, the use of the same U_{1s1s} correlation function in Ψ_e as in Ψ_g represents a reasonable first approximation.

A. Generalized oscillator strengths

Let us now examine the characteristics of our $f(K)$ curves. Except at the value $K=0$, a comparison with other workers would not appear to be possible. It is seen from Fig. 1 that the $f(K)$ curves obtained from the average of the correlated L, $V1$ and $V2$ calculations are all of essentially similar shape. As Z becomes larger, we see a progressive decrease in the value of $f(K)$ for small K. For $K>1.5$, however, the order of the $f(K)$ curves in Fig. 1 is seen to have been reversed since, as Z increases, the transition density spans fewer oscillations of the operator $\sum_{j=1}^{N} \times \exp(iKz_j)$ in Eq. (2), for example, and thus gives rise to a smaller degree of cancellation within the integral expression for $\mathcal{E}(K)$. When K is sufficiently large, the cancellation causes each of our $f(K)$ curves to tend to zero. Finally, we also note that, as Z increases, ΔE will decrease to zero due to the degeneracy of the ^1S and ^1P states which occurs in the hydrogenic limit of $Z\rightarrow\infty$.

From the individual L, $V1$, and $V2$ curves shown in Fig. 2 for selected ions, we see that for large K the L and $V2$ results for $f(K)$ converge. For small values of K, we observe that $f_L(K)$ is greater than either $f_{V1}(K)$ or $f_{V2}(K)$. With the exception of the correlated results for Be, see Table II, this observation is valid for all ions for both correlated and uncorrelated calculations. When $K=0$, an equivalence occurs between the $V1$ and $V2$ values—as is clear from inspection of Eqs. (3) and (4). The relative spread of the correlated L, $V1$, and $V2$ curves with respect to their average becomes smaller as Z decreases suggesting that, overall, our $f(K)$ values for low Z may be more reliable than those for high Z. Such a conclusion is, of course, based on the customary assumption that consistency between results obtained using "length" and "velocity" formulas gives some measure of their reliability.

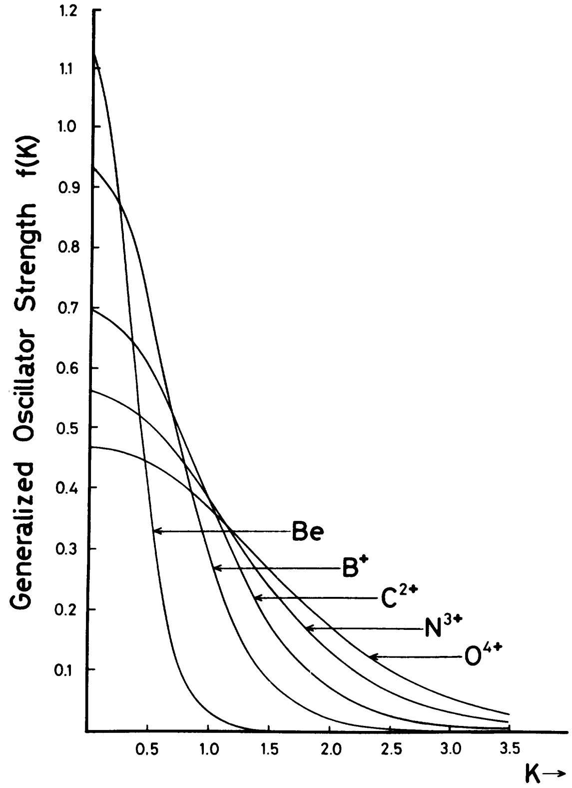

FIG. 1. Generalized oscillator strengths $f(K)$ for the ^1S-^1P transition of the Be-like ions obtained from the average of the L, $V1$ and $V2$ values derived from correlated wave functions.

Inspection of Table III reveals that our correlated results for $f(0)$ are in pleasing agreement with experiment over the whole Z range and, in addition, we note that our "velocity" values are generally superior to our "length" values. This latter observation may be a reflection of our inclusion of K-shell correlation effects in both the ground and excited states. Comparison with the best correlated calculations of Burke *et al.*[14] and also with the results of recent correlated studies by Nicolaides *et al.*[15] indicate that, in general, the present $f(0)$ values are in the closest agreement with experiment.

The influence of electron correlation on $f(K)$ for the $(1s^22s^2)\,^1S\rightarrow(1s^22s2p)\,^1P$ transition of the Be-

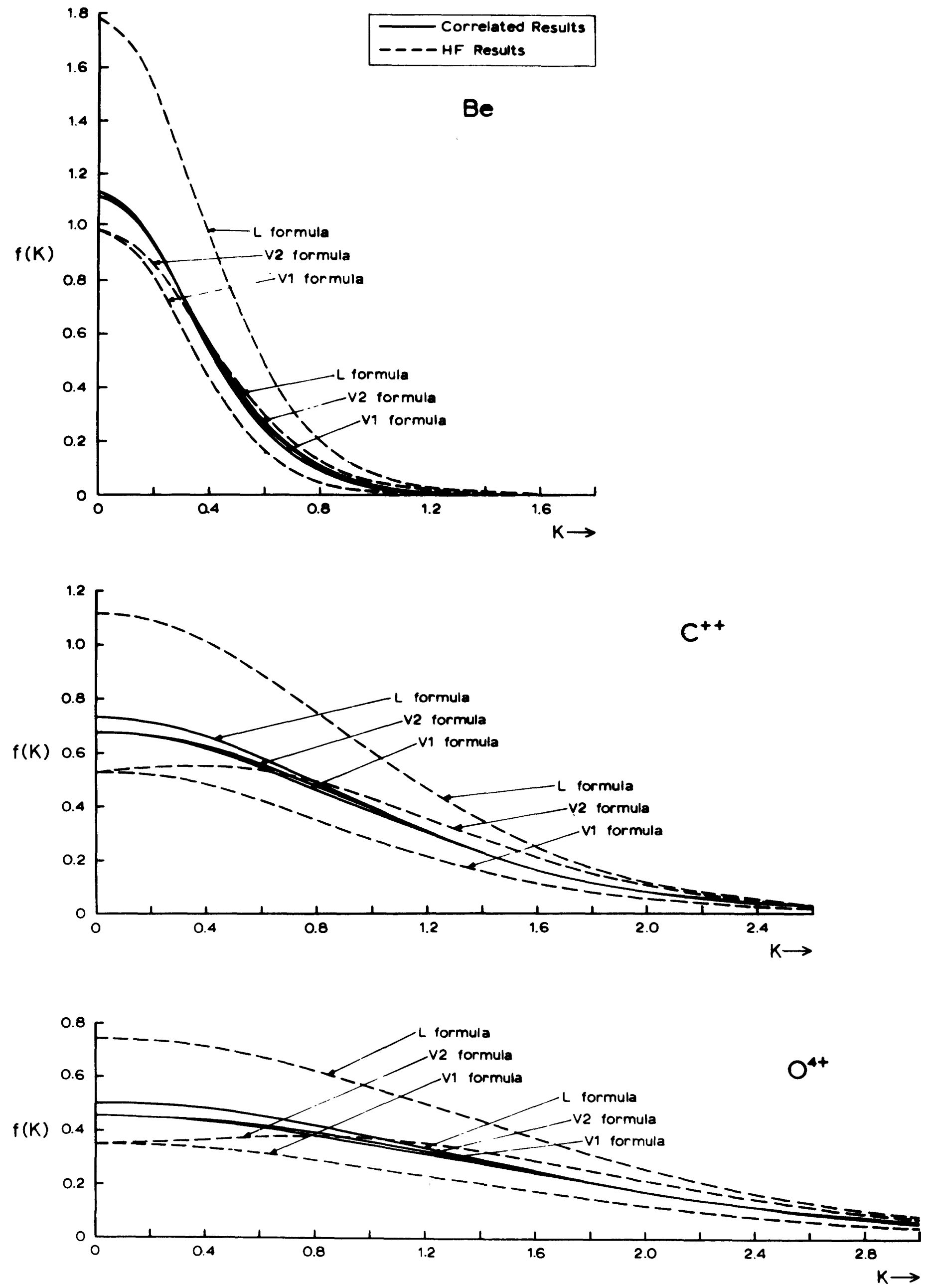

FIG. 2. Generalized oscillator strengths $f(K)$ for Be, C^{++}, and O^{4+} calculated using the L, $V1$, and $V2$ formulas. Results derived from correlated and uncorrelated wave functions are shown by solid and dashed lines, respectively.

like ions was found to have a dramatic effect. In Fig. 2 it is seen that, for small K, the "length" and "velocity" values differ by almost a factor of 2 when HF wave functions are used. However, the introduction of correlation into the description of Ψ_g and Ψ_e reduces this discrepancy to about 11% for $Z=8$ and to only 2% when $Z=4$. A striking improvement in the agreement amongst the L, $V1$, and $V2$ results also occurs over the whole K range for each ion.

We shall now comment on the correlation-induced changes which occur for the individual formulations of $f(K)$. For each ion, the $f_L(K)$ values were decreased in magnitude over the whole range of K whereas the reverse situation arose for the $V1$ formulation. For $V2$, however, the results for each ion revealed that correlation effects cause an increase in the generalized oscillator strength

TABLE II. Generalized oscillator strengths for the ${}^1S$-${}^1P$ transition of Be for three formulations of $\mathcal{E}(K)$ using HF and correlated wave functions.

Wave functions $\mathcal{E}(K)$ / K	Uncorrelated (HF) L	Uncorrelated (HF) $V1$	Uncorrelated (HF) $V2$	Correlated L	Correlated $V1$	Correlated $V2$
0.0	1.7812	0.9840	0.9840	1.1119	1.1319	1.1319
0.1	1.7122	0.9349	0.9515	1.0654	1.0805	1.0802
0.2	1.5228	0.8025	0.8601	0.9382	0.9413	0.9410
0.3	1.2575	0.6241	0.7266	0.7622	0.7511	0.7532
0.4	0.9697	0.4416	0.5746	0.5744	0.5524	0.5587
0.5	0.7033	0.2857	0.4273	0.4045	0.3773	0.3878
0.6	0.4838	0.1700	0.3010	0.2684	0.2417	0.2543
0.7	0.3183	0.0934	0.2025	0.1693	0.1466	0.1591
0.8	0.2021	0.0477	0.1312	0.1025	0.0852	0.0958
0.9	0.1248	0.0226	0.0827	0.0601	0.0479	0.0560
1.0	0.0755	0.0084	0.0510	0.0344	0.0264	0.0321
1.1	0.0450	0.0041	0.0311	0.0194	0.0144	0.0181
1.2	0.0266	0.0016	0.0187	0.0108	0.0079	0.0102
1.3	0.0156	0.0006	0.0113	0.0060	0.0044	0.0057
1.4	0.0091	0.0002	0.0067	0.0033	0.0025	0.0032
1.5	0.0053	0.0001	0.0040	0.0019	0.0015	0.0018
1.6	0.0031	0.0000	0.0024	0.0010	0.0009	0.0010
1.7	0.0018	0.0000	0.0014	0.0006	0.0006	0.0006
1.8	0.0011	0.0000	0.0009	0.0003	0.0004	0.0003
1.9	0.0006	0.0000	0.0005	0.0002	0.0003	0.0002
2.0	0.0003	0.0000	0.0003	0.0001	0.0002	0.0001
2.1	0.0002	0.0000	0.0002	0.0001	0.0001	0.0001
2.2	0.0001	0.0000	0.0001	0.0000	0.0001	0.0000
2.3	0.0001	0.0000	0.0001	0.0000	0.0001	0.0000
2.4	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
2.5	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000

at small K and a decrease at large K. These trends can be seen in Fig. 2 for the selected ions Be, C^{++}, and O^{4+}. Comparing the relative magnitude of the changes within each formulation, it was found that, at small K, the greatest percentage shift was, quite markedly, always associated with the L formula. When $K > 1.5$, the relative changes in both the "length" and "velocity" values were, with the exception of Be (see Table II), roughly of the same order of magnitude.

B. Inelastic-scattering cross sections

The use of the first Born approximation for the calculation of inelastic scattering cross sections becomes increasingly unreliable as the scattering target becomes more highly ionized. Consequent-

TABLE III. A comparison with experiment of the optical oscillator strengths, $f(0)$, for the ${}^1S$-${}^1P$ transition of the Be-like ions when calculated from correlated wave functions using the L and V formulas.

Source	Formula	Be	B^+	C^{++}	N^{3+}	O^{4+}
Present work	L	1.1119	0.9678	0.7341	0.5958	0.5036
	V	1.1319	0.9163	0.6790	0.5429	0.4527
Burke, Hibbert, and Robb(a)	L	1.4237	1.0480	0.7930	0.6293	0.5250
	V	1.3862	1.0064	0.8047	0.5954	0.4922
Nicolaides, Beck, and Sinanoğlu(b)	L	1.25	1.00	0.760	0.605	0.513
	V	1.14	1.07	0.780	0.631	0.525
Experiment		1.21 ± 0.03(c) 1.08 ± 0.05(d)	0.83 ± 0.09(e) 0.73 ± 0.07(f) 0.9 ± 0.2(g)	0.65 ± 0.03(h)	...	0.42 ± 0.05(i)

(a) Reference 14.
(b) Reference 15.
(c) Reference 16.
(d) Reference 17.
(e) Reference 18.
(f) Reference 19.
(g) Reference 20.
(h) Reference 21.
(i) Reference 22.

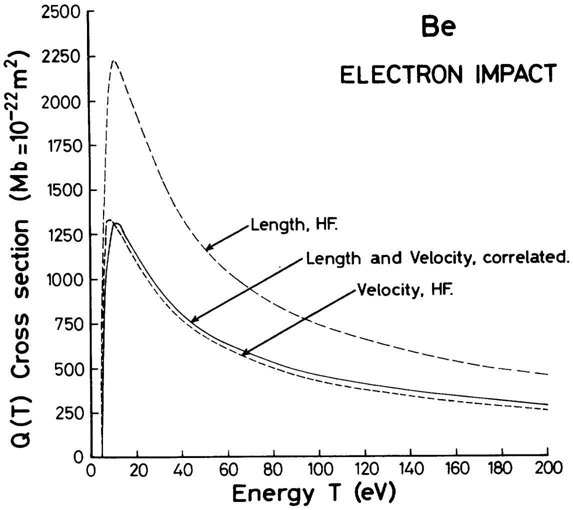

FIG. 3. Inelastic scattering cross section $Q(T)$ for the ${}^1S$-${}^1P$ transition of Be on electron impact using the L and $V2$ formulas. Solid and dashed curves are derived from correlated and uncorrelated wave functions, respectively.

ly, in the present work, $Q(T)$ for both proton and electron scattering was evaluated only for Be. For each projectile, correlated and uncorrelated calculations were performed using the corresponding results for both $f_L(K)$ and $f_{V2}(K)$; the integration in Eq. (6) was carried out by standard numerical procedures. As far as we know, no comparable results exist for the inelastic scattering cross sections of either protons or electrons from a Be target.

Figures 3 and 4 show that both cross sections rise rapidly from a threshold energy, pass through a fairly sharp maximum, and then exhibit a steady fall in magnitude with increasing projectile energy. When the ground and excited states are described by HF wave functions the discrepancy between the L and $V2$ results is considerable whereas, after the introduction of our correlation terms U_{1s1s} and U_{2s2s}, the curves for $Q_L(T)$ and $Q_{V2}(T)$ become graphically indistinguishable—except for a small separation in the energy region 5–30 keV which occurs for the proton scattering curve. Inspection of the correlated results in Tables IV and V does indicate, however, that, for each projectile, $Q_L(T) > Q_{V2}(T)$ at small T and, at large T, the order becomes reversed. Further, by comparison with the significant shifts which occur for the L-based curves, the $V2$ results would appear to be relatively insensitive to the use of correlated wave functions. Hence, if the graphical agreement between our correlated L and $V2$ results is indicative of their reliability compared with experiment, the uncorrelated $V2$ values for each interaction would seem, on the whole, to be surprisingly acceptable. A similar observation has also been noted by Kennedy and Kingston[3] in their examination of He. Clearly, since near-HF wave functions can now be obtained with relative ease, it would be convenient if such an observation could be shown to possess generality.

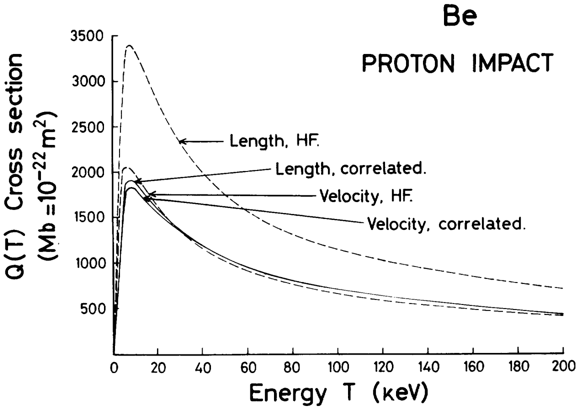

FIG. 4. Inelastic scattering cross section $Q(T)$ for the ${}^1S$-${}^1P$ transition of Be on proton impact using the L and $V2$ formulas. Solid and dashed curves are derived from correlated and uncorrelated wave functions, respectively.

IV. SUMMARY

Generalized oscillator strengths $f(K)$ have been calculated for the $(1s^2 2s^2)\,{}^1S \rightarrow (1s^2 2s 2p)\,{}^1P$ transition for the $Z = 4$–8 series of Be-like ions. For each ion, results were obtained using the "length" equation and two versions of the "velocity" formulation, here referred to as L, $V1$, and $V2$, respectively. An agreement amongst such results, when using approximate wave functions, is often taken as a measure of their reliability, although the occurrence of a chance agreement must always be kept in mind. Following the many-electron theory of Sinanoğlu, electron correlation was introduced into the K and L shells for the ground-state wave functions and the K shell for the excited-state wave functions by means of intrashell pair correlation functions U_{1s1s} and U_{2s2s}. To enable us to judge the importance of such correlation effects, values for $f(K)$ were also determined by using a Hartree-Fock description for both states. Details of wave functions, both correlated and uncorrelated, their energies, and several expectation values are being reported in a separate paper. For Be, the $f(K)$ values were used, within the first Born approximation, to determine the total inelastic scattering cross section $Q(T)$, where T is the incident energy of the projectile, for both proton and electron impact.

TABLE IV. Inelastic electron scattering cross sections $Q(T)$ for the ${}^1S$-${}^1P$ transition of Be (measured in units of 10^{-22} m^2).

Wave functions $\mathcal{E}(K)$ T(eV)	Uncorrelated (HF)		Correlated	
	L	$V2$	L	$V2$
6.0	1372.09	847.88	766.68	730.46
7.0	1860.28	1136.11	1055.72	1013.06
8.0	2076.76	1257.70	1191.12	1148.69
9.0	2178.00	1310.66	1258.79	1218.48
10.0	2219.20	1328.80	1290.06	1252.41
15.0	2118.51	1249.76	1251.47	1225.60
20.0	1919.21	1123.48	1142.42	1123.94
25.0	1737.89	1012.36	1039.27	1025.46
30.0	1585.18	920.20	950.96	940.28
35.0	1457.53	843.88	876.44	867.96
40.0	1349.99	780.00	813.27	806.40
45.0	1258.40	725.84	759.21	753.57
50.0	1179.46	679.34	712.46	707.77
55.0	1110.77	639.00	671.66	667.73
60.0	1050.44	603.66	635.75	632.43
65.0	996.95	572.39	603.85	601.03
70.0	949.18	544.52	575.31	572.91
75.0	906.25	519.51	549.63	547.58
80.0	867.45	496.93	526.39	524.63
85.0	832.21	476.46	505.26	503.76
90.0	800.05	457.79	485.96	484.67
95.0	770.53	440.67	468.22	467.13
100.0	743.32	424.92	451.87	450.94
200.0	447.72	254.57	273.35	273.67
300.0	327.55	185.79	200.37	200.89
400.0	261.66	148.19	160.26	160.82
500.0	219.58	124.22	134.60	135.16
600.0	190.05	107.42	116.58	117.12
700.0	168.03	94.91	103.13	103.65
800.0	150.90	85.19	92.66	93.16
900.0	137.15	77.39	84.24	84.72
1000.0	125.85	70.98	77.32	77.78

TABLE V. Inelastic proton scattering cross sections $Q(T)$ for the ${}^1S$-${}^1P$ transition of Be (measured in units of 10^{-22} m^2).

Wave functions $\mathcal{E}(K)$ T(keV)	Uncorrelated (HF)		Correlated	
	L	$V2$	L	$V2$
1.0	666.31	464.09	282.93	265.39
2.0	1872.07	1229.41	925.26	866.13
3.0	2620.93	1676.67	1373.43	1293.56
4.0	3029.02	1906.66	1637.38	1551.08
5.0	3240.83	2016.95	1786.28	1700.31
6.0	3340.12	2061.05	1865.86	1783.16
7.0	3373.60	2067.72	1903.26	1824.97
8.0	3367.83	2052.85	1914.49	1840.92
9.0	3338.27	2025.53	1909.23	1840.33
10.0	3294.36	1991.12	1893.53	1829.03
15.0	3004.66	1791.94	1754.44	1707.37
20.0	2722.70	1610.86	1603.57	1567.77
25.0	2483.49	1461.33	1470.85	1442.63
30.0	2283.80	1338.43	1357.94	1335.07
35.0	2116.05	1236.25	1261.96	1243.02
40.0	1973.54	1150.10	1179.75	1163.78
45.0	1851.00	1076.44	1108.62	1094.98
50.0	1744.51	1012.73	1046.52	1034.73
55.0	1651.07	957.03	991.81	981.53
60.0	1568.30	907.86	943.20	934.16
65.0	1494.45	864.10	899.71	891.72
70.0	1428.14	824.90	860.57	853.46
75.0	1368.19	789.54	825.12	818.76
80.0	1313.68	757.45	792.82	787.12
85.0	1263.89	728.17	763.28	758.13
90.0	1218.20	701.36	736.13	731.48
95.0	1176.14	676.70	711.11	706.89
100.0	1137.25	653.93	687.95	684.11
200.0	704.55	402.36	428.64	428.00
300.0	523.23	297.88	319.13	319.26
400.0	420.66	239.04	256.96	257.35
500.0	353.91	200.85	216.41	216.91
600.0	306.98	174.04	187.86	188.41
700.0	272.10	154.13	166.62	167.18
800.0	245.01	138.70	150.12	150.69
900.0	223.30	126.33	136.87	137.44
1000.0	205.43	116.17	125.97	126.53

With the exception of $f(0)$, the optical oscillator strength, no other comparisons with our $f(K)$ values are available. In that instance, not only is correlation found to be essential for consistency to be achieved between the "length" and "velocity" results but, over the whole Z range, our correlated values for $f(0)$ compare very well indeed with experiment. This is noticeably so for the V results, thus lending support to the comments of Burke *et al.* that, for this formulation of $f(0)$ in particular, an allowance for core correlation in the wave functions can be of importance.

The relative spread of the correlated L, $V1$, and $V2$ values for $f(K)$ about their average value decreases over the whole K range as Z becomes smaller thus suggesting increased reliability. The almost graphical indistinguishability amongst the $f(K)$ results for a low-Z value was found to be dramatically dependent on the introduction into the wave functions of our correlation terms U_{1s1s} and U_{2s2s}. Throughout the series, electron correlation causes its greatest change in the $f(K)$ values when K is small and this is particularly apparent for the L formula; at large K, the magnitude of the change for any given ion is of roughly similar order for each of the three formulations.

The graphical agreement between the correlated "length" and "velocity" based curves for $Q(T)$ is very striking for both proton and electron impact. As expected from the behavior of the $f(K)$ curves, the L-based values for $Q(T)$ show a marked sensitivity to the introduction of electron correlation. By comparison, the $V2$ values for both projectiles are relatively insensitive to correlation, the HF results being, in general, only slightly smaller than the correlated values.

As far as we can judge, the correlated results presented here for the Be-like ions are sufficiently encouraging for us to extend our use of intrashell pair correlated wave functions to the determination and examination of photoionization cross sections. A report of this work is now nearing completion.

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