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Inelastic Scattering of Fast Electrons from Simple Closed Shell Atoms. I. He, Be*

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The inelastic collision of fast electrons with ground state closed shell atoms is investigated within the context of First Born Approximation and Random Phase Approximation. Generalized oscillator strengths and total cross sections for $1^1S \rightarrow n^1D$ transitions in He and $1^1S \rightarrow n^1S$ in Be are evaluated and discussed.

Key words: Electron inelastic scattering from He and Be.

1. Introduction

The knowledge of absolute values for inelastic cross sections of elementary processes has recently become increasingly important in research fields as different as plasma and atmospheric physics, radiation physics and astrophysics. There has been, in particular, in the last few years, a growing development of both experimental and theoretical techniques with the intent of attaining detailed

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information about inelastic collision processes between high-energy electrons and atomic systems. The crucial quantity involved in the evaluation of First Born Approximation (FBA) differential cross sections for inelastic scattering of a charged particle is the so-called generalized oscillator strength [1–3], which can be regarded as the response of an atomic (or molecular) system to a sudden change in the momentum of its electrons. The evaluation of this transition property requires the knowledge of the wavefunctions for both ground and excited states of the system under consideration; since these wavefunctions are most frequently known only imperfectly (especially for excited states), their approximate nature raises reasonable doubts on the reliability of the results, which appear in various cases quite sensitive to the choice of the wavefunctions employed [4–6].

In this paper we propose to calculate generalized oscillator strengths (GOS) and related inelastic scattering total cross sections for electron scattering from ground state He and Be atoms, in the First Born Approximation, by using the Random Phase Approximation (RPA) [7–10]. As well known, this approach avoids the need for separately computing ground- and excited-state wavefunctions, leading directly to transition properties of atoms and molecules, while retaining in general the proper physical effects needed for quantitative accuracy of the final results.

The choice for such simple systems like Helium and Beryllium has been suggested by our desire of checking the validity of the approach (FBA + RPA), in view of its extension to molecular systems, through possible comparison with other very recent theoretical treatments as well as accurate experimental results. At the same time we have been enabled to verify, in a simple way, the one-centre portion of a general computer program for evaluating Fourier transforms of charge distributions described in terms of STO's, along the lines of a recently proposed approach [11].

2. Theory

The generalized oscillator strength $F_{fi}(q)$ for a transition of an N-electron atom from the initial state $|i\rangle$ to the final state $|f\rangle$ is defined as (atomic units are used throughout this paper unless differently indicated)

$$F_{fi}(q) = \frac{2}{q^2} E_{fi} \left| \langle f | \sum_{j=1}^{N} \exp(i\boldsymbol{q} \cdot \boldsymbol{r}_j) | i \rangle \right|^2 \tag{1}$$

where $\boldsymbol{q} = \boldsymbol{k}_i - \boldsymbol{k}_f$ is the momentum transfer which occurs during the scattering process and $E_{fi} = E_f - E_i$ the excitation energy from the state $|i\rangle$ to the state $|f\rangle$ of the target.

Within the First Born Approximation, the differential cross section for inelastic scattering of a fast charged (structureless) projectile (mass M_p, charge Z_p) from an atomic target is related to $F_{fi}(q)$ by

$$\frac{d\sigma_{fi}}{d\Omega} = \frac{2}{q^2} (M_p Z_p)^2 \frac{|\boldsymbol{k}_f|}{|\boldsymbol{k}_i|} \frac{F_{fi}(q)}{E_{fi}}. \tag{2}$$

The total inelastic scattering cross section

$$\sigma_{fi} = \int \frac{d\sigma_{fi}}{d\Omega} d\Omega = 2\pi \int_0^{\pi} \frac{d\sigma_{fi}}{d\Omega} \sin\theta \, d\theta \tag{3}$$

by using simple kinematic arguments, can be cast into the form

$$\sigma_{fi} = \frac{\pi M_p Z_p^2}{E_p E_{fi}} \int_{(k_f - k_i)^2}^{(k_f + k_i)^2} \frac{F_{fi}(q^2)}{q^2} d(q^2) \tag{4}$$

where $E_p = k_i^2/2M_p$ is the kinetic energy of the impinging projectile.

The *ab initio* prediction of FBA total cross sections is therefore essentially reduced to the evaluation of the transition properties E_{fi} and $F_{fi}(q^2)$; the integration appearing in Eq. (4) can, in fact, be carried out conveniently after expressing $F_{fi}(q^2)$ in the analytical form first suggested by Lassettre [12–15].

Details about the RPA method, by which we have approached in the present paper the evaluation of E_{fi} and $F_{fi}(q^2)$, are available in many papers (see, for instance, Refs. [7–10]) and will not be recalled.

3. Results

Although we have performed RPA calculations for several final states of He and Be pertaining to ^1S, ^1P and ^1D symmetries, in this paper only results for the transitions $1^1S \rightarrow n^1D$ ($n = 3, 4, 5$) in He and $(1s)^2(2s)^2 1^2S \rightarrow (1s)^2(2s)(ns)^1S$ ($n = 3, 4, 5$) in Be are presented. The results for some transition properties of He and Be are collected in Table 1 and Table 2, respectively; they have been obtained by stating the RPA problem in a matrix form, the involved hole and particle states being associated with occupied and virtual MO's solutions to the HF equations in the V^N potential [19–21]. The HF MO's were, in turn, built up in terms of extended basis sets of STO's with properly chosen quantum numbers and orbital exponents. For both He and Be, our computed excitation energy values are in complete agreement with those obtained by other authors [16, 22] using

Table 1. RPA transition properties of some ^1D final states of He atom

Transition	Excitation energy (a.u.)			$(dF_{n0}/dq^2)_{q=0}$ (a.u.)		
	Present paper	MSM[a]	Expt.[b]	Present paper	ACRZ[c]	BKK[d]
$1^1S \rightarrow 3^1D$	8.624 (−1)	8.624 (−1)	8.480 (−1)	9.27 (−3)	9.1 (−3)	8.94 (−3)
$1^1S \rightarrow 4^1D$	8.867 (−1)	8.867 (−1)	8.724 (−1)	4.77 (−3)	4.7 (−3)	
$1^1S \rightarrow 5^1D$	8.980 (−1)	8.979 (−1)	8.837 (−1)	2.54 (−3)	2.6 (−3)	

[a] See Ref. [16].
[b] Moore, C. E.: Atomic Energy Levels, Natl. Bur. Stds. Circ. No. 467 (U.S. GPO, Washington, D.C., 1949).
[c] See Ref. [17].
[d] Value deduced by the present authors from data appearing in Ref. [18].

Table 2. RPA transition energies for some ^1S final states of Be atom

Transition	Energy (a.u.) Present paper	SWD[a]	Expt.[b]
$(1s)^2(2s)^2\,{}^1S \rightarrow (1s)^2(2s)(3s)^1S$	2.249 (−1)	2.2485 (−1)	2.491 (−1)
$(1s)^2(2s)^2\,{}^1S \rightarrow (1s)^2(2s)(4s)^1S$	2.668 (−1)	2.6683 (−1)	2.973 (−1)
$(1s)^2(2s)^2\,{}^1S \rightarrow (1s)^2(2s)(5s)^1S$	2.839 (−1)	2.8382 (−1)	3.159 (−1)
$(1s)^2(2s)^2\,{}^1S \rightarrow (1s)(2s)^2(3s)^1S$	4.602	4.6011	
$(1s)^2(2s)^2\,{}^1S \rightarrow (1s)(2s)^2(4s)^1S$	4.680	4.6796	

[a] See Ref. [21].
[b] See footnote b of Table 1.

equivalent, although formally different approaches and can thus be regarded free from basis set effects: as a consequence, their discrepancy with respect to experimental data reflects only inherent flaws of the RPA method. In Table 1, in addition to excitation energies we have reported values for $(dF_{n0}/dq^2)_{q=0}$, the initial slope of the generalized oscillator strength versus the (square) transferred impulse q^2 (see Eq. (1)). This quantity which is proportional to the quadrupole oscillator strength $2E_{nD,1S} \cdot |(\sum_j r_j^2 \cdot P_{20}(\hat{r}_j))_{nD,1S}|^2$, is expected to be a sensitive test for the approximate model employed, in the case of optically forbidden transitions [3, 23]. The excellent agreement with recent calculations by Amusia et al. [17], who have exactly solved the RPA problem by integrating numerically the relevant time-dependent HF equations [24, 25], is obvious. For the transition $1^1S \rightarrow 3^1D$, an accurate $(dF/dq^2)_{q=0}$ value is available from calculations of Bell et al. [18] in terms of correlated wavefunctions of high quality: its comparison with the RPA estimates is quite favourable and supports the reliability of our computations. Because of the lack of comparison terms, in the case of Be we have not presented any values for the derivative $(dF_{nS,1S}/dq^2)_{q=0}$, which is proportional to the monopole oscillator strength $2E_{nS,1S}|(\sum_j r_j^2)_{nS,1S}|^2$.

Generalized oscillator strength (GOS) values for a few transitions $1^1S \rightarrow n^1D$ in He and $1^1S \rightarrow n^1S$ in Be are plotted versus q^2 in Figs. 1 and 2, respectively. The qualitative behaviour of the curves is easily understood considering Eq. (1) as $q^2 \rightarrow \infty$ and taking into account that for optically forbidden excitations $F_{n0}(0) = 0$. While our RPA values for the GOS relative to the transitions in He atom are in good agreement with previous accurate calculations [18], comparisons are lacking in the case of Be, for which we are unaware of existing GOS data relative to excitations $1^1S \rightarrow n^1S$. In view of the close agreement between our results (not presented here) and those obtained by Amusia et al. [26] for some low-lying states of Be pertaining to the symmetries ^1P and ^1D, our generalized oscillator strengths for the (monopole) transitions $1^1S \rightarrow n^1S$ in Be (Fig. 2) are to be considered as converged to the correct RPA values; to this regard we recall, incidentally, that there are not particular troubles encountered in solving the RPA problem for bound-bound transitions between states both of S symmetry by the approach pursued in this paper, contrary to what occurs in the procedure worked out in Ref. [26].

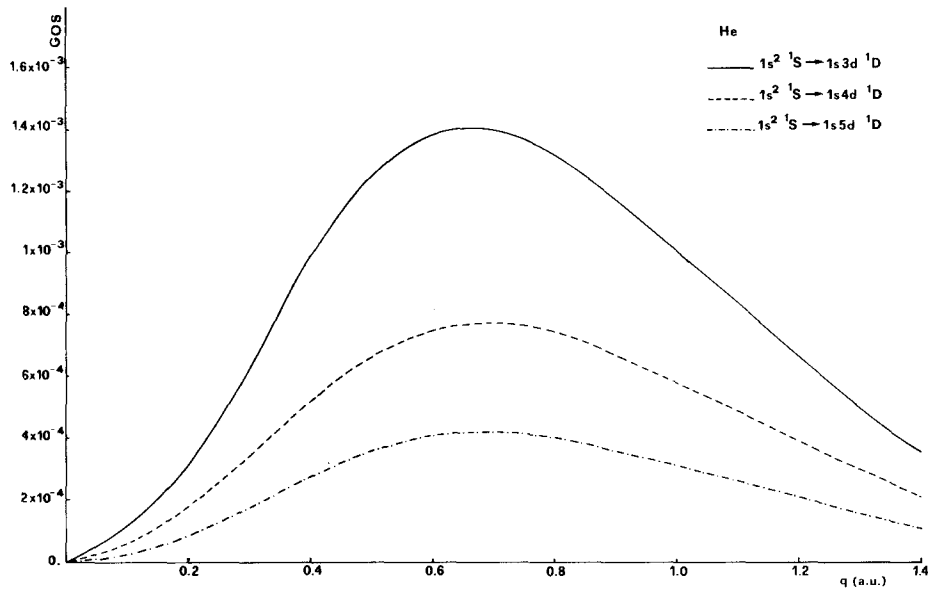

Fig. 1. RPA generalized oscillator strengths versus q^2 (a.u.) for the transitions $1^1S \rightarrow n^1D$ ($n = 3, 4, 5$) of He atom

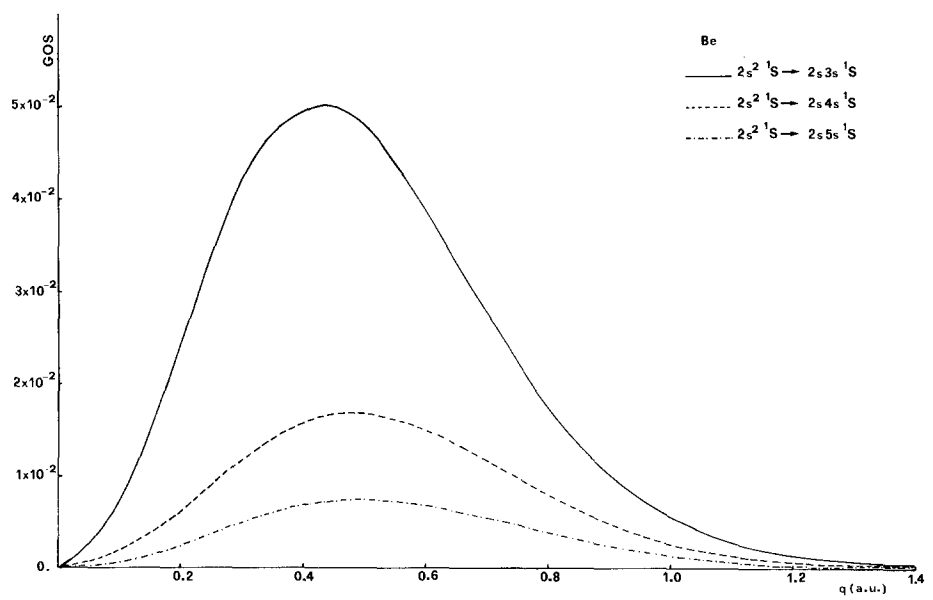

Fig. 2. RPA generalized oscillator strengths versus q^2 (a.u.) for the transitions $(2s)^2 \rightarrow (2s)(ns)$ ($n = 3, 4, 5$) of Be atom

Some caution should be used before accepting indiscriminately RPA estimates for transition properties. This is particularly true in the case of Be, because the two hole-two particle excitations rejected in the RPA model play a definitely important role when dealing with atoms of the alkaline-earth group. This assertion is readily understood on considering that the HF approximation $|(1s)^2(2s)^2\rangle$ to the ground state wavefunction of Be is a rather modest one, since it ignores important mixing effects arising from the (non-dynamical) interaction with the (rather low-lying) doubly excited configuration $|(1s)^2(2p)^2(^1S)\rangle$ [27, 28]; introducing correlation effects of this kind for the ground state and the excited state as well (so as to make allowance, in a balanced way, for the overall correlative correction) requires the overcoming of the one hole-one particle excitation model.

Total cross section data for He and Be are collected in Table 3 and Table 4, respectively, for several values of the incident electron energy. In view of the high energies involved, exchange contributions to the First Born amplitude are expected to be negligible and have not been taken into account. The values reported for the cross sections reflect obviously the accuracy of the basic generalized oscillator strengths: in face of the good agreement for He, which is immediately recognized by comparing RPA and accurate results to each other, for Be we are in the

Table 3. Total cross section values (a_0^2 units) for inelastic scattering e–He

E_{inc} (eV)		$1^1S \rightarrow 3^1D$	$1^1S \rightarrow 4^1D$	$1^1S \rightarrow 5^1D$
200	Present paper	0.1824 (−2)	0.9643 (−3)	0.4986 (−3)
	BKK[a]	0.1838 (−2)	0.98 (−3)	0.54 (−3)
400	Present paper	0.9689 (−3)	0.5119 (−3)	0.2643 (−3)
	BKK	0.9739 (−3)	0.52 (−3)	0.29 (−3)
500	Present paper	0.7843 (−3)	0.4143 (−3)	0.3139 (−3)
	BKK	0.7878 (−3)	0.42 (−3)	0.23 (−3)
1000	Present paper	0.4014 (−3)	0.2120 (−3)	0.1094 (−3)
	BKK	0.4028 (−3)	0.21 (−3)	0.12 (−3)
2000	Present paper	0.2030 (−3)	0.1072 (−3)	0.5534 (−4)
	BKK	0.2036 (−3)	0.11 (−3)	0.60 (−4)

[a] Ref. [18].

Table 4. Total cross section values (a_0^2 units) for inelastic scattering e-Be

E_{inc} (eV)	$(2s)^2 \rightarrow 2s3s$	$(2s)^2 \rightarrow 2s4s$	$(2s)^2 \rightarrow 2s5s$
200	0.267	0.716 (−1)	0.297 (−1)
400	0.135	0.361 (−1)	0.150 (−1)
500	0.108	0.290 (−1)	0.120 (−1)
1000	0.543 (−1)	0.145 (−1)	0.60 (−2)
2000	0.272 (−1)	0.73 (−2)	0.30 (−2)

position of stating that the results of Table 4 are almost surely close to the RPA values for the total cross sections corresponding to transitions $1^1S \rightarrow n^1S$: the relation between RPA and accurate results is still to be explored.

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