

Oscillator strengths for the magnesium isoelectronic sequence*

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The relativistic random-phase approximation is used to calculate the excitation energies and absorption oscillator strengths for the $3s^2\ ^1S_0-3s3p\ ^1P_1$, $-3s4p\ ^1P_1$, $-3s5p\ ^1P_1$, and $-3s3p\ ^3P_1$ transitions of selected elements of the magnesium isoelectronic sequence through nuclear charge $Z = 92$. The results are compared with previous theoretical and experimental values. The data plotted as a function of Z^{-1} enable us to study deviations from the predictions of the nonrelativistic Z -expansion theory.

I. INTRODUCTION

Accurate absorption oscillator strengths for highly stripped atoms are needed in astrophysics for the determination of solar abundances, temperatures, and densities and in the study of laboratory plasmas both for diagnostic purposes and for the determination of the effects of impurities on controlled thermonuclear fusion.

In order to calculate reliable values for transition rates and oscillator strengths, the effects of interelectron correlation must be taken into account. The nonrelativistic random-phase approximation¹ (RPA) has been very successful in including the most important correlation effects for systems with small nuclear charges (Z), but as the nuclear charge increases along the isoelectronic sequence, relativistic effects become important also.^{2,3} A random-phase approximation treating relativistic effects nonperturbatively (RRPA) has been applied to the calculation of oscillator strengths of the resonance transitions of elements of the helium^{4,5} and beryllium⁶ isoelectronic sequences, as well as to transitions between excited states of heliumlike ions.⁷ A relativistic calculation of oscillator strengths enables the study of systematic trends to be continued into the high Z end of the isoelectronic sequence where nonrelativistic calculations break down. For low Z elements, where relativistic effects are expected to be unimportant, a relativistic calculation has the virtue that forbidden transitions are obtained in the same manner as allowed transitions.

In this paper, we calculate the excitation energies and absorption oscillator strengths for the allowed resonance transitions $3s^2\ ^1S_0-3s3p\ ^1P_1$, $-3s4p\ ^1P_1$, $-3s5p\ ^1P_1$, and for the intercombination transition $3s^2\ ^1S_0-3s3p\ ^3P_1$ of elements of the magnesium isoelectronic sequence. We use the RRPA in a frozen core approximation which neglects correlations with the $1s$, $2s$, and $2p$ inner-shell electrons.

II. THEORY

The equations of the RRPA are derived using the time-dependent Hartree-Fock (TDHF) method.⁸ The ground state of an N -electron closed-shell atom is described by a single determinant constructed of the N Dirac-Hartree-Fock (DHF) orbitals $u_i(\vec{r})$. An external field $A_+e^{-i\omega t} + A_-e^{i\omega t}$ of frequency ω induces perturbations $w_{i\pm}$ in the orbitals u_i which then take the form

$$u_i(\vec{r}) + w_{i+}(\vec{r})e^{-i\omega t} + w_{i-}(\vec{r})e^{i\omega t}. \quad (1)$$

Using the variational principle

$$\{\delta\Psi(t), (H - i\partial/\partial t)\Psi(t)\} = 0,$$

where

$$H = \sum_{i=1}^N \vec{\alpha}_i \cdot \vec{p}_i + \beta_i m - \frac{Ze^2}{r_i} + \sum_{i>j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

is the Dirac Hamiltonian in natural units for an N electron atom, we obtain the zero-order equations, which are just the usual DHF equations, by equating to zero the terms containing neither the external field nor the perturbations. The first-order equations, obtained by linearizing in the perturbations and the external field, and separately equating the coefficients of $\exp(\pm i\omega t)$ equal to zero, are the RRPA equations

$$(h_0 + V - \epsilon_i \mp \omega)w_{i\pm} = (A_{\pm} - V_{\pm}^{(1)})u_i, \quad i = 1, 2, \dots, N, \quad (2)$$

where

$$h_0 = \vec{\alpha} \cdot \vec{p} + \beta m - e^2 Z/r,$$

$$Vw_i = \sum_{j=1}^N e^2 \int \frac{d^3r'}{|\vec{r} - \vec{r}'|} [(u_j^* u_i)'] w_i - (u_j^* w_i) u_j,$$

$$V_{\pm}^{(1)} u_i = \sum_{j=1}^N e^2 \int \frac{d^3r'}{|\vec{r} - \vec{r}'|} [(u_j^* w_{j\pm})' u_i + (w_{j\pm}^* u_j) u_i - (w_{j\pm}^* u_i) u_j - (u_j^* u_i) w_{j\pm}]$$

with A_{\pm} the amplitude of the external perturbation

of frequency $\pm\omega$ and ϵ_i the orbital eigenvalue of the i th DHF equation.

An eigenvalue problem for the atomic excitation energies ω_k and the eigenfunctions $w_{i k \pm}$ is obtained from the set of homogeneous equations which results from setting the perturbing external field, A_{\pm} , equal to zero in Eqs. (2). Normalization of the eigenfunctions is such that

$$\sum_{i=1}^N (\langle w_{i k+} | w_{i k+} \rangle - \langle w_{i k-} | w_{i k-} \rangle) = 1. \quad (3)$$

The transition rate from an excited state k to the ground state 0 by emission of a single photon, for electric multipole radiation, is given by

$$A_{k \rightarrow 0} = 8\pi \alpha \omega_k \left| \sum_{i=1}^N (\langle u_i | \vec{a}_{J M}^{(1)*} \cdot \vec{\alpha} | w_{i k+} \rangle + \langle u_i | \vec{\alpha} \cdot \vec{a}_{J M}^{(1)} | w_{i k-} \rangle) \right|^2, \quad (4)$$

where J and M are the photon angular momentum quantum numbers and where

$$\vec{a}_{J M}^{(1)} = [j_J'(\omega r) + j_J(\omega r)/\omega r] \vec{Y}_{J M}^{(1)}(\hat{r}) + [J(J+1)]^{1/2} j_J(\omega r) \vec{Y}_{J M}^{(1)}(\hat{r})/\omega r \quad (5)$$

is the vector potential of the multipole field in the Coulomb gauge with j_J a spherical Bessel function and $Y_{J M}^{(1)}$ vector spherical harmonics. For electric multipole radiation, a gauge transformation can be performed resulting in the replacement of $\vec{\alpha} \cdot \vec{a}_{J M}^{(1)}$ in Eq. (4) by $b_{J M} + \vec{\alpha} \cdot \vec{c}_{J M}$, where

$$b_{J M} = i \left(\frac{J+1}{J} \right)^{1/2} \left(j_J(\omega r) - \frac{\omega r j_{J+1}(\omega r)}{J+1} \right) Y_{J M}(\hat{r}),$$

$$\vec{c}_{J M} = \frac{\omega r j_J(\omega r)}{[J(J+1)]^{1/2}} \hat{r} Y_{J M}(\hat{r}).$$

With the former choice of gauge, the matrix element of Eq. (4) reduces in the nonrelativistic limit to the velocity form of the dipole matrix element, while with the latter choice, the matrix element reduces to the length form.⁹ As in the nonrelativistic random-phase approximation,^{1(b)} both forms are equivalent in the RRPA.⁵

By adopting the frozen core approximation, we reduce the problem from one involving eleven channels to one involving only the two virtual excitation channels $3s_{1/2} - n p_{1/2}$ and $3s_{1/2} - n p_{3/2}$. Such a simplifying procedure has been successful in retaining the important interelectron correlation effects while reducing the numerical complexity in previous calculations.^{6,10} For all transitions described in this work, we calculate the oscillator strengths with both choices of gauge. Since the inner-shell correlation effects are neglected, the length form should be the more reliable because of the greater sensitivity of the velocity form to

conditions close to the nucleus.⁶ The difference between the length and velocity results is an indication of the importance of inner-shell correlation effects.

The RRPA equations are solved iteratively beginning with the zero-order approximation for the energies and oscillator strengths that represents an intermediate coupling Dirac-Hartree-Fock solution. The nonrelativistic designations 1P_1 and 3P_1 are used to label the intermediate coupling solutions. As in Ref. 6, the Breit interaction is neglected. The reduction of the RRPA equations and a procedure for their numerical solution have been described in previous papers.^{5,6}

III. RESULTS AND DISCUSSION

Tables I, II, and III present the RRPA results for the $3s^2 \ ^1S_0 - 3s3p \ ^1P_1$, $-3s4p \ ^1P_1$, and $-3s5p \ ^1P_1$ transitions. They contain also the calculated Dirac-Hartree-Fock intermediate coupling results as well as values taken from the literature. A more extensive tabulation of comparison values for the neutral member is presented in Table IV. Table V compares the RRPA oscillator strengths for the resonance transition with the results of other relativistic calculations. The RRPA excitation energies for the intercombination transition $3s^2 \ ^1S_0 - 3s3p \ ^3P_1$ are of low accuracy (the error ranging from 22% for Cl VI to 13% for Fe XV) and the differences between the length and velocity forms of the oscillator strengths are sizable. Because of the uncertain accuracy of the oscillator strengths for these particular transitions, we present only a sample of our 3P_1 results in Table VI, along with semiempirical oscillator strengths^{5,6} obtained by correcting for the difference between the theoretical and experimental singlet-triplet energy separation.

For low values of the nuclear charge, where relativistic effects are small, the transition energy can be written^{27,28}

$$\Delta E = \epsilon_0 Z^2 + \epsilon_1 Z + \epsilon_2 + \epsilon_3 Z^{-1} + \dots$$

with $\epsilon_0 = 0$ if $\Delta n = 0$, where n is the principal quantum number of the active electron. It is instructive to plot $\Delta E/Z$ as a function of Z^{-1} for transitions in which the principal quantum number is unchanged and to plot $\Delta E/Z^2$ when there is a change in n (cf. Fig. 1).

The 3P_1 curve shows a departure from linearity as Z increases above 33. Both the 4^1P_1 and 5^1P_1 curves are slightly concave upward throughout the low and moderate Z elements, with a sharper increase in slope as the nuclear charge increases above $Z = 50$. These increases in slope at high Z are attributable to relativistic effects. Because of

TABLE I. $3s^2\ ^1S_0-3s3p\ ^1P_1$. RRPA excitation energies (in a.u.) and oscillator strengths (length form) compared with DHF intermediate coupling results and other values. A(B) denotes $A \times 10^B$.

Z	Excitation energy				Oscillator strength			
	RRPA	DHF	TDHF (RPA)	EXP	RRPA	DHF	TDHF (RPA)	Other
12	0.1496	0.1314	0.1492 ^a	0.1597 ^b	1.67	1.91	1.665 ^a	1.81 ± 0.18 ^d
13	0.2667	0.2433	0.2653	0.2727	1.85	2.10	1.877	1.84 ± 0.18
14	0.3745	0.3525	0.3716	0.3776 ^c	1.73	2.04	1.739	1.70 ± 0.17
15	0.4782	0.4591	0.4734	0.4793 ^b	1.59	1.91	1.591	1.60 ± 0.16
16	0.5796	0.5637	0.5725	0.5793	1.47	1.79	1.457	1.46 ± 0.15
17	0.6799	0.6670	0.6697	0.6787	1.36	1.66	1.342	1.28 ± 0.13
18	0.7798	0.7696	0.7658	0.7779	1.27	1.55	1.248	1.21 ± 0.12
20	0.9798	0.9746		0.9773	1.11	1.37		1.09 ± 0.11
22	1.1825	1.1816		1.1801 ^e	9.95(-1)	1.22		
24	1.3903	1.3930		1.3879	9.02(-1)	1.10		
26	1.6052	1.6112	1.5111	1.6035 ^f	8.27(-1)	1.01	7.83(-1)	8.3(-1) ^f
28	1.8297	1.8385		1.8285 ^g	7.67(-1)	9.30(-1)		
29	1.9463	1.9564			7.41(-1)	8.96(-1)		
30	2.0663	2.0777			7.17(-1)	8.65(-1)		7.08(-1) ^h
36	2.8795	2.8965			6.11(-1)	7.25(-1)		6.03(-1)
42	3.9273	3.9474			5.49(-1)	6.38(-1)		5.40(-1)
54	7.2596	7.2795			5.09(-1)	5.68(-1)		5.02(-1)
74	20.2087	20.2185			6.16(-1)	6.52(-1)		6.12(-1)
79	25.9631	25.9697			6.68(-1)	7.01(-1)		6.84(-1) ⁱ
92	49.1440	49.1420			8.43(-1)	8.69(-1)		8.42(-1) ^h

^a Stewart, Ref. 10.

^b Moore, Ref. 11(a).

^c Moore, Ref. 11(b).

^d Wiese, Smith, and Miles, Ref. 12.

^e Fawcett and Peacock, Ref. 13.

^f Cowan and Widing, Ref. 14.

^g Fawcett and Hayes, Ref. 15.

^h Cheng and Johnson, Ref. 16.

ⁱ Cowan, Ref. 17.

these relativistic effects, the leading term of the Z expansion of the transition energy takes the form²⁹

$$\Delta E/Z = (\epsilon_1 + Z^3 \alpha^2 \epsilon_r) + \dots, \quad \Delta n = 0,$$

$$\Delta E/Z^2 = (\epsilon_0 + Z^2 \alpha^2 \epsilon_r) + \dots, \quad \Delta n \neq 0.$$

For all transitions considered, the difference between the RRPA and DHF intermediate coupling energies becomes smaller as the nuclear charge increases. The difference of 12% for Mg I in the 3^1P_1 transition is reduced to 1% by Ar VII. For the 4^1P_1 transition the difference is already 1% for the second member of the sequence while for the 5^1P_1 transition it is 1% for the neutral member.

The time-dependent Hartree-Fock (RPA) calculations of Stewart¹⁰ on the 3^1P_1 and 4^1P_1 transitions provide a direct comparison with the RRPA calculations when relativistic effects can be neglected. The RRPA excitation energies are within 2% of the nonrelativistic values for all elements calculated by Stewart for both transitions with the exception of the 3^1P_1 transition of Fe XV for which our value is 6% higher. Our Fe XV value agrees closely with the measured value of Cowan and Widing¹⁴ as

well as with their value calculated taking into account relativistic effects and configuration interaction. The RRPA energies for the allowed transitions are in good agreement with the experimental values for all but the most weakly ionized elements of the isoelectronic sequence.

Figure 2 presents the calculated oscillator strengths in graphical form as a function of Z^{-1} , as suggested by the expression for the oscillator strength in the nonrelativistic Z expansion method

$$f = f_0 + f_1 Z^{-1} + f_2 Z^{-2} + \dots$$

with f_0 involving radial integrals over hydrogenic wave functions.

In the region where relativistic effects are expected to be small, say $Z < 30$, the curves display the typical behavior as a function of Z^{-1} .³⁰ Proceeding from high to low Z^{-1} , the RRPA curve for the $3^1S_0-3^1P_1$ transition attains a maximum at Al II, after which it decreases steadily toward the nonrelativistic hydrogenic value of zero. The $3^1S_0-4^1P_1$ transition oscillator strengths pass through a minimum at Si III and the $3^1S_0-5^1P_1$ transition oscillator strengths pass through a minimum at Al II.

TABLE II. $3s^2 1S_0-3s4p^1P_1$. RRPA excitation energies (in a.u.) and oscillator strengths (length form) compared with DHF intermediate coupling results and other values. $A(B)$ denotes $A \times 10^B$.

Z	Excitation energy				Oscillator strength			
	RRPA	DHF	TDHF (RPA)	EXP	RRPA	DHF	TDHF (RPA)	Other
12	0.2023	0.1968	0.2021 ^a	0.2248 ^b	1.64(-1)	1.29(-1)	1.83(-1) ^a	1.25(-1) ^d
13	0.4611	0.4547	0.4599	0.4872	9.67(-3)	3.06(-2)	2.5(-3)	2.7(-3)
14	0.7774	0.7713	0.7748	0.8041 ^c	6.36(-3)	1.08(-3)	1.7(-2)	3.11(-2)
15	1.1471	1.1414	1.1427	1.1733 ^b	3.92(-2)	6.00(-3)	5.9(-2)	8.44(-2)
16	1.5688	1.5634	1.5606		8.10(-2)	2.74(-2)	1.01(-1)	1.37(-1)
17	2.0415	2.0365	2.0260		1.24(-1)	5.62(-2)	1.41(-1)	9.16(-2)
18	2.5650	2.5603	2.5457	2.5805	1.64(-1)	8.80(-2)	1.81(-1)	
20	3.7641	3.7597		3.7923 ^e	2.35(-1)	1.51(-1)		
22	5.1662	5.1621		5.1939	2.94(-1)	2.08(-1)		
24	6.7728	6.7688		6.8022 ^b	3.38(-1)	2.54(-1)		
26	8.5858	8.5819	8.4718	8.602 ^f	3.70(-1)	2.91(-1)	4.22(-1)	5.0(-1) ^f
28	10.6077	10.6038		10.632 ^g	3.92(-1)	3.18(-1)		
29	11.6978	11.6939		11.720	3.99(-1)	3.28(-1)		
30	12.8412	12.8373			4.05(-1)	3.37(-1)		
36	20.8451	20.8413			4.17(-1)	3.63(-1)		
42	30.8879	30.8840			4.10(-1)	3.66(-1)		
54	57.6591	57.6552			3.79(-1)	3.48(-1)		
74	126.2469	126.2427			2.91(-1)	2.73(-1)		
79	149.2703	149.2660			2.62(-1)	2.46(-1)		
92	223.9457	223.9410			1.79(-1)	1.68(-1)		

^aStewart, Ref. 10.

^eEkberg, Ref. 19.

^bMoore, Ref. 11(a).

^fCowan and Widing, Ref. 14.

^cMoore, Ref. 11(b).

^gFeldman, Katz, Behring, and Cohen, Ref. 20.

^dVictor, Stewart, and Laughlin, Ref. 18.

TABLE III. $3s^2 1S_0-3s5p^1P_1$. RRPA excitation energies (in a.u.) and oscillator strengths (length form) compared with DHF intermediate coupling results and other values. $A(B)$ denotes $A \times 10^B$.

Z	Excitation energy			Oscillator strength		
	RRPA	DHF	EXP	RRPA	DHF	Other
12	0.2238	0.2216	0.2492 ^a	4.16(-2)	3.68(-2)	2.86(-2) ^c
13	0.5412	0.5386	0.5735	6.33(-5)	4.86(-3)	8 (-4)
14	0.9440	0.9414	0.9775 ^b	8.09(-3)	2.72(-4)	2.45(-2)
15	1.4258	1.4233	1.4583 ^a	2.30(-2)	6.40(-3)	
16	1.9838	1.9814		3.80(-2)	1.66(-2)	
17	2.6167	2.6144		5.17(-2)	2.79(-2)	
18	3.3239	3.3217		6.41(-2)	3.91(-2)	
20	4.9599	4.9579	5.0009 ^d	8.42(-2)	5.94(-2)	
22	6.8912	6.8893	6.9666	9.89(-2)	7.55(-2)	
24	9.1187	9.1168		1.09(-1)	8.76(-2)	
26	11.6442	11.6423		1.15(-1)	9.59(-2)	
28	14.4699	14.4681		1.19(-1)	1.01(-1)	
29	15.9963	15.9944		1.20(-1)	1.03(-1)	
30	17.5988	17.5970		1.20(-1)	1.05(-1)	
36	28.8383	28.8365		1.20(-1)	1.09(-1)	
42	42.9454	42.9436		1.18(-1)	1.09(-1)	
54	80.3659	80.3641		1.11(-1)	1.04(-1)	
74	174.4096	174.4077		9.14(-2)	8.71(-2)	
79	205.3614	205.3594		8.47(-2)	8.08(-2)	
92	303.7250	303.7229		6.36(-2)	6.07(-2)	

^aMoore, Ref. 11(a).

^cVictor, Stewart, and Laughlin, Ref. 18.

^bMoore, Ref. 11(b).

^dEkberg, Ref. 19.

TABLE IV. RRPA oscillator strengths for Mg I compared with values obtained by other methods. A(B) denotes $A \times 10^B$.

n^1P_1	RRPA	DHF	TDHF (RPA)	Model potential ^c	"Frozen-cores" ^d	Electron-beam phase-shift ^e	Beam-foil ^f	Hook ^g
3	1.67	1.91	1.67 ^a	1.66 ^b	1.72	1.76	1.86 ± 0.29	1.67 ± 0.15 ^f
4	1.64(-1)	1.29(-1)	1.83(-1)	1.50(-1)	1.25(-1)	1.19(-1)	1.8 ± 0.4(-1)	1.07 ± 0.02(-1) ^g
5	4.16(-2)	3.68(-2)	...	3.54(-2)	2.86(-2)	2.73(-2)	5.5 ± 1(-2)	2.27 ± 0.12(-2)

^aStewart, Ref. 10.^bAmusia, Cherepkov, Pavlin, Radojević, and Živanović, Ref. 21.^cVictor, Stewart, and Laughlin, Ref. 18.^dSaraph, Ref. 22.^eSmith and Liszt, Ref. 23.^fAndersen, Desesquelles, Jessen, and Sørensen, Ref. 24.^gMitchell, Ref. 25 (obtained from relative f values based on $f = 1.72$ for 3^1P_1).TABLE V. RRPA oscillator strengths for the resonance transition compared with the results of other relativistic calculations. L denotes length form; V denotes velocity form. A(B) denotes $A \times 10^B$.

Ion	RRPA		Multiconfiguration Hartree-Fock ^a		Parametric potential ^b		"HFR" ^c	Superposition of configurations ^d
	f_L	f_V	f_L	f_V	f_L	f_V	f	f
Mg	1.67	1.64	1.73	1.79	1.64	2.02		
Ar ⁺⁶	1.27	1.28	1.25	1.24	1.17	1.07	1.309	
Fe ⁺¹⁴	8.27(-1)	8.51(-1)	8.18(-1)	8.25(-1)	7.9(-1)	6.9(-1)	8.50(-1)	8.18(-1)
Kr ⁺²⁴	6.11(-1)	6.32(-1)	6.03(-1)	6.11(-1)			6.19(-1)	6.05(-1)
Mo ⁺³⁰	5.49(-1)	5.66(-1)	5.40(-1)	5.47(-1)			5.50(-1)	5.43(-1)
Xe ⁺⁴²	5.09(-1)	5.21(-1)	5.02(-1)	5.07(-1)			5.07(-1)	5.08(-1)
W ⁺⁶²	6.16(-1)	6.21(-1)	6.12(-1)	6.14(-1)			6.25(-1)	6.14(-1)

^aCheng and Johnson, Ref. 16.^bAymar and Luc-Koenig, Ref. 3(c).^cCowan, Ref. 17.^dWeiss, Ref. 26.TABLE VI. $3s^2 \ ^1S_0 - 3s3p \ ^3P_1$. RRPA excitation energies (in a.u.) and oscillator strengths (length form) for magnesiumlike chlorine, titanium, and iron compared with other values. Semiempirical oscillator strengths (EMP) are obtained by multiplying the RRPA values by $E(\text{EXP})\Delta E^2(\text{RRPA})/E(\text{RRPA})\Delta E^2(\text{EXP})$ where E and ΔE are the triplet energies and singlet-triplet energy differences, respectively. A(B) denotes $A \times 10^B$.

Z	E(RRPA)	ΔE (RRPA)	E(EXP)	ΔE (EXP)	f (RRPA)	f (EMP)	f (other)
17	0.3658	0.3141	0.4463 ^a	0.2324 ^{a,b}	8.61(-5)	1.92(-4)	1.8(-4) ^c
22	0.6946	0.4879	0.7920 ^a	0.3881 ^{a,d}	6.97(-4)	1.26(-3)	
26	0.9698	0.6354	1.0920 ^e	0.5115 ^e	2.17(-3)	3.77(-3)	3.3(-3) ^c

^aEkberg, Ref. 19.^bMoore, Ref. 11(a).^cCheng and Johnson, Ref. 16.^dFawcett and Peacock, Ref. 13.^eCowan and Widing, Ref. 14.

The curves then increase with decreasing Z^{-1} . Relativistic effects cause departures from the non-relativistic predictions at higher Z .

For all three allowed resonance transitions, the RRPA length and velocity results are in close agreement, except near the minima in the 4^1P_1 and 5^1P_1 curves. They are in harmony with the nonrelativistic TDHF values of Stewart for the $3^1S_0-3^1P_1$ transition for small Z . The oscillator strengths given by Wiese, Smith, and Miles¹² for $Z \leq 20$ are estimated to have an uncertainty of less than 10%;

the RRPA results are in good agreement with these values.

Uncertainties in the theoretical oscillator strengths are expected to be large for those transitions for which the oscillator strength curves are near minima due to cancellation in the radial matrix elements and configuration interaction effects.^{3(c), 18, 30(b)} Thus, agreement among the values calculated by different authors for the low Z elements of the $3^1S_0-4^1P_1$ transition is less satisfactory than for the $3^1S_0-3^1P_1$ transition. For the

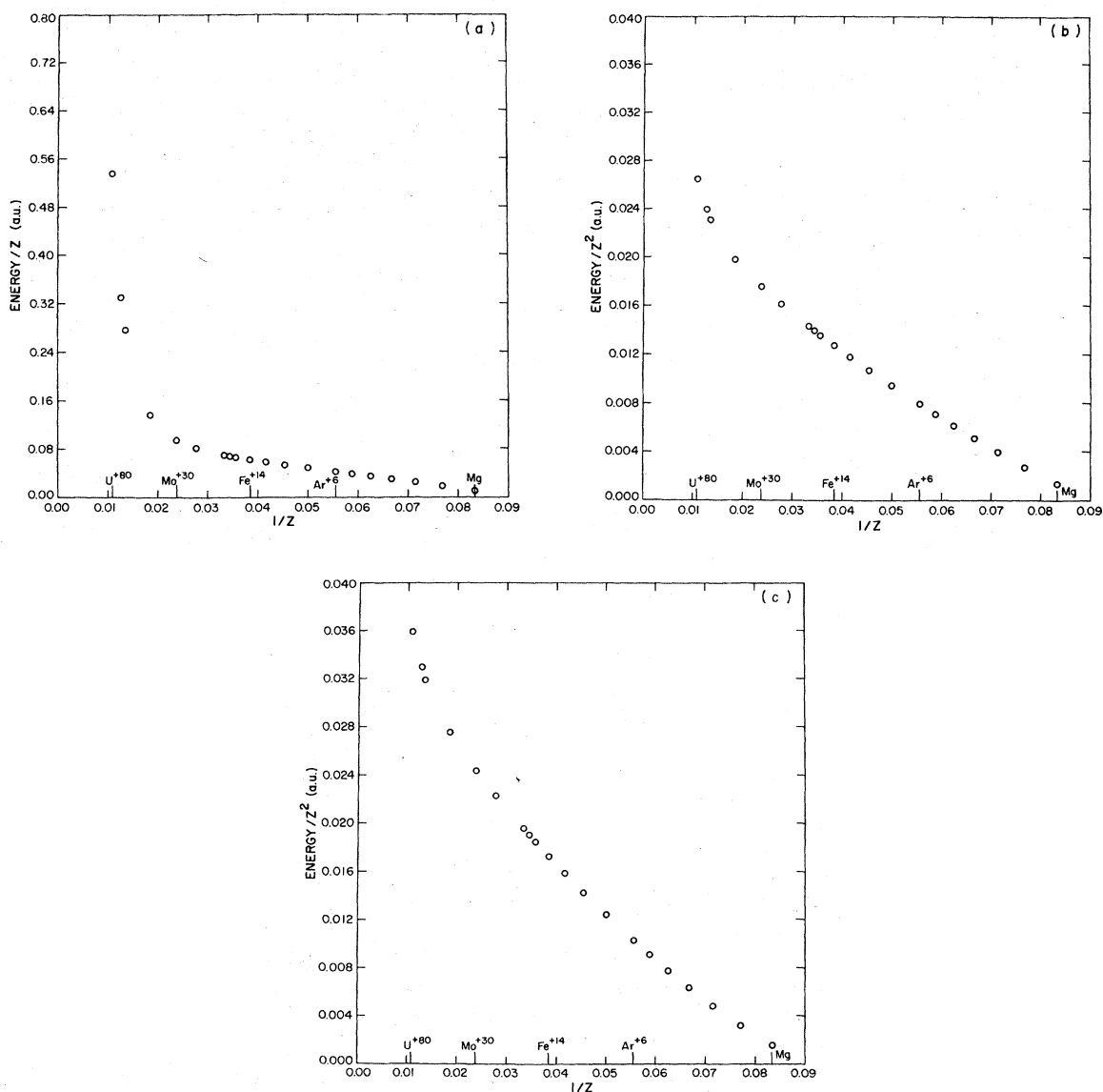


FIG. 1. (a) $3s^2\ ^1S_0-3s3p\ ^1P_1$. RRPA excitation energy in a.u., divided by the nuclear charge as a function of Z^{-1} . (b) $3s^2\ ^1S_0-3s4p\ ^1P_1$. RRPA excitation energy in a.u., divided by the square of the nuclear charge as a function of Z^{-1} . (c) $3s^2\ ^1S_0-3s5p\ ^1P_1$. RRPA excitation energy in a.u., divided by the square of the nuclear charge as a function of Z^{-1} . On the scale to which the graphs have been drawn, the corresponding DHF results coincide with the RRPA data points.

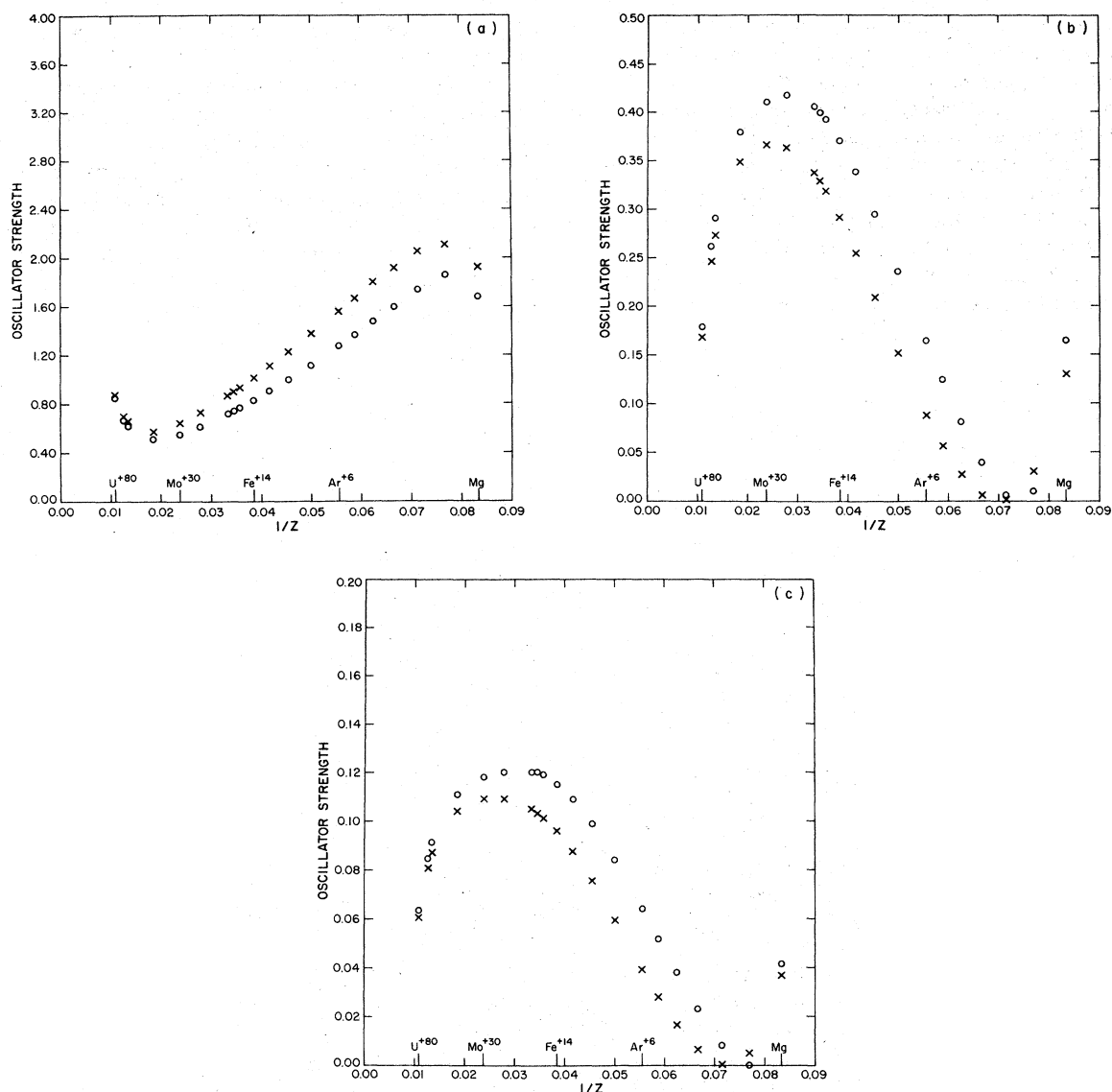


FIG. 2. Oscillator strength as a function of Z^{-1} for the (a) $3s^2 1S_0 - 3s3p^1P_1$, (b) $3s^2 1S_0 - 3s4p^1P_1$, and (c) $3s^2 1S_0 - 3s5p^1P_1$ transitions. \circ , RRPA; \times , DHF.

4^1P_1 transition, the difference between the RRPA and TDHF values of Stewart is of the order of 10% for Mg I and Ar VII, while for elements closer to the minimum [Fig. 2(b)] the difference is a factor of 3 or 4. Whereas the RRPA value for Mg I for the 3^1P_1 transition is in excellent agreement with the nonrelativistic RPA calculations of Amusia, Cherepkov, Pavlin, Radojević, and Živanović²¹ in which correlations with the L -shell electrons are taken into account, the RRPA values for the 4 and 5^1P_1 transitions are respectively 9% and 15% greater than the corresponding RPA values. The differences may be largely attributed to

the sensitivity of the transition matrix element to small changes in the wave function for elements for which the oscillator strength versus Z^{-1} curve is near a minimum. The RRPA values for Mg I for the 4^1P_1 and 5^1P_1 transitions lie between the experimentally determined values of Smith and Liszt²³ and of Mitchell.²⁵

The line strength S is related to the oscillator strength by

$$f = \frac{2}{3} (\Delta E/g) S,$$

where g is the degeneracy of the initial state and ΔE is the transition energy. In the Z -expansion

method, the line strength is written in the form

$$S = S_0 Z^{-2} + S_1 Z^{-3} + S_2 Z^{-4} + \dots$$

As given by the nonrelativistic charge expansion calculations of Crossley and Dalgarno,³¹ S_0 equals 271.65 and S_1 equals 3915.1 for the $3s^2 \ ^1S_0 - 3s3p \ ^1P_1$ transition. For U^{+80} , the RRPA value of $Z^2 S$ for this transition is 218 as compared to the nonrelativistic value of 320, indicating that the high- Z departure of the resonance transition oscillator

strength from the nonrelativistic prediction is attributable to the relativistic corrections to the excitation energy rather than to the transition integral.

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