YU ISSN 0015—3206
FZKAAA 16 (4) 321 (1984)

A NOTE ON OSCILLATOR STRENGTHS FOR THE ATOMS OF LITHIUM AND BERYLLIUM WITHIN RANDOM-PHASE APPROXIMATION WITH EXCHANGE

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Received 15 December 1983
Revised manuscript received 5 July 1984
UDC 539.18

Original scientific paper

The oscillator strengths for the transitions from the inner $1s^2\,2s\,(^2S) \rightarrow 1s^2\,v\,p\,(^2p)$ and outer $1s^2\,2s\,(^2S) \rightarrow 1svp\,(^1p)\,2s\,(^2p)$ subshell of Li atom as well as from the outer subshell of Be atom $1s^2\,2s^2\,(^1S) \rightarrow 1s^2\,2svp\,(^1p)$ are calculated up to the first and second order of the Random-Phase Approximation with Exchange (*RPAE*). Exclusion principle violating (*EPV*) contribution to the oscillator strengths up to the second order is computed too. The obtained values are in satisfactory agreement with available experimental data.

1. Introduction

It is well known that the many-body effects in the photoexcitation of heavier atoms (as well as at some other atomic phenomena) can be treated successfully

within *RPAE*[1,2,3]. On the other hand, the many-body perturbation theory is generally applicable at the lightest atoms[4,5,6,7]. Amusia et al.[8] showed, in this connection, that the *RPAE* can be applied even to a system with small number of particles. In a previous paper[9] we explained why the *RPAE* can be employed in the case of a system which cannot in any way be treated as a dense electron gas. Here we give the results (in atomic units) of our further investigations.

TABLE 1

Transition	*L*	*V*	*L*	*V*
	Zero order		up to first order	
$1s \rightarrow 2p$	0.3440	0.3212	0.3440	0.3368
$3p$	0.0539	0.0497	0,0527	0.0520
$4p$	0.0187	0,0173	0,0183	0.0180
	up to second order		*RPAE*	
$1s \rightarrow 2p$	0.3446	0.3393	0.3454	0.3388
$3p$	0.0528	0.0521	0.0528	0.0523
$4p$	0.0183	0.0181	0.0183	0.0181

The oscillator strengths for the inner subshell of Li atom up to the first and second order of *RPAE*, respectively. The *RPAE* and *HF* values of oscillator strengths are taken from Refs. 10 and 8.

TABLE 2

Transition	*L*	*V*	*L*	*V*
	Zero order		up to first order	
$2s \rightarrow 2p$	0.7658	0.7960	0.7625	0.7643
$3p$	0.0034	0.0026	0.0035	0.0035
$4p$	0.0035	0.0030	0.0036	0.0036
	up to second order		*RPAE*	
$2s \rightarrow 2p$	0.7332	0.7631	0.7638	0.7521
$3p$	0.0037	0.0035	0.0041	0.0041
$4p$	0.0036	0.0036	0.0039	0.0039
	Experiment			
$2s \rightarrow 2p$	0.753	(3%)		
$3p$	0.00552	(10%)		
$4p$	0.0048	(10%)		

The oscillator strengths for the outer subshell of Li atom up to the first and second order of the *RPAE*. The *RPAE* and *HF* values of oscillator strengths are taken from Refs. 10 and 8. The experimental values are from Ref. 11.

2. *Results*

In Table 1 we give the values of the oscillator strengths for the inner subshell of Li atom, up to the first and second order of the *RPAE*, respectively. The oscil-

lator strengths in *HF* approximation and in the *RPAE* are cited here (as well as in Tables 2 and 3) for the sake of comparison. They are taken from Refs. 10 and 8. One can see that oscillator strengths generally decrease with increasing photon energy. The mean value (of two forms) is growing in the following order of approximations: Hartree-Fock approximation (*HF*), first order of *RPAE*, second order of *RPAE* and *RPAE*. The first order of *RPAE* is close enough to the *RPAE*. The calculated values of the oscillator strengths for the outer subshell of Li atom, up to the first and second order of the *RPAE*, are presented in Table 2. The oscillator strength (mean value) gradually grows in the above-mentioned sequence of approximations, except for the transition $2s \rightarrow 2p$. The *RPAE* values are, of course, the closest to the experiment. One can also see that already the first order of the *RPAE* gives the satisfactory results. The discrepancy between two forms L (L and V form) serves us as a criterion of the validity of our procedure. The two forms must coincide in the *RPAE*. They differ in *HF* approximation because of the non-locality of the potential in this case. The experimental values are taken from Ref. 11. In Table 3

TABLE 3

Transition	L	V	L	V
	Zero order		up to first order	
$2s \rightarrow 2p$	1.9003	1.0144	1.4127	1.2509
$3p$	0.1064	0.0317	0.0559	0.0442
$4p$	0.0156	0.0023	0.0057	0.0038
	up to second order		*RPAE*	
$2s \rightarrow 2p$	1.4767	1.2588	1.4496	1.2707
$3p$	0.2201	0.0224	0.0250	0.0233
$4p$	0.0006	0.0010	0.0012	0.0011
	RPAE without *EPV* part		Experiment	
$2s \rightarrow 2p$	1.4024	1.2508	1.34 ± 0.05	
$3p$	0.0584	0.0408		
$4p$	0.0064	0.0033		

The oscillator strengths for the outer subshell of Be atom up to the first and second order of *RPAE*. The *RPAE* and *HF* values of oscillator strengths are taken from Refs. 10 and 8. The values of oscillator strengths in *RPAE* without *EPV* part are given too. The experimental value is from Ref. 12.

one has the oscillator strengths for the outer subshell of Be atom. The only one experimental value, corresponding to the transition $2s \rightarrow 2p$, is of Martinson et al.[12]. So we could say that the oscillator strength for this transition is described good enough by the first order of the *RPAE*. One can also see that the omission of the *EPV* part in the *RPAE* oscillator strength does not decrease the discrepancy between the experiment and the theory. The experimental value is just in between the *RPAE* value and the *RPAE* value without the *EPV* part. Table 4 contains the *EPV* part of the contribution to the dipole matrix element in *RPAE*, for different transitions, up to the second order of the *RPAE*, for the inner and outer subshell

of Li atom and for the outer subshell of Be atom. The *EPV* part for the outer subshell of Li atom is zero. For the inner subshell of Li atom the *EPV* part is slight. In the case of Be atom (outer subshell) *L*-form of the *EPV* part, corresponding to the transition $2s \rightarrow 3p$, is only one which becomes significant.

TABLE 4

Atom	Transition	*L*	*V*
Li	$1s \rightarrow 2p$	−0.00081	−0.00252
	$3p$	−0.00008	−0.00055
	$4p$	0.00003	−0.00015
Li	$2s \rightarrow 2p$	0	0
	$3p$	0	0
	$4p$	0	0
Be	$2s \rightarrow 2p$	0.03966	0.00331
	$3p$	−0.14489	−0.02132
	$4p$	−0.07448	−0.00113

The *EPV* part of the contribution to the dipole matrix element in the *RPAE* for the inner and outer subshell of Li atom and for the outer subshell of Be atom.

In conclusion we could say that the *RPAE* can be applied to a system with small number of particles. It would not be strange because the *RPAE* is the last approximation, in the expanding range of approximations, which retains in a way one-particle character. Let us just recall that it can be formulated as time-dependent *HF* approximation. The reason for applicability of this approximation to such a system is that the lowest orders of this approximation (already the first order) exhaust it (in the case of photoabsorption). In other words, the many-electron correlations, being described by higher-order diagrams in the many-body perturbation theory, are small, what we can expect. The *EPV* diagrams, which do not describe any physical process, emerge in the second order of the many-body perturbation theory and are the greatest in this order. In the first order we have only apparently *EPV* diagrams.

Acknowledgment

One of the authors (M. B.) wishes to express his deep gratitude to M. Tica for the great deal of numerical work.

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BILJEŠKA O OSCILATORNIM JAČINAMA ZA ATOME LITIJUMA I BERILIJUMA U OKVIRU APROKSIMACIJE SLUČAJNIH FAZA SA IZMJENOM

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Originalni znanstveni rad

Izračunate su oscilatorne jačine za prelaze sa unutrašnje $1s^2\,2s\,(^2S) \rightarrow 1s^2\,vp\,(^2P)$ i vanjske $1s^2\,2s\,(^2S) \rightarrow 1svp\,(^1P)\,2s\,(^2P)$ podljuske atoma Li kao i vanjske podljuske atoma Be $1s^2\,2s^2\,1S) \rightarrow 1s^2\,2svp\,(^1P)$ do prvog i drugog reda Aproksimacije slučajnih faza sa izmjenom (*RPAE*). Takođe su proračunati doprinosi oscilatornim jačinama koji narušavaju Paulijev princip isključenja (*EPV*) do drugog reda. Dobijene vrijednosti su u zadovoljavajućoj saglasnosti sa raspoloživim eksperimentalnim podacima.

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