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Atomic Lithium Excitation by Electron Impact

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ABSTRACT

Bethe approximation had been used to compute the excitation cross section in term of the diploe oscillator strength for some allowed transitions between energy levels of Li-atom collide with electrons with impact energy range (2-2000) eV. We also compute the radiation transition probability and lifetime. Our results for all calculations we had done were compared with the available theoretical and experimental data.

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اثارة ذرة الليثيوم بتأثير الالكترون

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الـــخُـــلاصـــة

تم استخدام تقريب Bethe لحساب المقطع العرضي للإثارة في حد قوة مذبذب ثنائي القطب لبعض الانتقالات المسموح بها بين مستويات الطاقة من ذرة الليثيوم عند تصادمها مع الإلكترونات ذات مدى طاقة التأثير (2-2000) eV. و نحسب أيضا احتمالية الانتقال الإشعاعي وزمن الانتقال. تمت مقارنة نتائجنا لجميع الحسابات التي أجريناها مع البيانات النظرية والتجريبية المتاحة.

الكلمات المفتاحية:

أثارة
مقطع عرضي
ذرة الليثيوم
تأثير الإلكترون
تقريب بيث

1. INTRODUCTION

Alkaline group elements such as lithium are of great interest in astrophysics as well as in diagnosing the plasma. A lot of lines which appears in lithium spectrum had been identified in the solar spectrum [1].

In the theoretical side early work was done represented by working on computing the

oscillator strength for these lines done by Fock and Petrashen [2], where they used in their treatment the wave functions of self-consistent field. Also the excitation cross section is performed by Williams et. al [3], where they calculate the excitation cross section at a limited number of electron impact energies. In the experimental side, Leep and Gallagher [4], Zajonc and Gallagher [5] were measured the excitation cross section for 2s-state to 2p-state for neutral lithium collide with electrons.

The importance of studying inelastic scattering is coming from that the need is increasing for reliable and accurate computational cross section data in many fields like astrophysics, physics of radiation, and plasma physics [6]. In the inelastic interactions of neutral atoms -in ground and excited states- with electrons, the information of cross sections are very important and has fundamental interest. A database of theoretical cross sections for inelastic collision of lithium atoms with electrons in the ground and excited states have been proposed by Schwinzer et. al [7]. To derive accurate cross sections for all inelastic excitation processes for lithium atoms colliding with single electrons they used sophisticated theoretical methods of calculations. The results of these methods were tested critically against the available newest experimental measurements data.

The computation of atomic transition probabilities for allowed electric dipole lines of Li-atom, were performed by Wiese et. al [8]. The critical data compilations were included transitions between ground state and some excited states and between excited states itself. The wave functions of Hartree-Fock for 2s, 2p, 3s, 3p, and 3d states of Li-atom were computed by a wide-range method. The followed procedure represented by depend the method of analytic self-consistent field. Oscillator strengths for some transitions between these states were calculated using the dipole length formula.

In this paper, Bethe approximation which play as a correct for the behavior of the Born approximation at high energies was used to calculate the excitation cross section for the scattering of electrons from lithium atom. The generated cross section is based on the calculated oscillator strength which in turn was produced from the given Hartree-Fock wave functions. Also we calculate the transition probability and lifetime between the states under investigation. Our results for all the preceding calculations were compared with available theoretical and measurements data, and in general the comparison was good

2. THEORY

In the excitation process for atoms by fast electrons from its initial (*i*) state to final (*f*) or excited state. The integral cross section which performed using Born approximation where the generalized oscillator strength (GOS) plays a crucial role [9-10], can be expressed as:

$$\sigma_n^{Born} = \frac{4\pi a_\circ^2}{T/R}\frac{R}{E_n}\int_{(K_{\min}a_\circ)^2}^{(K_{\max}a_\circ)^2} f_n(K)\, d\ln(Ka_\circ)^2 \quad \ldots. (1)$$

$$f_n(K) = \frac{E_n}{R}\frac{\left|\left\langle f\left|\sum_j e^{i\vec{K}\cdot\vec{r}_j}\right|i\right\rangle\right|^2}{(Ka_\circ)^2} \quad \ldots(2)$$

Where $f_n(K)$ is the (GOS), E_n is the excitation energy for the transition from the initial state to the final state, $\vec{K}$ is the momentum transfer, $a_\circ$ is the Bohr radius, $\vec{r}_j$ is the position of the *jth* electron in the target, R is the Rydberg energy and T is the incident electron energy. $K_{\max}$ and $K_{\min}$ are the limits of the momentum transfer given by

$$(K_{\min}a_\circ)^2 \approx \frac{E_n^2}{4TR} \equiv Q_{\min} \quad \ldots(3a)$$

$$(K_{\max}a_\circ)^2 \approx \frac{4T}{R} \equiv Q_{\max} \quad \ldots(3b)$$

Bethe cross section work as the leading portion of the approximated Born cross section, and it given in terms A_n and B_n parameters as

$$\sigma_n = \frac{4\pi a_\circ^2}{T/R}[A_n \ln(\frac{T}{R}) + B_n] \quad \ldots(4)$$

$$A_n = f_n R/E_n = \frac{\left|\left\langle f\left|\sum_j \vec{r}_j\right|i\right\rangle\right|^2}{3a_\circ^2} \quad \ldots(5)$$

$$B_n = A_n \ln(\frac{4Q_\circ R^2}{E_n^2}) \quad \ldots(6)$$

Where f_n is the optical oscillator strength and $Q_\circ$ is the cutoff parameter between $Q_{\min}$ and $Q_{\max}$.

As a Slater determinant here is the total wavefunction [11]:

$$\Psi = \Re(\phi_i \ldots \phi_f) \quad \ldots. (7)$$

Where $\Re$ is the anti-symmetrizing factor, *n* is the electrons number, and ϕ_i, ϕ_f, are the spin-orbit (one-electron functions). The orbitals to each other are orthogonal were assumed, so the spin-orbit can hold as the same. In term of the basis functions the orbital $\phi_{n\ell}$ can be expanded according to

$$\phi_{n\ell} = \sum_i c_n^i \chi_{i\ell} \quad \ldots (8)$$

The one-electron functions have a radial part is expressed in analytic form with a summation of the Slater-type orbitals

$$P_{n\ell} = \sum_{i=1}^{k} c_{in\ell} N_i r^{p_i} e^{-\xi_i r} \quad \ldots (9)$$

Where, $c_{in\ell}$ is the expansion coefficient and ξ is the orbital exponent.

$$N_i = (\frac{2(\xi_i)^{2p_i+1}}{(2p_i)!}) \quad \ldots (10)$$

In Table I, we present the Hartree-Fock wave functions for 2s-state taken from Ref. [11], 2p, 3s, 3p, and 3d-states taken from Ref. [1], which are Hartree-Fock wavefunctions for lithium atom.

The radiative transition probability in (sec^{-1}) for the state (*f*) is given by [12]:

$$A_f = \sum_i A_{fi} \quad \ldots (11)$$

$$A_{fi} = \frac{1}{2}\alpha^3 \frac{g_i}{g_f} \Delta E^2 f_{if} \quad \ldots (12)$$

(the Einstein's A-coefficient).

Where g_i, g_f are the factors of statistical weight, and α is the fine structure constant.

The life time of a state is given by

$$\tau_f = \frac{1}{A_f} \quad \ldots (13)$$

Table I: Values of Slater-Type parameters of Li atomic orbitals

Orbital	Power of r	Orbital Exponent	Expansion Coefficient
2s	1	2.47673	-0.14629
	1	4.69873	-0.01516
	2	0.3835	0.00377
	2	0.66055	0.98053
	2	1.07	0.10971
	2	1.632	-0.11021
3s	1	3.0	0.06705
	3	9.6	-0.00026
	3	3.38	0.0103
	3	2.52	-0.01308
	3	1.24	-0.18005
	3	0.757	-0.52505
	3	0.345	1.61032
	4	0.345	-0.41164
2p	2	1.5	0.13268
	4	2.12	0.04423
	4	1.275	0.3247
	4	0.785	0.50651
	4	0.566	0.16116
3d	3	1.0	0.34768
	5	0.98	0.01989
	5	0.6	0.27677

	5	0.404	0.43910
	5	1.762	-0.00004

3. RESULTS AND DISCUSSION

The cross section have been calculated for some possible excitation processes of $e^- + Li(n\ell) \rightarrow e^- + Li(n'\ell)$ with $n = 2,3$, and $n' = 2,3$. Those cross sections were performed in term of the dipole oscillator strength for allowed transitions with impact energy range from 2 eV to 2 keV.

In figure (1) the present work (P.W.) of the excitation cross section (EXCS) of lithium atom with the transition state $2s(^2S) \rightarrow 2p(^2P^o)$ has been compared with the theoretical calculations of Stone et. al [13], Schweinzer et. al [7], and the experimental measurements of Leep and Gallagher [4], Williams et. al [3], and Vuskovic et. al [14]. The agreement between our results of EXCS and theoretical one was very good and also was with the experimental data were very good but with Vuskovic data the agreement was reliable. It is worth to mention that that Stone group has implemented the scaled plane-wave Born approximation and they used the Dirac-Fock wavefunctions. Whereas Schweinzer group has depends advanced close-coupling computations which in turn provided them a new standard of good quality for the transitions between the ground and excited states and between the excited states itself.

In figures (2), (3), and (4) our results of the EXCS for Lithium atom with transitions between the excited states $2p(^2P^o) \rightarrow 3s(^2S)$, $2p(^2P^o) \rightarrow 3d(^2D)$, and $3s(^2S) \rightarrow 3p(^2P^o)$, all have been compared with Schweinzer et. al [7]. In general the agreement in figure (2) was good for impact energy stranded between (15-2000) eV, and in figure (3) the agreement was very good for impact energy stranded between (7-2000) eV. Whereas in figure (4) unfortunately the comparison was not successful and the results of agreement was occasional.

In this paper we also computed the radiation transition probability and life time for the states under investigation, where we tabulate it in table II, and moreover the oscillator strength.

4. CONCLUSION

We present in this paper the results for EXCS, transition probability, and lifetime of lithium atom collide with electrons at impact energies between 2eV and 2000eV. The EXCS were performed in term of the oscillator strength using the Bethe approximation which in turn was successful in dealing with the excitation process for Li-atom by fast electrons. Our computed results show a good agreement with theoretical and experimental data which had compared with. Some differences appears in fig.(4) for 3s→3p transition, because of the smallness of the calculated oscillator strength which in turn effects the value the calculated cross section.

Table II: The calculated oscillator strength, transition probability (sec^{-1}), and life time (sec) for some allowed states

Transition	Excitation Energy(eV) Ref.[1]	Oscillator Strength	Transition probability $\times 10^7$	Life time$\times 10^{-7}$
$2s(^2S) \rightarrow 2p(^2P^o)$	1.841	0.757	0.98	1.07
$2p(^2P^o) \rightarrow 3s(^2S)$	1.493	0.228	1.659	0.603
$2p(^2P^o) \rightarrow 3d(^2D)$	1.989	0.757	1.951	0.513
$3s(^2S) \rightarrow 3p(^2P^o)$	0.463	0.244	0.019	52.6

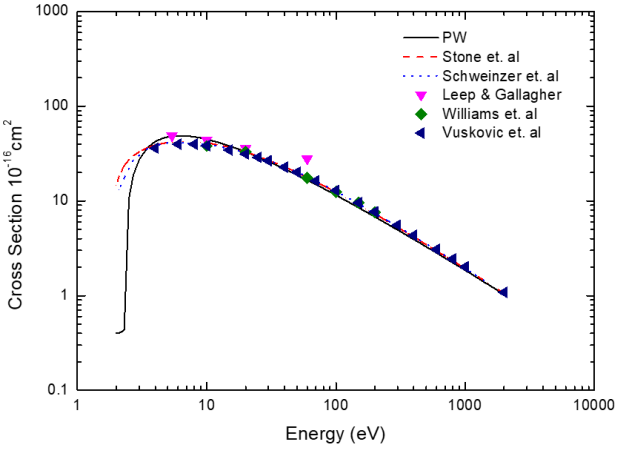

Figure 1. EXCS for inelastic e⁻+Li scattering for 2s→2p transition

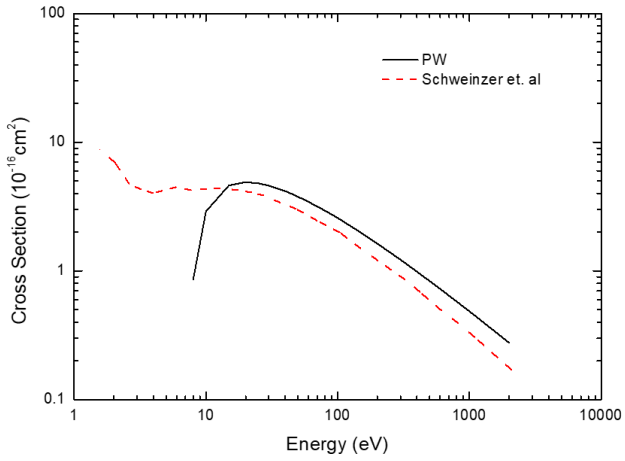

Figure 2. EXCS for inelastic e$^-$+Li scattering for 2p⟶3s transition

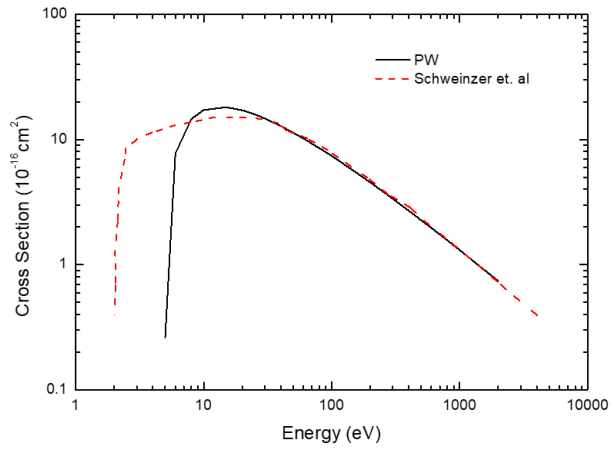

Figure 3. EXCS for inelastic e$^-$+Li scattering for 2p⟶3d transition

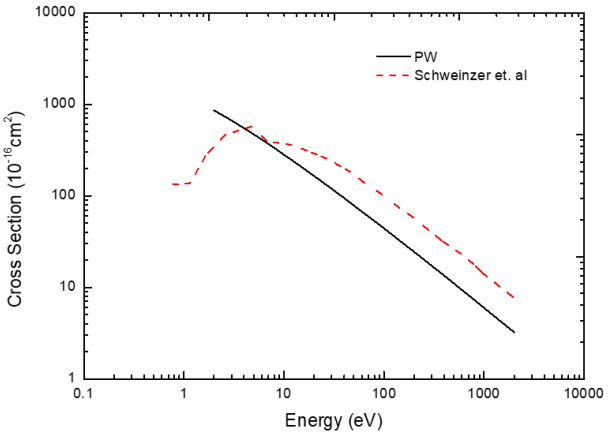

Figure 4. EXCS for inelastic e$^-$+Li scattering for 3s⟶3p transition

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