

Electron-Impact Excitation of Lithium

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Electron-impact excitation cross sections for the resonant transition ($2s-2p$) in the lithium atom have been calculated under the Born approximation for incident energies up to 60 eV. The polarization of the target atom caused by the incident charged particle is considered by modifying the target wave function. The exchange has also been included via the Ochkur approximation. The cross sections obtained here are compared with the other theoretical calculations and the experimental data.

INTRODUCTION

A number of theoretical studies of the $2s-2p$ excitation of lithium atoms by electron impact have been made¹⁻⁴ using quantal and classical approximations. In the alkali-metal atom, the polarization of the target system by the incident charged particle plays an important role. Such a polarization has not been taken into account in previous calculations of inelastic-collision cross sections in the alkali atoms. However, in the elastic scattering of electrons by alkali atoms, the effect of polarization has been studied by various authors.⁵⁻⁷ Llyod and McDowell⁸ have included the polarization effects in the study of inelastic collisions with hydrogen atoms by following an approach similar to that of Callaway *et al.*⁹ They have calculated the electron-impact excitation cross section of the $2s$ and $2p$ states of hydrogen from the ground state using two types of approximations. In one of the approximations they have taken the polarization of the atom in terms of the change in the wave functions of the target atom caused by the incident electron, whereas in the other type of approximation the effect of polarization and distortion are included in the scattered-electron wave function, treating the atomic wave function as unaltered. In both of these approximations the important effect of polarization to the first order has been included and leads to an improvement over the first-order Born approximation as exhibited in their calculations of hydrogen.

In the present paper we have calculated the electron-impact excitation cross section for the $2s-2p$ transition in lithium using the Born approximation and incorporating the effects of polarization, which are quite important for alkali atoms. Our approximation is very similar to the first type of approximation of Llyod and McDowell, but it differs in the procedure of including the polarization. We have adopted the simple approach of Stone⁶ for considering the contribution of polarization of the system. In this approach we neglect the effect of polarization on the wave functions of the scattered particle and

consider the distortion of the atomic functions only. Incorporating both of these distortions will render the calculations very difficult. In this procedure the polarization is determined by assuming that the atomic wave functions are of the form given by perturbation theory. The coefficient giving the coupling to the higher states is obtained by minimizing the energy of the atom. The effect of exchange has also been included through the Ochkur approximation.¹ The present approximation is reasonable because it takes into account both the polarization and exchange effects in the Born approximation.

THEORY

The perturbation of the atomic wave function by the incident electron and the total wave function of the system can be expressed as

$$\Psi(1, 2) = [\Psi_0(\vec{r}_2) + \beta(\vec{r}_1) \Psi_1(\vec{r}_2)] F(\vec{r}_1) \pm \Psi_0(\vec{r}_1) F(\vec{r}_2), \quad (1)$$

where $\Psi_0(\vec{r}_2)$ is the ground-state wave function of the atom and $\Psi_1(\vec{r}_2)$ is the first-excited-state wave function. $\beta(\vec{r}_1)$ is the coefficient giving the coupling to higher states. \vec{r}_1 and \vec{r}_2 are the position vectors of the incident and atomic electrons. $F(\vec{r}_1)$ is the scattered-electron wave function.

In Eq. (1) we have not chosen a properly symmetrized wave function. In effect we have ignored the exchange effects associated with the distortion of the atom. Exchange has been introduced as if the atom were not polarized, while polarization is included as if exchange did not take place. This is done mainly to simplify the calculation, but this simplification should not introduce significant errors in the result. The polarization of the wave function is small at distances below $3a_0$ where exchange is most important.⁶

The cross section for the excitation of the n th state of the atom from its ground state is given by

$$Q_{2s-nl} = (k_f/k_0) \int \frac{1}{4} (|T_{if}^+|^2 + 3|T_{if}^-|^2) d\hat{k} (\pi a_0^2), \quad (2)$$

where

$$k_f^2 = k_0^2 - \Delta E_{if}, \quad \vec{k} = \vec{k}_0 - \vec{k}_f. \quad (3)$$

\vec{k}_0 and \vec{k}_f are the initial and final momenta of the incident electron and ΔE_{if} is the threshold energy for excitation. The plus and minus signs refer to the singlet and triplet states of the total systems, respectively. T_{if} is given by

$$T_{if} = (1/2\pi) \langle \phi_m(\vec{r}_2) e^{i\vec{k}_f \cdot \vec{r}_1} | V | \Psi(1, 2) \rangle. \quad (4)$$

$V = (1/r_1 - 1/r_2 - 1/r_1)$ is the interaction potential, $\phi_m(\vec{r}_2)$ is the wave function of the m th state of the atom, and $\Psi(1, 2)$ is the total wave function of the system given by Eq. (1).

In the Born approximation we write

$$F(\vec{r}_1) = e^{i\vec{k}_0 \cdot \vec{r}_1}. \quad (5)$$

Therefore we have

$$\Psi(1, 2) = [\Psi_0(\vec{r}_2) + \beta(\vec{r}_1) \Psi_1(\vec{r}_2)] e^{i\vec{k}_0 \cdot \vec{r}_1} \pm \Psi_0(\vec{r}_1) e^{i\vec{k}_0 \cdot \vec{r}_2}. \quad (6)$$

Using this value of $\Psi(1, 2)$ in Eq. (4), we get

$$T_{if}^\pm = I_1 + I_2 \pm I_3,$$

where

$$I_1 = (1/2\pi) \langle \phi_m(\vec{r}_2) e^{i\vec{k} \cdot \vec{r}_1} | V | \Psi_0(\vec{r}_2) \rangle, \quad (7)$$

$$I_2 = (1/2\pi) \langle \phi_m(\vec{r}_2) e^{i\vec{k} \cdot \vec{r}_1} \beta(\vec{r}_1) | V | \Psi_1(\vec{r}_2) \rangle, \quad (8)$$

$$I_3 = (1/2\pi) \langle \phi_m(\vec{r}_2) e^{i(\vec{k}_0 \cdot \vec{r}_2 - \vec{k}_f \cdot \vec{r}_1)} | V | \Psi_0(\vec{r}_1) \rangle, \quad (9)$$

$$\beta(\vec{r}_1) = \beta(r_1) y_{10}(\theta_1, \phi_1)$$

and r_1, θ_1, ϕ_1 are the polar coordinates of \vec{r}_1 . Following the Ochkur approximation, I_3 reduces to

$$I_3 = (2/k_0^2) \langle \phi_m(\vec{r}_1) | e^{i\vec{k} \cdot \vec{r}_1} | \Psi_0(\vec{r}_1) \rangle. \quad (10)$$

CALCULATION OF β

The coupling coefficient $\beta(r_1)$ is calculated following the procedure of Stone. $\beta(r_1)$ is so chosen that the energy E_A of the atom is the minimum, i. e.,

$$\frac{\partial E_A}{\partial \beta} = 0,$$

where

$$E_A = \frac{\langle \Psi_0 + \beta \Psi_1 | H_A + V | \Psi_0 + \beta \Psi_1 \rangle}{\langle \Psi_0 + \beta \Psi_1 | \Psi_0 + \beta \Psi_1 \rangle}. \quad (11)$$

H_A is the Hamiltonian of the atom and $V(r_1, r_2)$ is the interaction of the atomic electron with the incident electron. The coefficient β is given by

$$\frac{\beta}{1 - \beta^2} = - \frac{V_{01}}{E_1 - E_0 + V_{11} - V_{00}}, \quad (12)$$

where

$$V_{if}(r_1) = \langle \Psi_0 | -2/r_1 + 1/|\vec{r}_2 - \vec{r}_1| | \Psi_f \rangle.$$

The function $\beta(r)$ is always negative; thus it correctly represents the effects of the polarization potential.

All the integrals occurring in Eqs. (2), (7)–(10), and (12) have been evaluated numerically. The wave function for the ground state of lithium is taken from Roothaan *et al.*¹⁰ and for the excited state from Stone.⁶

RESULTS AND DISCUSSION

The results of the present calculation for the $2s-2p$ transition in lithium by electron impact have

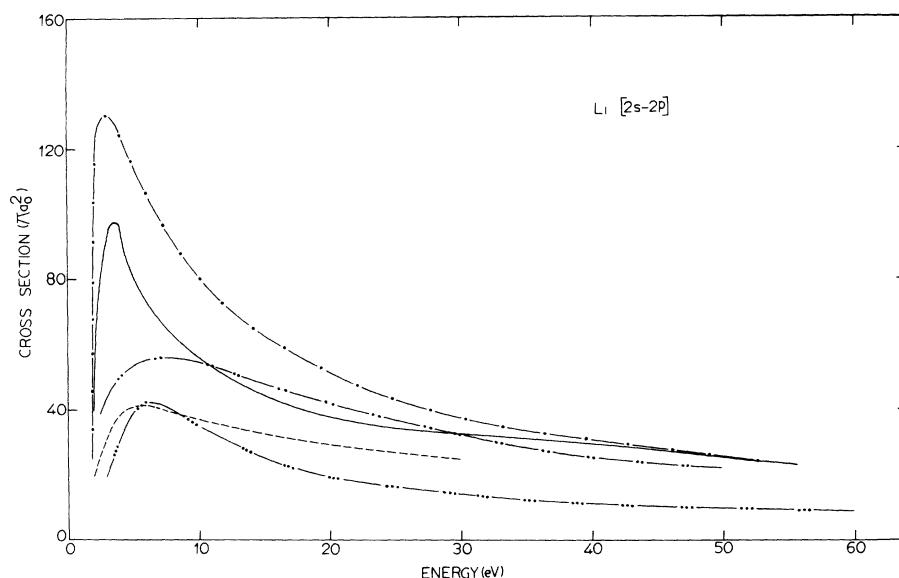


FIG. 1. Electron-impact excitation cross section of the $2s-2p$ state of Li. (—) Present calculations; (---) first-Born-approximation calculations; (-·-·-) close-coupling calculations; (-·-·-) classical binary-encounter calculations; (- - -) experimental data.

been shown in Fig. 1 for energies up to 60 eV. We have also compared our results with the close-coupling calculations of Burke and Taylor,³ the first-Born-approximation calculation of Vainshtein *et al.*,² the classical binary-encounter calculation of the authors,⁴ and the measurements of Hughes and Hendriskson.¹¹ It is seen that the present calculations which are based on the polarized Born approximation including exchange yield a value of the cross section that is lower than the first-Born-approximation calculation in the low- and intermediate-energy region. Near the threshold the reduction in the cross section is about 20%. In the intermediate-energy region the present calculations give a good agreement with the experimental data and close-coupling calculations. At higher energies (≈ 55 eV) the present calculations merge with the first-Born-

approximation calculations. The close-coupling calculations also tend to agree closely with the present calculations at higher energies. This is because the effect of polarization is less important at high energies. The inclusion of exchange in the polarized Born approximation produces a rather small exchange effect for the $2s-2p$ excitation of lithium. Thus we conclude that the inclusion of polarization improves the first-Born-approximation cross section in the low- and intermediate-energy range.

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Energies of s Eigenstates in a Static Screened Coulomb Potential*

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Energies of the $1s$, $2s$, $3s$, and $4s$ states are obtained by a perturbation calculation and by a one-parameter variational calculation for a two-particle system interacting through a static screened Coulomb potential. The variational results are practically identical with those recently obtained by Rogers, Graboske, and Harwood by the numerical integration of the wave equation, except in the region very close to the critical screening.

I. INTRODUCTION

The static screened Coulomb potential (SSCP)

$$V(r) = -e^2 e^{-\alpha r} / r, \quad (1.1)$$

where α is a screening parameter, occurs in several fields of physics. In nuclear physics it goes under the name of the Yukawa potential (with e^2 replaced by another coupling constant), and in plasma physics it is commonly known as the Debye-Hückel potential. Equation (1.1) also describes the potential of an impurity in a metal and in a semiconductor. The significance of α in these different contexts is, of course, all different.

During the last few years a number of studies¹⁻¹⁴ have been carried out to calculate the energy levels of an electron in such a potential and also to determine the number of bound states. Since the Schrödinger equation for Eq. (1.1) is not solvable analytically, the aforesaid investigations have employed perturbation theory,^{6,13} the variational method,^{2-4,12} and the actual numerical integration^{5,9,14} of the differential equation. Of these, the recent results of Rogers *et al.*,¹⁴ obtained by numerical techniques, are of high accuracy over a wide range of the screening parameter and cover 45 eigenstates. In the present paper we show that at least for " s " states, using analytical methods, one can