Pramāṇa – J. Phys., Vol. 25, No. 2, August 1985, pp. 175–177.

The effect of exchange in autoionization processes

J P MOHANTY, C S SINGH and D K RAI

Department of Physics, Banaras Hindu University, Varanasi 221005, India

MS received 30 March 1985; revised 17 May 1985

Abstract. The effect of including distortion (with and without exchange) in the wavefunction for the continuum electron while calculating the probability of autoionization of $2s^2\,{}^1S$, $2s2p\,{}^{1,3}P$, $2p^2\,{}^1D$ and $2p^2\,{}^1S$ states of He and Li^+ has been studied.

Keywords. Autoionization; doubly-excited state; continuum; distortion.

PACS No. 33·80

In this paper we have studied the effect of including the distortion in the continuum wavefunction for the ejected electron while calculating the decay probability of five low lying autoionizing states ($2s^2\,{}^1S$, $2s2p\,{}^{1,3}P$, $2p^2\,{}^1D$ and $2p^2\,{}^1S$) of the He and Li^+. Separate calculations have been performed including distortion (with and without exchange) as well as a pure coulombic wave from the continuum electron.

The probability of autoionization has been evaluated using the formula given by Wentzel (1927) from time-independent perturbation theory. The calculation is based on the method suggested by Wu (1944). Simple constants determined by Slater's rule have been used to represent the doubly-excited states. The continuum electron is assumed to move in the static potential of the ion (He^+ or Li^{++}) and when a partial wave expansion to its wavefunction ψ_k is made in the form

$$\psi_k = k^{-1/2} r^{-1} \exp[i(\delta_l + \eta_l)]\, U_l(k, r) P_l(\cos\theta), \tag{1}$$

where k is the momentum vector of the continuum electron, $(\delta_l + \eta_l)$ is the total phase shift, $P_l(\cos\theta)$ is the Legendre polynomial of degree l we find that the radial part $U_l(k, r)$ satisfies the differential equation (Wu 1944)

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - 2V_{st}\right) U_l(k, r) = W(r) U_l(r), \tag{2}$$

where V_{st} is the static potential of the ion and the term $W(r)U_l(r)$ arises due to exchange and $W(r)$ is known as the exchange potential.

The boundary conditions for $U_l(k, r)$ are

$$U_l(k, r) \to 0, \qquad r \to 0 \tag{3}$$

and

$$U_l(k, r) = (2/\pi)^{1/2} \sin\left(kr - \frac{1\pi}{2} + \frac{z}{k} \ln 2kr + \eta_l(k) + \delta_l\right), \quad r \to \infty \tag{4}$$

here $z = Z - 1$, Z being the charge of the nucleus.

The radial equation (2) for the continuum electron is solved by a non-iterative procedure due to Marriot (1958), the normalization being obtained by comparison with the JWKB solution (Burgess 1963). Three different choices have been made for $U_l(k, r)$. In the first choice both the exchange as well as the static potential terms are retained in the radial equation (2) while it is solved for $U_l(k, r)$. In the second choice we have neglected $W(r)$ and solved the equation with only the static potential. The third choice for $U_l(k, r)$ corresponds to a pure Coulomb function and is obtained by neglecting the exchange potential term and retaining only the electron-nucleus interaction term of the static potential in equation (2). Corresponding to these three solutions three separate calculations have been performed for the decay probability. The integration have been made numerically using a 3-point Simpson rule. The computer program which we developed for this purpose incorporates some parts of a program developed by McDowell *et al* (1974) for distorted wave calculations.

The results of our calculation for He and Li^+ are given in table 1. We see that the effect of exchange is very large in the case of $2s^2\ ^1S$ and $2p^2\ ^1S$ states of helium. In the case of $2p^2\ ^1S$ the results obtained with the inclusion of exchange are 3–4 times smaller than that obtained when the exchange is neglected. For $2s^2\ ^1S$ decay the result obtained including exchange is nearly two times greater than that obtained when the exchange is neglected. In the cases of the states $2s\,2p\ ^1P$ and $2p^2\ ^1D$ the inclusion of exchange has a very small effect. On the contrary for the decay of the $2s\,2p\ ^1P$ state the probability neglecting exchange is nearly 1·5 times greater than that obtained including exchange. In the case of Li^+ the effect of including exchange potential together with the static potential as the cause of distortion for the continuum electron is comparatively smaller. This is due to fact that in this case the static potential of the ion becomes more predominant.

From the comparison of our results we infer that in the case of neutral atoms continuum wavefunction including exchange effects is necessary for a good description. The importance of exchange decreases as ionic charge increases.

Table 1. Decay probability of different autoionizing states of He and Li^+.

States	He			Li^+		
	Distortion with exchange	Distortion without exchange	Coulomb wave	Distortion with exchange	Distortion without exchange	Coulomb wave
$2s^2\ ^1S$	$0·125^{16}$*	$0·623^{15}$		$0·174^{16}$	$0·109^{16}$	
$2s\,2p\ ^3p$	$0·927^{13}$	$0·143^{14}$	$0·165^{14}$	$0·126^{14}$	$0·171^{14}$	$0·195^{14}$
$2s\,2p\ ^1P$	$0·703^{14}$	$0·833^{14}$	$0·713^{14}$	$0·122^{15}$	$0·130^{15}$	$0·120^{15}$
$2p^2\ ^1D$	$0·850^{14}$	$0·846^{14}$	$0·850^{14}$	$0·113^{15}$	$0·113^{15}$	$0·113^{15}$
$2p^2\ ^1S$	$0·258^{15}$	$0·907^{15}$		$0·761^{15}$	$0·120^{16}$	

* Superscript denotes the power of ten by which the number is to be multiplied.

References

Burgess A 1963 *Proc. Phys. Soc.* **81** 442
Marriot R 1958 *Proc. Phys. Soc.* **72** 121
McDowell M R C, Morgan L A Myerscough V P 1974 *Comp. Phys. Commun.* 7 38
Wentzel G 1927 *Z. Phys.* **43** 524
Wu T Y 1944 *Phys. Rev.* **66** 291