Electron capture in collisions between protons and the ions He$^+$ and Li$^{+,2+}$ calculated using a new united-atom model

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Abstract. A new theoretical approach to calculate electron capture cross sections for ion–ion collisions in the intermediate energy region is developed. The impact parameter Schrödinger equation is solved by using an expansion in a two-state orthogonal basis which contains the charge $Z(R)$ of the 'united atom'. The electron capture amplitude is expressed in an analytic form for low capture probabilities and the peak point approximation. Our results for H$^+$+He$^+$ and H$^+$+Li$^+$ agree well with experimental data in the ranges 30–200 keV and 70–300 keV respectively. The results are compared with other theoretical results and quite a good agreement is obtained.

1. Introduction

Electron capture for ion–ion collision is one of the important processes in a plasma. The reactions

$$H^+ + He^+(1s) \rightarrow H + He^{2+} \tag{1}$$

$$H^+ + Li^{2+}(1s) \rightarrow H + Li^{3+} \tag{2}$$

$$H^+ + Li^+(1s^2) \rightarrow H + Li^{2+}(1s) \tag{3}$$

are very interesting in thermonuclear fusion research. Recently, many theoretical studies on electron capture processes from He$^+$ and Li^{2+} by protons have been reported. Errea *et al* (1987) studied reaction (1) using a molecular approach. Reading *et al* (1982a, b) calculated the capture cross sections for reactions (1) and (2) in the ranges 25–500 keV and 50–200 keV, respectively, by using the perturbative 'one-and-a-half-centred' *expansion method* (POHCE). Winter (1986, 1987) studied the first two reactions by using a Sturmian basis with 19–45 pseudostates at energies 17.5–200 keV. The capture cross sections for reaction (2) were obtained by Ermolaev and McDowell (1987) who adopted the coupled-state impact parameter codes, with 32 and 59 atomic orbitals respectively, for the energy region 17.5–3000 keV lab. Bransden and Noble (1981) used atomic orbital expansion to study reaction (1) for energies 4–230 keV. The continuum distorted-wave approximation (CDW) was used to compute the capture cross sections for reactions (1) and (2) by Mukherjee and Sil (1980). However, the agreement among theories as well as between theories and experiments is rather poor in the intermediate energy region.

For reaction (3), the existing theoretical methods are POHCE (Reading *et al* 1982b), classical trajectory Monte Carlo (CTMC) (Olson and Salop 1977) and the CDW approximation (Banyard and Shirtcliffe 1979, 1980). On the other hand, Sewell *et al* (1980) reported their experimental data for the electron capture for energies from 70–250 keV. However, there exists a large discrepancy between the above theories and the experimental findings.

Most of the above theories utilized a big basis to reflect the coupling between projectiles and targets, and the choice of the basis affects greatly theoretical results. However, Bransden and Noble (1981) have pointed out that, for the above reactions, the most important states are H(1s) and the 1s states of hydrogenic ions.

In this paper we take into account the 'united-atom' model suggested by Campos *et al* (1983). The charge $Z(R)$ of the 'united atom' may be written in the form

$$Z(R) = Z_t + \rho(R)Z_p$$

where Z_t and Z_p are the charges of the targets and the projectiles respectively, R is the internuclear distance and $\rho(R)$ is a 'weight factor' which will be determined by using the variational principle. The factor $\rho(R)$ varies from zero to unit when R varies from infinity (the separated-atom limit) to zero (the united-atom limit). That is, the charge of the 'united atom' changes from Z_t to $Z_t + Z_p$. In this model we choose the ground states of the 'united-atom' and the projectile to construct an orthogonal basis.

Our notation is as follows: r_1 and r_2 are the position vectors of the active electron with respect to the nuclei of the target and the projectile respectively, R is the vector of the projectile relative to the target and z_R is the component of R in the direction of the projectile velocity v. We assume that the projectile is moving along a straight path with impact parameter b, so we have $R = b + vt = b + z_R$ and $b \cdot v = 0$. Channel marks j and k refer to the initial and final channels of the reaction respectively.

Atomic units are used unless otherwise stated.

2. Theory

2.1. Formulae

Firstly, we determine the parameter $Z(R)$. When the internuclear distance is R and the electron is in the ground state of the 'united-atom', i.e. in the channel j, the electronic wavefunction is

$$U_j(r_1, R) = \pi^{-1/2}[Z(R)]^{3/2} \exp(-2Z(R)r_1). \tag{4}$$

In the impact parameter method, the electronic Hamiltonian is

$$\hat{H}(r_1, R) = \left(-\tfrac{1}{2}\nabla_{r_1}^2 - \frac{Z}{r_1}\right) + \left(\frac{Z - Z_t}{r_1} - \frac{Z_p}{r_2}\right) + \frac{Z_t Z_p}{R}. \tag{5}$$

Defining an average energy E_j

$$E_j = \langle U_j(r_1, R)|\hat{H}|U_j(r_1, R)\rangle \tag{6}$$

and substituting (4) and (5) into (6), we obtain the average energy

$$E_j = \tfrac{1}{2}Z^2 - (Z_t Z + Z_p/R) + Z_p(Z + 1/R)\exp(-2ZR) + Z_t Z_p/R. \tag{7}$$

where Z is still a variable parameter depending on the internuclear distance R. Before transfer, the electron is always in the ground state of the 'united atom'. So we adopt the variational principle $\partial E_j/\partial Z = 0$ to optimize the parameter Z

$$Z = Z_t + Z_p(1 + 2RZ) \exp(-2RZ) \tag{8}$$

which ensures that E_j is always the lowest energy level of the 'united atom' for arbitrary R. The extra terms in (8) really represent an effective screening of the target. Now the charge parameter Z, for each given R, is a solution of the non-linear equation (8).

After transfer, i.e. the electron is in the 1s orbital of the projectile, the electronic wavefunction $U_k(r_2)$ is an exact 1s function of the hydrogen atom with charge Z_p. The wavefunctions with plane-wave translation factors are of the following form

$$V_j(r_1, t) = U_j(r_1, R) \exp(-iqv \cdot r - \tfrac{1}{2}iq^2v^2t) \tag{9}$$

$$V_k(r_2, t) = U_k(r_2) \exp(i(1-q)v \cdot r - \tfrac{1}{2}i(1-q)^2v^2t) \tag{10}$$

where r is a vector of the electron relative to the mass centre of two nuclei, $q = M_p/(M_t + M_p)$ and M_t and M_p are the masses of the target and the projectile. So we have $r_1 = r + qR$ and $r_2 = r - (1-q)R$.

Obviously, the wavefunctions V_j and V_k are not orthogonal functions. In order to expand the impact parameter wavefunction $\Phi(r_1, t)$, we must construct a new function $\chi_k(r_2, t)$

$$\chi_k(r_2, t) = A_k(t)[V_k(r_2, t) - V_j(r_1, t)N_{jk}(t)] \tag{11}$$

which is orthogonal to $V_j(r_1, t)$. The normalization factor $A_k(t)$ and the overlap integral $N_{jk}(t)$ are

$$A_k(t) = (1 - |N_{jk}|^2)^{-1/2} \qquad N_{jk}(t) = \langle V_j(r_1, t)| V_k(r_2, t)\rangle. \tag{12}$$

$\Phi(r_1, t)$ is then expanded as

$$\Phi(r_1, t) = c_j(t)V_j(r_1, t) \exp(-iE_t t) + b_k(t)\chi_k(r_2, t) \exp(-iE_p t) \tag{13}$$

where $E_t = -\tfrac{1}{2}Z_t^2$ and $E_p = -\tfrac{1}{2}Z_p^2$. The coefficients c_j and b_k obey the normalization condition

$$|c_j(t)|^2 + |b_k(t)|^2 = 1. \tag{14}$$

The scattering process is described by the time-dependent Schrödinger equation

$$(i \partial/\partial t - \hat{H})\Phi(r_1, t) = 0. \tag{15}$$

Substituting (13) into (15) and taking into account low capture probabilities, i.e. let $c_j(t) \simeq 1$, we get the amplitude equation

$$i\dot{b}_k(t) = V_{kj} \exp(i\varepsilon t) \tag{16}$$

where $\dot{b}_k(t)$ is the time differentiation of the amplitude $b_k(t)$ and $\varepsilon = \tfrac{1}{2}(Z_t^2 - Z_p^2)$. The matrix element V_{kj} in (16) is defined as

$$V_{kj} = \langle \chi_k|\hat{H} - i \partial/\partial t| V_j\rangle = A_k^*(t)[\bar{N}_{kj} - N_{kj}D_j(R)] - \langle \chi_k|i \partial/\partial t|V_j\rangle \tag{17a}$$

with

$$\bar{N}_{kj} = \left\langle V_k \left| \frac{Z - Z_t}{r_1} - \frac{Z_p}{r_2} \right| V_j\right\rangle \tag{17b}$$

$$N_{kj} = N_{jk}^* \tag{17c}$$

$$D_j(R) = Z(Z - Z_t) - \frac{Z_p}{R}[1 - (1 + ZR) e^{-2ZR}]. \tag{17d}$$

The last term in (17a) may be ignored compared with other terms. So the amplitude b_k in (16) takes the following simple form

$$b_k(b) = \frac{1}{iv} \int_{-\infty}^{+\infty} dz_R \, V_{kj} \exp(i\varepsilon\eta z_R) \tag{18}$$

where $\eta = 1/v$. At the intermediate–high energies, the overlap integral $|N_{jk}|$ is much less than unity. So we have $A_k(t) \simeq 1$. Now we utilize the Fourier transform

$$\frac{1}{r} \exp(-cr) = \frac{1}{2\pi^2} \int d\mathbf{Q} \, \frac{\exp(-i\mathbf{Q} \cdot \mathbf{r})}{c^2 + Q^2} \tag{19}$$

and insert (17a)–(17d) into (18) by using (4), (9), (10) and (19). Equation (18) then contains the integral $\int d\mathbf{r}_1 \, d\mathbf{Q} \, d\mathbf{Q}' \, dz_R$. The integral $\int d\mathbf{r}_1$ may be performed and yields a three-dimensional delta function $\delta(\mathbf{Q}' - \mathbf{Q} - \mathbf{v})$ by which we can perform the integral $\int d\mathbf{Q}'$. Next, the integral $\int d\mathbf{Q} = \int d\mathbf{q} \, dQ_z$, in which $\mathbf{q}$ and Q_z are the transverse and longitudinal components of the momentum respectively, and the two-dimensional integral $\int d\mathbf{q}$ may be carried out analytically by using the Laplace transform and the table of integrals of Gradshteyn and Ryzhik (1980). Finally, we get the following integral

$$b_k(b) = \frac{2^3 Z_p^{5/2}}{iv} \int dQ_z \, dz_R \, I(Q_z, R) \exp(i(\varepsilon\eta + \tfrac{1}{2}v - Q_z)z_R) \tag{20}$$

with

$$I(Q_z, R) = Z^{3/2}[(Z - Z_t)I_{12}(Q_z, R) - ZI_{21}(Q_z, R) - 2ZD_j(R)I_{22}(Q_z, R)] \tag{21}$$

$$I_{12}(Q_z, R) = \frac{1}{\Delta^2}\left(K_0(ab) - K_0(cb) - \frac{b}{2c}\Delta K_1(cb)\right) \tag{22a}$$

$$I_{21}(Q_z, R) = \frac{1}{\Delta^2}\left(K_0(cb) - K_0(ab) + \frac{b}{2a}\Delta K_1(ab)\right) \tag{22b}$$

$$I_{22}(Q_z, R) = \frac{1}{\Delta}[I_{21}(Q_z, R) - I_{21}(Q_z, R)] \tag{22c}$$

where $a^2 = Z^2 + (Q_z - v)^2$, $c^2 = Z_p^2 + Q_z^2$, and $\Delta = c^2 - a^2$. The functions $K_0(x)$ and $K_1(x)$ are the zeroth order and the first-order change variable Bessel functions respectively. It may be checked that the function $I(Q_z, R)$ is much less than unity for any values of Q_z and R. Thus, the oscillating factor $\exp(i(\varepsilon\eta + \tfrac{1}{2}v - Q_z)z_R)$ makes the integral in (20) tend to zero except for points near $Q_z = \varepsilon\eta + \tfrac{1}{2}v$. That is, the maximum contribution for the amplitude b_k is taken from these points. We then get an analytical expression for the amplitude b_k by adopting the peak point approximation at $Q_z = \varepsilon\eta + \tfrac{1}{2}v$,

$$b_k(b) = \frac{2^4 Z_p^{5/2}}{iv} I(Q_z = \varepsilon\eta + \tfrac{1}{2}v, b, z_R = 0)$$

$$= \frac{2^4 Z_p^{5/2}}{iv} Z^{3/2}[(Z - Z_t)I_{12}(b) - ZI_{21}(b) - 2ZD_j(b)I_{22}(b)] \tag{23}$$

where the function $I_{mn}(b)$ is obtained by making $Q_z = \varepsilon\eta + \tfrac{1}{2}v$ and $z_R = 0$ in (22a)–(22c). Now the total 1s–1s cross section is

$$\sigma_{1s-1s} = 2\pi \int_0^\infty db \, b|b_k(b)|^2. \tag{24}$$

The integral in (24) is calculated by means of a numerical method and it converges rapidly. Usually, we need only integrate for the impact parameter b up to a few multiples of the first Bohr radius.

2.2. Connections with other Born approximation

The amplitude $b_k(b)$ in (18) may be divided into two parts

$$b_k(b) = b_k^{(1)}(b) + b_k^{(2)}(b) \tag{25}$$

where

$$b_k^{(1)}(b) = \frac{1}{iv} \int dz_R \exp(i\varepsilon\eta z_R) \left\langle V_k \left| \frac{Z_p}{r_2} - D_j(R) \right| V_j \right\rangle \tag{26}$$

$$b_k^{(2)}(b) = \frac{1}{iv} \int dz_R \exp(i\varepsilon\eta z_R) \left\langle V_k \left| \frac{Z - Z_t}{r_1} \right| V_j \right\rangle. \tag{27}$$

If we do not consider the 'united-atom' model, we will have $Z = Z_t$ and $b_k^{(2)} = 0$. Then $b_k(b) = b_k^{(1)}(b)$ is the amplitude obtained by Bates (1958) by neglecting the distortion of the electron wavefunction in the nuclear field of the projectile and the target and the overlap effect between wavefunctions in the initial and final states. For the capture from the K shell of the target to the K shell of the projectile, $D_j(R)$ is

$$D_j(R) = -\frac{Z_p}{R} [1 - (1 + Z_t R) \exp(-2Z_t R)]. \tag{28}$$

If we ignore the non-orthogonality between the wavefunctions in the initial and the final states, the amplitude $b_k^{(1)}$ changes into the OBK (Oppenheimer–Brinkman–Kramers) result.

If we take into account the 'united-atom' model, the wavefunction $V_j(\mathbf{r}_1, t) = V_j^0(\mathbf{r}_1, t)(Z/Z_t)^{3/2} \exp(-\rho(R)Z_p r_1)$, $V_j^0(\mathbf{r}_1, t)$ is the undistorted wavefunction in the initial state. The factor $(Z/Z_t)^{3/2} \exp(-\rho(R)Z_p r_1)$ describes the distortion of the electron wavefunction by the nuclear field of the projectile. That is, $b_k^{(1)}$ is an amplitude considered for the distortion of the initial wavefunction and the correction for non-orthogonality of the basis functions. $b_k^{(2)}$ in (27) is a second-order term.

In addition, the present idea is partially related to the idea of Campos *et al* (1983). However, we have modified their method by introducing Standard translation factors in (9)–(10) and choosing an undistorted final-state function $U_k(\mathbf{r}_2)$ which is similar to $U_j(\mathbf{r}_1, R)$ in the paper of Campos *et al*. We think that these modifications are very important for non-resonant collisions at the intermediate energies.

3. Results

3.1. $H^+ + He^+$ and $H^+ + Li^{2+}$

The present results are given in table 1. The entry of σ_{total} is obtained by multiplying σ_{1s-1s} by 1.2, which comes from the OBK approximation for the capture into all discrete states of a hydrogen atom. Comparisons with other theoretical and experimental results are plotted in figure 1. It can be seen that the present calculations for $H^+ + He^+$ are

Table 1. The electron capture cross sections for reactions $H^+ + He^+$ and $H^+ + Li^{2+}$. σ_{1s-1s} and σ_{total} are the capture cross sections for the electron captured into the 1s orbital and all discrete states of the hydrogen atom respectively. The unit is 10^{-18} cm^2.

|	$H^+ + He^+$		$H^+ + Li^{2+}$	
E (keV)	σ_{1s-1s}	σ_{total}	σ_{1s-1s}	σ_{total}
30	20.99	23.72†	0.31	0.37
40	21.81	26.17	0.55	0.66
50	20.85	25.02	0.79	0.95
75	15.75	18.90	1.26	1.51
100	11.08	13.30	1.49	1.79
125	7.73	9.28	1.53	1.84
150	5.47	6.56	1.46	1.75
175	3.91	4.69	1.34	1.61
200	2.84	3.41	1.19	1.43

† $\sigma_{total} = 1.13\sigma_{1s-1s}$ at 30 keV according to Errea (1987).
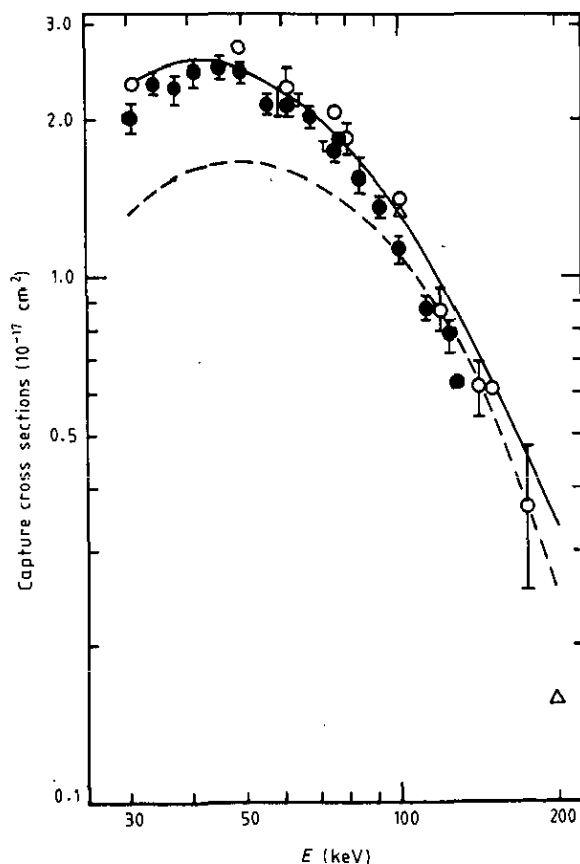
Figure 1. Total cross sections for electron capture from $He^+(1s)$ by H^+ as a function of the projectile energy. Theory: ——, present work; ○, Sturmian basis (Winter 1986, 1987); ●, POHCE (Reading *et al* 1982a); – – – –, AO8 (Bransden and Noble 1980); △, CDW (Mukherjee and Sil 1980). Experiment: ⊕, Rinn *et al* (1985); ⊖, Watts *et al* (1986).

in quite good agreement with the experimental findings reported by Rinn *et al* (1985) in the range of energy 30–100 keV, the maximum difference of about 10% occurs at 30 keV. Our cross sections are about 10% higher than Rinn's data above 100 keV, but agree very well with the data provided by Watts *et al* (1986) who remeasured the reaction (1) from 60 to 180 keV lab. The present calculations accord well with POHCE (Reading *et al* 1982a) result at 75 keV, but the latter is about 25% lower than ours at 130 keV. The results of a Sturmian basis with 19–35 pseudostates (Winter 1986, 1987) agree well with our results for the entire energy region calculated. The capture cross sections obtained from the eight-state atomic basis (Bransden and Noble 1981) give very good agreement with ours and experiments over 100 keV, but they are much lower than experiments at energies 30–100 keV. Mukherjee and Sil (1980) obtained CDW cross sections which are in agreement with our results within experimental error at energies 100 and 200 keV.

Figure 2 shows the 1s–1s cross sections for $H^+ + Li^{2+}$. There are no experimental data available. The result of a 32 atomic orbital expansion (Ermolaev *et al* 1987) is about 30% higher than our calculation at 50 keV. However, the situation is reversed at 30 and 150 keV. Both results accord well within 13% for energies 87.5 and 100 keV. The POHCE (Reading *et al* 1982b) results are 17% larger than ours at 50 and 100 keV, but 17% lower at 200 keV. Results calculated by using a Sturmian basis with 26–45 pseudostates (Winter 1986, 1987) agree well with our cross sections for the entire energy region calculated except for 75 and 100 keV where Sturmian results are 17% higher than our capture cross sections. However, there exists an obvious difference between the Sturmian approximation and the present method for the peak energy to which the maximum capture cross section corresponds. The former has a peak at 100 keV, but the latter peaks at 125 keV which is just what is predicted by the OBK approximation.
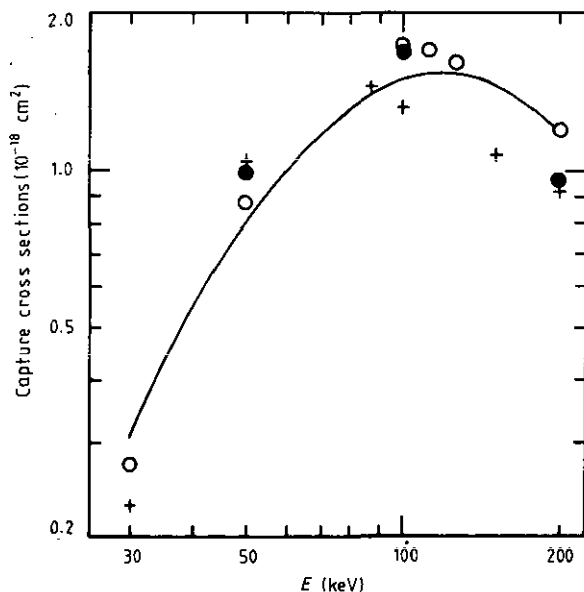
Figure 2. 1s–1s cross sections for electron capture from Li^{2+} (1s). Theory: ●, ○, as figure 1; +, AO32 (Ermolaev *et al* 1987).

3.2. $H^+ + Li^+$

Li^+ is the simplest multielectron target for ion–ion collision. We utilize the independent-electron model in which the correlation term between the electrons and the Coulomb interaction from the nucleus are replaced by their average

$$-\frac{Z_t}{r_1} - \frac{Z_p}{r_2} + \frac{1}{r_{12}} = -\frac{Z_t^{\text{eff}}}{r_1} - \frac{Z_t^{\text{eff}}}{r_2}$$

where r_i is the distance of the ith electron relative to the target nucleus. Then the wavefunction of the lithium ion Li^+ is a simple product of the hydrogenic wavefunctions

Table 2. Similar to table 1 for the reaction $H^+ + Li^+$. The column POHCE corresponds to the POHCE results and column Sewell to the data of Sewell *et al* (1980).

E (keV)	σ_{1s-1s}	σ_{total}	POHCE	Sewell
50	14.19	17.03		
60	14.84	17.81		
70.86	14.78	17.74	12.33	21.9 ± 3.4
80	14.26	17.11		
94.86	13.02	15.62	10.26	19.4 ± 2.2
100.57	12.48	14.98		18.1 ± 2.0
134.86	9.20	11.04	6.65	15.1 ± 0.9
166.86	6.73	8.08	4.56	10.0 ± 1.2
194.3	5.14	6.17	3.34	
210.29	4.37	5.24		6.0 ± 1.8
252.57	2.92	3.50	1.80	3.6 ± 1.7
400	0.84	1.01	0.45	
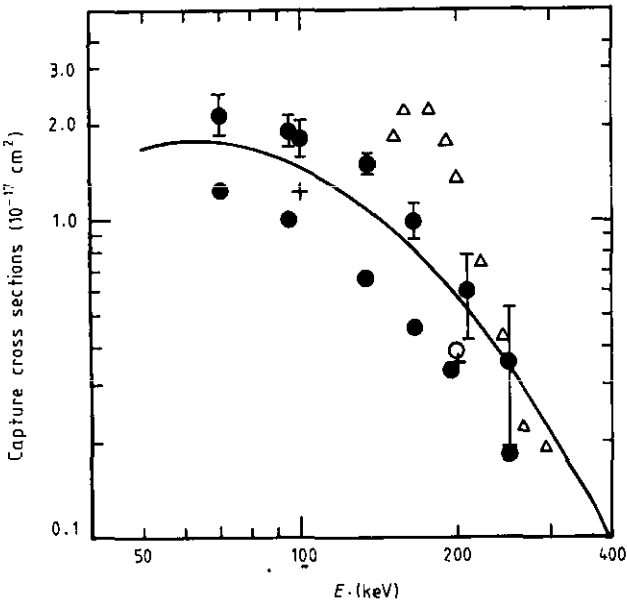
Figure 3. Similar to figure 1 for electron capture from $Li^+(1s^2)$. Theory: O, +, CDW (Banyard and Shirtcliffe 1979, 1980); $\triangle$, CTMC (Olson and Salop 1977). Experiment: ●, Sewell *et al* (1980).

with the effective charge Z_t^{eff} which is chosen so as to adjust the first ionization potential to the experimental finding. So the charge Z_t in the above equations is replaced by Z_t^{eff} and the total 1s–1s capture cross section in (24) is mutiplied by two because of the two 1s electrons for Li$^+$.

Our total capture cross sections for H$^+$ + Li$^+$ are given in table 2. In figure 3 we present our results as a function of the impact energy and also show other theoretical values and experimental data. From figure 3 it can be seen that our capture cross sections are in close agreement with experimental data (Sewell *et al* 1980) within 9% for the energy region from 70 to 252 keV except for 135 keV, where our value is 26% lower than the measurement. Moreover, our capture cross section reaches its maximum at about 60 keV, which is in good accord with the experimental trend and the prediction of the OBK approximation. The POHCE (Reading *et al* 1982b) results somewhat underestimate the observed values for the entire region calculated and so do the CDW results (Banyard and Shirtcliffe 1979, 1980). Compared with the experiment, however, CTMC (Olson and Salop 1977) results have an obviously different trend.

In conclusion, we have developed a new method to calculate electron capture cross sections under the 'united-atom' model. This method not only has very simple numerical computation, but also it gives a good agreement with experiment and other theories. Therefore we consider that this method should be tested for other collision reactions.

Acknowledgments

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