Differential cross section for the excitation of hydrogenlike ions from He^+ to C^{5+} by low-energy-electron impact

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A close-coupling calculation with 1*s*, 2*s*, and 2*p* states has been carried out for the 1*s*-2*s*,2*p* excitations of hydrogenlike ions by electrons with an energy lower than 2.5 times the excitation energy. Differential cross sections show a strong dependence on both nuclear charge and impact energy, especially for the 1*s*-2*s* excitation. A scaling relation for differential cross sections is well satisfied for the 1*s*-2*p* transition. A comparison is made between the present result and other theoretical calculations.

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Excitation processes of atomic ions by electron impact are of great importance in applications to astrophysics, laser technologies, and thermonuclear fusion plasmas. Differential cross sections (DCS) of these processes have been the subject of considerable recent interest from a theoretical point of view. In particular, the DCS in collisions between electron and H-like ions are instructive to elucidate the mechanism of the collision processes, because the collision systems are the simplest prototype of similar, but more complicated ones.

To the authors' knowledge, the first calculation of DCS was carried out by Berrington *et al.* [1] for the excitation of 2*s* state of He^+ at $X \simeq 1$ within a framework of the *R*-matrix theory. Here, X is the impact energy divided by excitation threshold energy (3 Ry in the case of He^+). Recently, a systematic study along an isoelectronic sequence was made by Nakazaki and Itikawa [2] on the 1*s*-2*s*,2*p* excitations of H-like ions at $X \geq 2$ in the Coulomb-Born (CB) and the Coulomb-Born-Oppenheimer (CBO) approximations. This sutdy was followed by Srivastava *et al.* [3], who made a calculation on the excitation of the 2*p* state of He^+ at $X=2$ in the distorted-wave exchange approximation (DWXA) method.

In this Brief Report, the excitations of the 2*s* and 2*p* states of H-like ions from He^+ to C^{5+} by electrons with energy of $1<X<2.5$, have been examined theoretically by using the close-coupling (CC) approximation proposed by Eisner and Seaton [4] (referred to as I, hereafter). In actual calculations, the computer code IMPACT of Crees *et al.* [5] has been employed. The energy matrix elements H_{jj}, of the two-electron system and the algebraic coefficients of a_{ij}, b_{ij}, $f_{ii'}$, and $g_{ii'}$ [see Eqs. (6.2), (6.4), and (6.5) of I], which are required as input for IMPACT, have been computed with the computer codes RIAS [6] and WEIGHTS [7], respectively.

Numerical calculations have been carried out by taking into account the 1*s*, 2*s*, 2*p*, 3*s*, 3*p*, and 3*d* states of H-like ions in the CC expansion. Inclusion of the $n=3$ states reduces DCS in magitude by 18% and 17% for the 1*s*-2*s* and 1*s*-2*p* transitions, respectively, but has no effect on the change of DCS in shape except for the cases where the resonances in series converging to the $n=3$ ion states occur [8]. Besides, the six-state CC calculation is very time consuming. Therefore, the simpler three-state (1*s*, 2*s*, and 2*p*) CC approximation is employed in this study.

With the use of IMPACT we can obtain R matrix defined as

$$\mathbf{F}(r)\rightarrow k^{-1/2}[\sin\xi+(\cos\xi)\mathbf{R}] \quad \text{as } r\rightarrow\infty \ , \tag{1}$$

where, for each channel i,

$$\xi_i=k_i r-\tfrac{1}{2}\ell_i\pi+(z/k_i)\ln(k_i r)+\sigma_i, \quad z=Z-1 \ , \tag{2}$$

with k_i the wave number of electron of the channel, ℓ_i the orbital quantum number, and σ_i $[=\arg(\ell_i+1-iz/k_i)]$ the Coulomb phase shift. Collision strength for the transition $i\rightarrow f$ is defined as

$$\Omega(i\rightarrow f)=\frac{1}{2}\sum_{S,L,\pi}\sum_{l,l'}(2S+1)(2L+1)|T_{fi}(ll';SL\pi)|^2 \tag{3}$$

with T matrix

$$\mathbf{T}=2i\mathbf{R}/(\mathbf{I}-i\mathbf{R}) \ , \tag{4}$$

where ll' refers, for a given $LS\pi$, to the set of channels which include the ionic states i and f.

In Table I, the results of scaled collision strength $Z^2\Omega$ with respect to the nuclrar charge Z are listed for the 1*s*-2*s* and 1*s*-2*p* excitations of the He^+ to C^{5+} ions. Similar CC calculations are available in the case of He^+. For the 1*s*-2*p* transition, the present results are in close agreement with the three-state CC calculations of Hayes and Seaton [9]. For the 1*s*-2*s* excitation, the present results exactly agree with the three-state CC calculations of Berrington *et al.* [1] just above the threshold energy. The plot of $Z^2\Omega$ in Refs. [1] and [9] shows a monotonic behavior. However, a similar plot of $Z^2\Omega$ in the present calculation shows a shoulder in the range of X from 1.06 to 1.5; although less clear it is still discernible. The present results are within a numerical error of 1% estimated from the symmetry of the R matrix. A slightly larger discrepancy of 5% exists at $X=1.01$, compared with the calculation of Hayes and Seaton. This might be due to a difference between theirs and ours in the calculation of the two-electron energy matrix $H_{jj'}$. The cross section is very

TABLE I. Scaled collision strength $Z^2\Omega$ with respect to nuclear charge Z for the 1s-2s,2p excitations. X is the impact energy divided by excitation energy.

	He^+		Le^{2+}		Be^{3+}		B^{4+}		C^{5+}	
X	2s	2p	2s	2p	2s	2p	2s	2p	2s	2p
1.0017	0.770	1.45								
1.0033	0.766	1.46								
1.05	0.775	1.84	0.754	2.58	0.706	2.85	0.679	2.94	0.671	2.99
1.0667	0.773	1.94								
1.33	0.726	3.06								
1.5	0.677	3.44	0.642	3.61	0.649	3.65	0.660	3.66	0.670	3.67
2.0	0.641	4.21	0.649	4.33	0.667	4.38	0.682	4.40	0.693	4.41
2.5	0.658	4.93	0.672	5.02	0.690	5.06	0.704	5.10	0.714	5.12

sensitive to it just above the threshold energy. Another reason for this discrepancy may be considered to come from the choice of tabular points for the integration of radial functions. We have used 84 tabular points to achieve an error of 1% in DCS. In the calculation of Ω, much less tabular points, say 20, are usually used.

At impact energy near threshold region in the 2s-2p coupling effect is appreciably sensitive and the scaling relation is broken. At higher energies, $X \geq 1.5$, however, the relation is satisfied within an error of 9% for the 1s-2s excitation and of 7% for the 1s-2p.

In order to compute the DCS with the computer code DCS2 of Onda *et al.* [10], the R matrix was transformed into the R' matrix with Coulomb phase shift defined by

$$\mathbf{F}(r) \rightarrow k^{-1/2}[\sin\xi' + (\cos\xi')\mathbf{R}'] ,$$

$$\xi' = \xi - \sigma \quad \text{as } r \rightarrow \infty . \tag{5}$$

We can readily obtain a relation between matrices $\mathbf{R}$ and $\mathbf{R}'$

$$\mathbf{R}' = [\sin\sigma + (\cos\sigma)\mathbf{R}]/[\cos\sigma - (\sin\sigma)\mathbf{R}] . \tag{6}$$

Figures 1 and 2 show the DCS for the 1s-2s and 1s-2p transitions of the He^+ ion at the impact energies of 3.005, 3.01, 3.20, and 3.99 Ry. Compared with the DCS for the 1s-2s excitation of Berrington *et al.* [1], the present results show that the backward scattering becomes more dominant. The DCS for the 1s-2p excitation is nearly symmetric at the scattering angle of 90° at low energy and becomes peaked at 0°, as the collision energy increases.

In order to check the convergence of the partial wave expansion, the 1s-2p DCS at 3.99 Ry, as a typical example, was calculated with R matrices up to a maximum total orbital angular momentum $L_{max}=20$. For the energies considered here, R matrices up to a maximum total $L_{max}=10$ were sufficient to give reliable DCS within an error of 1%.

Although the integrated cross section of Berrington *et al.* for the 1s-2s excitation agrees well with the present

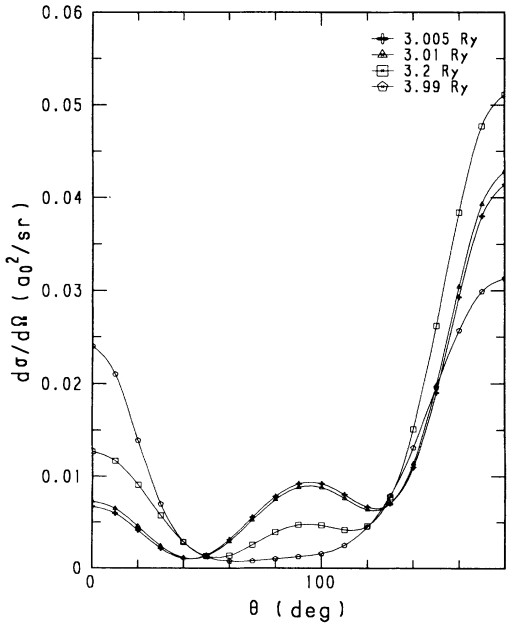

FIG. 1. Differential cross section for the 1s-2s excitation of He^+.

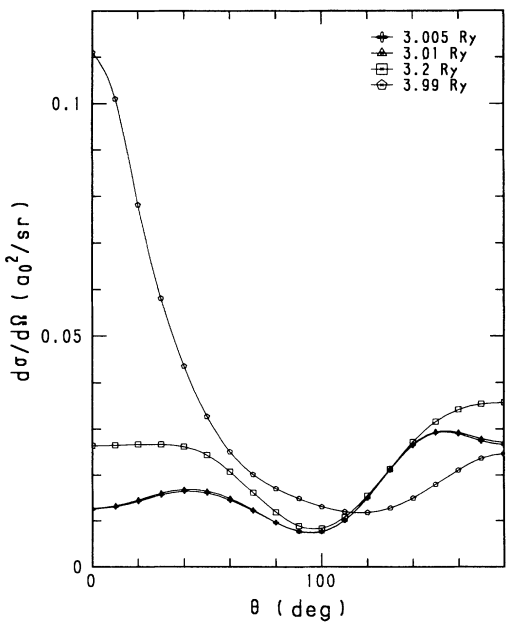

FIG. 2. Differential cross section for the 1s-2p excitation of He^+.

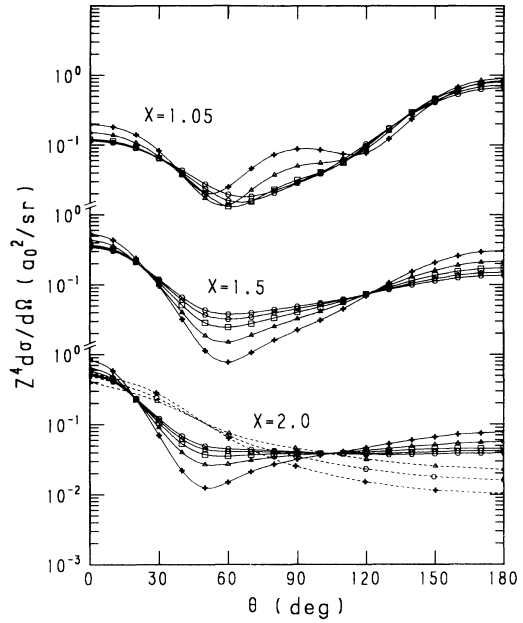

FIG. 3. Scaled differential cross section $Z^4 d\sigma/d\Omega$ with respect to nuclear charge Z for the 1s-2s excitation. The symbols of cross, triangle, square, pentagon, and hexagon are for the He^+, Li^{2+}, Be^{3+}, B^{4+}, and C^{5+} ion, respectively. Dotted curves with $X=2.0$ show the Coulomb-Born calculation by Nakazaki and Itikawa in Ref. [2].

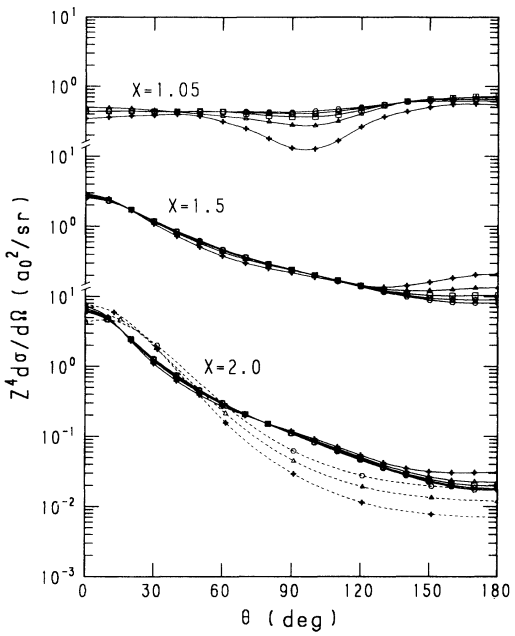

FIG. 4. The same as Fig. 3 but for the 1s-2p transition.

calculation, the DCS are quite different from each other. This is due to the fact that the Coulomb phase shift was not correctly dealt with in Ref. [1], because we can get the same results as theirs when the R matrix, instead of the R' matrix, is applied to the original version of the computer code of Salvini [11].

Scaled DCS, $Z^4 d\sigma/d\Omega$, is plotted in Fig. 3 for the 1s-2s transition of the He^+ to C^{5+} ions at the energies $X=1.05$, 1.5, and 2.0. In this cases, R matrices up to $L_{max}=14$ were computed. At $X=1.05$, the scaled DCS of He^+ and Li^{2+} show a different behavior, that is, there appears a maximum at about 90°, corresponding to that on the DCS curve (see Fig. 1). This feature is strongly dependent on both the nuclear charge Z and the collision energy, because there appears no maximum in the case of $Z \geq 3$ and a minimum instead appears on the scaled DCS curve at the higher energies. In the CB and CBO calculations at $X=2.0$ of Nakazaki and Itikawa, such a minima is not predicted. It is considered, therefore, that inclusion of the 2s-2p coupling is effective and indispensable in the calculation of DCS. As the collision energy increases, the forward scattering becomes more probable than the backward scattering, as expected. The exchange effect in large-angle scattering is more enhanced than in the CBO approximation.

Figure 4 is the same as Fig. 3 but for the 1s-2p transition. R matrices up to $L_{max}=23$ were computed in this case. At $X=1.05$, the DCS is almost isotropic except for the case of He^+, where a minimum around 90° is discernible. As the collision energy increases, the 2s-2p coupling is less effective and the scaling relation is well satisfied except for large scattering angle, $\theta \geq 120°$, compared with the DCS for the 1s-2s excitation. In a recent article of Srivastava *et al.* [3] a comparison has been made among the DCS for the exctiation of the 2p state of He^+ at $X=2$ calculated in the CB, CBO, and DWXA approximations (see Fig. 7 in Ref. [3]). The present result is in good accord with the DWXA calculation, although the former is two times greater than the latter at the scattering angle of 90°. This difference may be due to the effect of the 2s-2p coupling.

We have examined scaled DCS of the excitations to the 2s and 2p states of H-like ions from He^+ to C^{5+} in the three-state close-coupling approximation with the $n=2$ states. This is because inclusion of the higher-n states is not so effective as in other positive ions [12] with more than one electron. A comparison has been made between the present calculation and the CB, CBO, and DWXA calculations. However, in order to study the accuracy of the approximation, comparison of the present result with experimental measurements is an excellent way. But, there are no measurements for these ions available at present.

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