K-matrix Correction of B, CB Cross-Sections

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1 Introduction

There are two approaches in the calculations of excitation and ionization of atoms and ions by electrons.

A. Sophisticated *CC-type* methods, such as *R-matrix* [1] and *CCC* [2]. They usually provide sufficiently accurate results. However, there are some disagreements and questions in particular cases.

B. Rather simple *Born-type* (1. order) methods – *B* (Born), *CB* (Coulomb-Born) with possible inclusion of exchange and normalization.

Generally, cross sections obtained by *A*-methods are preferable, but they are available for a very limited number of transitions and atoms. Fast calculations for many transitions required for atomic data in diagnostic code are in fact unreliable. Therefore, use of the *B*-methods is necessary. For example, using the code **ATOM** one can calculate as many cross sections and rate coefficients as necessary with minimal preparation.

Unfortunately, the accuracy of calculations by simple *CB* methods is often insufficient. To create real databases it is important to understand the physical reasons for errors and to develop sufficiently simple ways of correcting them. One very efficient way is the *K*-matrix method. It is based on a 1. order *B* (*CB* for ions) calculation of the matrix **K** for a given set of transitions

$$K_{\Gamma\Gamma'} = \langle\ ,\ |U|\ ,\ '\rangle\ ,\quad ,\ = a\epsilon l S_T L_T \tag{1}$$

where a is a set of target quantum numbers, ϵl are incident electron energy and orbital momentum, and $S_T L_T$ are total angular momenta of the system. The Born K-matrix is used for the calculation of **S**-matrix and cross section $\sigma(a_0 - a_1)$:

$$\mathbf{S}(K) \ = \frac{\mathbf{I} + i\mathbf{K}(B)}{\mathbf{I} - i\mathbf{K}(B)} \tag{2a}$$

$$\sigma(a_0 - a_1\,|K\,) = \sum_{l_0 l_1 S_T L_T} \frac{[S_T L_T]^2}{[S_0 L_0]^2}\,|S(\ ,\ _0,\ ,\ _1\,|K\,) - I(\ ,\ _0,\ ,\ _1)|^2 \tag{2b}$$

where K, B in the argument denote K-matrix and B approximations. $[SL]^2 \equiv (2S+1)(2L+1)$.

The full K-matrix approach is released in the coupled programs **ATOM-AKM**. They can be run on PC-486 and require about 10 minutes for 10 channels (transitions) in 10-20 energy points.

In the present report, we demonstrate two effects – normalization and channel interaction – which can be readily described by the K-matrix method.

2 Normalization

The effect of normalization is related to the unitarity of the S-matrix (conservation of incident particle flux). It can considerably decrease cross sections of strong transitions, such as $nl_0 - nl_1$. Less evident is the similar decreasing effect for all other $nl_0 - n'l'$ transitions, in particular *weak* ones.

The pure normalization effect can be described by an approximate K-matrix in the one-row – one-column form :

$$\mathbf{K} = \left\{ \begin{array}{cccc} 0 & ,_0,' & ,_0,'' & \dots \\ ,',_0 & 0 & 0 & 0 \\ ,'',_0 & 0 & 0 & 0 \\ \dots & 0 & 0 & 0 \end{array} \right\} \tag{3}$$

In this case, Eq. 2 can be solved and we obtain:

$$\sigma(a_0 - a_1|K) = \sum_{l_0 l_1 S_T L_T} \frac{\sigma(,_0,_1|B)}{[1 + D(,_0)]^2}, \quad D(,_0) = \sum_{a'l'} K^2(,_0,')^2 \,. \tag{4}$$

One can see from Eq. 4 the influence of strong transitions on the weak ones due to the sum in D. Moreover, for a given initial state, a_0, the normalizing factor $(1 + D)^2$ is the same for all final states. From now on we call the approximation given by Eqs. 3-4 *normalized Born BNm*, where m is the number of states a' in the sum for D.

One important consequence is the normalization effect for *all transitions from the excited states.* As an illustration, we show in Fig. 1-2 the excitation and ionization cross sections in He from the $2s^1S$ state. B and $BN8$ (all nl, $n = 2, 3, 4$) cross sections are obtained by the code **ATOM**. CCC data are from [2]. $BN8$ results are considerably closer to CCC as compared to B. One can see in Fig. 3 that the normalization effect for ionization is similar to that of excitation.

There is a large difference from experimental data for transitions from He metastables. As a rule, measured cross sections (for example see [3]) are a few times (up to an order) larger than calculated by any method . A typical example is shown in Fig. 4. The reason for such a discrepancy is not clear. Maybe it is worthwhile noting that the presence of a rather small number of atoms in the $2p^3P$ state ($\sim$10% of $2s^3S$) might explain this disagreement (Fig. 4).

3 Interaction of Channels

The normalization effect decreases cross sections. Use of the full K-matrix in Eq. 2a yields more complicated results. Besides normalization it provides channel interaction, which manifests itself by:

i. Transitions through intermediate levels; for example $1s - 2p - 3d$;

ii. Change of $\sigma(E)$ due to the interaction of many levels.

$1s - 2p - 3d$ is a rather pure example of transitions through intermediate levels. Due to the dipole interaction in both stages, $\sigma(1s - 3d)$ is considerably larger than the one obtained by the B method. The case of the $2s - 3d$ transition is more complicated: the effect of the two-stage dipole transition is partly compensated by the normalization effect (which is absent for transitions from $1s$ state). This is manifested by the $K36$ curve in Fig. 3. Channel interactions of many levels leads to a further decrease of the cross section (curve $K74$).

All these effects are even more pronounced in the case of the transition $2s - 4f$, see Fig 4.

4 Conclusion

Born-type methods (CB for ions) together with the many-channel K-matrix take into account effects of normalization and channel interactions and provide reasonable cross sections. Use of these methods in the code **ATOM** and complex **ATOM-AKM** give the possibility of a fast and comparatively simple calculation of cross sections and rate coefficients for as many transitions as necessary.

References

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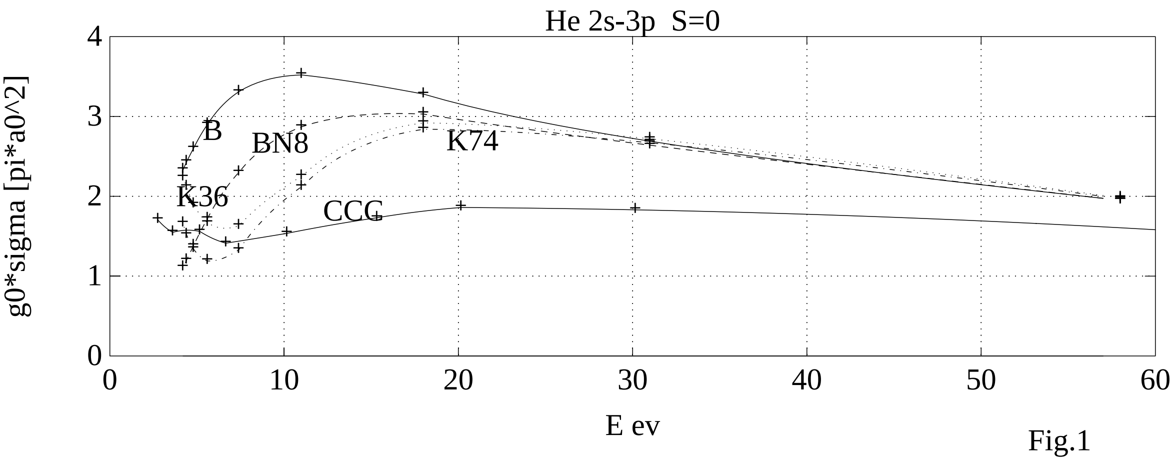
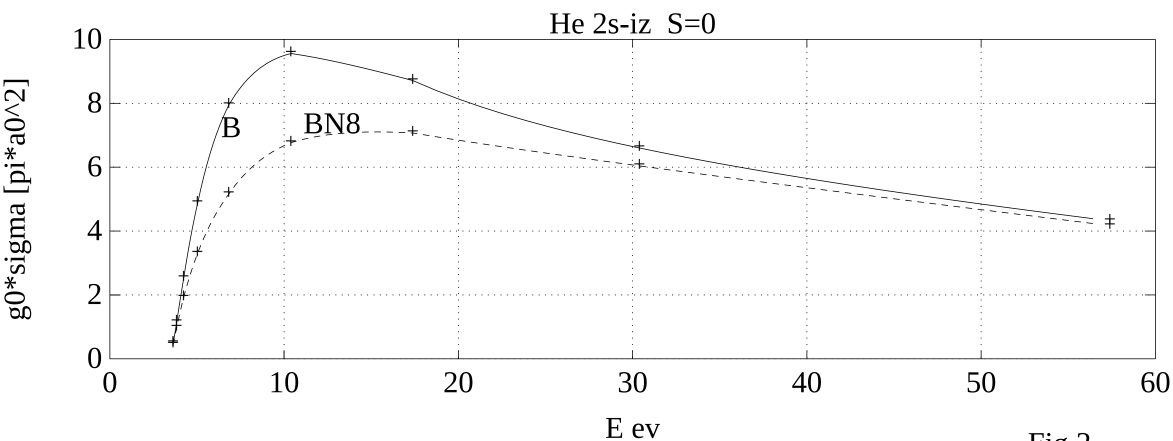

He 2s-3p S=0
g0*sigma [pi*a0^2]
E ev
B
BN8
K74
K36
CCC
0
1
2
3
4
10
20
30
40
50
60
Fig.1


He 2s-iz S=0
g0*sigma [pi*a0^2]
E ev
B
BN8
0
2
4
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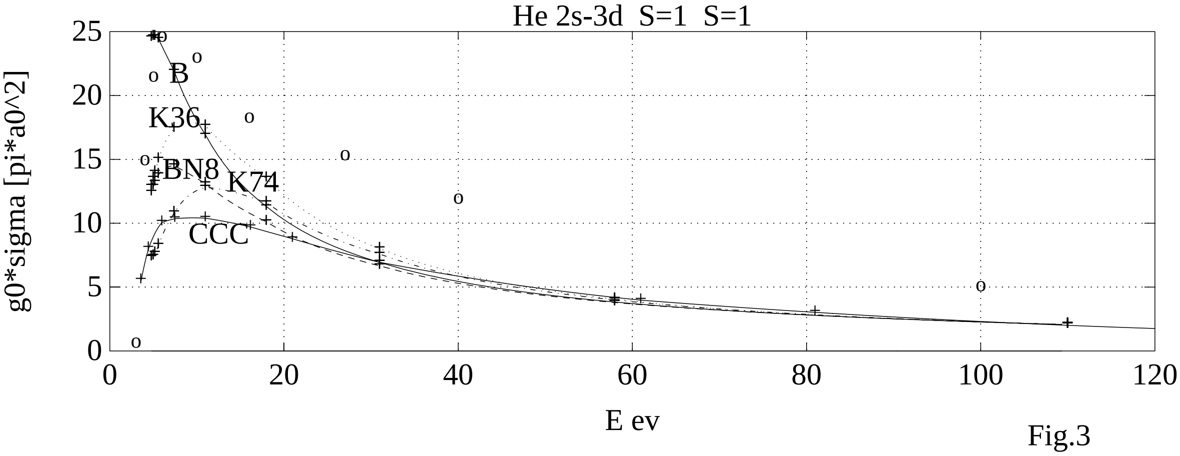
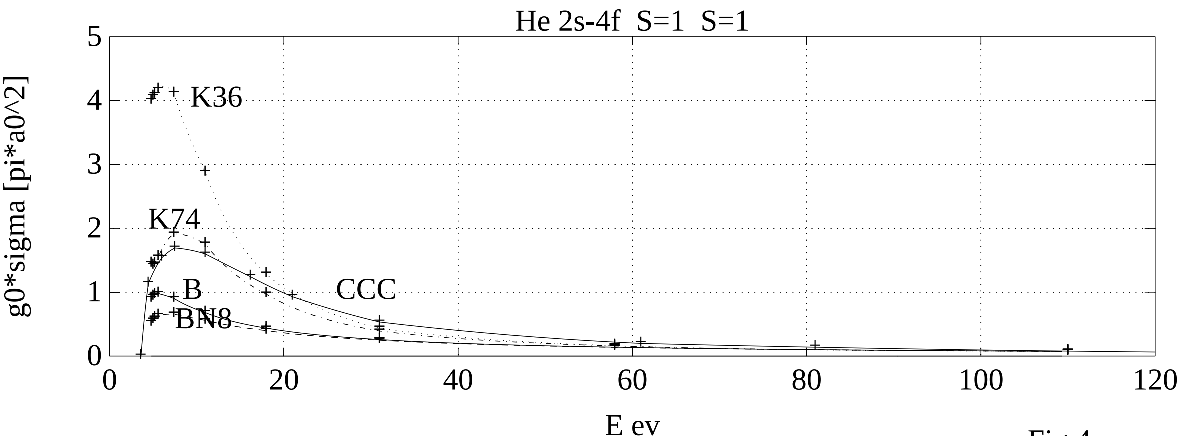
50
60
Fig.2



He 2s-3d S=1 S=1
g0*sigma [pi*a0^2]
E ev
B
K36
BN8
K74
CCC
0
5
10
15
20
25
0
20
40
60
80
100
120

Fig.3



He 2s-4f S=1 S=1
g0*sigma [pi*a0^2]
E ev
K36
K74
B
BN8
CCC
0
1
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3
4
5
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20
40
60
80
100
120

Fig.4