# **An approximate description of the double capture process**  in  $\overline{He^{2}}$ <sup>+</sup> + He collisions with static correlation  $\star$

**G. Deco\*\* and N. Griin** 

Institut für Theoretische Physik der Justus-Liebig-Universität, W-6300 Giessen, Federal Republic of Germany

Received 10 May 1990; final version 7 January 1991

**Abstract.** It is shown that the process of resonant double electron capture in high energy  $He^{2+} + He$  collisions can be approximately described by a sum over products of one-electron CDW amplitudes. The summation coefficients are determined by stationary ground-state calculations with CI wavefunctions. Total and differential cross sections are calculated and compared with experimental values.

PACS:  $34.10.+X$ ;  $34.70.+e$ 

# **1. Introduction**

For the simultaneous capture of both electrons in  $He^{2+}$ on He collisions at impact energies around and above 0.5 MeV some total cross sections have been measured several years ago  $[1-4]$ . New data on the total capture cross section beyond 1.2 MeV were published by de Castro Faria et al. [5]. At these high energies no differential data in the projectile angle had been published. Recently, Schuch et al. [6] published differential measurements at 1.5 MeV together with total cross sections for 1.5, 4 and 6 MeV impact energies. In this latter work, also an comparison was made with the results of a formula which approximates the amplitude for the double capture process as a sum over products of one-electron capture amplitudes. These amplitudes were calculated in the continuum distorted wave (CDW) approximation. The weight factors of these products were obtained in a static configuration interaction (CI) calculation of the bound He ground-state.

All other known theoretical calculations treat the double capture process essentially in the independent particle approximation.

Theisen and McGuire [7] use a two state atomic expansion for one active electron to be captured. Gayet et al. [8] and Gayet [9] apply the perturbation method

within the CDW model. The one-electron bound-state wavefunctions are of Hartree-Fock type or even hydrogenic. Crothers and McCarrol [10] describe the two electron bound ground-state by a correlated wavefunction of Pluvinage-type [11] but calculate only single electron transfer within the CDW model. The authors mentioned use independent partile statistics to obtain the results for double electron transfer.

The aim of the present work is to justify the method mentioned above and applied in the work by Schuch et al. [6]. In the next Sect. we give the details of our derivation and compare in the last Sect. with experimental and other theoretical values.

# **2. Theory**

## *2.1. The description of the ground-state*

We use atomic units. The ground-state solution of the stationary Schrödinger equation

$$
H\Psi = E\Psi \tag{1}
$$

with the two-electron Hamiltonian

$$
H = -\frac{1}{2}A_1 - \frac{1}{2}A_2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}
$$
 (2)

is attacked by the CI method. Z is the nuclear charge  $(=2$  for He) and  $r_1$ ,  $r_2$  and  $r_{12}$  are the distances from the nucleus and the interelectronic distance. With this Hamiltonian we may separate the spatial from the spin part in the wavefunction

$$
\Psi(\mathbf{r}_1, \mathbf{r}_1; s_1, s_2) = \Phi(\mathbf{r}_1, \mathbf{r}_2) \cdot \chi_{\text{singlet}}(s_1, s_2). \tag{3}
$$

For the <sup>1</sup>S ground-state  $\Phi$  is symmetric and has to represent a total angular momentum of zero. We expand  $\Phi$ in a sum of products of one-electron functions which themselves are solutions of an one-electron equation with a *l*-dependent effective nuclear charge.

<sup>\*</sup> Work supported by GSI (Darmstadt) and BMFT (06 GI 709)

<sup>\*\*</sup> Permanent address: Siemens, W-8044 Unterschleißheim, Federal Republic of Germany

$$
\left(-\frac{1}{2}\Delta - \frac{(l+1)\bar{Z}}{r}\right)\phi_{n,l,m;\bar{Z}}(\mathbf{r}) = \varepsilon_{nl;\bar{Z}}\,\phi_{n,l,m;\bar{Z}}(\mathbf{r}),\tag{4a}
$$

$$
\varepsilon_{n,l;\bar{Z}} = -\frac{\bar{Z}^2 (l+1)^2}{2 n^2}.
$$
\n(4b)

Instead of (4 a) we will in the following also use the shortcut notation

$$
\left(-\frac{1}{2}\Delta - \frac{\overline{Z}_k}{r}\right)\phi_k(\mathbf{r}) = \varepsilon_k \phi_k(\mathbf{r}).\tag{4c}
$$

This set of one-electron functions is orthonormal and complete, in principle with inclusion of the continuum. Our choice of the effective nuclear charge in the form  $(l+1)Z$  is a little bit more restrictive than an also possible, totally free variation for every  $l$  value. But, the latter procedure would lead to high effective charges, simulating high one-electron energies. For those energies the CDW formalism, which we apply in the final Sect., will no longer work at impact energies in which we are interested (see for instance [9J on this point). We may write for a S-state

$$
\Phi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{n_1, l; n_2, l} C_{n_1, l; n_1, l} \frac{(1 + \delta_{n_1, n_2}(1/2 - 1))}{1/2(2l + 1)}
$$

$$
\cdot \sum_{m} (-1)^m \{ \phi_{n_1, l, m; \bar{z}}(\mathbf{r}_1) \phi_{n_1, l, -m; \bar{z}}(\mathbf{r}_2) + (1 - \delta_{n_1, n_2}) \phi_{n_1, l, m; \bar{z}}(\mathbf{r}_2) \phi_{n_2, l, -m; \bar{z}}(\mathbf{r}_1) \}
$$
(5)

or with evident abbreviations and much shorter

$$
\phi(\mathbf{r}_1, \mathbf{r}_2) = \sum_k C_k \phi_{k_1}(\mathbf{r}_1) \phi_{k_2}(\mathbf{r}_2).
$$
 (6)

A finite sum of the form (5) or (6) is equivalent to a CI treatment of the  ${}^{1}S$  ground-state. The real coefficients  $C_k$  and the nonlinear parameter  $\overline{Z}$  are determined variationally.

## *2.2. The approximation of the double electron transition amplitude*

We treat the nuclear motion classically in the impact parameter approximation with straight line trajectories. The vector for the internuclear distance is given by

$$
\mathbf{R}(t) = \mathbf{b} + \mathbf{v}t \tag{7}
$$

where v is the relative velocity and **b** the impact parameter. The motion of the two electrons is governed by the time-dependent Schrödinger equation. We take the nuclear centre of mass as origin of the electron coordinates  $r$  and denote by an index  $T$  or  $P$  the coordinates from the target and projectile nucleus, respectively. The transition amplitude for the two-electron exchange is

$$
a_{2e} = \lim_{t \to \infty} \langle \chi_f | \Psi_i^+ \rangle. \tag{8}
$$

Here,  $\Psi_t^+$  is the exact solution of the Schrödinger equation

$$
\left(H_{\text{total}} - i\frac{\partial}{\partial t}\right)\Psi_{i}^{+}(\mathbf{r}_{1}, \mathbf{r}_{2}, t) = 0\tag{9}
$$

with

$$
H_{\text{total}} = -\frac{1}{2}A_1 - \frac{1}{2}A_2 - \frac{Z_T}{r_{T_1}} - \frac{Z_T}{r_{T_2}} - \frac{Z_P}{r_{P_1}} - \frac{Z_P}{r_{P_2}} + \frac{1}{r_{12}}.
$$
 (10)

For the He<sup>2+</sup> +He standard system  $Z_T = Z_p = 2$ . The connection with the initial situation of two bound electrons at the target is given by

$$
\lim_{t \to -\infty} \Psi_i^+(r_1, r_2, t) = \chi_i(r_1, r_2, t). \tag{11}
$$

For  $\chi_i$  we put

$$
\chi_i(\mathbf{r}_1, \mathbf{r}_2, t) = L^+(\mathbf{r}_{P_1}) L^+(\mathbf{r}_{P_2}) \Phi_T(\mathbf{r}_{T_1}, \mathbf{r}_{T_2}, t) e^{-i(\frac{v}{2})^2 t - i\frac{\mathbf{v}}{2} \cdot (\mathbf{r}_1 + \mathbf{r}_2)}.
$$
\n(12)

 $\Phi_T$  describes the ground-state of the target as given by (6) and we have

$$
\Phi_T(\mathbf{r}_{T_1}, \mathbf{r}_{T_2}, t) = \Phi(\mathbf{r}_{T_1}, \mathbf{r}_{T_2}) \cdot e^{-iE} g^t \tag{13}
$$

with the (variationally determined) ground-state energy  $E_g$ . The CDW distortion factors  $L^+$  take account of the Coulomb boundary conditions.

$$
L^{+}(\mathbf{r}_{P}) = e^{\pi \nu_{P/2}} \Gamma(1 - i \nu_{P}) \, {}_{1}F_{1} \left( i \nu_{P}, 1, i(\nu r_{P} + \mathbf{v} \cdot \mathbf{r}_{P}) \right) \tag{14}
$$

 $v_P = Z_P/v$  and  $_1F_1$  is the hypergeometric function. The motion of the target electrons relative to the origin is included in the translational factors of (12).  $\chi_f$  is built up in very much the same way as  $\chi_i$ .

$$
\chi_f = L^-(\mathbf{r}_{T_1}) L^-(\mathbf{r}_{T_2}) \Phi_P(\mathbf{r}_{P_1}, \mathbf{r}_{P_2}, t) e^{-i\left(\frac{v}{2}\right)^2 t + i\frac{\mathbf{v}}{2}\cdot(\mathbf{r}_1 + \mathbf{r}_2)} \qquad (15)
$$

$$
L^{-}(\mathbf{r}_{T}) = e^{\pi \mathbf{v}_{T/2}} \Gamma(1 + i \mathbf{v}_{T}) \, {}_{1}F_{1}(-i \mathbf{v}_{T}, 1, -i(vr_{T} + \mathbf{v} \cdot \mathbf{r}_{T})) \tag{16}
$$

with  $v_T = Z_T/v$ .

We remark that we have from  $(1)$ ,  $(2)$ ,  $(4)$ ,  $(6)$  and the equation for  $\phi_p$  corresponding to (13)

$$
\sum_{k} c_{k} \left[ -\Delta \varepsilon_{k} + (\overline{Z}_{P,k_{1}} - Z_{p}) \frac{1}{r_{P_{1}}} + (\overline{Z}_{P,k_{2}} - Z_{P}) \frac{1}{r_{P_{2}}} + \frac{1}{r_{12}} \right] \cdot \phi_{k_{1}}(\mathbf{r}_{P_{1}}) \phi_{k_{2}}(\mathbf{r}_{P_{2}}) e^{-iE} g^{t} = 0 \tag{17}
$$

with  $\Delta \varepsilon_k = E_{g} - \varepsilon_{k_1} - \varepsilon_{k_2}$ .

This equation holds true if the expansion of (6) is exact and is fulfilled in a variational sense if we truncate the expansion (6) for practical calculations.

Let us define a one-electron scattering wavefunction  $\psi_k^-$  (r, t) by imposing the fulfillment of

$$
\left(-\frac{1}{2}\Delta - \frac{Z_T}{r_T} - \frac{\overline{Z}_{P,k}}{r_P}\right)\psi_k^-(\mathbf{r},t) = i\frac{\partial}{\partial t}\psi_k^-(\mathbf{r},t)
$$
(18)

341

with the asymptotic condition

$$
\lim_{t \to +\infty} \psi_k^-(\mathbf{r}, t) = L^-(\mathbf{r}_T) \phi_k(\mathbf{r}_P) e^{-i\varepsilon_k t + i\frac{\mathbf{v}}{2} \cdot \mathbf{r} - i\frac{v^2}{8}t}.
$$
 (19)

Because of (19), (15) we may equally well write for  $a_{2e}$ 

$$
a_{2e} = \lim_{t \to +\infty} \sum_{k} c_k \langle \psi_{k_1}^-(\mathbf{r}_1, t) \psi_{k_2}^-(\mathbf{r}_2, t) e^{-iA\epsilon_k t} | \Psi_i^+ \rangle. \tag{20}
$$

Here, as well as in (8) the brackets mean integration over the electronic coordinates. In the following it is of some advantage to use the Dirac notation for the abstract state vectors. Thus, indicating merely the timedependence we have

$$
|\Psi_t^+(t)\rangle = |\chi_i(t)\rangle + \int_{-\infty}^{+\infty} dt' G^+(t-t')
$$

$$
\cdot \left\{ \left( H_{\text{total}}(t') - i \frac{\partial}{\partial t'} \right) | \chi_i(t') \rangle \right\} \tag{21}
$$

with the retarded Greenfunction  $G^+$  obeying

$$
\left(H_{\text{total}}(t) - i\frac{\partial}{\partial t}\right)G^{+}(t) = -\delta(t) \quad \text{for } t > 0
$$
  

$$
G^{+}(t) = 0 \quad \text{for } t < 0.
$$
 (22)

We may define for every index-combination  $(k_1, k_2)$  in the sum of (20) one retarded Greenfunction  $G^+_{k_1,k_2}(t)$  by

$$
\left(H_{0;k_1,k_2}-i\frac{\partial}{\partial t}\right)G_{k_1,k_2}^+(t)=-\delta(t) \quad \text{for } t>0
$$
  

$$
G_{k_1,k_2}^+(t) =0 \quad \text{for } t<0
$$
 (23)

where we take  $H_{0;k_1,k_2}$  to be the operator

$$
H_{0;k_1,k_2} = \frac{p_1^2}{2} + \frac{p_2^2}{2} - \frac{Z_T}{r_{T_1}} - \frac{Z_T}{r_{T_2}} - \frac{\overline{Z}_{P,k_1}}{r_{P_1}} - \frac{\overline{Z}_{P,k_2}}{r_{P_2}} + E_g - \varepsilon_{k_1} - \varepsilon_{k_2}.
$$
\n(24)

We have underlined the parts which by means of (18) evolve  $|\psi_{k_1}^-\rangle e^{-i\epsilon_{k_1}t}$  in time. Further, we note that the difference

$$
H'_{k_1,k_2} = H_{\text{total}} - H_{0;k_1,k_2} = -A\varepsilon_k + (\overline{Z}_{P,k_1} - Z_P) \frac{1}{r_{P_1}} + (\overline{Z}_{P,k_2} - Z_P) \frac{1}{r_{P_2}} + \frac{1}{r_{12}}
$$
(25)

is just the expression appearing in  $(17)$ . In  $(21)$  we insert for  $G^+(t-t')$  the identity

$$
G^{+}(t-t') = G_{k_1,k_2}^{+}(t-t') + \int_{-\infty}^{+\infty} dt'' G_{k_1,k_2}^{+}(t-t'')
$$
  
 
$$
\cdot H'_{k_1,k_2}(t'') G^{+}(t''-t')
$$
 (26)

and the result is used to obtain from (20) for the transition amplitude

$$
a_{2e} = \lim_{t \to \infty} \left\{ \sum_{k} C_{k} \left\langle \psi_{k_{1}}^{-}(t) \psi_{k_{2}}^{-}(t) e^{-i \Delta \varepsilon_{k} t} | \chi_{i}(t) \right\rangle \right.+ \sum_{k} C_{k} \int_{-\infty}^{+\infty} dt' \left\langle \psi_{k_{1}}^{-}(t) \psi_{k_{2}}^{-}(t) e^{-i \Delta \varepsilon_{k} t} | G_{k_{1},k_{2}}^{+}(t-t') \right.\cdot \left( H_{\text{total}}(t') - i \frac{\partial}{\partial t'} \right) | \chi_{i}(t') \right\)+ \sum_{k} C_{k} \int_{-\infty}^{+\infty} dt' \int_{-\infty}^{+\infty} dt''\left\langle \psi_{k_{1}}^{-}(t) \psi_{k_{2}}^{-}(t) e^{-i \Delta \varepsilon_{k} t} | G_{k_{1},k_{2}}^{+}(t-t'') \right.\cdot H_{k_{1},k_{2}}'(t') G^{+}(t''-t') \left( H_{\text{total}}(t') - i \frac{\partial}{\partial t'} \right) | \chi_{i}(t') \right\rangle= a^{(0)} + a^{(1)} + a^{(2)}.
$$
\n(27)

The first term  $a^{(0)}$  vanishes since for  $t \to \infty \chi_i$  is a target state and  $\psi_{k_1}^-\psi_{k_2}^-$  is then located at the projectile nucleus. For the second term  $a^{(1)}$  we note that the action of  $G_{k_1,k_2}^+(t-t')$  can be taken to the left and because of (23) and  $(24)$  we get

$$
a^{(1)} = -i \sum_{k} C_{k} \int_{-\infty}^{+\infty} dt' \langle \psi_{k_{1}}^{-}(t') \psi_{k_{2}}^{-}(t') e^{-iA\epsilon_{k}t'}|
$$

$$
\cdot \left( H_{\text{total}}(t') - i \frac{\partial}{\partial t'} \right) | \chi_{i}(t') \rangle.
$$
 (28)

We apply the operator  $H_{total}$  to the left. (18) together with the definition of  $H'_{k_1,k_2}$  by (25) lead to

$$
\langle \psi_{k_1}^-(t') \psi_{k_2}^-(t') e^{-iA\epsilon_k t'} | H_{\text{total}}(t') \rangle
$$
  
= 
$$
-i \frac{\partial}{\partial t'} \langle \psi_{k_1}^-(t') \psi_{k_2}^-(t') e^{-iA\epsilon_k t'} |
$$
  
+ 
$$
\langle \psi_{k_1}^-(t') \psi_{k_2}^-(t') e^{-iA\epsilon_k t'} | H'_{k_1,k_2}(t').
$$
 (29)

Therefore, for a part of the integrand in (28) the time integration can be performed. Noting again that at the upper time-limit we have orthogonality of  $\psi_{k_1} \psi_{k_2}$  with  $\chi_i$  we end with

$$
a^{(1)} = \lim_{t \to -\infty} \sum_{k} C_{k} \langle \psi_{k_{1}}^{-}(t) \psi_{k_{2}}^{-}(t) e^{-i\Delta e_{k}t} | \chi_{i}(t) \rangle
$$
  
\n
$$
-i \sum_{k} C_{k} \int_{-\infty}^{+\infty} dt' \langle \psi_{k_{1}}^{-}(t') \psi_{k_{2}}^{-}(t')
$$
  
\n
$$
+ e^{-i\Delta e_{k}t'} | H'_{k_{1},k_{2}}(t') | \chi_{i}(t') \rangle
$$
  
\n
$$
= a^{(1,1)} + a^{(1,2)}.
$$
 (30)

In the first contribution,  $a^{(1,1)}$ , we replace  $\chi_i$  with the help of (12), (13) and (6) by a sum (in coordinate representation)

$$
\chi_i(\mathbf{r}_1, \mathbf{r}_2, t) = \sum_j C_j \tilde{\chi}_{j_1}(\mathbf{r}_1, t) \tilde{\chi}_{j_2}(\mathbf{r}_2, t) e^{-iE_{\mathbf{g}}t}
$$
(31)

$$
\tilde{\chi}_j(\mathbf{r},t) = L^+(\mathbf{r}_P) \phi_j(\mathbf{r}_T) e^{-i\frac{\mathbf{v}^2}{2}\mathbf{r} - i\frac{\mathbf{v}^2}{8}t}.
$$
\n(32)

Therefore we have

$$
a^{(1,1)} = \lim_{t \to -\infty} \sum_{k,j} C_k C_j \langle \psi_{k_1}^- e^{i s_{k_1} t} | \tilde{\chi}_{j_1} \rangle \langle \psi_{k_2}^- e^{i s_{k_2} t} | \tilde{\chi}_{j_2} \rangle. \tag{33}
$$

Thus, at least one part of the exact two-electron transition amplutide is expressable as a sum over products of one-electron amplitudes. For the third term  $a^{(2)}$  in (27) we only remark that one can get rid of the Green function  $G_{k_1,k_2}^+(t-t'')$  in applying it to the left which yields

$$
a^{(2)} = -i \sum_{k} C_{k} \int_{-\infty}^{+\infty} dt' \int_{-\infty}^{+\infty} dt'' \langle \psi_{k_{1}}^{-}(t'') \psi_{k_{2}}^{-}(t'') e^{-iA\epsilon_{k}t''} -H_{k_{1},k_{2}}(t'')...
$$
(34)

where the dots stand for the remainder from  $(27)$ .

If the one particle transition amplitudes of (33) are calculated in a first order - in our case: in the CDWapproximation  $-$ , one has

$$
\lim_{t \to -\infty} \langle \psi_{k_1}^{-} e^{i\epsilon_{k_1}t} | \tilde{\chi}_{j,T} \rangle = -i \int_{-\infty}^{+\infty} dt \langle \psi_k^{-} e^{i\epsilon_{k}t} | W_k | \tilde{\chi}_{j,T} \rangle
$$
  

$$
\simeq -i \int_{-\infty}^{+\infty} dt \langle \tilde{\chi}_{k,P} | W_k | \tilde{\chi}_{j,T} \rangle
$$
  

$$
= a_{\text{CDW};1}^{-k} e
$$
 (35)

 $W_k$  is the perturbation,  $\tilde{\chi}_{j,T}$  is defined by (32) with an additional index T, reminding of the localisation at the target. From (19) the definition of  $\tilde{\chi}_{k,P}$  as a distorted projectile one-electron wavefunction is evident. Performing this CDW-approximation for  $a^{(1,1)}$  it is only consequent to replace also in the remaining terms  $a^{(1,2)}$  and  $\hat{a}^{(2)}$  the exact one-electron scattering functions  $\psi_k^-$  by their asymptotic limit given in (19). But then in both,  $a^{(1,2)}$  and  $a^{(2)}$ , a sum of the form given in (17) arises. Consequently, we drop these terms in the approximation. This means in effect that we have

$$
a_{2e} \simeq a_{\text{CDW}}^{(1,1)} = \sum_{k,j} C_k C_j a_{\text{CDW},1e}^{j_1 \to k_1} a_{\text{CDW},1e}^{j_2 \to k_2}.
$$
 (36)

Since the amplitude depends only on  $|\mathbf{b}| = b$  the total cross section in the impact parameter approximation is obtained from the amplitude  $a(b)$  by

$$
\sigma = 2\pi \int_{0}^{\infty} d\ b \ b |a(b)|^{2}.
$$
 (37)

The differential cross section for the angular behaviour of the projectile in the laboratory system can be expressed for our transition as

$$
\frac{d\sigma}{d\Omega} = M^2 v^2 \bigg|_0^{\infty} db \, b^{\left(1+i2\frac{Z_T Z_p}{v}\right)} J_0 \left(2M v b \sin\frac{\Theta}{2}\right) a(b) \bigg|^2. \tag{38}
$$

 $M$  is the projectile mass,  $\Theta$  the laboratory polar scattering angle and  $J_0$  the Bessel function of lowest order. The phase factor in the integrand takes care of the nuclear interaction (see for instance  $\lceil 12 \rceil$ ).

Table 1. Results of CI-calculations for the  ${}^{1}S$  ground-state of He; see text for further explanation

Ansatz	One electron functions (notation: nl)		Energy
(1)	1 s	1.6875	$-2.84766$
(2)	1s, 2s, 2p, 3d	1.7661	$-2.87136$
(3)	1s, 2s, 3s, 4s; 2p, 3p, 4p; 3d	1.7899	$-2.87646$



**Fig.** L Cross sections for double capture differential in the angle of the scattered projectile for He<sup> $2+$ </sup> + He collisions at 1.5 MeV laboratory energy. The dots are experiments [6]. The curves corresponds to the different static wavefunctions of Table 1. The dashed curve is the result of folding the full curve with the experimental resolution

#### **3. Results and conclusions**

We applied our formalism to the reaction  $He^{2+}$  $+He(1^1S) \rightarrow He(1^1S) + He^{2+}$  that is to say the resonance double electron exchange between the groundstates of the He target and projectile nucleus. For the static CI calculations we give only the results of the finite expansions which were also used for the approximation of the amplitude via (36).

The lines (1), (2), and (3) of Table 1 differ in the number of one-electron functions used in the CI-ansatz. Line (1) means that we have used one function of the configuration  $(1s)^2$  and in line (3) we have 17 functions: 10 for  $(ns, n's)$ ; 6 for  $(np, n'p)$  and one for  $(3d)^2$  configurations, respectively. It is clear that we can do much better as far as the total energy is concerned. But as the results for the differential and total cross sections reported below already show a fairly good convergence behaviour we did not increase the static basis.

To calculate the one-electron CDW-amplitudes of (36) we used the published codes of Belkic et al. [12, 13] with slight modifications.

Figure 1 shows a comparison between the calculated differential cross section using the ansatz  $(1)$ ,  $(2)$ , or  $(3)$ of Table 1, respectively, with the experimental measurement of Schuch et al.  $[6]$ . The impact energy is 1.5 MeV. The theoretical values demonstrate the rapid convergence mentioned above. The agreement with the experi-

Table 2. Total cross section in  $cm<sup>2</sup>$  for double charge transfer in  $He<sup>2+</sup> + He$  collisions. The results using three different CI calculations are compared with the experiment of Schuch et al. [6]

$E_{\rm lab}$	Theory with CI			Experiment
MeV	(1)	(2)	(3)	Г6 I
1.5	$1.1 \cdot 10^{-20}$	$1.44 \cdot 10^{-20}$	$1.52 \cdot 10^{-20}$	$1.0 \cdot 10^{-20}$
	$2.9 \cdot 10^{-24}$	$4.27 \cdot 10^{-24}$	$4.82 \cdot 10^{-24}$	$1.3 \cdot 10^{-24}$
6	$6.54 \cdot 10^{-26}$	$1.0 \cdot 10^{-25}$	$1.1 \cdot 10^{-25}$	$0.54 \cdot 10^{-25}$



Fig. 2. Total double capture cross sections for  $\text{He}^{2+}$  + He collisions as function of the impact energy. Full curve: this work; dotted curve: independent-particle approximation (IPA) with HF orbitals [8]; dashed curve: IPA with hydrogenic orbitals [8]. Experiments: dots: [3]; squares: [4]; asterixes: [1]; triangle: [6]; open circles: [5]

ment is good. In principle it is necessary to fold the theoretical values with the experimental angular resolution function [6]. The effect of this folding procedure is a subpression of the theoretical curves for small projectile scattering angles, as can be seen by the dashed curve in Fig. 1. Values for angles beyond 0.1 mrad are negligibly influenced by the folding procedure. The experimental data points for angles below 0.1 mrad may be too high because of inclusion of the radiative electron capture contribution (see [6]). No finer structure seems to be present in the data which could be an evidence for a dynamical correlation effect. For instance a Thomas peak for double electron transfer would appear at an angle of  $\theta_{\rm lab} = 2.4 \cdot 10^{-4}$ . But the small hump in the experiment as well as in the theory near this angle can not serve as a confirmation. Obviously the experimental result of an integration over the angles should yield a total cross section which lies above the theoretical one. This is not the case as can be seen from the first line of Table 2. In this Table our values are compared with the total cross sections measurements of the same group (Schuch et al. [6]). The reason is that the experiments for differential and total cross sections were performed independently from one another. It is believed [6] that the measured total cross sections are about 30% too low. Thus, the mentioned discrepancy is a sign of the difficulties to measure the process in question with high accuracy. The theoretical values for the highest energies given show also rapid convergence and are roughly in agreement with the experiment.

Finally, Fig. 2 gives the comparison of calculations with ansatz (3) for moderately high energies with further experiments and with two independent-particle CDW approximations of Gayet et al. [8] which differ by approximating the final electron wavefunction either by a product of hydrogenic (upper curve) or HF orbitals (lower curve) whereas the initial orbitals are of HF-type. It should be mentioned that our results with ansatz (1)  $((1s)<sup>2</sup>$ -configuration alone) are quite similar to the lower curve.

From this and also from the comparison of the columns labeled (1) and (3) of Table 2 we conclude that the better description of the initial and final wavefunctions by static correlations plays always a role, even at the highest energies.

We are highly indebted to Dr. Antone Satin for fruitful discussions and for providing us with a version of a program to calculate one-electron CDW amplitudes.

### **References**

- 1. Nikolaev, V., Fatewa, L., Dimitriev, I., Teplova, Ya.: Sov. Phys. JETP. 14, 67 (1962)
- 2. Berkner, K., Pyte, R, Stearns, W., Warren, I.: Phys. Rev. 166, 44 (1968)
- 3. Pivovar, L., Novikov, M., Tabaev, V.: Sov. Phys. JETP 15, 1035  $(1962)$
- 4. McDaniet, E., Flamery, M., Ellis, H., Eisele, F.L., Pope, W.: US army missile research and development command report H, 78 (1977)
- 5. de Castro Faria, N.V, Freire, F.L., de Pinho, A.G.: Phys. Rev. A37, 280 (1988)
- 6. Schuch, R., Vogt, IL, Justiniano, E., Deco, G., Griin, N.: J. Phys. B 24, L133 (1991)
- 7. Theisen, T.C., McGuire, J.H.: Phys. Rev. A20, 1406 (1979)
- 8. Gayet, R., Rivarola, R., Salin, A.: J. Phys. B 14, 2421 (1981)
- 9. Gayet, R.: J. Phys. (Paris) Colloq. C1, 50, 53 (1989)
- 10. Crothers, D.S.F., McCaroll, R.: J. Phys. B 20, 2835 (1987)
- 11. Pluvinage, P.: Ann. Phys. (NY) 5, 145 (1950)
- 12. Rivarola, R., Miraglia, J.: J. Phys. B 15, 2221 (1982)
- 13. Belkić, Dz., Gayet, R., Salin, A.: Comput. Phys. Commun. 30, 193 (1983)