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Theoretical study of single and double charge transfer in He^{2+}-He collisions at kilo-electron-volt energies in a diabatic molecular representation

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A 15-state diabatic molecular expansion, covering channels up to 2*s* and 2*p* excitations, has been used to study single and double charge transfer in He^{2+}-He($1s^2$) collisions at kilo-electron-volt energies. The aim of the work has been to explore the usefulness of this type of diabatic molecular basis for eventual use in benchmark calculations, electron translation factors not being included in this low-energy calculation. Our results for single and double electron capture agree very well with experiment up to relative velocities of ~0.5–0.6 a.u. For single capture into the ground state the series can be truncated early with very little effect, but for double capture the truncation cannot be done. A probable connection with correlated two-electron motion is discussed.

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I. INTRODUCTION

In low-energy ion-atom collisions involving a single active electron, the use of adiabatic molecular wave functions was initiated by Bates, Massey, and Stewart [1] and has had a long history. Diabatic states were introduced by Lichten [2] for the same purpose and, because they cannot be rigorously defined, many criteria have been proposed [3–9] to incorporate the fact that electrons cannot adjust themselves to the nuclear motion in a quasimolecular collision complex as easily as in a stable molecule.

In a practical close-coupling calculation, we have to truncate the diabatic series after a finite number of terms. As Smith [4] pointed out, an early truncation of a diabatic series has to be paid for by a price—namely, sacrifice of configuration interaction. Since in the one-electron picture configuration interaction is the only way to take account of electron correlation, this gives rise to a probability that for two-electron processes that involve direct (rather than sequential) two-electron exchange and/or excitation, (e.g., [10]), early truncation of diabatic series can lead to neglect of electron correlation.

We have used in this paper a diabatic molecular representation to study single and double charge transfer in He^{2+}-He collisions at low energies (relative velocity <1 a.u.). The reaction channels are given at the beginning of Sec. IV. The diabatic basis has been constructed similarly as in an earlier work [11] devoted to single charge transfer in He^{+}-He collisions. The double capture process is resonant and involves an exchange of two electrons. We find that our results demonstrate the above effect of diabatic basis truncation for this two-electron process.

The plan of the paper is as follows. In Sec. II we define the diabatic basis and set up the coupled equations in the impact-parameter formulation. The techniques used for numerically solving these coupled equations are outlined in Sec. III. In Sec. IV we present our results. Finally, our conclusions are summarized in Sec. V.

II. THEORY

We are using atomic units throughout unless otherwise specified. First expand the total wave function of the collision complex in a body-fixed (e.g., [4]) molecular basis,

$$\Psi(\mathbf{r},\mathbf{R}(t))=\sum_k c_k(t)\psi_k(\mathbf{r},R)\ . \tag{1}$$

Then in the semiclassical impact-parameter approximation, the time-dependent Schrödinger equation becomes (see [11] for details)

$$i\frac{dc_j}{dt}=\sum_k (H_{jk}+P_{jk}+Q_{jk})c_k\ , \tag{2}$$

where

$$H_{jk}=\langle\psi_j|H_{el}|\psi_k\rangle\ ,$$

$$P_{jk}=\frac{vz}{R}\left\langle\psi_j\left|-i\frac{\partial}{\partial R}\right|\psi_k\right\rangle\ ,$$

$$Q_{jk}=\frac{vb}{R^2}\left\langle\psi_j\left|-i\frac{\partial}{\partial\theta}\right|\psi_k\right\rangle\ ,$$

where $z=vt$ and b is the impact parameter. (There is an obvious misprint in the last line of Eq. (7) in [11].)

For use in (1) and (2) we now define a diabatic molecular basis as in [11],

$$\psi(\mathbf{r},R)=\underline{U}(R=\infty)\underline{S}(R)\phi(r,\zeta(R=\infty);R)\ , \tag{3}$$

where ψ and ϕ are column vectors, ζ are the orbital exponents, $\underline{S}(R)$ is the Schmidt orthonormalization matrix and $\underline{U}$ diagonalizes $\langle\underline{S}\phi|H_{el}|\underline{S}\phi\rangle$ at large R. The individual diabatic configurations ϕ are constructed with linear-combination-of-atomic-orbitals molecular orbitals

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TABLE I. Basis functions (normalized) used to construct the diabatic molecular wave functions (1). The symbol $\{A,B\}$ denotes the spatially symmetric (singlet) combination $(A_1B_2+A_2B_1)(\alpha_1\beta_2-\alpha_2\beta_1)$ where α,β are "up" and "down" spin functions and A,B are spatial MO's.

Singlet g-states

$$\phi_1=\frac{1}{\sqrt{2}}[\sigma_g(1s)^2-\sigma_u(1s)^2]$$
$$\phi_2=\frac{1}{\sqrt{2}}[\sigma_g(1s)^2+\sigma_u(1s)^2]$$
$$\phi_3=\tfrac{1}{2}[\{\sigma_g(1s)\pi_g(2p_+)\}-\{\sigma_u(1s)\pi_u(2p_+)\}]$$
$$\phi_4=\tfrac{1}{2}[\{\sigma_g(1s)\pi_g(2p_+)\}+\{\sigma_u(1s)\pi_u(2p_+)\}]$$
$$\phi_5=\tfrac{1}{2}[\{\sigma_g(1s)\sigma_g(2s)\}-\{\sigma_u(1s)\sigma_u(2s)\}]$$
$$\phi_6=\tfrac{1}{2}[\{\sigma_g(1s)\sigma_g(2s)\}+\{\sigma_u(1s)\sigma_u(2s)\}]$$
$$\phi_7=\tfrac{1}{2}[\{\sigma_g(1s)\sigma_g(2p_0)\}-\{\sigma_u(1s)\sigma_u(2p_0)\}]$$
$$\phi_8=\tfrac{1}{2}[\{\sigma_g(1s)\sigma_g(2p_0)\}+\{\sigma_u(1s)\sigma_u(2p_0)\}]$$

Singlet u-states

$$\phi_9=\frac{1}{\sqrt{2}}\{\sigma_g(1s)\sigma_u(1s)\}$$
$$\phi_{10}=\tfrac{1}{2}[\{\sigma_g(1s)\pi_u(2p_+)\}-\{\sigma_u(1s)\pi_g(2p_+)\}]$$
$$\phi_{11}=\tfrac{1}{2}[\{\sigma_g(1s)\pi_u(2p_+)\}+\{\sigma_u(1s)\pi_g(2p_+)\}]$$
$$\phi_{12}=\tfrac{1}{2}[\{\sigma_g(1s)\sigma_u(2s)\}-\{\sigma_u(1s)\sigma_g(2s)\}]$$
$$\phi_{13}=\tfrac{1}{2}[\{\sigma_g(1s)\sigma_u(2s)\}+\{\sigma_u(1s)\sigma_g(2s)\}]$$
$$\phi_{14}=\tfrac{1}{2}[\{\sigma_g(1s)\sigma_u(2p_0)\}-\{\sigma_u(1s)\sigma_g(2p_0)\}]$$
$$\phi_{15}=\tfrac{1}{2}[\{\sigma_g(1s)\sigma_u(2p_0)\}+\{\sigma_u(1s)\sigma_g(2p_0)\}]$$

(MO's) built up with a minimal Slater basis. The center of mass coincides with the center of charge for a symmetric system, and has been chosen as the origin of the coordinates. Obviously, at large R, ψ coincides with the adiabatic basis.

Afrosimov *et al.* [12] and Shah, McCallion, and Gilbody [13] have carried out extensive measurements of single and double charge transfer in He^{2+}-He collisions. In particular, Afrosimov *et al.* give cross sections for single charge transfer into different channels,

$$He(1s^2)+He^{2+}\rightarrow He^+(1s)+He^+(nl) \tag{4}$$

with $n=1,2,3,4$. For $n>2$, though, the cross sections are quite small, and we have chosen a diabatic basis whose separated-atom energies cover the spectrum for $n=1$ and 2 completely. Tables I and II show the basis functions ϕ_i together with the theoretical separated-atom limits and the calculated separated-atom energies at internuclear distance $R=50$ a.u. These energies were obtained by variation of the orbital exponents at this value of R.

We now "freeze" the exponents and the $\underline{U}$ matrix at $R=50$ a.u. to form the diabatic basis (3) extending over all R. Because an adiabatic basis must be formed by variationally minimizing the energies at all R, the "diabatic" character of this basis becomes more apparent towards small R. Also, as shown in [11], this basis is a close approximation to Smith's [4] "standard" radial diabatic basis in that the radial coupling matrix $\underline{P}$ is negligible throughout. The angular couplings $\underline{Q}$ have been evaluated by standard methods (see [14] for details). It may be noted from Table II that our diabatic states go over correctly to the separated-atom limits. Since for this system the definition of one-electron translation factors (ETF's) become problematical for molecular states that dissociate into $He^+ + He^+$ channels, we have chosen to omit the ETF's from our calculations, which are restricted to low energy anyway.

III. CALCULATIONAL DETAILS

The coupled equations (2) finally assume the form

$$i\frac{dc_j}{dt}=\sum_{k=1}^{15}c_k(H_{jk}+Q_{jk})\ . \tag{5}$$

A unitary transformation

$$C_j=c_j\exp\left[i\int_{-\infty}^{t}H_{jj}dt\right] \tag{6}$$

TABLE II. Separated-atom behavior of the basis states.

Basis functions	Separated-atom limit	Energy (a.u.) Calculated at $R=50$ a.u.	From Ref. [26]
ϕ_1	$\{1s_A(1)1s_B(2)\}$	-3.98000	-3.97963
ϕ_2	$[1s_A(1)1s_A(2)+1s_B(1)1s_B(2)]$	-2.85153	-2.90335^a
ϕ_3	$\{1s_B(1)2p_{+A}(2)\}-\{1s_A(1)2p_{+B}(2)\}$	-2.47999	-2.47978
ϕ_4	$\{1s_A(1)2p_{+A}(2)\}-\{1s_B(1)2p_{+B}(2)\}$	-2.12228	-2.12363
ϕ_5	$\{1s_A(1)2s_B(2)\}+\{1s_B(1)2s_A(2)\}$	-2.47385	-2.47978
ϕ_6	$\{1s_A(1)2s_A(2)\}+\{1s_B(1)2s_B(2)\}$	-2.14039	-2.14576
ϕ_7	$\{1s_B(1)2p_{0A}(2)\}-\{1s_A(1)2p_{0B}(2)\}$	-2.47998	-2.47978
ϕ_8	$\{1s_A(1)2p_{0A}(2)\}-\{1s_B(1)2p_{0B}(2)\}$	-2.12208	-2.12363
ϕ_9	$[1s_A(1)1s_A(2)-1s_B(1)1s_B(2)]$	-2.85122	-2.90335^a
ϕ_{10}	$\{1s_A(1)2p_{+B}(2)\}+\{1s_B(1)2p_{+A}(2)\}$	-2.48002	-2.47978
ϕ_{11}	$\{1s_A(1)2p_{+A}(2)\}+\{1s_B(1)2p_{+B}(2)\}$	-2.12259	-2.12363
ϕ_{12}	$\{1s_B(1)2s_A(2)\}-\{1s_A(1)2s_B(2)\}$	-2.47401	-2.47978
ϕ_{13}	$\{1s_A(1)2s_A(2)\}-\{1s_B(1)2s_B(2)\}$	-2.14048	-2.14576
ϕ_{14}	$\{1s_B(1)2p_{0A}(2)\}+\{1s_A(1)2p_{0B}(2)\}$	-2.47970	-2.47978
ϕ_{15}	$\{1s_A(1)2p_{0A}(2)\}+\{1s_B(1)2p_{0B}(2)\}$	-2.12208	-2.12363

[a] For this separated-atom limit, the best single-zeta energy $=-2.847656$ hartree, while the Hartree-Fock energy $=-2.86168$ hartree [27].

eliminates the diagonal elements of $\underline{H}$ from (5), leaving

$$i\frac{dC_j}{dt}=\sum_{\substack{k\neq j\\ k=1}}^{15} C_k(H_{jk}+Q_{jk})\exp\left[i\int(H_{jj}-H_{kk})\right]dt\ . \qquad (7)$$

Because of the choice of the origin at the center of the internuclear line, the g and u subsets of the coupled equations (7) separate. The equations were solved by the Bulirsch-Stoer method [15] which was programmed to preserve unitarity to within 4–5 parts in 10^4 (or better). Choosing the initial boundary conditions $c_k(t=-\infty)$ to match with the entrance channel in (4), the probabilities for the different charge-transfer channels were obtained as follows:

(i) Single charge transfer to the ground state [$n=1$ in (4)]:

$$P=\tfrac{1}{2}|c_1(+\infty)|^2\ . \qquad (8a)$$

(ii) Double charge transfer (resonant channel):

$$P=\tfrac{1}{2}|c_2(+\infty)-c_9(+\infty)|^2\ . \qquad (8b)$$

(iii) Single charge transfer to excited channels, e.g., $nl=2s$ in (4):

$$P=\tfrac{1}{2}|c_5(+\infty)\pm c_{12}(+\infty)|^2\ , \qquad (8c)$$

with the + (−) sign for target (projectile) excitation. Cross sections for the different processes were then obtained by standard methods. Calculations were done on a 32-bit personal computer using double precision arithmetic.

IV. RESULTS AND DISCUSSION

We have computed the cross sections for the following charge-transfer reactions:

(i) Single capture:

$$\mathrm{He}_A(1s^2)+\mathrm{He}_B^{2+}\rightarrow\mathrm{He}_A^{+}(1s)+\mathrm{He}_B^{+}(1s) \qquad (9a)$$

$$\rightarrow\mathrm{He}_A^{+}(1s)+\mathrm{He}_B^{+}(nl) \qquad (9b)$$

$$\rightarrow\mathrm{He}_A^{+}(nl)+\mathrm{He}_B^{+}(1s) \qquad (9c)$$

$$(nl=2s,2p_0,2p_\pm).$$

(ii) Resonant double capture:

$$\mathrm{He}_A(1s^2)+\mathrm{He}_B^{2+}\rightarrow\mathrm{He}_A^{2+}+\mathrm{He}_B(1s^2) \qquad (10)$$

at laboratory energies up to ~25 keV/amu. Channels for target *as well as* projectile excitations have been ignored.

Figures 1(a) and 1(b) show a few diabatic Hamiltonian matrix elements. In principle, for an infinitely large number of configurations, these curves should yield the "exact" adiabatic potentials of He^{2+}-He on diagonalization; in practice, with a basis set truncated before $n=3$, such a comparison would have only a qualitative value. Nevertheless, we compare in Fig. 2, a few diagonalized potential curves obtained from our diabatic curves with the adiabatic eigenvalues taken from Gao *et al.* [16]. Except at very small R, the agreement is generally fairly good.

We reiterate, however, that the usefulness of our (finite) diabatic basis lies not in this quantum chemistry aspect, but rather in its ability to predict quantitative cross sections. As already mentioned, Afrosimov *et al.* [12(a)] have given the different channel (nl) cross sections for reactions (9). Figure 3 shows the cross sections for the single capture to the ground state, i.e., the channel (9a) above. The experimental data of Ref. ~~[12(a)] and the~~ theoretical results of Fulton and Mittleman [17] are shown for comparison. Also shown are the results of a parallel three-state calculation [18] where the g states ϕ_1, ϕ_2 and the u state ϕ_9 were retained. Theoretical results for this reaction have also been presented by Harel and Salin [19] and Gramlich, Gruen, and Scheid [20]. The re-

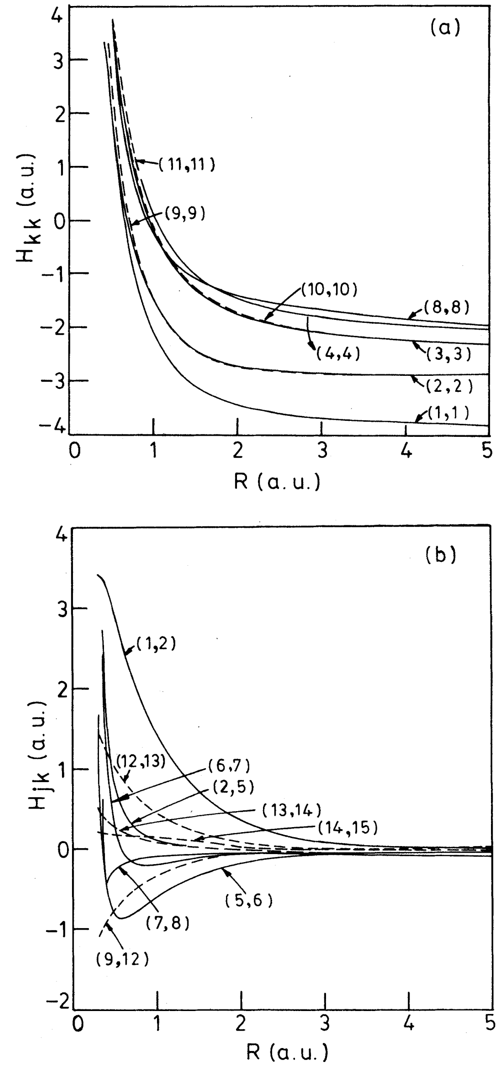

FIG. 1. (a) Some typical diabatic diagonal Hamiltonian matrix elements (H_{kk}) for the basis (3) of the text plotted against internuclear distance (R). Full-line curves for g states; dotted curves for u states. For numbering of the states $|k\rangle$ see Table I. (b) Some typical diabatic off-diagonal Hamiltonian matrix elements (H_{jk}). Full-line curves for g-g elements; dotted curves for u-u elements.

sults in [19] (not shown) practically coincide with our results; Gramlich, Gruen, and Scheid used Gaussian orbital expansions, and their results differ markedly from ours at low energies.

It is seen that for energies up to 5 keV/amu the present results agree very well with experiment. This proves the usefulness of this diabatic expansion at low energies. Also, the observation made by Zygelman *et al.* [21] that "a molecular state expansion without electron translation factors is a valid low-energy approximation" is borne out by our results. Note that our three-state results are very good at low energies, although they tend to overshoot the 15-state results towards the higher energies. This can probably be traced back to the observation made by Kimura and Lane [22] that "a calculation with a small basis set generally overestimates the cross section because of reflection of the flux within the given space."

In Fig. 4 we show the experimental data of a *total* single charge-transfer cross section [12b] together with our calculated results of charge transfer into channels

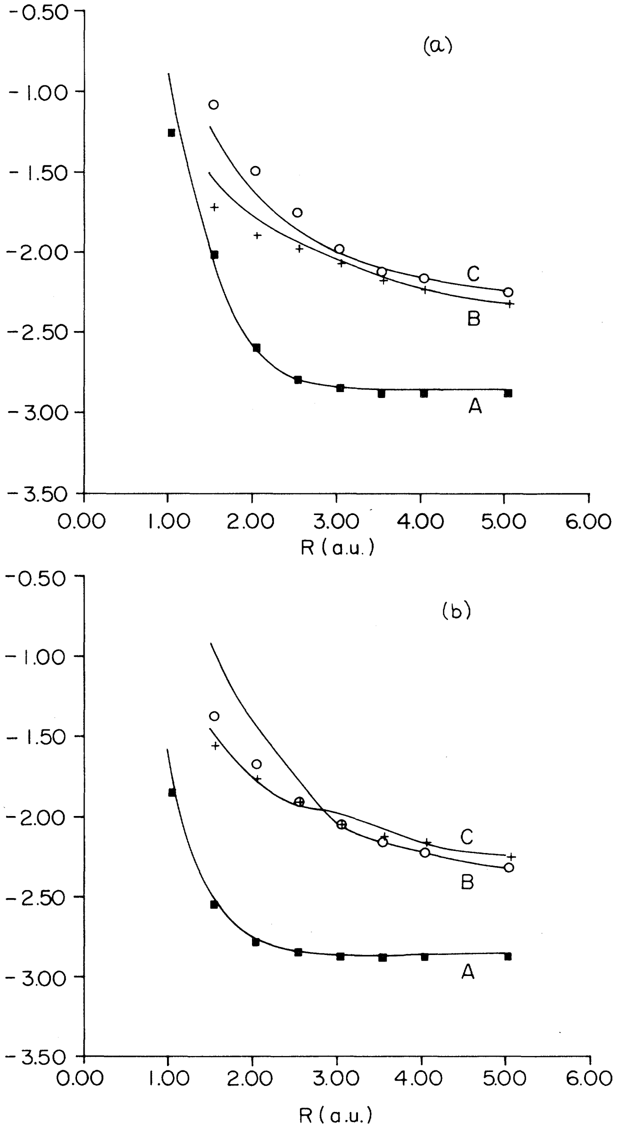

FIG. 2. (a) Comparison of diagonalized potential curves obtained from our results with eigenvalues read off from corresponding ${}^1\Sigma_g$ adiabatic curves given by Gao *et al.* [16] for the He^{2+}-He system. Curves *A*, *B*, and *C* dissociate to $He^{2+}+He(1s^2)$, $He^+(1s)+He^+(2p)$, and $He^+(1s)+He^+(2s)$, respectively. Symbols: $2\,{}^1\Sigma_g$ of Fig. 2 Ref. [16] (■); $3\,{}^1\Sigma_g$ (+); $4\,{}^1\Sigma_g$ (○). (b) Same as (a) for ${}^1\Sigma_u$ states. Symbols: ${}^1\Sigma_u$ of Fig. 2 Ref. [16] (■); $2\,{}^1\Sigma_u$ (○); $3\,{}^1\Sigma_u$ (+).

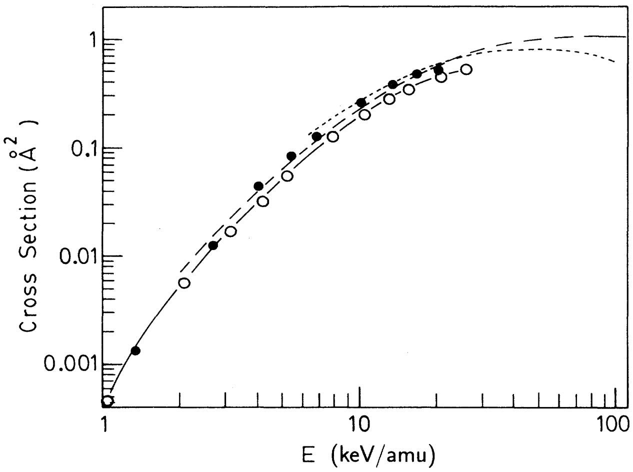

FIG. 3. Single-charge-transfer cross sections for reaction (9a) plotted against the collision energy. Open circles: present calculation (15-state basis); dashed line three-state calculation; dotted line: Fulton and Mittleman [17]; dark circles: Afrosimov's data [12(a)].

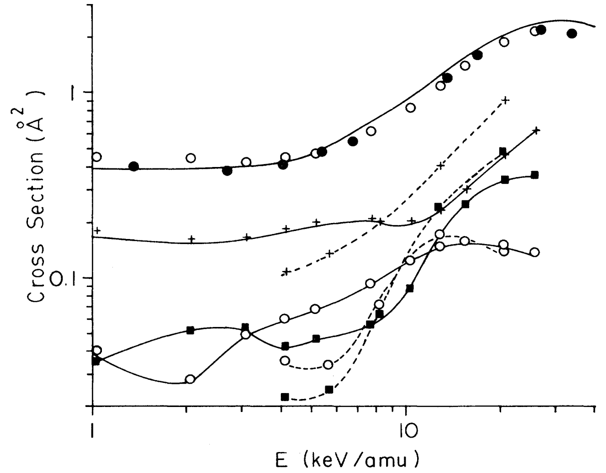

FIG. 4. Total and partial cross sections for single-electron capture. *Upper curves:* open circles, present calculation [summed over Eqs. (9a)–(9c)]; dark circles, Afrosimov's data; solid line, Kimura and Lane [22]. *Lower curves:* projectile (target) excitation. Symbols joined by full lines give our results; those joined by dashed lines give results of Fritsch [24]. Legend of symbols: projectile 2*s* excitation (■); projectile 2*p* excitation (+); target 2*s* excitation (○).

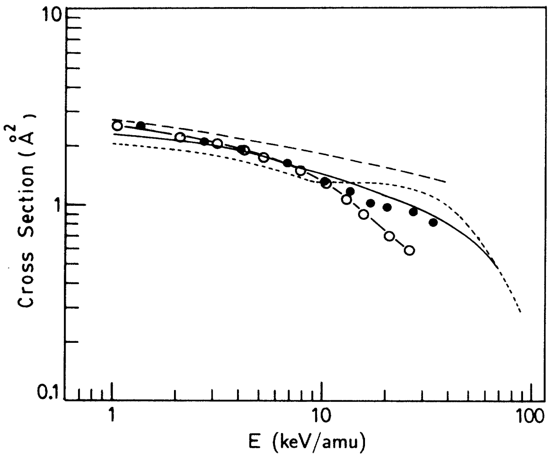

FIG. 5. Double-charge-transfer cross sections for reaction (10) plotted against collision energy. Open circles: present calculation (15-state basis); dashed line: three-state calculation; solid line: Kimura and Lane [22]; dotted line: Fulton and Mittleman [17]; dark circles: Afrosimov's data [12b].

(9a)–(9c) combined. Once again, the agreement is quite good. The theoretical results of Kimura [23], who used a "traveling" MO expansion including excitation channels up to $(3s,3p)$, are also shown. The figure also shows more detailed comparison of our $2s$ and $2p$ excitation cross sections with the recent work of Fritsch [24], who used a traveling atomic-orbital basis expansion. Fairly good agreement of the energy dependence of the projectile $(2s,2p)$ excitation and the target $(2s)$ excitation above 8 keV/amu is observed between the present results and the results of Fritsch [24].

The resonant double capture results are shown in Fig. 5, which also shows the experimental data of Afrosimov *et al.* [12b], our three-state calculations, and the theoretical results of Fulton and Mittleman [17] and of Kimura [23]. Up to energies of 10 keV/amu the agreement with experiment of our 15-state results is striking. We also find that our three-state calculations fail to reproduce the experimental data, although the general trend of variation with energy is correct.

An analysis of this feature of the three-state calculation, namely, its success to reproduce the single-charge-transfer data and its failure for double charge transfer leads us to the following conclusion. The symmetric resonant process involves a large probability of a *two-electron transfer,* and if we extend the generally accepted Bates-Lynn model [25] of resonant charge transfer to this case, the collision dynamics involves a two-electron correlated oscillation between the states ϕ_2 and ϕ_9. However, within this one-electron orbital model, a proper account of correlated behavior of the two electrons can only be obtained via configuration interaction, and this is exactly what is sacrificed when our diabatic basis is truncated early, as discussed earlier in this paper. This shows that while for single-charge-transfer collisions a diabatic series can be truncated early (so long as the relevant exit channels are not left out), for double charge transfer this cannot be done in general.

V. CONCLUSIONS

We explore in our paper the usefulness of a diabatic molecular basis expansion for a two-electron ion-atom collision system. We find that for single electron transfer into ground state as well as into excited states, the diabatic basis is useful. We also feel that if electron translation factors are properly incorporated, this diabatic basis can be used for benchmark calculations. Our studies show that for processes where correlated two-electron motion is important, the diabatic close-coupling series must retain enough terms for a proper configuration interaction, whereas for single-electron-transfer processes, the series can be truncated early so long as the exit channels are included.

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[1] D. R. Bates, H. S. W. Massey, and A. L. Stewart, Proc. R. Soc. London, Ser. A **216**, 437 (1953).
[2] W. Lichten, Phys. Rev. **131**, 229 (1963).
[3] T. F. O'Malley, Phys. Rev. **162**, 98 (1967); J. Chem. Phys. **51**, 322 (1969).
[4] F. T. Smith, Phys. Rev. **179**, 111 (1969).
[5] M. Barat and W. Lichten, Phys. Rev. A **6**, 211 (1972).
[6] J. Eichler, U. Wille, B. Fastrup, and K. Taulbjerg, Phys. Rev. A **14**, 707 (1976).
[7] J. B. Delos, Rev. Mod. Phys. **53**, 287 (1981).
[8] T. M. Kereselidze and B. I. Kikiani, Zh. Eksp. Teor. Fiz. **87**, 741 (1984) [Sov. Phys. JETP **60**, 423 (1984)].
[9] A. Russek and R. J. Furlan, Phys. Rev. A **39**, 5034 (1989).
[10] R. K. Janev and H. Winter, Phys. Rep. **117**, 267 (1985).
[11] T. K. Rai Dastidar and K. Rai Dastidar, Chem. Phys. Lett. **85**, 229 (1982). The same diabatic basis has been used by S. Ganguly, K. Rai Dastidar, and T. K. Rai Dastidar, Phys. Rev. A **31**, 1171 (1985); **33**, 3060 (1986).
[12] (a) V. V. Afrosimov, A.A. Basalaev, G. A. Leiko, and M. N. Panov, Zh. Eksp. Teor. Fiz. **74**, 1605 (1978) [Sov. Phys. JETP **47**, 837 (1978)]; (b) V. V. Afrosimov, G. A. Leiko, Yu. A. Mamaev, and M. N. Panov, *ibid.* **67**, 1329 (1974) [**40**, 661 (1974)].
[13] M. B. Shah, P. McCallion, and H. B. Gilbody, J. Phys. B **22**, 3037 (1989).
[14] T. K. Rai Dastidar, K. Rai Dastidar, and M. Guha, Chem. Phys. **43**, 189 (1979).
[15] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T.

Vetterling, *Numerical Recipes* (Cambridge University Press, Cambridge, 1986).
[16] R. S. Gao, C. M. Dutta, N. F. Lane, K. A. Smith, R. F. Stebbings, and M. Kimura, Phys. Rev. A **45**, 6388 (1992).
[17] M. J. Fulton and M. H. Mittleman, Proc. Phys. Soc. London **87**, 669 (1966).
[18] C. Chaudhuri, S. Sanyal, and T. K. Rai Dastidar, Pramana J. Phys. **43**, 175 (1994).
[19] C. Harel and A. Salin, J. Phys. B **13**, 785 (1980).
[20] K. Gramlich, N. Gruen, and W. Scheid, J. Phys. B **22**, 2567 (1989).
[21] B. Zygelman, D. L. Cooper, M. J. Ford, A. Dalgarno, J. Gerratt, and M. Raimondi, Phys. Rev. A **46**, 3846 (1992).
[22] M. Kimura and N. F. Lane, Adv. At. Mol. Opt. Phys. **26**, 79 (1990).
[23] M. Kimura, J. Phys. B **21**, L19 (1988).
[24] W. Fritsch, J. Phys. B **27**, 3461 (1994).
[25] D. R. Bates and N. Lynn, Proc. R. Soc. London, Ser. A **253**, 141 (1959).
[26] C. E. Moore, *Atomic Energy Levels,* Natl. Bur. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) Circ. No. 467 (U.S. GPO, Washington, D.C., 1949), Vol. 1.
[27] E. Clementi and C. Roetti, At. Data Nucl. Data Tables **14**, 177 (1974).