

## §9. Multicenter Close-coupling Calculations for Ionization Processes

Toshima, N. (Univ. Tsukuba)  
Tawara, H.

The conventional two-center expansion, in which the total scattering wavefunction is expanded in terms of the eigenfunctions of the target and the projectile atoms, has been widely used for the study of ion-atom rearrangement collisions. However, the convergence of the basis functions becomes in some cases very slow and we need to employ a huge number of basis functions in order to obtain satisfactorily accurate cross sections. The triple-center expansion method was proposed by Anderson *et al.*<sup>1)</sup> in order to accelerate the convergence by incorporating the united atom wave functions explicitly into the basis functions. The method was studied further by Lin *et al.*<sup>2)</sup>, Winter and Lin,<sup>3,4)</sup> and Winter<sup>5)</sup> mainly for the calculations of ionization cross sections.

In this report we extend the two-center Gaussian-type-orbital-basis (GTO) coupled-channel method to a triple-center description. We adopt the impact parameter method; the relative motion of the heavy particles is described classically by a rectilinear trajectory with a constant velocity  $v$  in the impact-parameter representation. The time-dependent Schrödinger equation of a single-electron system,

$$\left[ H - i \frac{\partial}{\partial t} \right] \Psi(\mathbf{r}, t) = 0 \quad (1)$$

is solved numerically by introducing an expansion:

$$\begin{aligned} \Psi(\mathbf{r}, t) = & \sum_{i=1}^{N_T} a_i(t) \psi_i^T(\mathbf{r}_T, t) \\ & + \sum_{i=N_T+1}^{N_T+N_P} a_i(t) \psi_i^P(\mathbf{r}_P, t) \\ & + \sum_{i=N_T+N_P+1}^N a_i(t) \psi_i^C(\mathbf{r}_C, t), \end{aligned} \quad (2)$$

in terms of the target wave functions:

$$\psi_i^T(\mathbf{r}_T, t) = \phi_i^T(\mathbf{r}_T) \exp(-iE_i^T t), \quad (3)$$

the projectile wave functions:

$$\begin{aligned} \psi_i^P(\mathbf{r}_P, t) = & \phi_i^P(\mathbf{r}_P) \\ & \times \exp(-iE_i^P t + i\mathbf{v} \cdot \mathbf{r}_T - \frac{i}{2}v^2 t), \end{aligned} \quad (4)$$

and wave functions of a virtual atom on the third center C:

$$\begin{aligned} \psi_i^C(\mathbf{r}_C, t) = & \phi_i^C(\mathbf{r}_C) \\ & \times \exp(-iE_i^C t + i\mathbf{p}\mathbf{v} \cdot \mathbf{r}_T - \frac{i}{2}p^2 v^2 t). \end{aligned} \quad (5)$$

Here,  $\phi_i^T, \phi_i^P$  and  $\phi_i^C$  are the hydrogenic eigenfunctions with eigenvalues  $E_i^T, E_i^P$  and  $E_i^C$  of the Hamiltonians of the target T, projectile P and virtual atom C, respectively; and  $\mathbf{r}_T, \mathbf{r}_P, \mathbf{r}_C$  and  $\mathbf{r}$  are the electron coordinates measured from the three centers T, P, C, and from the coordinate origin, respectively. The third center C and its nuclear charge are arbitrary in principle. We choose C as the equiforce saddle point between the two nuclei, and the charge as that of the united atom, i.e.,

$$p = \frac{\sqrt{Z_T}}{\sqrt{Z_T} + \sqrt{Z_P}}, \quad (6)$$

$$Z_C = Z_T + Z_P. \quad (7)$$

Here,  $p$  is the ratio of the distances between T and C and between T and P, while  $Z_T, Z_P$  and  $Z_C$  stand for the charges on T, P and C, respectively. The eigenfunctions of each center are further expanded in terms of the Gaussian-type basis functions as

$$\phi_{nlm}(\mathbf{r}) = \sum_{\nu} c_{\nu}^{nl} e^{-\alpha_{\nu} r^2} r^{\ell} Y_{\ell m}(\hat{r}), \quad (8)$$

where the nonlinear parameters  $\alpha_{\nu}$  are generated as a modified geometrical progression. The coefficients  $c_{\nu}^{nl}$  are determined so as to diagonalize the atomic Hamiltonians of the target, projectile and virtual atom. Substitution of Eq. (2) into Eq. (1) gives coupled equations in a matrix form:

$$iS \frac{d\mathbf{a}}{dt} = \mathbf{V}\mathbf{a}, \quad (9)$$

where  $\mathbf{a}$  is the column vector of the expansion coefficients, while S and V are the overlap and interaction matrices defined as

$$S_{ij} = \langle \psi_i | \psi_j \rangle, \quad (10)$$

$$V_{ij} = \langle \psi_i | H - i\partial/\partial t | \psi_j \rangle. \quad (11)$$

All the matrix elements of S and V are calculated analytically in the same way as stated for the two-center expansion.<sup>6)</sup> This high analyticity is a great advantage of the GTO expansion method since three-center matrix elements appearing in  $V_{ij}$  are very complicated to handle and since the calculation in the representation of the Slater-type-orbital (STO) expansion is time-consuming.

### References

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