PHYSICAL REVIEW A VOLUME 39, NUMBER 5 MARCH 1, 1989

Practical criterion for the determination of translation factors. IV. Simplified norm method

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(Received 13 June 1988)

Closing the series on the use of the norm method as a practical criterion to determine translation factors, we report a considerable simplification of the computational effort involved in our method. We study the speed of convergence of the sum-over-states expression giving the norms, and the possible use as criteria of rough approximations obtained by truncating this sum to a few states. Our main conclusion is that the rough-approximation method would yield the same translation factors as the exact one, while involving a minimal additional programming effort to that of the evaluation of molecular energies and couplings, and being applicable to semianalytical as well as variational wave functions, state-dependent as well as common translation factors, and package as well as *ad hoc* molecular programs.

I. INTRODUCTION

It is by now well established that generalization of the molecular expansion method, with the introduction of translation factors[1-6] to correct for the so-called momentum-transfer problem, permits us to treat successfully charge-exchange processes in ion-atom collisions, at least up to the energy region where their cross section is maximal. On the other hand, it is also known that the translation-factor solution of the momentum-transfer problem is only of formal value[7,8] unless it is supported by a guiding criterion as to the appropriate form of the factors.

In recent articles[9-11] we proposed, and used, such a criterion to gauge the quality of a translation factor. For this, we introduced norms that measure the couplings between the (usually small number of) states included in a molecular expansion and the infinite set of those that are left out. It was shown in Ref. 9 how those norms could be calculated analytically for wave functions that are written in terms of Gaussian-type orbitals (GTO's). The sum of the squares of all discarded couplings, yielding the Euclidean norm, gauges the overall quality of the trial space, while a weighted norm is more useful when optimizing translation factors for particular collisional processes.

In Refs. 10 and 11 the norm criterion was employed to optimize the form of a common translation factor[12,13] (CTF), within a given trial space, and to compare different analytical forms; in particular, in Ref. 11 attention was devoted to CTF optimization in the important region of intermediate and large internuclear distances R. The ensuing translation factors were successfully employed in a large number of cross-section calculations.[14-20]

A practical limitation of our approach to determine translation factors, however, is that a separate (and involved) program needs to be written for each specific analytical trial form of these factors. We suspect that this feature has understandably deterred other workers from using our optimization method directly.

Furthermore, our optimization studies have perforce been restricted to the kind of basis sets (GTO's) and translation factors (CTF's) that are currently employed in our collisional calculations. We think it would be useful for workers who may choose to use, e.g., one-electron diatomic molecule (OEDM) orbitals instead of GTO's, plane-wave-type translation factors instead of CTF's, or other approximations to correct for the momentum-transfer problem, to be able to apply the norm criterion to establish comparisons, without a considerable programming effort.

With this aim in mind, we have studied ways of simplifying that effort so that it would involve the same kind of integrals as are required in the collisional calculation. For our numerical tests, we chose as a benchmark the often-used HeH^{2+} quasimolecule, the common translation factor of Errea *et al.*,[13] and a basis $\{\phi_n\}$ consisting of the $1s\sigma$, $2s\sigma$, $2p\sigma$, $3d\sigma$, and $3d\pi$ molecular orbitals.

The purpose of the present paper, which closes the series on the use of the norm method as a practical criterion for the determination of translation factors, is to expose the conclusions of our study. In particular, we shall address the following two questions that directly bear on simplifying the norm method.

(1) How fast does the sum over infinite states involved in the norm converge? Can one approximate this norm to a good precision with a finite number of terms, and if so, with which ones?

(2) How reliable is an optimization criterion based on a roughly approximated norm calculated by substituting the analytical evaluation by a direct truncated summation over couplings, so that only a 50% accuracy (or even worse) is reached?

In the following paragraph we shall state the main definitions that are required for our paper to be self-contained. In Secs. III and IV we shall present our results that permit us to answer (quite optimistically) both questions. Atomic units are used throughout.

II. DEFINITIONS

We first define the Euclidean and weighted norms, for a molecular approach modified with a CTF, and in an impact-parameter formalism. In this approach, the electronic wave function representing the colliding system is approximated by the ansatz

$$\psi=\sum_{k=1}^{K} a_k(t)\phi_k(\mathbf{r},t)\exp\left[iU-i\int_0^t E_k dt'\right] \tag{1}$$

with ϕ_k and E_k the HeH^{2+} molecular wave functions and energies for fixed nuclear positions, $\mathbf{r}$ the electron position vector, and $\exp(iU)$ the CTF. As in previous work,[10,11] we choose $k=1s\sigma$, $2s\sigma$, $2p\sigma$, $3d\sigma$, and $2p\pi$ (hence $K=5$). It is immaterial for the present purpose which form is chosen for the CTF; in fact, it could just as well be replaced by a noncommon translation factor. For the sake of computational simplicity, we have taken it to be that introduced by Errea *et al.*[13] This has the advantages of having been thoroughly analyzed in our previous studies[10] for a wide range of internuclear distances, and containing parameters to be optimized, which will help us to answer question (2) of the Introduction:

$$U=f(\mathbf{r},R)\mathbf{v}\cdot\mathbf{r}-\tfrac{1}{2}f^2(\mathbf{r},R)v^2t \ , \tag{2}$$

where

$$f=\frac{R}{R^2+\beta^2}[\mathbf{r}\cdot\hat{\mathbf{R}}+(p-p_0)]-(p-p_0) \tag{3}$$

is a so-called switching factor[12,21–23] modulating the electronic velocity as the electron passes from being attached to the helium nucleus, ($p=0$), to belonging to the proton ($p=1$). Transition probabilities are easily shown[13] to be independent of the position of this origin (the value of p). The common translation factor (2),(3) contains two adjustable parameters to be optimized: β, which defines the extent of the cutoff in the switching factor, and p_0, which defines the so-called[13] privileged origin of electronic coordinates (the origin for which $f\rightarrow 0$ when $R\rightarrow 0$).

As the internuclear distance R tends to infinity each term of expansion (1) fulfills the impact-parameter equation:

$$\left[i\frac{\partial}{\partial t}-H\right]\Phi=0 \ . \tag{4}$$

Following Ref. 5, we call P the projection operator onto the manifold spanned by the K molecular wave functions ϕ_k included in the expansion (1), and $Q=1-P$. One can then define the Euclidean norm of discarded couplings:

$$\begin{aligned}N_E&=\left|\sum_{k=1}^{K}\left\|Q\left[i\frac{\partial}{\partial t}-H\right]P\phi_k\exp\left[iU-i\int_0^t E_k dt'\right]\right\|^2\right|^{1/2}\\&=\left|\sum_{k=1}^{K}\sum\!\!\!\!\!\!\int_j\left|\left\langle\phi_j\exp\left[iU-i\int_0^t E_j dt'\right]\right|\left[i\frac{\partial}{\partial t}-H\right]\left|\phi_k\exp\left[iU-i\int_0^t E_k dt'\right]\right\rangle\right|^2\right|^{1/2} ,\end{aligned} \tag{5}$$

where the sum plus integral over j refers to the (infinite) set of states left out in expansion (1).

The norm N always vanishes for $R\rightarrow\infty$, and also vanishes for a whole trajectory when (and only when) the wave function (1) is the exact solution of Eq. (4). This was the basis for proposing[9] the minimization of N as a means of determining a CTF that optimizes the ansatz (1), in the sense that it minimizes the couplings between the molecular wave functions included in the expansion, and those spanning the complementary space that are orthogonal to these.

Minimization of the Euclidean norm (5) provides an overall optimization of the P subspace. An alternative, collision-specific approach is provided by minimization of the weighted norm:

$$N_w=\left|\sum_{k=1}^{K}w_k(t)\left\|Q\left[i\frac{\partial}{\partial t}-H\right]P\phi_k\exp\left[iU-i\int_0^t E_k dt'\right]\right\|^2\right|^{1/2} \tag{6}$$

of similar properties to N_E.[9,10] The choice $w_k=|a_k|^2$ weights each P-Q coupling according to the population of the corresponding P state. It can be shown that N_w provides an upper bound and an oscillation-averaged form of the deviation vector[24,25] between the exact and approximate solutions of Eq. (4).

In earlier work[10] we optimized both N_E, and N_w for $\mathrm{He}^{2+}+\mathrm{H}$ collisions. For the sake of generality, it is more convenient here to consider approximations useful for any collisional process involving the $1s\sigma$, $2s\sigma$, $2p\sigma$, $3d\sigma$, and $2p\pi$ orbitals of the HeH^{2+} quasimolecule. For this purpose, we introduce the partial norms

$$\begin{aligned}N(k)&=\left\|Q\left[i\frac{\partial}{\partial t}-H\right]P\phi_k\exp\left[iU-i\int_0^t E_k dt'\right]\right\|\\&=\left|\sum\!\!\!\!\!\!\int_j\left|\left\langle\phi_j\exp\left[iU-i\int_0^t E_j dt'\right]\right|\left[i\frac{\partial}{\partial t}-H\right]\left|\phi_k\exp\left[iU-i\int_0^t E_k dt'\right]\right\rangle\right|^2\right|^{1/2}\end{aligned} \tag{7}$$

so that one has

$$N_E=\left[\sum_{k=1}^{K} N(k)^2\right]^{1/2} \tag{8}$$

and

$$N_w=\left[\sum_{k=1}^{K} w_k N(k)^2\right]^{1/2} . \tag{9}$$

Furthermore, we define

$$N(k,J)=\left|\sum_{j=1}^{J}\left|\left\langle \phi_j' \exp\left[iU-i\int_0^t E_j' dt'\right]\right|\left[i\frac{\partial}{\partial t}-H\right]\left|\phi_k \exp\left[iU-i\int_0^T E_k dt'\right]\right\rangle\right|^2\right|^{1/2} , \tag{10}$$

which is the approximation to the partial norm $N(k)$ reached by truncating the infinite sum plus integral of Eq. (7) to J terms, and employing either the exact eigenfunctions ϕ_j of the electronic Hamiltonian or approximate wave functions ϕ_j' resulting from a variational calculation for this Hamiltonian. Below the ionization threshold, these latter functions ϕ_j' provide representations for (a finite number of) the HeH^{2+} bound electronic states—yielding good approximations for the lowest-lying ones, and increasingly inaccurate ones for the higher Rydberg terms. Above the ionization threshold, they yield[26] an L^2-integrable discretization of the continuum orbitals. We emphasize that, unlike the case of the exact norm (7), the evaluation of $N(k;J)$ in (10) is a trivial step that can be implemented in any standard calculation of molecular energies and couplings.

From completeness of the basis set used in the variational calculation, it follows that

$$N(k,J)\rightarrow N(k) \tag{11}$$

as $J\rightarrow\infty$.

The partial norms (10) yield the following approximate Euclidean and weighted norms:

$$N_E(J)=\left[\sum_{k=1}^{K} N(k,J)^2\right]^{1/2} , \tag{12}$$

$$N_w(J)=\left[\sum_{k=1}^{K} w_k N(k,J)^2\right]^{1/2} . \tag{13}$$

We now consider questions (1) and (2) in the Introduction.

III. CONVERGENCE OF THE NORM EXPANSION

Using the CTF of Eqs. (2) and (3), and a basis set ϕ_k ($k=1s\sigma,2s\sigma,2p\sigma,3d\sigma,2p\pi$), we calculated the partial norms $N(k;J)$ as functions of J, for several nuclear trajectories and impact energies. As an illustration, we present, in this work, results obtained for a nuclear trajectory with impact parameter 1.0 a.u., and impact energy of 25 keV amu^{-1}. We have checked that these conclusions obtained for this particular case also hold for other nuclear trajectories.

Incidentally, we notice that the corresponding relative nuclear velocity, $v=1$ a.u., is sufficiently large that terms in v^2, etc., play an important part in the optimization of translation factors in the molecular formalism.

In our molecular calculations, the wave functions ϕ_k were expanded in a two-center basis set of 49 GTO's, given in Table I. Since in the variational determination of those wave functions one obtains 49 eigenvalues and eigenvectors, convergence will be studied with J running from 1 to $49-K=44$. As mentioned in the previous section, the wave functions ϕ_j' thus obtained only provide good representations to the exact HeH^{2+} stationary states for the lowest eigenvalues; also, they only yield a finite number of approximate Rydberg state wave functions for energies less than the ionization threshold ($j\leq 24$ in our calculations), and they provide a discretization of the continuous orbitals for higher energies ($j>24$).

We present in Fig. 1 the values of $N(k;J)/N(k)$, $k=1s\sigma$, $2s\sigma$, $2p\sigma$, $3d\sigma$, and $2p\pi$, as functions of J, for an internuclear distance $R=3$ a.u., and in Fig. 2 the corresponding ratio for the Euclidean norm $N_E(J)/N_E$. The dependence of the accuracy reached upon the internuclear separation is exemplified in Fig. 3, where we plot $N_E(J=43)/N_E$ as a function of R. Calculations have been performed with the CTF of Eqs. (2) and (3), with $\beta=4.0$ and the privileged origin on the center of nuclear charge ($p_0=0.333$). For completeness, we indicate by an arrow in Fig. 1 the position of the ionization threshold.

The main conclusion to be drawn from Fig. 1 is that convergence is very good, reaching 98% of the value of N for $J=44$, even when, as mentioned above, the wave functions ϕ_j' of the highest excited states are very poor approximations to the exact ones ϕ_j. This fast conver-

TABLE I. Exponents of the Gaussian basis set used in the present calculation.

He			H	
α_{1s}	$\alpha_{2p_{z,x}}$	$\alpha_{3d_{z^2,x^2,xz}}$	α_{1s}	$\alpha_{2p_{z,x}}$
0.015	0.0150	0.0235	0.0075	0.010
0.030	0.0375	0.5280	0.0225	0.025
0.065	0.1050	0.1298	0.0730	0.075
0.140	0.3150	0.4083	0.2560	0.250
0.450	1.0000		0.9600	1.000
1.800	3.4000		3.8400	
10.000			16.5000	
75.000				

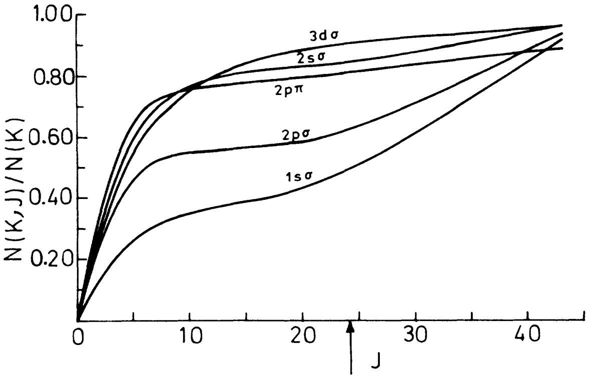

FIG. 1. Values of the ratio $N(k,J)/N(k)$ [Eqs. (7) and (10)] for $k = 1s\sigma$, $2p\sigma$, $2s\sigma$, $3d\sigma$, and $2p\pi$ as functions of the number of terms J included in the complementary space, for an internuclear distance $R = 3.0$ a.u., an impact parameter $b = 1.0$., a nuclear velocity $v = 1.0$ a.u., and the common translation factor of Eqs. (2) and (3) with $\beta = 4.0$ and $p_0 = 0.333$. The arrow indicates the position of the ionization threshold.

gence is partly due to the well-known over-completeness (basis-set superposition[27]) of a two-center expansion (Table I). On the other hand, when R increases, the GTO's centered on one atom become unable to span the atomic orbitals centered on the other, and as a result convergence is less good, as shown in Fig. 3. It is then fortunate that convergence is best for the region of intermediate distances where the form of the translation factor is totally unknown and where optimization is most critical.

A further significant result is that only about 50% accuracy in the norms is reached when the discretized continuum is ignored in the approximation $N(k;J)$ (i.e., for $J < 24$). Figure 1 shows that a large part of the norm comes, not only from the states lying next in energy, but also from those lying deep in the ionization continuum. This poses a problem when exact eigenfunctions of a one-electron Hamiltonian (such as OEDM's) are chosen as basis functions, since evaluation of nonadiabatic couplings with the corresponding continuum wave function is nontrivial.[28]

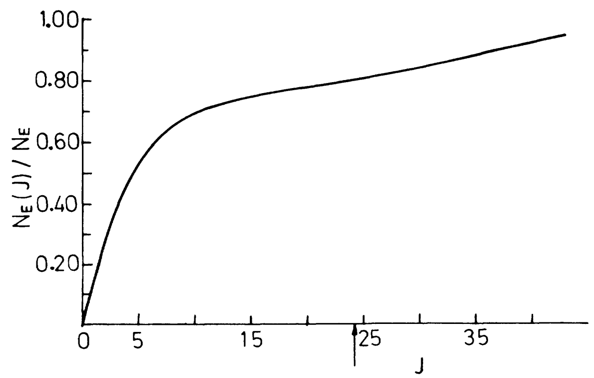

FIG. 2. Ratio $N_E(J)/N_E$ for the Euclidean norm [Eqs. (5) and (12)] as a function of the number of terms J included in the complementary space. The values for R, b, v, and the translation factor parameters are the same as in Fig. 1.

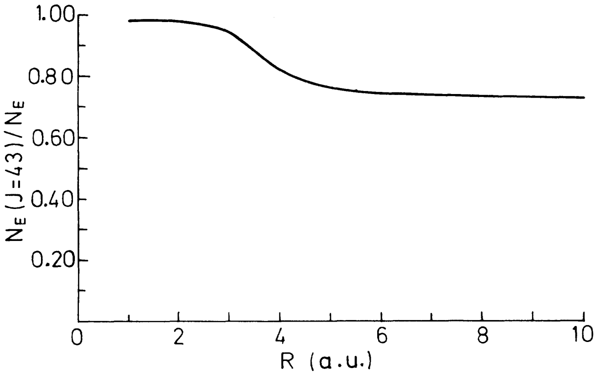

FIG. 3. Values of the ratio $N_E(J=43)/N_E$ as a function of the internuclear distance R. The values for b, v, β, and p_0 are the same as in Fig. 1.

To sum up, from Fig. 1 we conclude that a variational procedure can provide norms that are as exact as desired; for this, however, one should not neglect high-lying states that are obtained in the calculation.

IV. USE OF INACCURATE NORMS

We are here interested in ascertaining how an optimization procedure fares when it is carried out with a poor approximation to the norm [J small in Eqs. (10), (12), and (13)]—furthermore, with an approximation that is not even uniform with respect to R (as may be gleaned from Fig. 3). In order that our conclusions be valid for any weighted norm, we shall perform the comparison for some partial norms [Eq. (10)] as well as for the Euclidean one [Eq. (12)].

We display in Figs. 4(a) and 4(b) the values of the exact $N(1s\sigma)$, calculated analytically as in Ref. 10, for the same energy and nuclear trajectory as in Figs. 1–3, for two choices of privileged origin: (a) $p_0 = 0.333$ and (b) $p_0 = 1.0$ and for several values of the cutoff parameter β. The corresponding quantities for the $2p\sigma$ state are given in Figs. 5(a) and 5(b). We do not show the norms corresponding to the other P states, to avoid presenting too many figures that obey the same patterns and lead to the same conclusions; for completeness, we also present in Figs. 6(a) and 6(b) the values for the Euclidean norm N_E. A CTF optimization procedure would then involve combining the partial norms to yield either N_w [Eq. (9)] or N_E [Eq. (8)], and choosing the values of p_0 and β that yield the smallest norms.

To facilitate comparison, we present the corresponding approximate norms in Figs. 4(c) and 4(d) [$N(1s\sigma;J=8)$], Figs. 5(c) and 5(d) [$N(2p\sigma;J=8)$], and Figs. 6(c) and 6(d) [$N_E(J=8)$]. These quantities have been calculated in a straightforward way, by summing over the squares of the couplings that result in the variational treatment for the molecular wave functions. In this calculation the states involved in Eq. (10) are $j = 3s\sigma$, $3p\sigma$, $4d\sigma$, $4f\sigma$, $3d\pi$, $3p\pi$, $4f\pi$, and $3d\delta$; hence, no discretized continuum orbitals are involved in our approximate sum, and this

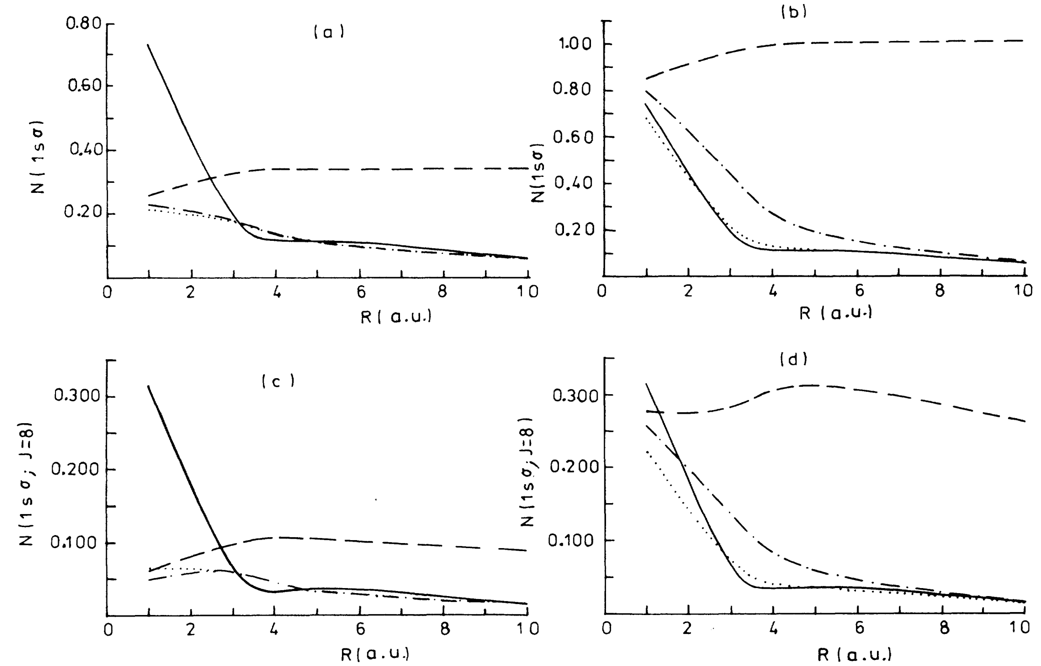

FIG. 4. Comparison of the exact $N(k=1s\sigma)$ [(a), (b)] and approximate $N(k=1s\sigma, J=8)$ [(c), (d)] partial norms as functions of the internuclear distance R, for two choices of the parameter p_0: $p_0=0.333$ [(a), (c)]; $p_0=1.0$, [(b), (d)], and for several values of the cutoff parameter β: $\beta=0.5$ (——); $\beta=2.0$ (· · · ·); $\beta=4.0$ (—·—·—). For comparison purposes, the norm values without translation factors (— — —) are also included. The impact energy and nuclear trajectory are the same as in Figs. 1–3.

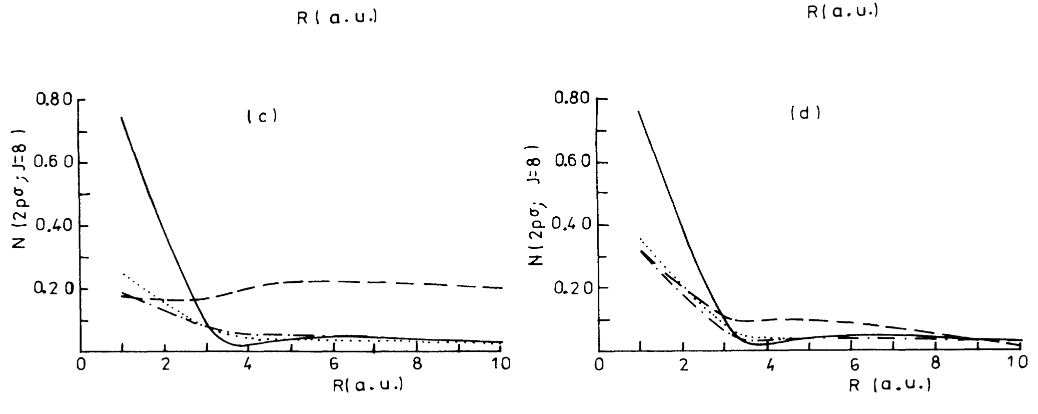

FIG. 5. Same as Fig. 4 for $k=2p\sigma$.

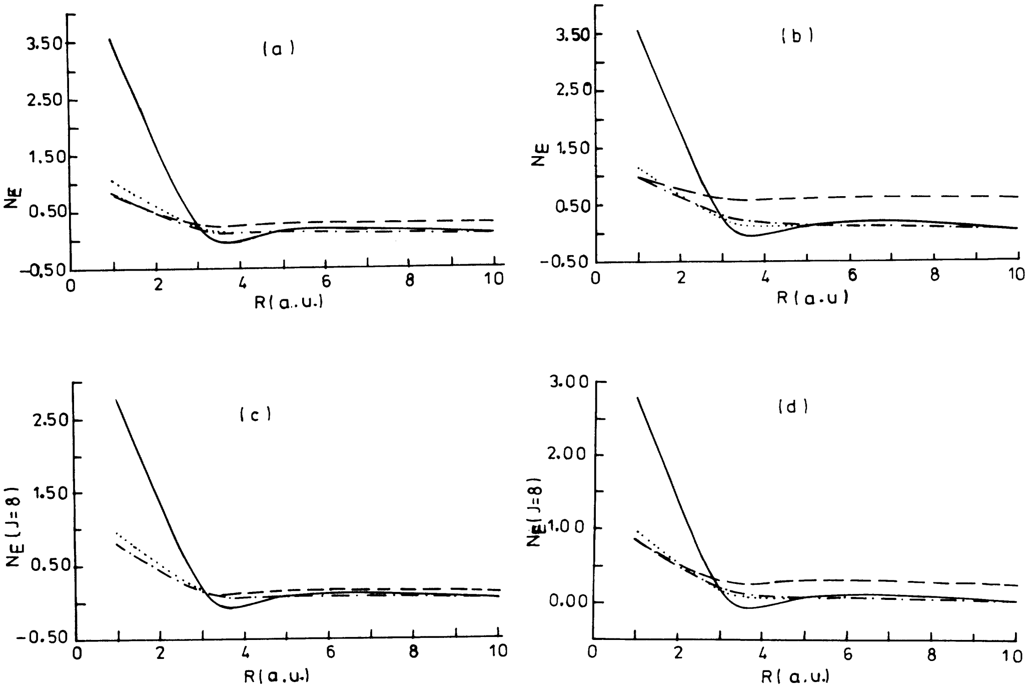

FIG. 6. Comparison of the exact N_E [Eq. (5)] and approximate $N_E(J=8)$ [Eq. (12)] as functions of the internuclear distance R. Same symbols as in Fig. 4 are used.

simplified procedure can be easily implemented when OEDM, or numerically evaluated, orbitals are employed.

We further notice that, according to Fig. 1, the choice $J=8$ in the approximate norms [Eq. (10)] only yields a 30% accuracy for $N(1s\sigma;J)$ and a 50% accuracy for $N(2p\sigma;J)$, at a distance $R=3$ a.u., the approximation becomes worse for larger R. As a consequence, the numbers involved in the exact (Figs. 4(a), 4(b), 5(a), 5(b), 6(a), and 6(b)] and rough [Figs. 4(c), 4(d), 5(c), 5(d), 6(c), and 6(d)] calculations are quite different. However, in an optimization procedure what is important is not these absolute numbers but their relative variation when the parameters are changed. For this purpose, we have rescaled the figures that correspond to the rough norms.

Comparison between Figs. 4(a), 4(b), 5(a), 5(b) and 4(c), 4(d), 5(c), 5(d), as well as between Figs. 6(a), 6(b) and 6(c), 6(d), respectively, provides a striking proof that, to optimize translation factors, roughly approximated norms will perfectly do, whether one uses the Euclidean or any weighed norm as a criterion. Small differences between exact and approximate norms are smaller than significant variations with respect to the CTF parameters, or between different forms of the CTF, and are immaterial in the optimization procedure.

V. CONCLUSIONS

In the present work we report a considerable simplification of the computational effort involved in using the Euclidean and weighted norms as criteria to determine translation factors.

Taking as benchmark the common translation factor of Errea *et al.*[13] and a basis of HeH^{2+} five molecular orbitals, we have investigated the speed of convergence of the sum over states involved in the norm expression, by comparing the exact value for this expression with the approximations reached by truncating it.

The main conclusion from those studies is that convergence is fast (reaching 98% accuracy in our calculations) for the most critical region of small to intermediate internuclear distances, *provided* that the molecular states with energies lying in the ionization continuum are included in the sum. This conclusion is very encouraging in view of the considerable programming effort involved in the exact evaluation of the norms, and especially in view of applying the method to more sophisticated translation factors, and to the many electron case. On the other hand, it poses a problem when semianalytical or numerical wave functions are employed, as in the OEDM approach.

Next, and foremost, we have tested the usefulness, as criteria, of patently inaccurate norms, such as obtained by truncating to a few terms their sum-over-states expression. Our main result is that, at least for the benchmark case analyzed here, although the accuracy reached in the truncation may be as poor as 30–50%, the translation factors obtained by minimizing the inaccurate norms would be practically indistinguishable from those obtained from minimizing the exact norms. In this respect, it should be borne in mind that the purpose of evaluating N_E or N_w is not to provide accurate values for these quantities, but to supply a quantitative criterion to determine translation factors.

The simplified finite sum-over-states criterion requires a minimal amount of computational effort. Moreover, since it does not involve continuum states, it may be applied to any kind of molecular wave function (and also to atomic wave functions), and to any kind of translation factor, whether common or state dependent.

Because of the previous characteristics, we hope that the present work will stimulate the checking, whenever necessary, of the procedures employed to cope with the momentum-transfer problem. As explicitly proved by Errea *et al.*,[8] to eliminate the known drawbacks of the perturbed stationary states approach, it is not sufficient to introduce translation factors (or reaction coordinates) in the collisional calculation, since dependence on the functional form of the factors can be larger than the origin dependence of the results obtained without them.

ACKNOWLEDGMENTS

This research has been partially supported by the Comisión Asesora de Investigación Cientifica y Técnica, Project No. 890/84.

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