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Calculated cross section for photoionization from the 1π and 3σ orbitals of hydrogen fluoride

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The photoionization cross section for the two highest-lying orbitals of hydrogen fluoride has been calculated both using a single-center spherical-wave approximation for the continuum electrons and using Tchebychev moment-analysis calculations. The results from the two computational schemes are in good agreement for channels where there is small possibility of partial waves of different l quantum numbers being mixed. Where such mixing can take place, inadequacies of the spherical-wave approach show up as large discrepancies between results calculated using the length and the velocity forms of the transition operator.

I. INTRODUCTION

The last decade has seen an increasing interest in the photoionization cross sections of atoms and molecules, spurred by the study of molecules in interstellar space, the search for high-energy lasers, and the increased availability of synchrotron radiation for investigating these cross sections. Theory and computational techniques have reached the point where quantitative predictions of atomic photoionization cross section can be made. However, the treatment of molecular photoionization is still in a developmental stage. One of the main problems here is the lack of a convenient description of the outgoing continuum electron.

Several computational schemes for treating molecular photoionization have been suggested.[1-7] In the present paper we shall use the single-center expansion method where continuum orbitals are represented as spherical waves expanded about a molecular center. While this method previously has provided reasonable results for some simple systems,[1,8] it is clear that the approximations inherent in the scheme may cause difficulties in application to more general molecular systems. It is therefore of interest to explore the possibilities of the single-center spherical-wave expansion further and to determine the limitations of the method.

Recently calculations of Auger transition rates in hydrogen fluoride using single-center spherical-wave continuum orbitals have been shown to give results in satisfactory agreement with experiment.[9] However, the energy range of the Auger electrons in HF is from 590 to 650 eV, and thus beyond the energy region where most of the oscillator strength of the molecule would be expected. It is therefore not immediately clear that the single-center expansion will be a suitable approach to the calculation of the photoionization cross section of HF, and the present work is an attempt at evaluating the usefulness of this method for such calculations.

The HF molecule should provide a reasonable test case because its electron distribution tends to be centered about the F nucleus. A detailed discussion of charge distributions in first-row hydrides has been given by Bader, Keaveny, and Cade[10] who state, "The HF molecule of all the first-row hydrides approaches most nearly the limiting ionic structure H^+A^-." It is therefore natural to compare results obtained on HF with corresponding results from Ne, the isoelectronic atom, a system which has been exhaustively investigated.[11,12] In particular, we will concentrate on the HF photoionization corresponding to ionization from the $2p$ level which dominates the photoionization cross section of Ne. Assuming electric-dipole selection rules, ionization from the $2p$ level can go to continuum orbitals of s or d symmetry (which we will denote ks or kd orbitals) with the kd channel accounting for the bulk of the photoionization cross section. For HF, which has the electronic ground-state configuration $(1\sigma^2 2\sigma^2 3\sigma^2 1\pi^4)^1\Sigma^+$, the corresponding ionization goes either from the 1π orbital to $k\sigma$, $k\pi$, or $k\delta$, giving the final states $(1\sigma^2 2\sigma^2 3\sigma^2 1\pi^3 k\delta^1)^1\Pi$, $(1\sigma^2 2\sigma^2 3\sigma^2 1\pi^3 k\pi^1)^1\Sigma^+$, and $(1\sigma^2 2\sigma^2 3\sigma^2 1\pi^3 k\sigma^1)^1\Pi$; or from 3σ to $k\sigma$ or $k\pi$ with the final states $(1\sigma^2 2\sigma^2 3\sigma^1 1\pi^4 k\sigma^1)^1\Sigma^+$ and $(1\sigma^2 2\sigma^2 3\sigma^1 1\pi^4 k\pi^1)^1\Pi$. In a spherical-wave expansion one would expect the d wave to dominate, in analogy with the Ne case; in particular the 1π to $k_d\delta$ (denoting the $l=2$ component of a continuum orbital with δ symmetry) should be the dominant channel.

In the present investigation we have calculated the photoionization cross section for a number of these outgoing channels. As suggested by the discussion in the previous paragraph, we have concentrated on the d wave or $l=2$ component of the continuum orbitals. However, for the 1π to $k\sigma$

channel, we have also calculated the contribution from the s wave. The s wave will, of course, also contribute in the 3σ to $k\sigma$ channel, but this contribution is expected to be small, and its magnitude may be estimated from the calculation for the 1π to $k\sigma$ channel. On the basis of the Ne results we do not expect a large contribution from the partial p waves, the cross section for the $2s$ to kp channel of Ne being an order of magnitude smaller than the $2p$ cross section.

We do not know of any experimental measurements of the photoionization cross section for HF except for the points from Ne I and He I measurements by Debies and Rabalais.[13] To obtain an indication of the reliability of our results we have performed Tchebychev moment-analysis calculations in parallel with the single-center expansion calculations. Section II of this article deals with the computational details of the two methods used. The computational results are presented and discussed in Sec. III, while Sec. IV contains some concluding remarks. It should be noted that the calculations presented here are in a lowest-order independent-particle scheme; no attempt has been made to discuss the effect of higher-order correlations. Also, all calculations are carried out in a fixed-nuclei approximation with an internuclear distance of 1.7328 bohr.

II. COMPUTATIONAL DETAILS

A. The single-center expansion

Our single-center calculations take as their starting point the self-consistent field (SCF) wave function for hydrogen fluoride given by Cade and Huo.[14] Their calculation which uses an extensive STO (Slater-type-orbital) basis is believed to be close to the Hartree-Fock limit. This function is expanded in spherical harmonics about the fluorine atom going up to $l=18$ for the σ orbitals and $l=17$ for the π orbitals.[15] The one-particle Hamiltonian for the free electron is obtained by coupling the continuum orbital of the outgoing electron and the ionized molecular system to the right symmetry for the final state. This Hamiltonian is then partitioned using the set of spherical harmonics centered on F. We approximate the continuum orbital by writing it in the form $R_{\epsilon l}(r) \times Y_{lm}(\theta, \phi)$. The final-state many-electron wave function has the spin $\frac{1}{2}$ of the core coupled to the spin $\frac{1}{2}$ of the outgoing electron to give $S=0$. This many-electron continuum state is used to derive a Hartree-Fock equation for $R_{\epsilon l}(r)$ given by

$$h_{ll}(r)R_{\epsilon l}(r) = \epsilon R_{\epsilon l}(r)\,, \tag{1}$$

where $h_{ll}(r)$ is the Hartree-Fock operator for this restricted problem where the continuum orbital involves only one $Y_{lm}(\theta, \phi)$. For further details on the derivation and solution of Eq. (1), see Refs. 1 and 9. As expected in Hartree-Fock calculations, h_{ll} contains nonlocal exchange terms. These terms lead to differences in results calculated with the Hartree-Fock "length" and "velocity" matrix elements defined below.

The continuum orbitals are normalized such that

$$R_{\epsilon l}(r) \to \frac{1}{r}\cos\left(kr + \delta_l + \frac{1}{k}\ln 2kr - \tfrac{1}{2}(l+1)\pi\right) \tag{2}$$

as $r \to \infty$, with $k=\sqrt{2\epsilon}$. With this normalization of the continuum orbitals the partial photoionization cross sections as a function of photon energy, ω, is given in atomic units as

$$\sigma_{lm}(\omega) = \frac{8\pi\omega}{3ck}\left|\left\langle \Psi_{flm}\middle|\sum_i \vec{r}_i\middle|\Psi_0\right\rangle\right|^2 . \tag{3}$$

Here Ψ_0 is the initial state, in our case the HF ground state, and Ψ_{flm} represents a final state of the system where the residual ion is coupled to a continuum orbital of the form $R_\epsilon(r)Y_{lm}(\theta, \phi)$. To obtain the total cross section it is necessary to sum over all possible l and m.

Alternatively, the partial cross section may also be expressed using the velocity form of the matrix element, as

$$\sigma_{lm}(\omega) = \frac{8\pi}{3\omega ck}\left|\left\langle \Psi_{flm}\middle|\sum_i \nabla_i\middle|\Psi_0\right\rangle\right|^2 . \tag{4}$$

Equations (3) and (4) give identical results when Ψ_f and Ψ_0 are exact eigenstates of the full many-body Hamiltonian. While agreement between results calculated using the two forms of the transition matrix element does not guarantee accuracy, noticeable discrepancies, on the other hand, are indicative of poor overall accuracy. We have therefore included both length and velocity results for all channels.

In accordance with the introductory remarks on the relative importance of the various contributions to the partial cross sections our calculations concentrate mainly on the $l=2$ or d-wave channels for the outgoing electron. Ionization potentials, where needed, were taken from the work of Shaw and Thomas as 16.05 eV for 1π and 19.28 eV for 3σ.[16]

B. The Tchebychev analysis

The use of the Stieltjes and Tchebychev moment analysis for calculating photoionization cross sections, as well as the actual computational implementation of these methods has been discussed extensively elsewhere (see, e.g., Refs. 3 and 12, and reference therein). Therefore only a brief outline will be presented here. We relate the photoionization cross section to the oscillator strength den-

sity at ϵ, $g(\epsilon)$, by

$$\sigma(\omega) = (2\pi^2/c)g(\epsilon)\,. \tag{5}$$

In the Tchebychev approach $g(\epsilon)$ is computed by differentiating the cumulative oscillator strength constructed from the poles and residues of a rational fraction involving polynomials $Q_n(z)$ and $P_n(z)$ constructed from recurrence relations of the type

$$Q_n(z) = (1 - \alpha_n z)Q_{n-1}(z) - z^2\beta_{n-1}Q_{n-1}(z)\,. \tag{6}$$

The coefficients α_n and β_n are calculated from a pseudospectrum obtained by diagonalizing a one-electron Hamiltonian representing a $V^{(n-1)}$ frozen core potential in an extended basis-set space.

In the present calculation the pseudospectra have been calculated using the STO integral-UIBMOL SCF package described previously.[17,18] The program package has been suitably modified for producing pseudospectra to be used with the Tchebychev analysis. Our starting point is again the basis set given by Cade and Huo[14] which we augment by a number of basis orbitals to describe the outgoing electron. The additional basis functions must be chosen to give the best possible coverage of the continuum; in particular this means that one should have a fairly dense pseudospectrum in the region just above the threshold where the cross section changes most rapidly. The coverage is, however, limited by the danger of linear dependencies in the basis sets used. For the $k\delta$ channel a (16, 8, 8, 13) basis, i.e., 16δ, $8\pi_+$, $8\pi_-$, and $13\delta_+$ orbitals, was used to obtain a 13-point pseudospectrum. For $k\pi$ channels a (16, 8, 19) basis gave an 18-point spectrum. For $k\delta$ channels, 23 points were obtained from a (26, 8, 8) basis. As an illustration the exponents of one of the basis sets, as well as the pseudospectrum obtained with this basis, are presented in Table I.

The medium-sized calculations presented here depend heavily on the extrapolation of the α_n and β_n sequences described previously.[3,12,19] In most of the calculations the sequence has been extrapolated from $n = 3$ corresponding to the use of 6 converged moments. With our present program we are not able to achieve a substantially larger number of converged moments. Also for the Tchebychev analysis we have calculated cross sections using both the length and the velocity formalism.

The two computational approaches to molecular photoionization used in this work both describe the residual ion in a frozen core $V^{(n-1)}$ static exchange approximation, and should be of comparable accuracy in this respect. Any discrepancies between results obtained with the two methods should therefore be chiefly attributable to the different treatment of the continuum states.

TABLE I. The 1π to $k\pi$ transition. Basis functions used in the π space and calculated pseudospectrum for this transition. All quantities in atomic units. (Functions with negative n quantum numbers are centered on hydrogen.) Numbers in parentheses indicate powers of ten.

Basis set			Pseudospectrum		
	Quantum numbers			Transition moments	
Orbital exponent	N	L	Transition energy	Velocity form	Length form
1.3584	2	1	0.4587	1.22(−05)	1.01(−05)
2.3291	2	1	0.4834	6.09(−06)	4.35(−06)
4.2615	2	1	0.5340	1.67(−02)	1.54(−02)
9.2974	2	1	0.5460	4.42(−03)	4.22(−03)
2.1338	3	2	0.6061	1.00(−04)	8.75(−05)
2.7937	4	3	0.6914	3.90(−02)	3.92(−02)
1.7706	−2	1	0.7042	7.17(−02)	7.30(−02)
3.3205	−3	2	0.7595	2.37(−02)	2.49(−02)
4.5000	3	2	0.9810	7.95(−02)	8.83(−02)
1.0200	3	2	1.0152	8.14(−2)	8.44(−02)
0.8312	3	2	1.5443	2.88(−01)	3.35(−01)
0.6773	3	2	2.3237	1.01(−04)	4.73(−04)
0.5519	3	2	3.2539	2.68(−01)	3.04(−01)
0.4497	3	2	4.4524	6.96(−04)	4.73(−04)
0.3665	3	2	4.5580	4.26(−04)	6.79(−04)
0.2986	3	2	8.6497	1.52(−02)	1.67(−02)
0.2433	3	2	10.9058	6.01(−02)	6.87(−02)
0.1622	3	2	35.9694	4.93(−07)	5.40(−05)
0.1081	3	2			

III. RESULTS AND DISCUSSION

A. The 1π to $k\delta$ channel

On purely statistical grounds one would expect this channel to account for a large part of the total photoionization cross section. On the other hand, this is also the channel where the single-center expansion might be expected to give the best results. The only possible photoionization channels for Ne which have an $l = 2$ component are the continuum d orbitals, and it is therefore a reasonable assumption that the mixing of other spherical waves into this channel will be small, i.e., that the $k_d\delta$ spherical wave provides a reasonable description of the outgoing electron. The calculated cross section (Fig. 1) shows agreement between single-center length and velocity forms which is as good as, or better than, that obtained in the numerical calculation of the $2p$ to kd cross section of Ne.[12,20] The cross sections obtained from the Tchebychev analysis are in good agreement with the single-center results, even better than for the previous Ne calculation.[12] Comparison between the two calculations should, however, be made bearing in mind that the Ne calculation used Gaussian-type orbitals, while Slater-type orbitals are employed in the present work. The Tchebychev

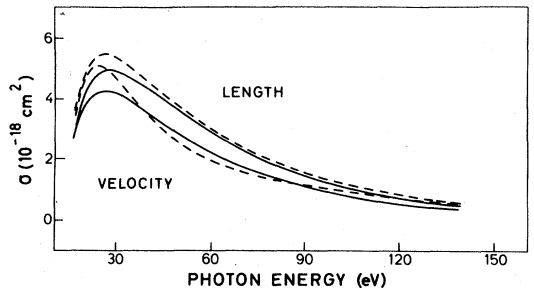

FIG. 1. Calculated photoionization cross section for HF 1π to $k_d\delta$ solid curve: single-center results. Dashed curve: Tchebychev results.

results are characteristically higher than the single-center results in the area around the maximum. This behavior is also observed in the Ne calculations. A possible cause of this may be an insufficient number of values for the pseudospectrum in this region of rapid change, preventing the moment analysis from describing the curve with the required accuracy. This behavior is a general feature of all the calculations presented here, as well as for the previous Ne calculation, and may be an inherent weakness in the medium-size Tchebychev calculations carried out by us. It is also noticeable that while the velocity form gave the best agreement between Tchebychev and single-center results for the Ne calculation, the length form generally gives the better agreement in the present work. This may at least partly be ascribed to the use of Slater-type orbitals giving a better description of the long-range behavior of atomic orbitals.

B. The 1π to $k\pi$ channel

The remarks of the previous section about the mixing of spherical waves applies to this channel as well, with the exception of possible interference by a p wave. However, the 1π orbitals have no $2s$ character, and by analogy with the Ne case, the contribution from a possible p wave should be in-

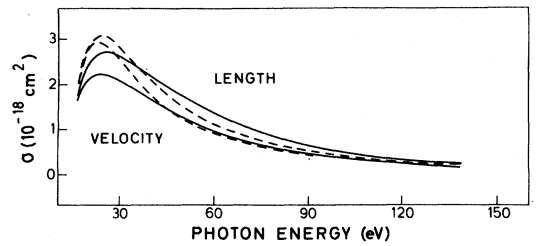

FIG. 2. Calculated photoionization cross section for HF 1π to $k_d\pi$ solid curve: single-center results. Dashed curve: Tchebychev results.

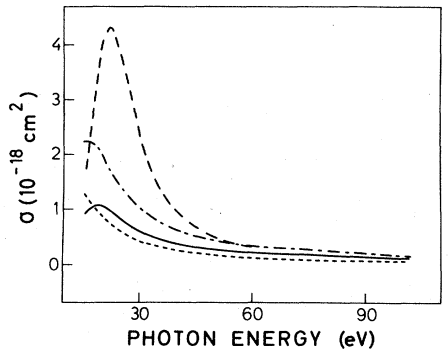

FIG. 3. Calculated photoionization cross section for HF 1π to $k\sigma$ length form. Solid curve: single-center 1π to $k_d\sigma$; dotted curve: single-center 1π to $k_s\sigma$; Dash-dot curve: total single-center 1π to $k\sigma$ cross section; Dashed curve: Tchebychev results.

significant. We therefore believe that also for this channel the $k_d\pi$ continuum orbital may be used to describe the outgoing electron. The single-center cross-section curves in Fig. 2 certainly show agreement between length and velocity which is of the same quality as the $2p$ to kd cross section for Ne. The remarks made above about agreement between Tchebychev and single-center calculation apply to this channel as well.

C. The 1π to $k\sigma$ channel

The $2p$ to ks channel photoionization cross section of Ne is of the same magnitude as the $2p$ to kd channel close to threshold, suggesting a possible mixing of the s and d waves in the 1π to $k\sigma$ channel for HF close to threshold. We have therefore calculated the cross section for the s wave as well as the d wave for this channel. The results are presented in Figs. 3 and 4. Only in this chan-

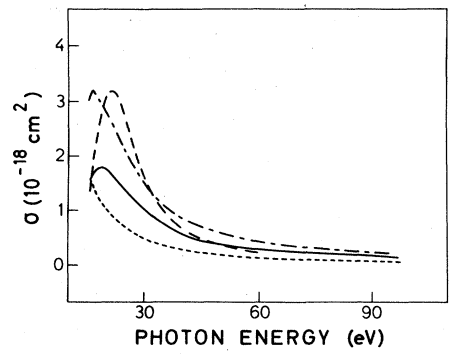

FIG. 4. Calculated photoionization cross section for HF 1π to $k\sigma$ velocity form. Solid curve: single-center 1π to $k_d\sigma$; Dotted curve: single-center 1π to $k_s\sigma$; Dash-dot curve: total single-center 1π to $k\sigma$ cross section; Dashed curve: Tchebychev results.

nel is the length form of the cross section lower than the velocity form. For the s wave this is only marginally so, but for the d wave the discrepancy is 40% in the peak area, giving a discrepancy of up to 30% in the total 1π to $k\sigma$ cross section calculated as the sum of these two.

In both the $1\pi \rightarrow k\sigma$ and $3\sigma \rightarrow k\sigma$ channels the 4σ orbital is expected to give significant contributions close to threshold. However, it is not clear that this orbital dominates since the coefficients of many orbitals are large for the diffuse contributions and have alternating signs.

For this channel the Tchebychev calculation using the length form gives a very sharp peak centered around 30 eV which deviates strongly from the single-center results whereas the two calculations using the velocity form show reasonable agreement. The Tchebychev curves also give some (clearly unphysical) oscillations at higher energies; we have therefore only included results for energies below 70 eV in Figs. 3 and 4. Oscillations of this type are usually indicative of the use of nonconverged moments in the moment analysis. However, extending the basis sets to the limits of our present computer programs does not smooth out the results. For this channel we may have encountered problems of the type described by Nesbet who found that two weakly coupled channels may give rise to highly irregular results in the moment analysis if care is not taken to separate these.[21] In the present case, we have attempted to distinguish two or more separate pseudospectra on the basis of the main spherical-wave component. We are not able to unambiguously separate pseudospectra in this manner. Thus, clearly some other criteria are needed. At present we are uncertain as to what significance to attach to the Tchebychev results for this channel; a further investigation into this problem is therefore required.

D. The 3σ to $k\sigma$ channel

Also for this channel, mixing of the s and d waves is expected. In the single-center scheme we have only calculated the d-wave cross section (Fig. 5), we expect the s-wave contribution to show the same qualitative behavior as for the 1π to $k\sigma$ channel, giving a maximum contribution of approximately 0.7 Mb close to threshold. The large discrepancy between the single-center length and velocity results indicates that the spherical wave does not describe the outgoing electron correctly. For this $k\sigma$ channel the Tchebychev analysis provides a set of curves which show a reasonable agreement, and a shape which, although somewhat more peaked than the 1π to $k\pi$ and $k\delta$ channels, is

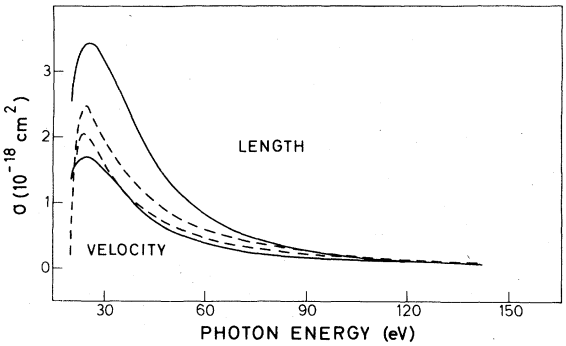

FIG. 5. Calculated photoionization cross section for HF 3σ to $k\sigma$. Solid curve: single-center results. Dashed curve: Tchebychev results.

quite similar to these. Also the curves show none of the high-energy oscillations seen for the 1π to $k\sigma$ channel. This is somewhat surprising because the two channels were calculated using the same basis set (26 σ orbitals and 8π orbitals). Thus the effects which cause the irregular high-energy Tchebychev results of the 1π to $k\sigma$ channel are somehow absent in the 3σ to $k\sigma$ channel.

E. The 3σ to $k\pi$ channel

For this channel the two types of calculations are in good agreement and both yield length and velocity results that are quite close (Fig. 6). There is a possibility of p- and d-wave mixing, caused by the $2s$ character of the HF 3σ orbital; evidently this is too small to cause any difficulties for either computational scheme.

F. The total cross section from the 1π and 3σ orbitals

Figures 7 and 8 show the total cross sections for photoionization from the 1π and 3σ orbitals of HF, as well as the sum of these. Due to the length-

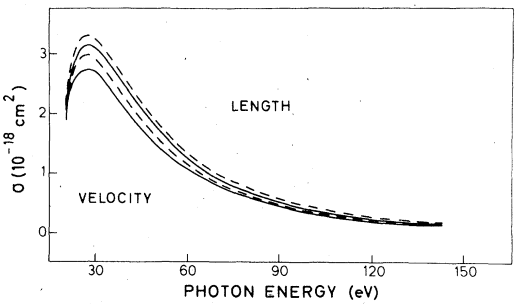

FIG. 6. Calculated photoionization cross section for HF 3σ to $k\pi$. Solid curve: single-center results. Dashed curve: Tchebychev results.

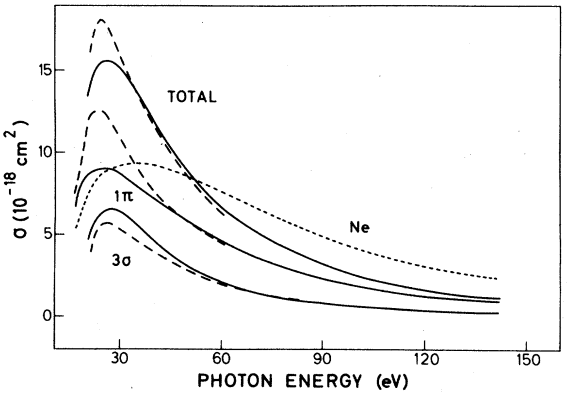

FIG. 7. Calculated cross sections for photoionization from the 1π and 3σ orbitals of HF. Length form. Solid curve: single-center results. Dashed curve: Tchebychev results. Dotted curve: corresponding cross section for Ne included for comparison.

velocity reversal for the 1π to $k\sigma$ channel, agreement between the two forms in the single-center calculation is fortuitously good, this also gives a somewhat deceptive length and velocity agreement for the total cross section. The Tchebychev results lie above the single-center results for all but the 3σ length forms, where the large single-center length result in the $k\sigma$ channel dominates. For that particular channel single-center results are probably low by approximately one Mb in the threshold region because of the neglected s wave; this, of course, also affects the total cross section. For ionization from the 1π orbital the large discrepancy between single-center and Tchebychev length results are mainly due to the sharply peaked

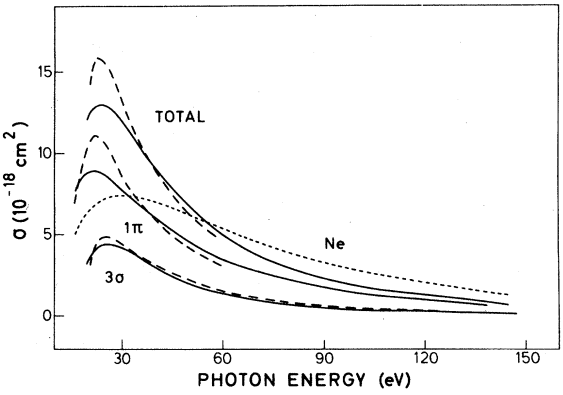

FIG. 8. Calculated cross sections for photoionization from the 1π and 3σ orbitals of HF. Velocity form. Solid curve: single-center results. Dashed curve: Tchebychev results. Dotted curve: corresponding cross section for Ne included for comparison.

Tchebychev cross section for the $k\sigma$ channel. For the reasons noted under the discussion of that channel, Tchebychev results are shown only up to 60 eV for the 1π cross section and for the total.

Also shown in Figs. 7 and 8 are the Ne $2p$-photoionization cross sections from atomic numerical Hartree-Fock calculations (unpublished results by Carter), which, except for the length and velocity discrepancy, are in good agreement with calculations accounting for higher-order effects.[11] At energies below 50 eV the HF cross section fits nicely between the Ne results and the cross section for water calculated by Williams and Langhoff.[22] The OPW calculations by Debies and Rabalais[13] give cross sections that are an order of magnitude too small, as was the case for water. It is noteworthy, though, that the OPW calculations give a qualitatively correct picture of the relative behavior of the Ne, HF, and H_2O photoionization cross section.

IV. CONCLUDING REMARKS

In the present work we have investigated the photoionization cross sections from the 3σ and 1π orbitals of HF. Although no experimental data are available for comparison, our use of two independent computational schemes as well as the length and velocity forms of the transition moment operator enables us to draw conclusions as to the usefulness of the single-center expansion method, which is our main objective. The method appears to perform quite well as long as there is no possibility of mixing between different spherical waves in the outgoing channels. For these cases results using the length and velocity forms are in good agreement, the agreement being comparable to that obtained by numerical calculations on the analogous atomic system. Furthermore, for these cases the results are in good agreement with those obtained from Tchebychev moment analysis. Breakdown of the single-center scheme for the case where two spherical waves may mix in the outgoing channel is clearly indicated by the large length and velocity discrepancy observed in the calculation. This mixing of waves might be accounted for explicitly by the use of perturbation theory as applied by us previously[9] to the Auger transition rates of HF. This will be a formidable computational task.

As already noted, neither of the methods applied by us go beyond the Hartree-Fock level. The Tchebychev moment analysis may easily by extended to include also correlation effects by recasting the calculations in a configuration-interaction (CI) scheme, as already done by a number

of authors.[23-25] For the single-center expansion method the many-body formalism developed for atomic photoionization may be applied. For the calculation presented here, the moment-analysis approach has definite advantages in its ability to handle outgoing channels where different spherical waves may mix. However, with the present state of the art there is clearly a need for several high-quality computational schemes for calculating molecular photoionization cross sections.

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