Photodetachment cross sections of negative ions: The range of validity of the Wigner threshold law

John W. Farley
Department of Physics, University of Nevada, Las Vegas, 4505 Maryland Parkway, Las Vegas, Nevada 89154
(Received 31 July 1989)

The threshold behavior of the photodetachment cross section of negative ions as a function of photon frequency is usually described by the Wigner law. However, there is little theoretical guidance about the range or accuracy of the Wigner law. This paper reports the results of a model calculation using the zero-core-contribution (ZCC) approximation. Theoretical expressions for the leading correction to the Wigner law are developed, giving the range of validity of the Wigner law and the expected accuracy. The results, derived within the ZCC approximation, are relevant to extraction of electron affinities from experimental photodetachment data.

INTRODUCTION

In photodetachment, electromagnetic radiation is incident upon a negative ion, producing a free electron and a neutral. The photodetachment process can be written symbolically as

$$\hbar\omega + X^- \rightarrow X + e^- \ . \tag{1}$$

Photodetachment of H^- makes an important contribution to the opacity of the solar atmosphere in the infrared, as first realized by Wildt.[1] In the terrestrial atmosphere, photodetachment of anions affects the conductivity of the ionosphere, which, in turn, influences radio communications.[2]

Photodetachment is possible if the photon energy $\hbar\omega$ exceeds the electron affinity E, the binding energy of the electron to the neutral. Conservation of energy gives

$$\hbar\omega = E + \hbar^2 k^2/2m \ , \tag{2}$$

where $\hbar k$ is the linear momentum of the free electron.[3] The behavior of cross sections just above threshold (where $k=0$) has been a subject of experimental and theoretical interest for decades.

Threshold behavior has the greatest practical interest in the determination of electron affinities. Electron affinities can be extracted from experimental measurements of the photodetachment cross section as a function of photon energy. Superficially, it might appear that only the data closest to threshold is useful. However, since the cross section approaches zero slowly in the vicinity of threshold, the data taken closest to threshold has the worst signal-to-noise ratio. The proper procedure is to extrapolate to threshold, thereby making use of all the data. It is therefore important to know the correct functional form for use in the extrapolation process.

In 1948, Wigner[4] derived general expressions for the behavior of cross sections near threshold for various processes. An expression was derived for the asymptotic behavior of the photodetachment cross section just above threshold. The threshold behavior is determined by the long-range behavior of the potential. This can be justified intuitively, because a near-threshold electron reaches the large-r region with a very low velocity, and consequently spends a great deal of time at large r. This effect becomes more pronounced as threshold is approached; hence the long-range behavior of the potential becomes increasingly important as threshold is approached.

After photodetachment, the receding electron and the neutral are treated using a standard approach: The two-body three-dimensional problem is reduced to a one-body one-dimensional problem. As part of the reduction process, the electron mass is replaced by the reduced mass μ, and the physical potential $V(r)$ is replaced by an effective potential $V_{\text{eff}}(r)$, which is the sum of $V(r)$ and the centrifugal barrier term viz.,

$$V_{\text{eff}}(r) = V(r) + l(l+1)\hbar^2/2\mu r^2 \ , \tag{3}$$

where $\hbar l$ is the angular momentum of the outgoing electron. The premise of the Wigner photodetachment law is that the interaction between the departing electron and the neutral falls off faster than r^{-2} for large r. Therefore at large r the dominant term in V_{eff} is the centrifugal barrier term. The resulting Wigner threshold law[5] is

$$\sigma \rightarrow A k^{2l+1} \ , \tag{4}$$

where $\hbar k$ is the linear momentum of the outgoing electron and A is a normalization constant. The Wigner law has often been used to fit photodetachment data.

The Wigner law is a threshold law: It holds "near" threshold. There is little theoretical guidance about how close to threshold one has to be. The law is said to "hold" if the deviation between the law and reality is less than some arbitrary fraction. In other words, there is no theoretical guideline for either the range or the accuracy of the Wigner law. Presumably, the Wigner law is the first term in the expansion of the (unknown) exact solution, expressed in increasing powers of k. As the energy increases above threshold, the Wigner law begins to fail, because the unknown second term is an appreciable fraction of the first term. Hereinafter, we refer to the first

term, expressed in Eq. (4), as the "Wigner term" and the second term as the "leading correction."

This paper reports the results of a model calculation using the zero-core-contribution (hereinafter ZCC) approximation of Stehman, Woo, and co-workers, a well-established approximation which yields analytical expressions for photodetachment cross sections for a model atom of given core radius and electron affinity. By dealing with an analytically soluble problem, insights may be gained which are relevant to the full-fledged theoretical problem. By taking the near-threshold limit, expressions are obtained for the Wigner term and the leading correction. The correction term has not been obtained before. The range and accuracy are assessed, relative to the ZCC approximation, of the Wigner term and of the Wigner term with the leading correction. The inclusion of the leading correction results in an improved threshold law with improved range and accuracy (within the ZCC approximation). Finally, comparison is made with other theoretical results. The leading correction term obtained here is roughly the same size as the polarization term derived by O'Malley.

THEORY

ZCC approximation

The ZCC approximation of Stehman and Woo[6] is based on the following assumptions: (1) The many-electron wave functions of the initial and final states can be factored into wave functions of a single outer electron and of a frozen core of radius r_0 (2) the wave function of the core is unchanged during the photodetachment process, (3) the core makes no contribution to the photodetachment process, and (4) the potential vanishes outside the core. Bethe and Longmire[7] used this approach in 1950 to calculate the photodisintegration of the deuteron, and a decade later Ohmura and Ohmura[8] used it to calculate the photodetachment cross section of H^-. (The H^- system has been the subject of a more sophisticated treatment by Broad and Reinhardt[9]). These assumptions simplify the calculation by reducing the calculation of the matrix element to a one-dimensional problem.

The ZCC approximation is a semiempirical approach, with three input parameters: The electron affinity E, taken from experiment, the core radius r_0, taken from a Hartree-Fock calculation, and the orbital angular momentum L of the initial orbital. Superficially, it might appear that the electron affinity is best obtained from a large-scale computer calculation. However, calculation of electron affinities is difficult, even for the best routines on supercomputers.[10] Often, even the sign cannot be determined reliably. Consequently, the most reliable procedure is to take E from experiment.

The calculation can be performed in closed form, yielding an analytical expression for the photodetachment cross section as a function of photon energy. The model fits the experimental cross sections quite well for several atomic anions: Hydrogen and the alkali metals, carbon, oxygen, and (less well) iodine. The ZCC model was first developed for application to atomic anions, then extended[11] to the molecular anions O_2^- and S_2^-. An extended version of the ZCC model was applied to multichannel photodetachment of atomic species by Clodius, Stehman, and Woo,[12] and to photodetachment of the polyatomic system NO_2^- by the same authors.[13] The NO_2^- system has been studied recently by Lineberger and co-workers[14] using ultraviolet laser photoelectron spectrometry; they reinterpret the drift-tube experimental data of Woo *et al.*[15]

The ZCC approximation can be specialized to photodetachment from an s, p, or d orbital: $L=0$, 1, or 2. These cases include most atomic cases of practical interest.

Photodetachment from an s orbital

The final state is a p wave. The total cross section σ is

$$\sigma=(8\pi/3)\alpha(m\omega k/\hbar)R_{ps}^2 , \tag{5}$$

where

$$R_{ps}=N_0\exp(-\gamma r_0)[k^2(k^2+\gamma^2)^2]^{-1} \times\{[k^3(2-\gamma r_0)-\gamma^3 r_0 k]\cos kr_0 +[\gamma(\gamma^2+3k^2)+k^2 r_0(\gamma^2+k^2)]\sin kr_0\} . \tag{6}$$

The normalization factor N_0 is

$$N_0^2=2\gamma\exp(2\gamma r_0) , \tag{7}$$

and γ is

$$\gamma=(2mE)^{1/2}/\hbar . \tag{8}$$

The spatial extent of the initial wave function is roughly $1/\gamma$. For $E=1$ eV, $\gamma=0.5123$ Å^{-1}.

For small k, σ approaches

$$\sigma\rightarrow(8\pi/3)\alpha(m\omega/\hbar\gamma^4)[A_3(k/\gamma)^3+A_5(k/\gamma)^5] , \tag{9}$$

where

$$A_3=2(2+2x+x^2+x^3/3)^2 , \tag{10}$$

and

$$A_5=-4(2+2x+x^2+x^3/3) \times(4+4x+2x^2+2x^3/3+x^4/6+x^5/120) , \tag{11}$$

where x, the natural scaling parameter, is

$$x=\gamma r_0 . \tag{12}$$

The theory should be applicable for core radii smaller than the spatial extent of the initial wave function $1/\gamma$; i.e., $\gamma r_0<1$. The A_3k^3 term in Eq. (9) is the Wigner term and the A_5k^5 term is the leading correction.

Photodetachment from a p orbital

The final state can be either an s wave or a d wave. The cross section σ is

$$\sigma=(8\pi\alpha/9)(m\omega k/\hbar)(R_{sp}^2+2R_{dp}^2)\ , \tag{13}$$

where R_{sp} and R_{dp} are the matrix elements for outgoing s and d wave, respectively. R_{sp} and R_{dp} are given by the following expressions:

$$R_{sp}=\frac{N_1\exp(-\gamma r_0)}{\gamma k(r^2+k^2)^2}\{[k^3(1+\gamma r_0)+k\gamma^2(3+\gamma r_0)]\cos kr_0+[k^2\gamma^2 r_0+\gamma^3(2+\gamma r_0)]\sin kr_0\} \tag{14}$$

and

$$R_{dp}=-N_1\exp(-\gamma r_0)\{[k(3\gamma^4 r_0)+k^3(6\gamma^2+\gamma^3 r_0^2)+k^5(r_0+\gamma r_0^2)]\cos(kr_0)$$
$$+[-3\gamma^4+k^2(-6\gamma^2-\gamma^3 r_0+\gamma^4 r_0^2)+k^4(-3-3\gamma r_0+\gamma^2 r_0^2)]\sin(kr_0)\}/[\gamma k^3 r_0(k^2+\gamma^2)^2]\ , \tag{15}$$

where the normalization factor N_1 is given by

$$N_1^2=2\gamma x\exp(2x)/(x+2)\ . \tag{16}$$

Near threshold, as $k\to 0$, R_{sp}^2 has a constant term and a term quadratic in k, whereas R_{dp}^2 is negligible because its lowest-order term is quartic in k. The threshold behavior of σ is therefore

$$\sigma\to(8\pi\alpha/9)(m\omega/\hbar\gamma^4)[B_1(k/\gamma)+B_3(k/\gamma)^3]\ , \tag{17}$$

where B_1 and B_3 are given by

$$B_1=2x(x^2+3x+3)^2/(x+2) \tag{18}$$

and

$$B_3=-2x(3x+6)^{-1}(x^2+3x+3)$$
$$\times(x^4+5x^3+15x^2+30x+30)\ . \tag{19}$$

The B_1k term in Eq. (17) is the Wigner term and the B_3k^3 term is the leading correction.

Photodetachment from a d orbital

The total cross section σ is given by

$$\sigma=(8\pi/5)\alpha(m\omega k/\hbar)(2R_{pd}^2/3+R_{fd}^2)\ , \tag{20}$$

where R_{pd} and R_{fd} represent the radial integrals in the matrix elements giving p-wave and f-wave detachment, respectively. After a considerable amount of algebra, R_{pd} and R_{fd} can be expressed as

$$R_{pd}=\frac{N_2\gamma\exp(-\gamma r_0)}{\gamma^2+k^2}\left[\sin(kr_0)\left[\frac{3(k^2+\gamma^2)}{k^2\gamma^3 r_0}+\frac{3k^4+6k^2\gamma^2+\gamma^4}{k^2\gamma^2(k^2+\gamma^2)}+\frac{r_0}{\gamma}\right]\right.$$
$$\left.-\cos(kr_0)\left[\frac{r_0}{k}+\frac{3\gamma^2+k^2}{k\gamma(k^2+\gamma^2)}\right]\right]\ , \tag{21}$$

and

$$R_{fd}=N_2\gamma\exp(-\gamma r_0)\left[\sin(kr_0)\left[\frac{15(1+\gamma r_0)}{k^4\gamma^3 r_0}-\frac{3}{k^2\gamma^3 r_0}-\frac{(3k^2+2\gamma^2)(k^2+3\gamma^2)}{k^2\gamma^2(k^2+\gamma^2)^2}\right]\right.$$
$$\left.-\cos(kr_0)\left[\frac{15(1+kr_0)}{k^3\gamma^3 r_0^2}+\frac{4k^2+2\gamma^2}{k\gamma(k^2+\gamma^2)^2}-\frac{r_0}{k(k^2+\gamma^2)}\right]\right]\ . \tag{22}$$

The normalization constant N_2 is

$$N_2=\exp(x)[(2\gamma x^3)/(x^3+6x^2+12x+6x)]^{1/2}\ . \tag{23}$$

As $k\to 0$, the leading term in R_{fd} is cubic in k, giving a contribution $\sim k^7$ to σ, which is negligible. The resulting expression for the total cross section is

$$\sigma\to(16\pi\alpha/15)(m\omega/\hbar)N_2^2\exp(-2x)\gamma^{-7}r_0^{-2}$$
$$\times[C_3(k/\gamma)^3+C_5(k/\gamma)^5]\ , \tag{24}$$

where

$$C_3=(x^4/3+2x^3+5x^2+5x)^2\ , \tag{25}$$

and

$$C_5=(2x^4/3+4x^3+10x^2+10x)$$
$$\times(-x^6/30-4x^5/15-7x^4/6-3x^3/2-7x^2-7x)\ . \tag{26}$$

The C_3k^3 term in Eq. (24) is the Wigner term and the C_5k^5 term is the leading correction.

RESULTS

Analytical expressions were derived above for the Wigner term and the leading correction within the ZCC approximation. The expressions were coded in FORTRAN-77 and evaluated on a SUN 3/160 workstation. Three expressions are compared: The Wigner term alone, the Wigner term with the leading correction, and the exact ZCC expression. Figures 1(a)–1(c) show the results for photodetachment from an s, p, and d orbital, respectively. For simplicity the atom has an electron affinity E of 1.0 eV and a core radius r_0 of 1.0 Å. The consequences of varying r_0 and E are discussed below.

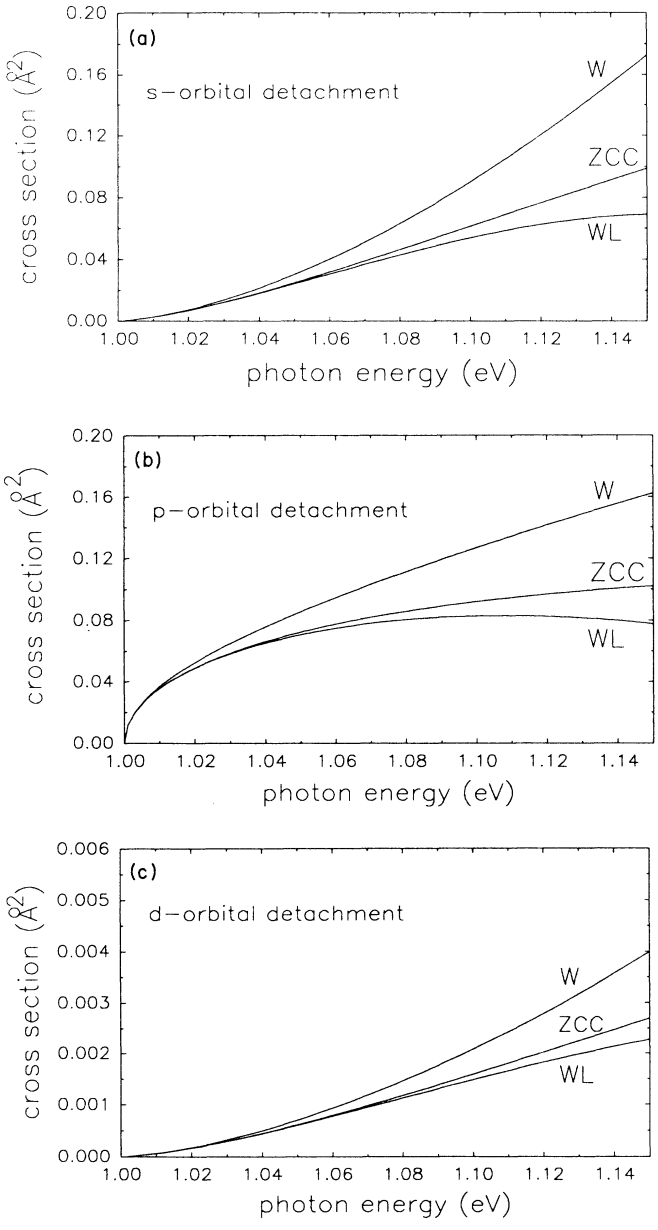

FIG. 1. Calculated photodetachment cross section for photodetachment. The core radius is 1.0 Å and the electron affinity is 1.0 eV. ZCC is the zero-core-contribution approximation, W is the Wigner term, and the WL is the sum of the Wigner term and the leading correction. (a) shows detachment from an s orbital, (b) from a p orbital, and (c) from a d orbital.

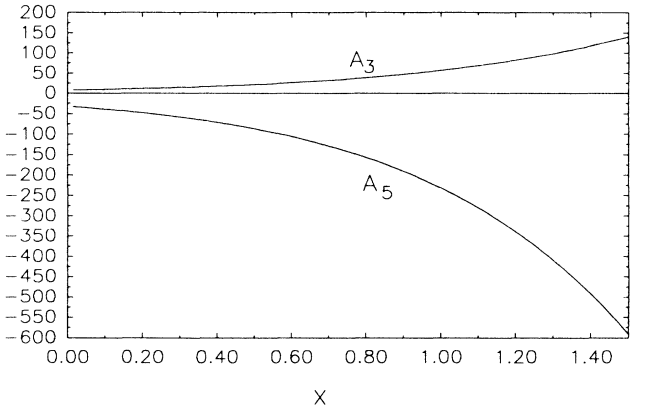

FIG. 2. Coefficients of the Wigner term and leading correction, for photodetachment from an s orbital, as function of $x \equiv \gamma r_0$. See Eqs. (10) and (11).

Figure 1 demonstrates several things: First, the ZCC approximation obeys the Wigner law at threshold: The curves converge at threshold. Second, there are significant deviations from the Wigner law within 50–100 meV of threshold. Third, the inclusion of the leading correction results in an important improvement in the range and accuracy of the Wigner law. Fourth, the accuracy of the Wigner law may be estimated by using the size of the leading correction: because the leading correction slightly overcompensates, the leading correction is an upper bound for the accuracy of the Wigner term.

The parameter $x \equiv \gamma r_0$ is a natural scaling parameter for the problem. Figures 2–4 display the coefficients as a function of x. The threshold coefficients may be derived for any atomic ion using these curves.

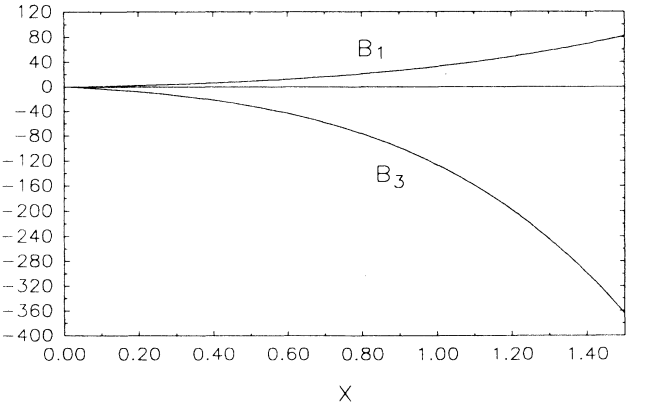

FIG. 3. Coefficients of the Wigner term and leading correction, for photodetachment from a p orbital, as a function of $x \equiv \gamma r_0$. See Eqs. (18) and (19).

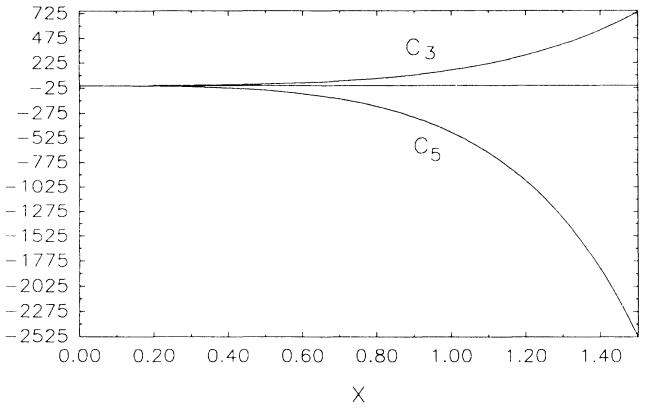

FIG. 4. Coefficients of the Wigner term and leading correction, for photodetachment from a d orbital, as a function of $x \equiv \gamma r_0$. See Eqs. (25) and (26).

The cross sections in Fig. 1 apply for an electron affinity E of 1.0 eV and a core radius r_0 of 1.0 Å. Figures 5(a)–5(c) display the results of varying r_0 for photodetachment from an s, p, and d orbital, respectively. Calculations have been performed for values of r_0 of 1.0 and 2.0 Å. The ZCC cross section and both approximations (Wigner, Wigner with leading correction) all increase with r_0. Consequently, the cross sections have been normalized to the ZCC cross section. Apart from an overall normalization factor, the results are insensitive to r_0.

The final question is the scaling of the results with the electron affinity E. The appropriate variable is the energy above threshold, normalized to the electron affinity. We denote this is as z,

$$z=(\hbar\omega-E)/E \ . \tag{27}$$

From Eqs. (2) and (8), $z=k^2/\gamma^2$. We have performed calculations of the cross section for photodetachment from s, p, and d orbitals, for E of 1.0 and 2.0 eV, with $r_0=1.0$ Å in all cases. The two cases have, of course, the same value of k from Eq. (2), and x differing by a factor of $\sqrt{2}$ from Eqs. (8) and (12). As in Fig. 5, we have normalized to the ZCC cross section, plotting W/ZCC and WL/ZCC as a function of z. The curves for $E=1.0$ and 2.0 eV fall on top of one another, differing by typically 0.1% at 50 meV above threshold. Such curves would be unresolved in journal artwork, and are therefore omitted.

Comparison with other theoretical work

Branscomb *et al.*[16] considered a square-well potential and derived threshold behavior of the cross section

$$\sigma \rightarrow k^{2l+1}(c_0+c_2k^2+\cdots) \ . \tag{28}$$

However, they did not explicitly evaluate any of the coefficients.

O'Malley[17] investigated the effect of long-range forces on the cross section near threshold. He considered a case in which the receding electron induces an electric dipole moment $\mathbf{p}=\alpha_p\mathbf{E}$ in the neutral core, where α_p is the polarizability of the neutral. Because $E=qr^{-2}$, we obtain a potential $V_{\rm pol}=-q\alpha_p r^{-4}$. The resulting behavior of the cross section near threshold is

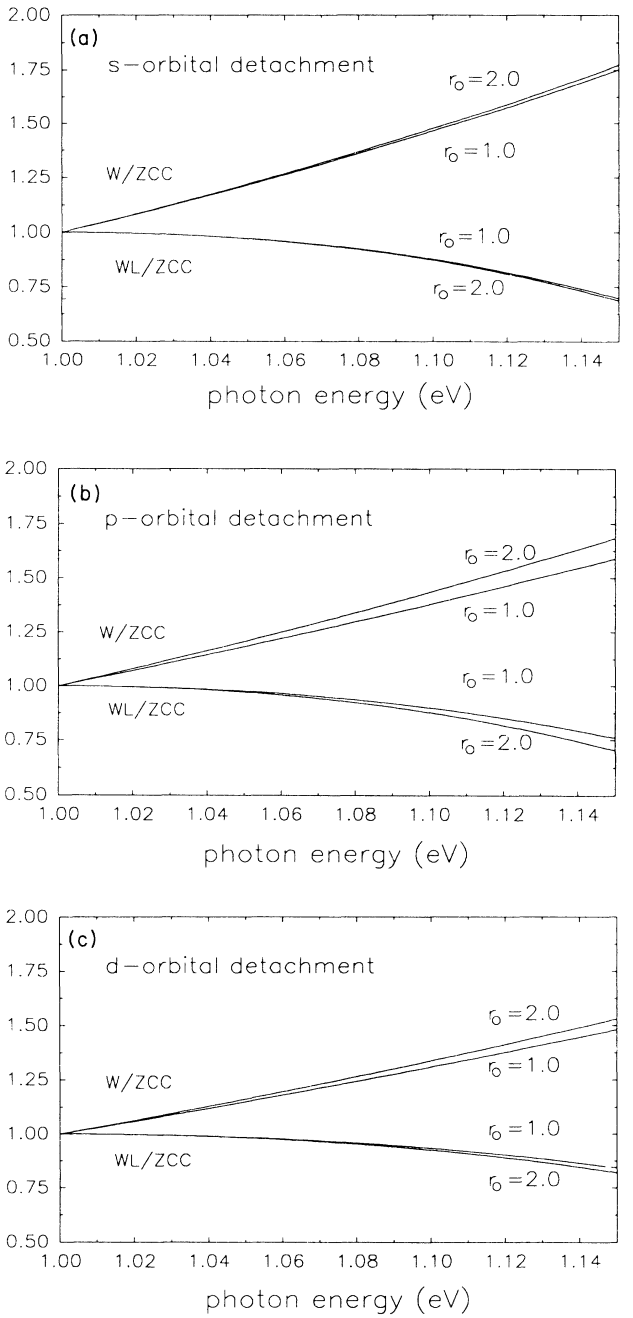

FIG. 5. Effect of varying r_0 from 1.0 to 2.0 Å on the photodetachment cross section. Shown are the Wigner term (W) and the Wigner term with the leading correction (WL). The cross sections have been normalized to the ZCC cross section. (a) shows detachment from an s orbital, (b) from a p orbital, and (c) from a d orbital.

$$\sigma(k)\rightarrow k^{2l+1}\{1-4\alpha_p k^2\ln(ka_0)/[a_0(2l+3)(2l+1)(2l-1)]+O(k^2)\}\ . \tag{29}$$

In the curly brackets { }, the first term signifies the Wigner term. The middle term, proportional to $k^2\ln k$, arises from the r^{-4} potential, and a_0 is the Bohr radius. (In Ref. 17, the polarization term appeared with the incorrect sign. The correct sign is used here.) The last term $O(k^2)$ is present for short-range potentials as well. The coefficient of the last term was not derived.

In the ZCC approximation, the potential is assumed to vanish outside $r=r_0$. Thus O'Malley's polarization term results from the inclusion of the r^{-4} potential, which is neglected in the ZCC approximation. In the limit of small polarizability of the neutral, $\alpha_p\rightarrow 0$, O'Malley's result passes over into our result.

As a practical matter, because $\ln k$ varies so slowly, the two terms, $k^2\ln k$ and k^2, have almost the same k dependence. It is very unlikely that experimental measurements will span a wide enough dynamic range of k with a large enough signal-to-noise ratio to distinguish reliably between the two k dependences. Therefore, a consistent treatment that goes beyond the Wigner term must include both the polarization term and the leading correction term.

Limitations of the model

If the neutral has a nonvanishing electric quadrupole moment, there will be an additional term in the threshold law, also derived by O'Malley. The numerical coefficient multiplying the quadrupole term is small enough that it may often be neglected, which we do here.

An apparent exception to the Wigner law was discovered theoretically by Engelking[18] to explain anomalous threshold behavior discovered experimentally[19] by Lineberger and co-workers in OH^-; namely, a cross section that obeys a power law $\sigma\sim k^x$, with $x<1$. In OH^-, the departing electron leaves behind a polar molecule with internal angular momentum along the dipole axis. Under these circumstances, there is an anisotropic potential between the departing electron and the rotating dipole, $V(r)=\boldsymbol{\mu}\cdot\hat{\mathbf{r}}/2r^2$. Since this potential has the same inverse square dependence as the centrifugal barrier, the two terms will have the same relative size at all distances r. Engelking realized that the assumptions underlying the Wigner law are violated in this case, because the centrifugal potential is not the dominant potential at large r. The Wigner law therefore does not hold. What is needed instead is a close-coupling calculation. Such a calculation has been carried out for OH^- by Engelking and Herrick.[20,21] In the present paper, it is assumed that it is the Wigner law that applies, and not the "Engelking exception."

CONCLUSIONS

Simple expressions have been derived which can be used to estimate the range and accuracy of the Wigner law. These expressions may be valuable for extrapolation of experimental data in order to extract electron affinities. The typical procedure is to assume a Wigner power law. As Mead and Lineberger remark,[22] one justifiable procedure involves fitting some theoretical form (i.e., the Wigner law) to data sets of successively smaller energy range. Sufficiently close to threshold, the constants obtained should be invariant to the range of the data. The expressions here can be used to improve the extrapolation procedure. Because Eqs. (8) and (12) involve the electron affinity, an iterative technique is indicated, converging when a self-consistent solution is obtained. The process would undoubtedly converge rapidly, because relatively small corrections to the electron affinity are involved. Threshold photodetachment is, of course, not the only way to obtain electron affinities: Photoelectron spectrometry has produced the majority of measured electron affinities.[23] However, threshold photodetachment is the most precise technique: The standard calibrating ion for photoelectron spectrometry is O^-, and the latest determination of its electron affinity by Neumark *et al.*[24] used later threshold photodetachment.

For simplicity, this paper has concentrated on atomic systems. However, as discussed above, the ZCC model has already been applied the molecular systems, and many researchers[25] have applied the Wigner threshold law to molecules. The formalism can therefore be extended to molecular systems as well.

ACKNOWLEDGMENTS

Assistance by Dave Draggon in programming and performing the plotting is gratefully acknowledged. Support for this work was provided by the National Science Foundation under Grant Nos. PHY87-19090 and PHY89-03387, by the U.S. Air Force Astronautics Laboratory under Contract No. F04611-87-K-0211, and by the NASA Planetary Atmospheres Program under Grant No. NAGW-1585.

[1]R. Wildt, Astrophys. J. **89**, 295 (1939); **93**, 47 (1941).
[2]H. S. W. Massey, *Negative Ions*, 3rd ed. (Cambridge University Press, London, 1976).
[3]The recoil energy of the neutral, a very small correction, has been neglected.
[4]Eugene P. Wigner, Phys. Rev. **73**, 1002 (1948).
[5]In Wigner's original work it is $A'[k/(\hbar\omega+k)]^{2l+1}$, but this is usually reduced to its leading term.
[6]R. M. Stehman and S. B. Woo, Phys. Rev. A **20**, 281 (1979).
[7]H. A. Bethe and L. Longmire, Phys. Rev. **77**, 647 (1950).
[8]T. Ohmura and H. Ohmura, Phys. Rev. **118**, 154 (1960).
[9]J. T. Broad and W. P. Reinhardt, Phys. Rev. A **14**, 2159 (1976).
[10]J. Simons and K. D. Jordan, Chem. Rev. **87**, 535 (1987); J. V. Ortiz, Int. J. Quantum Chem. **21**, 469 (1987).
[11]R. M. Stehman and S. B. Woo, Phys. Rev. A **23**, 2866 (1981).
[12]W. B. Clodius, R. M. Stehman, and S. B. Woo, Phys. Rev. A

27, 333 (1983).
[13]W. B. Clodius, R. M. Stehman, and S. B. Woo, Phys. Rev. A **28**, 760 (1983).
[14]Kent M. Ervin, Joe Ho, and W. Carl Lineberger, J. Phys. Chem. **92**, 5405 (1988).
[15]S. B. Woo, E. M. Helmy, P. Mauk, and A. Paszek, Phys. Rev. A **24**, 1380 (1981).
[16]L. M. Branscomb, D. S. Burch, S. J. Smith, and S. Geltman, Phys. Rev. **111**, 504 (1958).
[17]Thomas F. O'Malley, Phys. Rev. **137**, A1668 (1965).
[18]Paul C. Engelking, Phys. Rev. A **26**, 740 (1982).
[19]P. A. Schulz, R. D. Mead, P. L. Jones, and W. C. Lineberger, J. Chem. Phys. **77**, 1153 (1982).
[20]David R. Herrick and Paul C. Engelking, Phys. Rev. A **29**, 2421 (1984).
[21]P. C. Engelking and D. R. Herrick, Phys. Rev. A **29**, 2425 (1984).
[22]Roy D. Mead and W. Carl Lineberger, *Electron-Molecule Collisions and Photoionization Processes* edited by V. McKoy, H. Suzuki, K. Takayanagi and S. Trajmar (Verlag Chemie, Deerfield Becah, FL 1983), p. 1.
[23]H. Hotop and W. C. Lineberger, J. Phys. Chem. Ref. Data **14**, 731 (1985).
[24]D. M. Neumark, K. R. Lykke, T. Andersen, and W. C. Lineberger, Phys. Rev. A **32**, 1890 (1985).
[25]See, for example, K. J. Reed, A. H. Zimmerman, H. C. Andersen, and J. I. Brauman, J. Chem. Phys. **64**, 1368 (1976).