from 24.7–675.0 and 5.3–103.0 Torr, respectively, for neon-hydrogen and helium-hydrogen mixtures. However, at the higher pressures (>150 Torr for neon-hydrogen mixtures, >70 Torr for helium-hydrogen mixtures) an apparent violation of Paschen's law was observed; thus for constant p_0x values the breakdown potential increased significantly over its value at lower pressures.

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Final-State Effects in Atomic Processes: Photodetachment*†

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A formalism which corrects Born-approximation amplitudes for final-state effects in atomic scattering and detachment processes is developed from use of Jost function enhancement factors. The method leads to soluble integral equations of the Omnès type. Application is made to the photodetachment of negative oxygen ions ($\gamma+O^-\rightarrow O+e^-$), yielding an improved fit to recent experimental data. The theory is compared with earlier work of Klein and Brueckner.

I. INTRODUCTION

FINAL-state effects in atomic reactions may exert considerable influence on observed spectra. As a model we shall consider the effects of the interaction between the ejected electron and the residual atom in the photodetachment process $\gamma+O^-\rightarrow O+e^-$. Klein and Brueckner[1] studied this process using asymptotic phase-shifted continuum wave functions. Since their work, there has been considerable development in the theory of final-state interactions evolving from the early work of Watson,[2] and exploiting the analytic structure of scattering amplitudes and Jost functions. Although most of the formalism was developed for high-energy physics, it is equally applicable to other domains. Apart from the work of Gerjuoy and Krall[3] stemming from the investigations of Klein and Zemach,[4] little use of these recent methods has been made in atomic physics. The adaptation presented here is designed to provide maximum computational ease for low-energy processes.

Appendix A contains a brief review of the Jost function formalism and its relation to final-state interactions. In Sec. II the final-state corrections to the Born amplitude are shown to yield soluble integral equations of the Omnès type. Section III presents the solutions which are based on plausible assumptions for the analytic structure of the amplitude. An alternative method facilitates computation in some cases. The photodetachment process is formulated in Sec. IV as an example. Results of a sample numerical calculation are contained in Sec. V together with a comparison of the methods with those of Klein and Brueckner. Appendix B discusses alternate forms of the Born amplitude which may improve the accuracy of the formalism.

II. FINAL-STATE CORRECTIONS TO BORN AMPLITUDES

For processes such as detachment of a bound system, the scattering amplitude is given by

$$T=\int d^3r\psi_l^{-*}(q,r)V(r,k)\phi_B(r)\,, \tag{1}$$

where ψ_l^- is the continuum wave function for the detached system with momentum q, ϕ_B the bound state, and V the interaction depending parametrically on the incident momentum k. Energy conservation relates q, k, and the binding energy. Generally, the integral (1) is terminated at small r by the spatial extent of ϕ_B, or of the interaction V (as will be the case for large momentum transfers). In this case, the relation (A4) permits the substitution

$$\psi_l(q,r)\approx f_l^{-1}(-q)\psi_l^{(0)}(q,r) \tag{2}$$

which gives us the final-state enhancement

$$T(q)=f_l^{-1}(-q)T^B(q)\,, \tag{3}$$

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† Portions of this work were reported in University of California Lawrence Radiation Laboratory Report UCRL 10762 (1963), and in Bull. Am. Phys. Soc. **8**, 621 (1963).

[1] M. M. Klein and K. A. Brueckner, Phys. Rev. **111**, 1115 (1958).

[2] K. M. Watson, Phys. Rev. **88**, 1163 (1952).

[3] E. Gerjuoy and N. A. Krall, Phys. Rev. **119**, 705 (1960); **127**, 2105 (1962).

[4] A. Klein and C. Zemach, Ann. Phys. (N. Y.) **7**, 365 (1959).

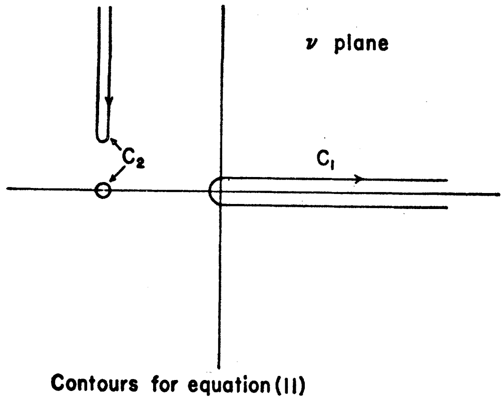

FIG. 1. Contours for Eq. (11).

where the Born amplitude is given by

$$T^B(q)=\int d^3r\psi_l^{(0)*}V\phi_B\,. \tag{4}$$

As explained in Appendix A, $f_l^{-1}(-q)$ as an enhancement is the analog of the wave function of the interacting final-state pair normalized to unity for no interaction. The asymptotic condition (A6) gives the expected limit

$$T(q)_{q\to\infty}\to T^B(q)\,. \tag{5}$$

The analytic structure in the energy $\nu(\nu=q^2)$ for the difference $T(\nu)-T^B(\nu)$ will be as follows: (1) Simple poles from the zeros of $D_l(\nu)=f_l(-q)$ which correspond to bound states of energy ν_i on the negative real axis with residue $\Gamma_i(\Gamma_i$ is related to the binding of the state $\phi_B)$,[5] (2) a branch cut on the positive real axis with discontinuity given by that of D^{-1}[cf. (A5)],

$$[D^{-1}]=2ie^{-i\delta(\nu)}\sin\delta(\nu)D(\nu)\,, \tag{6}$$

and (3) possible cuts arising from $T-T^B$. We shall assume these to be unimportant in the physical region ($\nu>0$, real). This last assumption may be studied by using (A8) in (1); since $\phi_l(q,r)$ is an entire function of q, it facilitates examination of the difference $\phi_l(q,r)-j_l(kr)$.

With this analytic structure, Cauchy's theorem then gives the integral equation for $T-T^B$ (using the reality of T^B):

$$T(\nu)=T^B(\nu)+\sum_i\frac{\Gamma i}{\nu-\nu_i}+\frac{1}{\pi}\times\int_0^\infty d\nu'\frac{e^{-i\delta(\nu')}\sin\delta(\nu')T(\nu')}{\nu'-\nu-i\epsilon}\,. \tag{7}$$

The subscript l denoting the relevant angular momentum is understood for all the functions appearing in (7).

[5] M. Goldberger and K. M. Watson, *Collision Theory* (J. Wiley & Sons, Inc., New York, 1964), Chap. IX.

III. SOLUTIONS TO THE EQUATION

Integral equations similar to (7) occur frequently in final state theory; their solution, studied by Omnès[6] and Muskhelishvili[7] is of the form

$$T(\nu)=T^B(\nu)+\sum_i\frac{\Gamma_i}{\nu-\nu_i}e^{u(\nu)-u(\nu_i)}+\frac{e^{u(\nu)}}{\pi}\times\int_0^\infty\frac{e^{-u(\nu')}\sin\delta(\nu')T^B(\nu')}{\nu'-\nu-i\epsilon}\,, \tag{8}$$

where

$$D(\nu)=e^{-u(\nu)},$$

and from (A5)

$$u(\nu)=\frac{1}{\pi}\int_0^\infty\frac{\delta(\nu')}{\nu'-\nu-i\epsilon}=\frac{P}{\pi}\int_0^\infty\frac{\delta(\nu')}{\nu'-\nu}+i\delta(\nu)=\rho(\nu)+i\delta(\nu)\,. \tag{9}$$

In (9), P denotes the principal part integration and δ is the scattering phase shift for the final-state particles in a state of definite angular momentum. The same solution is immediately obtained from the Chew-Mandelstam technique,[8] where T is assumed to be of the form N/D, with N and D real on the right and left real axes, respectively.

It may happen that T^B has especially simple branch cuts (or poles) which in general are in unphysical regions (in the ν plane) and do not overlap the right-hand cut of D. A dispersion relation for $D(\nu)T^B(\nu)$ would give (discontinuities are denoted by [ ])

$$T^B(\nu)D(\nu)=\frac{1}{2\pi i}\left\{\int_{C_1}d\nu'\frac{T^B(\nu')[D(\nu')]}{\nu'-\nu-i\epsilon}+\int_{C_2}\frac{[T^B(\nu')]D(\nu')}{\nu'-\nu-i\epsilon}\right\}, \tag{10}$$

where C_1 and C_2 surround the cuts (or poles) of D and T^B, respectively, as shown in Fig. 1. The first integrand is just the negative of that in (8), so an equivalent solution is, apart from the pole terms,

$$T(\nu)=\frac{e^{u(\nu)}}{2\pi i}\int_{C_2}\frac{[T^B(\nu')]e^{-u(\nu')}}{\nu'-\nu-i\epsilon}\,. \tag{11}$$

The form (11) has the advantage of involving $u(\nu')$ in unphysical regions, where from (9) it is seen to involve no principal part singularity, and is, in general, more rapidly convergent. When C_2 lies on the negative real axis, u is of the form

$$u(\nu)=\frac{1}{\pi}\int_0^\infty\frac{\delta(\nu')}{\nu'+\nu}d\nu'\,. \tag{12}$$

[6] R. Omnès, Nuovo Cimento 8, 316 (1958).

[7] N. I. Muskhelishvili, *Singular Integral Equations* (E. P. Noordhoff, Gronigen, Holland, 1953).

[8] G. Chew, *S-Matrix Theory of Strong Interactions* (W. A. Benjamin, Inc., New York, 1961).

In the next section some further computational advantages of (11) are discussed with examples.

IV. CALCULATIONAL APPROXIMATIONS AND EXAMPLES

For reference, we consider two examples. First, a process the photodisintegration of a deuteron would have a Born amplitude of the form[5]

$$T^B \approx \int r^2 dr \frac{\sin qr}{qr} \frac{\sin kr}{kr} \frac{e^{-\alpha r}}{r}, \tag{13}$$

with cuts in q^2 running from $\pm(i\alpha \pm k)$ to $\pm(i\infty \pm k)$, which become more unphysical as the spatial extent of the bound state decreases. In this example, the cut structure is not especially simple and the forms (8) or (11) are of comparable difficulty for a computer calculation.

The second example is the s-wave amplitude for the photodetachment of O^- in the dipole approximation to be discussed in detail in Sec. V. The Born term is of the form

$$T^B \approx (3\lambda + \lambda^{-1}\nu)/(\nu + \lambda^2)^2. \tag{14}$$

Here, the only singularity is a double pole at $\nu = -\lambda^2$ on the negative real axis. Thus, the solution (11) is trivially evaluated and is obviously preferable to the form (8).

Because high-energy phase shifts are seldom known accurately, and because inelastic processes set in at relatively low energies for atomic scattering, it is important to carefully examine the integrals occurring in (8) and (9). As can be seen from (8), the solution is unaffected by subtractions in u of the form

$$u(\nu) = u(\nu_0) + \frac{\nu - \nu_0}{\pi} \int_0^\infty \frac{\delta(\nu')}{(\nu' - \nu_0)(\nu' - \nu - i\epsilon)}, \tag{15}$$

which de-emphasize high-energy behavior at the price of increased dependence on the accuracy of the phase shifts at the subtraction point(s). Again, the form (11) leaves (13) without singularities in the physical region.

For many low-energy atomic scattering processes, an effective range and scattering length approximation for the phase shift

$$k \cot\delta = (1/\alpha) + \tfrac{1}{2} r_0 k^2 \tag{16}$$

may be used which gives a closed form[9] for the integral u in (9).

$$f_l(-k) = D_l(\nu) = (k + i\beta^+)/(k + i\beta^-), \tag{17a}$$

where

$$\beta^{\pm} = (1/r_0)[\pm 1 + (1 + (2r_0/\alpha))^{1/2}]. \tag{17b}$$

[This can determine more simply by constructing the S matrix from (16) and using (A7) and (A8).]

For the solution (11) which involves unphysical values of ν', $u(\nu')$ may be slowly varying about by some average value $u(\nu_0)$, and the integral calculated in the form

$$\int \frac{d^3 r e^{u(\nu_0) - u(\nu)} [T^B(\nu')]}{\nu' - \nu - i\epsilon}. \tag{18}$$

[9] R. Jost and W. Kohn, Phys. Rev. 87, 988 (1952).

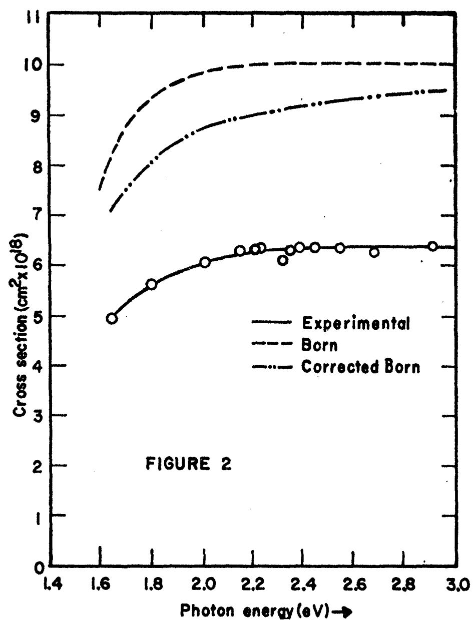

FIG. 2. Oxygen photodetachment cross sections.

It should be noted that the initial approximation (2) in Sec. II depends on a small r termination of the integral. Various forms for dipole matrix elements (length, velocity, acceleration), shown in Appendix B, give successively greater dependence on values of r near the origin.

V. PHOTODETACHMENT CALCULATION

The foregoing formalism is next applied to the photodetachment of negative oxygen ions. From Bates and Massey[10] the dipole matrix elements give

$$\sigma = \frac{8\pi}{3} \frac{mke^2\omega}{h^2 c} (M_s^2 + 2M_d^2),$$

$$M_s = \int_0^\infty u_s(r) u_{2p}(r) r^3 dr, \tag{19}$$

$$M_d = \int_0^\infty u_d(r) u_{2p}(r) r^3 dr,$$

where u_{2p} is the bound-state wave function; u_s and u_d are the $l=0$ and $l=2$ continuum functions. Since the dipole-matrix element emphasizes large r values, Klein and Brueckner[1] used the asymptotic form valid outside the force range,

$$u_l(r) = (1/kr) \sin(kr + \delta_l - l\pi/2) \tag{20}$$

[10] D. R. Bates and H. S. W. Massey, Trans. Roy. Soc. (London) A239, 269 (1943).

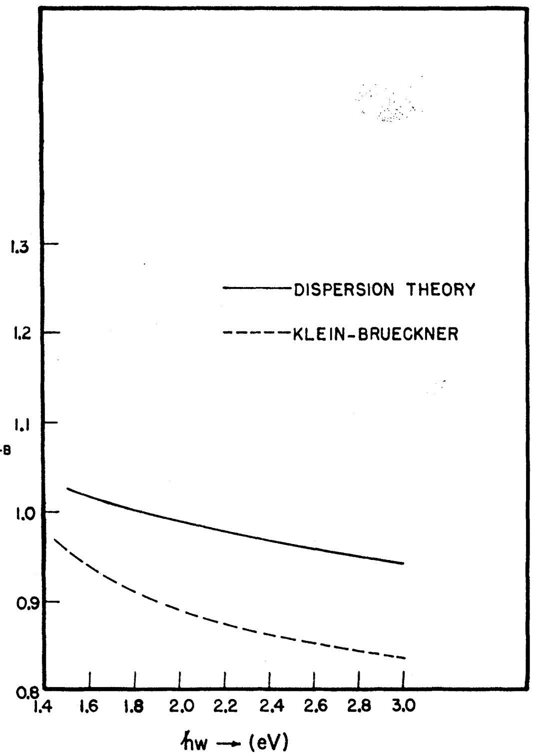

FIG. 3. Enhancement factors T/T^B of Eq. (22) versus photon energy.

together with the bound state

$$u_{2p}(r)=N(e^{-\lambda r}/r)[1+(1/\lambda r)]\,. \tag{21}$$

Since their work, the experimental situation has changed somewhat, the recent experiment photodetachment, given by Smith[11] is shown in Fig. 2, together with the Born approximation. The results of a sample calculation using Eq. (8) employing an effective range phase-shift parameterization is seen to correct the Born result towards the experimental curve. The effective range $r_0=2.7$ and scattering length $\alpha=-0.4$ (atomic units) used are in accord with the estimates of electron-oxygen scattering reported from experiment[11] and theory.[12]

The results are qualitatively similar to those of Klein and Brueckner: The final-state corrections modify the Born approximation toward the experimental data, but do not account for all the difference. As would be expected from a repulsive final-state phase shift,[5] the amplitude is decreased from its value with no interaction.

For this example it is interesting to explicitly exhibit the correction to the Born amplitude for the present formalism and that of Klein and Brueckner for the s-wave term (which dominates the calculation). From (19)–(21), with and without phase shift, and from evaluation of the residue of the double pole in (11) with the effective range term (16), we have

(a) Born approximation

$$T^B(\nu)=N(\nu+\lambda^2)^{-2}(3\lambda+\lambda^{-1}\nu)\,, \tag{22a}$$

(b) Klein-Brueckner

$$T^K(\nu)=T^B(\nu)\left[\cos\delta_s+\frac{2\lambda^2}{3\lambda+\lambda^{-1}\nu}\frac{\sin\delta_s}{k}\right], \tag{22b}$$

(c) dispersion relation

$$T(\nu)=T^B(\nu)\frac{D(-\lambda^2)}{D(\nu)}\left[1+\frac{2\lambda^2(\nu+\lambda^2)}{3\lambda^2+\nu}\frac{D'(-\lambda^2)}{D(-\lambda^2)}\right]. \tag{22c}$$

From (22c) and (9) it is seen that the amplitude bears the phase of the final-state interaction. This is an example of Watson's theorem[13,14] for final-state reaction processes. As a sample calculation of the results (22), we show in Fig. 3 the results for a reaction with typical parameters $\alpha=1.6$, $r=0.86$. An attractive interaction was used for this illustration because it is known that attractive final-state interactions have much greater sensitivity to energy than do repulsive interactions.[5,14] The binding 1.45 eV gives a value of $\lambda\,(\lambda^2=2mE_B/\hbar^2)$ of 0.0537 (atomic units). The results are as expected for an attractive interaction: The enhancement is greater for low energies.[2,5] The asymptotic limit (A6) shows that in (22c), the final-state effects affect the spectrum less at high energies.

A similar calculation for the photodetachment of H^-, a process of astrophysical interest, was inconclusive due to the extremely small relevant phase shifts and their present uncertain accuracy.[12]

CONCLUSIONS

The methods proposed for accommodating final-state interactions in atomic scattering and detachment processes derived from analytic properties of the relevant amplitudes, have been shown to yield integral equations which correct Born estimates when the final-state scattering phase shift is known. A sample calculation improves the agreement of the Born approximation with experiment.

ACKNOWLEDGMENTS

The author gratefully acknowledges the advice of Professor Kenneth M. Watson who suggested this study, and useful conversations with Dr. T. N. Truong and Dr. P. G. Burke concerning integral equations and atomic phase shifts, respectively.

[11] S. J. Smith, in *Proceedings of the Fourth International Conference on Ionization Phenomena in Gas, Uppsala, 1959*, edited by by N. R. Nilsson (North-Holland Publishing Company, Amsterdam, 1960), p. 219.

[12] P. G. Burke and H. M. Schey, Phys. Rev. **126**, 147 (1962).

[13] K. M. Watson, Phys. Rev. **95**, 228 (1954).

[14] J. Gillispie, *Final State Interactions* [Holden-Day, Inc., San Francisco, 1964 (to be published)].

APPENDIX A: JOST FUNCTIONS AND ENHANCEMENT FACTORS

Aspects of Jost functions relevant to final-state theory are briefly reviewed here. For a complete development the reader is referred to the review article of Newton[15] whose notation we follow. The Jost function[9,16,14] is defined as the limit

$$f_l(k)=\lim_{r\to 0}\frac{(kr)^l}{(2l-1)!!}f_l(k,r) \qquad \text{(A1)}$$

of the solution to the radial Schrödinger equation

$$\left[-\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)}{r^2}-k^2\right]\psi_l(k,r)=0\,, \qquad \text{(A2)}$$

with boundary condition

$$\lim_{r\to\infty} e^{ikr}f_l(k,r)=i^l. \qquad \text{(A3)}$$

The property of these functions most useful for final-states theory is expressed by the limit of the "physical" solutions

$$\frac{|\psi_l(k,r)|^2}{|\psi_l^{(0)}(k,r)|^2}\xrightarrow[r\to 0]{}\frac{1}{|f_l(-k)|^2}\,, \qquad \text{(A4)}$$

which relates the relative probability of a particle pair being at small separation with and without interaction; $\psi_l^{(0)}$ is the solution to (A2) with $V(r)=0$. This is just the wave function enhancement of Watson.[2] The function $f_l(-k)$ is the Fredholm[16] determinant, or equivalently, the D function of N/D techniques.[8] Thus, it provides a natural bridge between potential theory and dispersion relation methods.

The function f may be determined from the potential [9,15] or from the phase shift through the integral representation

$$f_l(-k)=D_l(\nu)=\exp\left[-\frac{1}{\pi}\int_0^\infty\frac{\delta_l(\nu')}{\nu'-\nu-i\epsilon}\right] \qquad \text{(A5)}$$

for $\nu=k^2$. The asymptotic limit

$$\lim_{k\to\infty} f_l(k)\to 1 \qquad \text{(A6)}$$

shows, as would be expected, that final-state effects vanish at high energies.

The phase of $f_l(k)$ is seen to be that of the S matrix from the relations

$$S_l(k)=\exp[2i\delta_l(k)]=f_l(k)/f_l(-k) \qquad \text{(A7)}$$

and the analytic continuation

$$f_l^*(-k^*)=f_l(k)\,. \qquad \text{(A8)}$$

Finally, the Jost function relates the "physical" solution (incoming plane waves and outgoing spherical waves) and the solution regular at the origin

$$\lim_{r\to 0}\phi_l(k,r)=\frac{k^{l+1}}{(2l+1)!!} \qquad \text{(A9)}$$

through[15]

$$\psi_l^+(k,r)=[k^{l+1}/f_l(-k)]\phi_l(k,r)\,. \qquad \text{(A10)}$$

The function ϕ, as defined by (A9) is an entire function of k[16] and thus especially useful for studying analytic properties.

APPENDIX B: DIPOLE MATRIX ELEMENTS

For dipole matrix elements, several forms equivalent for exact wave functions give emphasis on different regions of the amplitude integrations. The article of Geltman[17] contains a more complete discussion and further references.

Three forms, length, velocity, and acceleration give successively increased emphasis on small values of r in the wave functions as seen from the typical absorption coefficients.

$$\sigma_L=C_Lk(k^2+2I)\left|\int\psi_F{}^*z\phi_B d^3r\right|^2, \qquad \text{(B1)}$$

$$\sigma_V=C_Vk(k^2+2I)^{-1}\left|\int\psi_F{}^*(\partial/\partial z)\phi_B d^3r\right|^2, \qquad \text{(B2)}$$

$$\sigma_A=C_Ak(k^2+2I)^{-3}\left|\psi_F{}^*(z/r^3)\phi_B d^3r\right|^2, \qquad \text{(B3)}$$

where I is the ionization energy, ψ_F the free final state of momentum k, and ψ_B the bound state.

Generally, the length form (B1) enhances the validity of asymptotic approximations such as (26) of Klein and Brueckner, while velocity and acceleration forms enhance small r approximations such as (2). In our example of Sec. V, it was seen that for the parameters used the two approximations gave roughly equivalent results.

[15] R. Newton, J. Math. Phys. **1**, 319 (1960).
[16] R. Jost and A. Pais, Phys. Rev. **82**, 840 (1951).
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