THE VALIDITY OF THE SEMICLASSICAL METHOD FOR THE COUPLED CHANNEL ATOMIC SCATTERING PROBLEM †

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Abstract

The S-matrix elements for the two-channel atomic scattering system are not smoothly varying functions; hence some justification must be given for the application of the stationary phase approximation to the evaluation of scattering amplitudes for this system. For a specific example, we show that the contribution to the amplitudes from the region of rapid variation is negligible compared to the stationary phase value, since the region of rapid variation is small and the phases vary sufficiently slowly. The semiclassical interpretation of the oscillations in the elastic and inelastic cross sections as the "interference" between two classical trajectories is therefore a valid one.

I. INTRODUCTION

It has been convincingly shown[1] for a wide range of energies and the range of potentials commonly found in atomic scattering problems that the JWKB approximation is an excellent approximation to the S-matrix phase shifts. In the JWKB approximation each quantum mechanical phase shift $\delta(\ell,E)$ is approximated by the equivalent classical phase shift[2,3] $\Delta(\ell,E)$. The one-channel scattering amplitude $f(\theta,E)$ is then expressed as

$$f(\theta E) = (2ik)^{-1} \sum_{\ell} (2\ell + 1)(e^{2i\Delta(\ell,E)} - 1)\, P_{\ell}(\cos\theta) \equiv \sum_{\ell} A(\ell,\theta,E)$$

and the differential cross section as

$$\sigma(\theta,E) = \left| f(\theta,E) \right|^2 = \sum_{\ell} \left| A(\ell,\theta,E) \right|^2 + \text{interference terms.}$$

The cross section contains an infinite number of interference terms of which usually only a few are important. Modern computational techniques[1] enable us to calculate $f(\theta,E)$ and hence $\sigma(\theta,E)$ explicitly, given the phase shifts $\Delta(\ell,E)$. However, to obtain a physical picture of the scattering process, it is useful to approximate the scattering amplitude $f(\theta,E)$ by its stationary phase value, as essentially the contribution of one partial wave. The attractiveness of the full semiclassical treatment--JWKB approximation together with the stationary phase approximation--resides in the fact that the differential cross section considered as an integral over all trajectories[4] derives solely from the classical Newtonian trajectory. Quantum mechanical effects only occur at infinities and discontinuities of this classical cross section,[3] where the simple stationary phase approximation breaks down.

In the full semiclassical treatment we will say that the differential cross section derives from the classical trajectory. In more complicated situations, where there is more than one channel open for scattering, we can often talk of the quantum mechanical interference of these classical terms. For instance, in He^+ - He scattering[1] the scattering amplitude can be well approximated by a sum of two terms, one derived from the gerade trajectory, the other from the ungerade trajectory. The oscillations in the differential cross section are simply the result of the "interference" of these two trajectories. But this is a trivial case of two-channel scattering, since the two channels are effectively uncoupled. A much more interesting system is the inelastic He^+ - He scattering system. Mott and Massey[5] have argued persuasively that we can again analyze the cross sections in terms of the semiclassical picture, as the quantum mechanical interference of terms derived from classical trajectories. It is the purpose of this paper to examine whether, in fact, this picture is a useful and reliable picture of the dynamics of the process.

In section II we examine the question of how smoothly varying the integrand must be in order to apply the stationary phase method to the evaluation of an integral. In section III we consider a specific two-channel system and determine the S-matrix elements in a form that can readily be interpreted in terms of the semiclassical picture. These elements are not smoothly varying and consequently we examine how large the contribution from the region of rapid variation is compared to the stationary phase evaluation of the amplitude, ignoring the rapid change in the integrand. We find for a wide range of angles that this contribution is small because the region of variation is small and the phases are slowly varying. This latter fact implies that the stationary phase value is large. For more rapidly varying phases it is conceivable that the two magnitudes are comparable in size.

Following Green,[6] we use the Stueckelberg[7] solution for angular momentum (ℓ) much less than ℓ_c, where ℓ_c is the angular momentum corresponding to the coincidence of classical turning points and the crossing point for the two-channel potentials. For ℓ in the neighborhood of ℓ_c we solve a simple model in section IV and match the solution for this model with the Stueckelberg solution for $\ell < \ell_c$. This model in fact illustrates previous criticism [8,9] of the Stueckelberg solution. We find that matching requires that we amend the Stueckelberg phase τ by the addition of a phase whose magnitude depends on the details of the coupling potential. Further, the smoothly varying probability coefficients of Stueckelberg's solution turn out to be oscillatory in our model.

II. THE MULTICHANNEL S-MATRIX

We wish to calculate the elastic and inelastic differential cross sections for an n-channel, two-body nonrelativistic quantum mechanical system. Denoting the S-matrix at total energy E and total angular momentum ℓ by $S_{ij}(\ell,E)$, where $i,j = 1,\ldots,n$, we determine the scattering amplitudes[5] as

$$f_{ij}(\theta) = [2i(k_i k_j)^{1/2}]^{-1} \sum_{\ell} (2\ell + 1)(S_{ij} - \delta_{ij})P_{\ell}(\theta). \qquad (1)$$

For the one channel case, approximation techniques [2,3] have been evolved to reduce the summation to a single term, a process that essentially reduces the quantum mechanical calculation to a classical calculation. This semiclassical method involves making the following two approximations:

i) $P_{\ell}(\theta) \sim \left[\frac{2}{\ell\pi \sin\theta}\right]^{1/2} \sin\left[(\ell + \tfrac{1}{2})\theta + \frac{\pi}{4}\right]$ when $\sin\theta > \ell^{-1}$.

ii) The summation over ℓ is replaced by an integral.

Eq. (1) then becomes

$$f(\theta) \sim \left[\frac{2}{\pi \sin \theta}\right]^{1/2} (-4k)^{-1} \int_0^\infty d\ell\, (2\ell + 1)\, \ell^{-1/2} (e^{2i\delta(\theta,E)} - 1)$$

$$\left[e^{i[(\ell + \frac{1}{2})\theta + \pi/4]} - e^{-i[(\ell+\frac{1}{2})\theta + \pi/4]} \right] \qquad (2)$$

where $\delta(\ell,E)$ is the one-channel phase shift. We define $N^{\pm}(\ell,E)$ $\equiv 2\delta(\ell,E) \pm [(\ell + \frac{1}{2})\theta + \pi/4]$. The validity of these approximations requires at least that many partial waves contribute and that the important contributions derive from partial waves with large values of ℓ.

The final step is provided by the stationary phase approximation, the conditions for the validity of which we now examine. We consider the integral $I_{\pm}^{(\lambda)} = \int_0^\infty d\ell\, e^{iN\pm(\ell,E)}\, \ell^{\lambda}$ with $\lambda = 0$. If $\frac{dN\pm(\ell,E)}{d\ell} = 0$ for $\ell = \ell_{oi}$ $(i = 1,\ldots,k)$, then the stationary phase approximation states that

$$I_{\pm}^{(o)} \simeq \sum_i [iN''_{\pm}(\ell_{oi},E)]^{-1/2} e^{iN_{\pm}(\ell_{oi},E)}\, (2\pi)^{1/2} \qquad (3)$$

(where the prime indicates differentiation with respect to ℓ), provided that the ℓ_{oi}'s are well separated.

Let us consider the integral where $N_-(\ell,E)$ is such that $k = 1$. We first make the transformation $y = N_-(\ell,E)$ and, defining $g(y) \equiv N'_-(\ell,E)$, we determine

$$I_-^{(o)} = \int_{y_{o1}}^\infty dy\, g^{-1}(y)\, e^{iy} + \int_{y_{oo}}^{y_{o1}} dy\, g^{-1}(y)\, e^{iy} \qquad (4)$$

the limit y_{oo}, y_{o1} being defined in Fig. 1, where $N_-(\ell,E)$ for a purely repulsive potential is plotted. As ℓ tends to infinity, then $N_-(\ell,E)$ tends to $\ell\theta$ and $g(y)$ to θ. In the neighborhood of ℓ_{o1} we could approximate $N(\ell,E)$ by a quadratic (denoted by the dotted curve in Fig. 1) and correspondingly we could approximate $g(y)$ by $(2N''_-(\ell,E)(y - y_{o1}))^{1/2}$ in the

neighborhood of y_{01}. The integral $I^{(0)}_{-}$ would be well approximated using the quadratic approximation for g(y) and with the range of integration extended from y_{00} to $-\infty$ if (i) ℓ_{01} is sufficiently large that there is little variation of the $|y - y_{01}|^{-1/2}$ curve over a period of 2π at y_{00}, and (ii) the maximum is not a too asymmetric or narrow peak in that the change in the difference between the $N_{-}(\ell,E)$ curve and the quadratic approximation to that curve over a period of 2π in y is small. We know that as ℓ tends to infinity the quadratic approximation to g(y) and g(y) itself have different limits; if this difference is spread sufficiently thinly over each period of oscillation, then it does not give an extra contribution to the integral. Thus if we denote the quadratic approximation to g(y) by $g_q(y)$, then for all y we must have the condition $|(g(y + 2\pi) - g(y) - g_q(y + 2\pi) + g_q(y))| \ll 1$.

In general we need to evaluate the integral $I^{f}_{-} \equiv \int_0^\infty d\ell\, e^{iN_{-}(\ell,E)} f(\ell)$. I^{f}_{-} is only approximated by $f(\ell_{01})\, I^{(0)}_{-}$ if the following conditions hold;

i) In the neighborhood of y_{01} we can approximate $\tilde{f}(y) \simeq f(\ell)$ by $\tilde{f}(y) = f(\ell_{01}) + f'(\ell_{01})[\tfrac{1}{2}N''(\ell_{01},E)]^{-1/2}$ $\tilde{f}(y) = f(\ell_{01}) + f'(\ell_{01})$ $[\tfrac{1}{2}N''(\ell_{01},E)]^{-1/2}(y - y_{01})^{1/2}$. For $\tilde{f}(y)$ to be slowly varying in the neighborhood of y_{01}, the condition $f(\ell_{01})(N''(\ell_{01},E))^{1/2} \gg f'(\ell_{01})$ must be satisfied.

ii) For y not in the immediate vicinity of y_{01}, the condition $|f(y + 2\pi) - f(y)| \ll 1$ must be satisfied.

We will say that the function $f(\ell)$ is slowly varying if these two conditions are satisfied. For example, if $f(\ell) = \ell^{1/2}$, then $I^{(1/2)} \simeq I^{(0)} \ell_{01}^{1/2}$ only if ℓ_{01} is large and the peak is not too broad.

If the phase shift $\delta(\ell,E)$ is such as to satisfy these conditions, then for k = 1 we can, to a good approximation, determine $f(\theta)$ as

$$f(\theta) \simeq \left[\frac{1}{\sin\theta}\right]^{1/2} (+k)^{-1} \ell_{01}^{1/2} [iN''_{-}(\ell_{01},E)]^{-1/2} e^{iN_{-}(\ell_{01},E)}. \qquad (5)$$

We now examine the question as to whether and under what conditions we can apply the stationary phase approximation to inelastic systems. For simplicity we consider a two-channel system. The S-matrix is unitary and by virtue of time reversal invariance is symmetric in the angular momentum basis. We can therefore represent the two-channel S-matrix as

$$S = \begin{pmatrix} \rho_1 e^{i\theta_1} & , & \rho_2 e^{\frac{1}{2}i[(\theta_1+\theta_2) + (2n+1)\pi]} \\ \rho_2 e^{\frac{1}{2}i[(\theta_1+\theta_2) + (2n+1)\pi]} & , & \rho_1 e^{i\theta_2} \end{pmatrix} \qquad (6)$$

where $\rho_{1,2}$ are real and $\rho_2^2 + \rho_1^2 = 1$. If ρ_1 and ρ_2 were slowly varying functions of ℓ in the sense described, then we could apply the stationary phase method directly to the phases $\theta_{1,2} \pm [(\ell + \frac{1}{2})\theta + \pi/4]$ and $\frac{1}{2}[(\theta_1 + \theta_2) + (2n + 1)\pi] \pm [(\ell + \frac{1}{2})\theta + \pi/4]$. In general, however, ρ_1 and ρ_2 are not slowly varying functions of ℓ. In fact the Stueckelberg[7] solution to the inelastic atomic scattering problem gives ρ_2 as an oscillatory function and ρ_1 oscillatory about a nonzero mean value. In any event this parameterization of the S-matrix is not appropriate for our purpose, since our aim is not necessarily to calculate cross sections--this can be done by computer without any semiclassical approximation--but to derive a formalism that will interpret the cross sections

in terms of essentially classical quantities. We look for a parametrization of the S-matrix that has an obvious physical interpretation.

III. PARAMETERIZATION OF THE S-MATRIX

We restrict our considerations to the inelastic atomic scattering problem where the diabatic channel potentials V_{11} and V_{22} are both repulsive and the coupling potential V_{12} is only different from zero in a small neighborhood of the crossing point of the two channel potentials. We first introduce notation to simplify the discussion:

i) $P_1(r)$ ($p_2(r)$) is the classical radial momentum in channel 1 (channel 2).

ii) $p_1^0(r)$ ($p_2^0(r)$) is the classical radial momentum for free motion in channel 1 (channel 2).

iii) r_{t1} (r_{t2}) is the classical turning point in channel 1 (channel 2).

iv) r_{t1}^0 (r_{t2}^0) is the turning point for free motion in channel 1 (channel 2).

v) $\bar{\delta}_{1,2} \equiv \lim_{R\to\infty} \int_{[r_c]}^{R} dr\, p_{1,2}(r) - \int_{r_{t1,t2}^0}^{R} p_{1,2}^0(r)\, dr$, where $[r_c]$ denotes the maximum of r_c and $r_{t1,t2}$.

vi) $\chi_{1,2} = \int_{r_{t1,t2}}^{r_c} p_{1,2}(r)\, dr$ or zero if $r_{t1,t2} \geq r_c$.

vii) $\chi = \chi_1 - \chi_2$ and $\delta_{1,2} = \bar{\delta}_{1,2} + \chi_{1,2}$.

viii) $k_{1,2} = p_{1,2}(\infty)$.

ix) $\ell_c = r_c(k_1^2 - V_{11}(r_c))^{1/2}$.

x) $v_\ell(r_c)$ is the radial velocity at $r = r_c$.

xi) $\gamma(\ell,E) \equiv [\frac{1}{2}V_{12}(r_c)]^2 \left[\left|\frac{d}{dr}(V_{11}(r_c) - V_{22}(r_c)\right| v_e(r_c)\right]^{-1}$ or zero if $\ell \geq \ell_c$.

xii) $\cos^2\varphi = \exp(-2\gamma(\ell,E))$.

If we are to take the Mott and Massey semiclassical picture of the inelastic process seriously, we would expect the differential cross sections to involve "interference" between the possible classical trajectories, and we would expect the phases $\bar{\delta}_{1,2} \pm \chi_{1,2}$ to occur naturally in the S-matrix.

Let us first look at the eigenphase parameterization of the S-matrix. Any symmetric unitary matrix (S) can be diagonalized by a real orthogonal matrix. This can be seen most simply by writing S as $\exp(2i\Delta)$ where Δ is a real symmetric matrix. The real orthogonal matrix that diagonalizes Δ also diagonalizes S. For the two-channel case we can parameterize the U and D matrices as follows:

$$U = \begin{pmatrix} \cos\epsilon & \sin\epsilon \\ -\sin\epsilon & \cos\epsilon \end{pmatrix} \quad , \quad D = \begin{pmatrix} e^{2i\delta_A} & 0 \\ 0 & e^{2i\delta_B} \end{pmatrix} \tag{7}$$

and

$$S = \begin{pmatrix} e^{2i\delta_A}\cos^2\epsilon + e^{2i\delta_B}\sin^2\epsilon & \sin\epsilon\cos\epsilon(e^{2i\delta_A} - e^{2i\delta_B}) \\ \sin\epsilon\cos\epsilon(e^{2i\delta_A} - e^{2i\delta_B}) & e^{2i\delta_A}\sin^2\epsilon + e^{2i\delta_B}\cos^2\epsilon \end{pmatrix} \tag{8}$$

In the weak coupling limit, S_{11} and S_{22} are the S_{11} and S_{22} elements for the uncoupled problem to lowest order in the coupling constant. S_{12}, to lowest order, involves the phases $\delta_A = \bar{\delta}_1 + \chi_1$, $\delta_B = \bar{\delta}_2 + \chi_2$, whereas the semiclassical picture would require phases $\frac{1}{2}(\bar{\delta}_1 + \bar{\delta}_2) + \chi_1$ and $\frac{1}{2}(\bar{\delta}_1 + \bar{\delta}_2) + \chi_2$, since these are the classical phases for the classical trajectories. There is, however, a parameterization that involves these latter phases:

$$S = \begin{pmatrix} [\cos^2\varphi e^{2i\chi_1} + \sin^2\varphi e^{2i\chi_2}]\, e^{2i\bar{\delta}_1} & , \sin\varphi\cos\varphi\, e^{i(\bar{\delta}_1+\bar{\delta}_2)}[e^{2i\chi_1} - e^{2i\chi_2}] \\ \sin\varphi\cos\varphi\, e^{i(\bar{\delta}_1+\bar{\delta}_2)}\,[e^{2i\chi_1} - e^{2i\chi_2}], & [\sin^2\varphi e^{2i\chi_1} + \cos^2\varphi e^{2i\chi_2}]\, e^{2i\bar{\delta}_2} \end{pmatrix} \quad (9)$$

Whatever the real functions $\bar{\delta}_1$, $\bar{\delta}_2$, χ_1, χ_2, φ may be, the S-matrix of (9) is unitary. The solution that Stueckelberg obtained for the two-channel atomic scattering process was expressed in the form of (9) with the functions $\bar{\delta}_1$, $\bar{\delta}_2$, χ_1, χ_2, φ given explicitly at the head of this section. The surprising feature of this solution is that the $\cos^2\varphi$, $\sin^2\varphi$ functions are not oscillatory. The form of these functions is given in Fig. 2. The solution is only claimed to be valid for ℓ not close to ℓ_c. The solution of the equations for ℓ close to ℓ_c has been given by Nykhovskii et al.[10] This solution smooths out the discontinuities of Stueckelberg's solution, but the $\sin\varphi\cos\varphi$ and $\sin^2\varphi$ functions still fall rapidly to zero for $\ell > \ell_c$. This is also borne out by the model solved in section IV and by the empirical inelastic differential cross section.[11]

We will examine the Stueckelberg solution with the following values for the potentials and parameters of the system:

i) $V_{11} = 10^4 \exp(-r)\, r^{-1}\ \mathring{A}^{-2}$.

ii) $V_{22} = (20.4 \times 10^4) \exp(-4r)\, r^{-1}\ \mathring{A}^{-2}$.

iii) $V_{12}(r_c) = 500\ \mathring{A}^{-2}$.

iv) $k_1 \simeq k_2 = 200\ \mathring{A}^{-1}$.

v) $r_c = 1\ \mathring{A}$.

For ℓ in the region of ℓ_c we match Stueckelberg's solution with the solution of the model of section IV. This matching necessitates changing the phase in the S-matrix from $\chi_2 - \chi_1$ to $\chi_2 - \chi_1 + \pi$.

We first examine the elastic differential cross section and to simplify the argument we introduce additional notation:

i) $\delta_{11} \equiv \delta_1$, $\delta_{12} \equiv \delta_1 + (\chi_2 - \chi_1 + \pi)$.

ii) $N_{11,12}(\ell,E,\theta) = 2\delta_{11,12} - ((\ell + \frac{1}{2})\theta + \pi/4)$.

iii) $\ell_{11,12}$ is the solution of the equation $\theta = 2\frac{d}{d\ell}\delta_{11,12}$.

iv) $\left|\frac{d^2N_{11}(\ell,E,\theta)}{d\ell^2}\right|^{-1}(2\ell_{11}+1) \equiv k_1^2\,[\sigma_1^1\ 2\sin\theta]$.

v) $\left|\frac{d^2N_{12}(\ell,E,\theta)}{d\ell^2}\right|^{-1}(2\ell_{12}+1) \equiv k_1^2\,[\sigma_1^2\ 2\sin\theta]$.

The smoothness of the functions $\cos^2\varphi$, $\sin^2\varphi$ is determined in relation to the phases N_{11}, N_{12} and we plot phase N_{11} in Fig. 2 for various values of θ. If indeed the functions were smooth as defined in Section I, then the stationary phase method would allow us to write the elastic differential cross section as[6]

$$\sigma_{11}(\theta,E) = \cos^4\varphi(\ell_{11},E)(\sigma_1^1) + \sin^4\varphi(\ell_{12},E)(\sigma_1^2) + 2\sin^2\varphi(\ell_{12},E)\cos^2\varphi(\ell_{11},E)$$

$$\cos(N_{11}(\ell_{11},E) - N_{12}(\ell_{12},E))\ (\sigma_1^1)^{1/2}(\sigma_1^2)^{1/2} \qquad (10)$$

with upper and lower envelopes given by

$$\sigma_{11}^{\pm}(\theta,E) = [\cos^2\varphi(\ell_{11},E)(\sigma_1^1)^{1/2} \pm \sin^2\varphi(\ell_{12},E)(\sigma_1^2)^{1/2}]^2 \qquad (11)$$

For our specific system the phases δ_{11}, δ_{12} are monotonically increasing and the $\cos^2\varphi$, $\sin^2\varphi$ functions are rapidly varying in the range $180 < \ell < 200$. Before we can justify the use of the stationary phase approximation, we must indicate why the contribution to the amplitude from this region is unimportant. First let us consider those angles $\theta > \theta_c$ where θ_c($\sim$.15) corresponds to $\ell_{11} = \ell_c$. Consider for example $\theta = 0.40$ corresponding to $\ell_{11} \simeq 100$. For this value of ℓ both $\cos^2\varphi$ and $\sin^2\varphi$ are slowly varying functions. The ratio of the magnitude of the contribution from the range $180 < \ell < 200$ to the stationary phase value is essentially proportional to $n^{-1}(\Delta\ell)[N_1^1{}'(\ell_{11},E)]^{1/2}$. $\Delta\ell$ is an estimate of the width of the region in ℓ where $\cos^2\varphi$ and $\sin^2\varphi$ are rapidly varying and n is the number of oscillations of the phase N_{11} in that interval. Since for our system $N_1^1{}'$ is small (of the order 10^{-3}) then for n = 1 the correction to the stationary phase value from the region $180 < \ell < 200$ is about seven per cent. As θ decreases toward θ_c, then $N_1^1{}'$ becomes smaller together with n. Close to θ_c we can easily estimate the correction to the stationary phase value, since in the interval $180 < \ell < 200$ the phase is essentially constant. The correction is about 20 per cent. To within 10 per cent the stationary phase approximation is a good approximation for angles greater than $\theta \sim 0.25$

From equation (11) we can understand the circumstances under which the upper envelope σ_{11}^{+} can rise above the one-channel elastic cross section σ_1^1. For angles not close to θ_c, $\cos^2\varphi(\ell_{11},E)$ and $\sin^2\varphi(\ell_{12},E)$ are slowly varying and their sum is close to unity (ℓ_{12} is less than ℓ_{11}). For σ_{11}^{+} to rise above σ_1^1 for these angles, σ_1^2 must be greater than σ_1^1. As θ approaches θ_c the sum $\cos^2\varphi(\ell_{11},E) + \sin^2\varphi(\ell_{12},E)$ becomes markedly different from unity and for σ_{11}^{+} to rise above σ_1^1 for these angles σ_1^2 must again be greater than σ_1^1. The phenomenon does not occur for our potentials. If the phenomenon does occur, it is an indication of a significant difference in the shape of the two channel potentials in the crossing region.

Both from the form of $\cos^2\varphi$ and from obvious physical considerations, the effect of decreasing the potential V_{12}, increasing the difference in slopes of the channel potentials at r_c or increasing the energy is to lower the magnitude of the correction term relative to the stationary phase value.

Similarly we can examine the inelastic differential cross section and again we introduce additional notation. We define the following functions:

$$\delta_{01} = \tfrac{1}{2}(\delta_1+\delta_2) - \tfrac{1}{2}(\chi_2-\chi_1+\pi).$$

$$\delta_{02} = \tfrac{1}{2}(\delta_1+\delta_2) + \tfrac{1}{2}(\chi_2-\chi_1+\pi).$$

$$N_{01} = \delta_{01} - [(\ell+\tfrac{1}{2})\theta + \pi/4].$$

$$N_{02} = \delta_{02} - [(\ell+\tfrac{1}{2})\theta + \pi/4].$$

$\ell_{01}(\ell_{02})$ is the solution of the equation $\theta = 2\frac{d}{d\ell}\,\delta_{01}(\theta = 2\frac{d}{d\ell}\,\delta_{02})$.

$$\left|\frac{d^2N_{01}(\ell_{01},E)}{d\ell^2}\right|^{-1}(2\ell_{01}+1) = [\sigma_0^1\ 2\sin\theta]k_1^2.$$

$$\left|\frac{d^2N_{02}(\ell_{02},E)}{d\ell^2}\right|^{-1}(2\ell_{02}+1) = [\sigma_0^2\ 2\sin\theta]k_2^2.$$

The stationary phase approximation to the inelastic differential cross section $\sigma_{12}(\theta,E)$ is simply

$$\sigma_{12}(\theta,E) = \sin^2\varphi(\ell_{01},E)\ \cos^2\varphi(\ell_{01},E)\sigma_0^1 + \sin^2\varphi(\ell_{02},E)\ \cos^2\varphi(\ell_{02},E)(\sigma_0^2)$$
$$- 2\sin\varphi(\ell_{01},E)\ \sin\varphi(\ell_{02},E)\ \cos\varphi(\ell_{01},E)\ \cos\varphi(\ell_{02},E)(\sigma_0^1)^{1/2}$$
$$\cos(N_{01}(\ell_{01},E) - N_{02}(\ell_{02},E)) \qquad (12)$$

with the upper and lower envelopes given by

$$\sigma_{12}^{\pm}(\theta,E) = [\sin\varphi(\ell_{01},E)\ \cos\varphi(\ell_{01},E)(\sigma_0^1)^{1/2} \pm \sin\varphi(\ell_{02},E)\ \cos\varphi(\ell_{02},E)\ (\sigma_0^2)^{1/2}]^2 \tag{13}$$

These results were again also determined by Green.[6] For the sine and cosine functions and the phases, we match the Stueckelberg solution with the solution from the model in section IV in the transition region. The stationary phase approximation is a good approximation for angles in excess of 0.25, and hence we can analyze the oscillations in the inelastic cross section by means of Eq. (12). However, the simple stationary phase approximation is of no use in inferring parameters of the system from the behavior of the initial steep slope of the inelastic cross section.

IV. A TWO-CHANNEL MODEL

We study a particular model for two-channel atomic scattering that can be solved explicitly using the JWKB solutions for the uncoupled channels and that contains the salient features of the physical scattering system. We introduce this model to gain some insight into the behavior of the solutions for ℓ in the neighborhood of ℓ_c and for $\ell > \ell_c$. Also we wish to compare this model solution with the Stueckelberg solution for $\ell \ll \ell_c$, since there has been much discussion as to the correctness of that solution. In 1935 O. K. Rice[8] published a severe criticism of Stueckelberg's method and the whole question has again been raised in the detailed work of Thorson.[9] There are two major criticisms. The first is that Stueckelberg's method fails for this problem. In Kemble's language[12] there does not exist a good path round the singularities of the JWKB

approximation to enable us to match solutions for different ranges of the variable r. In fact Thorson has argued that the constraints on this path are so severe as to make its existence unlikely. Further, if such a path exists, then the matching conditions are too few in number to uniquely determine the solution. Stueckelberg's solution ignores this arbitrary phase, giving it a value zero.

We consider a two-channel potential problem in which the coupling potential $V_{12}(r)$ is a delta function interaction of strength A at radial distance $r = r_c$. The Schroedinger equations are

$$\left[-\frac{d^2}{dr^2} + V_{11} + \frac{\ell(\ell+1)}{r^2} - k_1^2\right] \psi_1^{\ell}(r) = A\psi_2^{\ell}(r)\ \delta(r-r_c) \tag{14}$$

$$\left[-\frac{d^2}{dr^2} + V_{22} + \frac{\ell(\ell+1)}{r^2} - k_2^2\right] \psi_2^{\ell}(r) = A\psi_1^{\ell}(r)\ \delta(r-r_c) \tag{15}$$

For simplicity we suppose that $k_1 \sim k_2 \equiv k$. Let us denote the solution to the uncoupled equation for channel 1,2 with the correct boundary condition at $r = 0$ by $\psi_{12,20}$ and the solution for the uncoupled channel 1,2 that has a behavior at infinity of $e^{+i[kr-\pi/2(\ell+1)]}\ \left[e^{-i[kr-\pi/2(\ell+1)]}\right]$ by $\psi_{11,21}(\psi_{12,22})$. The boundary conditions at $r = r_c$ are as follows:

$$\psi_{1,2}(r_c^+) = \psi_{1,2}(r_c^-) \quad \text{where } \psi_{1,2}(r_c^{\pm}) \text{ denotes } \lim_{\epsilon\to 0} \psi_{1,2}(r_c \pm \epsilon).$$

$$\frac{d}{dr}\psi_{1,2}(r_c^+) - \frac{d}{dr}\psi_{1,2}(r_c^-) = A\,\psi_{2,1}(r_c).$$

It is straightforward to evaluate the S-matrix elements and we state the result of that calculation:

$$S_{11} = (-)\left[\frac{(\psi_{10}\psi_{12}' - \psi_{10}'\psi_{12}) - \tilde{A}\,\psi_{12}}{(\psi_{10}\psi_{11}' - \psi_{11}\psi_{10}') - \tilde{A}\,\psi_{11}}\right] \tag{16}$$

$$S_{12} = (-)\ \frac{A\ \psi_{10}\psi_{20}}{(\psi_{20}\psi_{21}' - \psi_{21}\psi_{20}')}\ \frac{(\psi_{11}\psi_{12}' - \psi_{12}\psi_{11}')}{(\psi_{10}\psi_{11}' - \psi_{10}'\psi_{11}) - \tilde{A}\ \psi_{11}} \tag{17}$$

where

$$\tilde{A} = \frac{A^2\ \psi_{10}\psi_{20}\psi_{21}}{(\psi_{20}\psi_{21}' - \psi_{21}\psi_{20}')}\ . \tag{18}$$

All wave functions are to be evaluated at $r = r_c$. The prime on the wave functions indicates differentiation with respect to r. These matrix elements can be greatly simplified by using the fact that the Wronskian of any two solutions of our differential equation is a constant function of the variable r. We thus evaluate the Wronskians at $r = \infty$. For example, $(\psi_{10}\psi_{11}' - \psi_{10}'\psi_{11}) = (+i)e^{-i(\delta_1+\chi_1)}$ in the notation of section III. For $\ell \ll kr_c$ we find, using the JWKB solutions for uncoupled channels, that

$$S_{12} = (-2i)\ \frac{A_c \sin(\chi_1+\pi/4)\ \sin(\chi_2+\pi/4)\ e^{i(\delta_1+\delta_2)}}{1 + A_c^2\ \sin(\chi_1+\pi/4)\ \sin(\chi_2+\pi/4)\ e^{i(\chi_1+\chi_2-\pi/2)}} \tag{19}$$

where $A_c = A\ (p_1(r_c)p_2(r_c))^{-1/2}$. For $\ell \sim \ell_c$ the solutions are Airy functions rather than sine cosine functions. For $\ell \ll kr_c$ we find, using the JWKB solutions for uncoupled channels, that

$$S_{11} = (+)e^{2i\delta_1}\ \frac{1 - A_c^2 \sin(\chi_1+\pi/4)\sin(\chi_2+\pi/4)\ e^{i(\chi_2-\chi_1)}}{1 + A_c^2 \sin(\chi_1+\pi/4)\sin(\chi_2+\pi/4)\ e^{i(\chi_1+\chi_2-\pi/2)}}\ . \tag{20}$$

The numerical results for the system of section III are plotted in Fig. 2. We find, in particular, that the $\cos^2\varphi$ and $\sin^2\varphi$ functions are rapidly varying in the neighborhood of ℓ_c. In the range $180 < \ell < 200$, $\cos^2\varphi$ falls from unity to 0.5 and rises again to unity. Undoubtedly this violent functional behavior is accentuated by our choice of the delta

function coupling potential. However, a more realistic potential is still likely to give violent variation, since (1) the delta function solution joins the Stueckelberg solution smoothly at $\ell = 180$, (ii) for strong enough coupling $\cos^2\varphi$ is likely to fall to 0.5, and (iii) as ℓ is increased $\cos^2\varphi$ rises to unity when the tail of the Airy function starts to overlap the region where the coupling potential is nonzero. The smaller this region, the more rapidly $\cos^2\varphi$ rises to unity. The delta function model also indicates that the phase $\chi_2 - \chi_1$ should be adjusted, in this case to $\chi_2 - \chi_1 + \pi$.

In the region of validity of the Stueckelberg's solution we find from Eq. (20) that $\cos^2\varphi = 1 - A_c^2 (1 - \sin 2\chi_1)$ and hence $\cos^2\varphi$ is an oscillatory function, not a smoothly varying function as Stueckelberg found. It therefore seems that essential assumptions have been made about the details of the coupling interaction in the Stueckelberg model to render the solution so simple.

V. SUMMARY

We have examined the concept of smoothly varying functions in relation to the stationary phase approximation for evaluating scattering amplitudes. The S-matrix elements for the two-channel atomic scattering problem vary violently in the small region of interaction between the two channels. However, in spite of this rapid variation the contribution to the amplitude from this region is below ten per cent for a wide range of angles, because the region of rapid change is small and the second derivative of the phase at the secondary phase point is small. We

indicate for a specific model at what angle beyond the critical angle, indicating the onset of inelasticity, the stationary phase approximation becomes a good approximation. The interpretation of the oscillations in the elastic and inelastic cross sections as the "interference" of classical trajectories is a valid picture, at least for the types of potential we consider and provided that the Stueckelberg solution is a correct solution.

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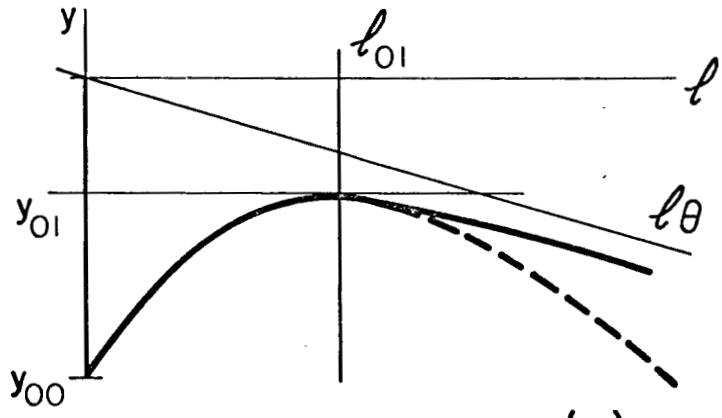
Figure Captions:

Fig. 1a The function $N_{-}(\ell, E, \theta)$

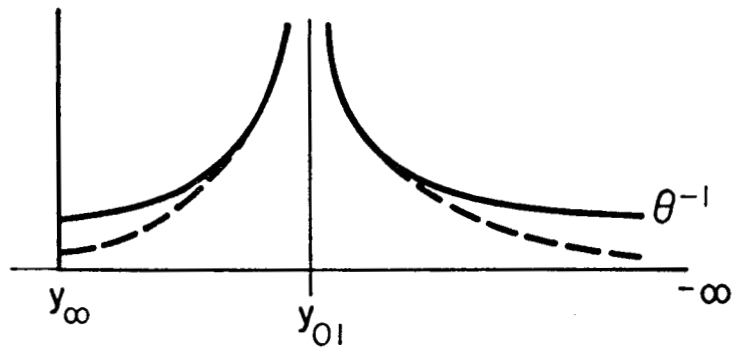
1b The function $|g(y)|^{-1}$

Fig. 2 Phase shift N_{11} and probability coefficients $\cos^2\varphi$, $\sin^2\varphi$ for the system of section III



(a)

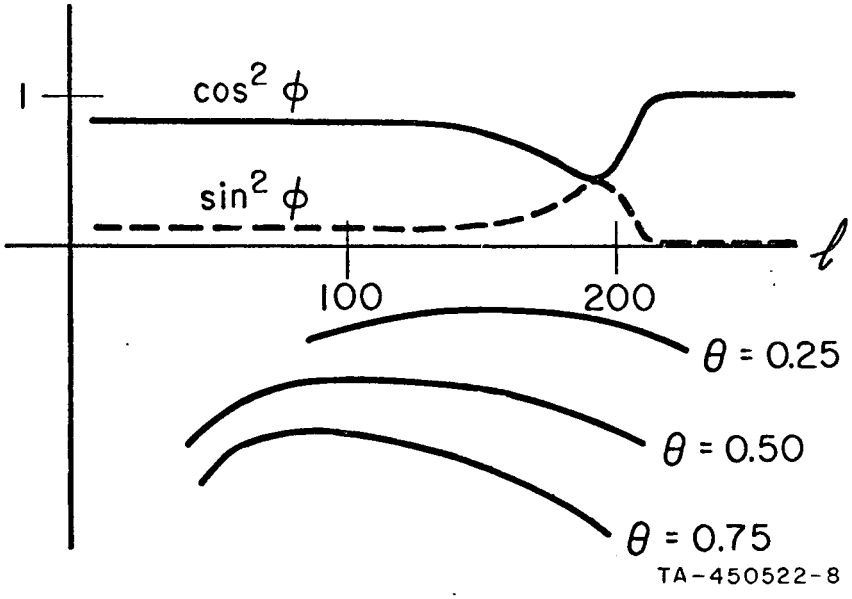
PLOT OF FUNCTION $N_-(\ell, E, \theta)$



(b)

PLOT OF FUNCTION $|g(y)|^{-1}$

TA-450522-7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sin² φ
100
200
ℓ
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θ = 0.50
θ = 0.75
TA-450522-8