Impact Expansions in Classical and Semiclassical Scattering*

FELIX T. SMITH, RAYMOND P. MARCHI, AND KENT G. DEDRICK
Stanford Research Institute, Menlo Park, California
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In the energy regime appropriate to classical and semiclassical atomic scattering theory, experimental data on differential cross sections $\sigma(\theta,E)$ and interference patterns are conveniently analyzed through the use of reduced variables such as $\tau=E\theta$, $\rho=\theta\sin\theta\sigma(\theta,E)$. In forward scattering, the reduced relationship is the leading term of an impact expansion of the type $\rho(\tau,E)=\sum_n E^{-n}\rho_n(\tau)$. The $\rho_n(\tau)$ are obtained by eliminating the impact parameter b from expansions of the classical scattering functions of the type $\tau(b,E)=\sum_n E^{-n}\tau_n(b)$, introduced by Lehmann and Leibfried. Backscattering data are to be analyzed through expansions such as $\sigma(\theta,E)=\sum_n(\pi-\theta)^{2n}\sigma_n(E)$, derived by eliminating b from expansions like $\pi-\theta=\varphi(b,E)=\sum_n b^{2n+1}\varphi_n(E)$. If the scattering arises from a potential $V(r)$, the coefficients $\tau_n(b)$, $\varphi_n(E)$, etc., are expressed in the form of integrals over the potentials which lend themselves to inversion procedures similar to Firsov's by which a lower bound to the potential can be extracted from the scattering data. In addition to deriving these expansions and testing them on several realistic interatomic potentials, we describe how the reduced variables they suggest can be applied to the presentation and analysis of experimental data.

A. INTRODUCTION

IN calculations of scattering phenomena at moderately high energies (in the kilovolt range, for instance) the so-called impact-parameter approximation has proven exceedingly useful.[1] In the usual treatments that approximation is based on the assumption that the motions of the heavy particles in the collision are to be treated not only classically but as if no deflection at all took place in the course of the collision. In addition to estimating total cross sections, the results of such calculations have been successfully applied to the analysis of small-angle differential-scattering experiments when such phenomena as charge exchange were under study.[2] Recently similar information has become available from experiments in differential scattering at comparatively large angles for which the usual assumptions of the impact-parameter method are clearly inapplicable.[3] Nevertheless, it has proved possible to analyze the data by methods which are a simple extension of those suggested by the simple forms of approximation. Clearly a further development of the underlying theory of the method is desirable, and it is to this task that the present work addresses itself.

Everhart and others have made considerable use of certain reduced variables for the presentation and analysis of scattering data obtained at small and moderate angles.[4] Of particular importance is the reduced scattering angle

$$\tau=E\theta,$$

where E is the kinetic energy and θ is the scattering angle, all of which we shall assume to be measured in the center-of-mass system. The reason for the success of this variable in particular is that it is in first approximation a function only of the impact parameter b of the collision. This simple relationship between τ and b has been used for some time in the theory of the collisions between fast ions and atoms of a solid lattice in radiation damage and sputtering, where it is known as the momentum approximation, and Lehmann and Leibfried showed that it is really the first term of an expansion in $1/E$.[5] Similarly, the other functions which enter into the analysis of scattering experiments such as the reduced cross section can be expressed as a similar series in which the successive terms are obtainable as functions of b alone.[6] (That work was done in ignorance of Lehmann and Leibfried's treatment.) Because the initial terms of these expansions are identical with the expressions of the impact parameter approximation, we have chosen to call such an expansion an impact expansion. Leibfried has also presented a complementary expansion which is useful particularly in the very wide-angle region or in the region of backscattering.[5] There are thus two expansions in effect, the forward impact expansion and the backward impact expansion. Lehmann and Leibfried originally derived these expansions by the use of contour integrals, and remarked that these can be transformed into integrals along the real axis after integrating by parts. We have found an alternative derivation which leads directly to the real integrals in question, and which facilitates the inverse process, the deduction of the potential from scattering data.

One of the purposes for which these expansions can be used is the presentation and analysis of experimental data. Obviously, the impact parameter is not one of the

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[1] E.g., D. R. Bates, *Atomic and Molecular Processes* (Academic Press Inc., New York, 1962), p. 578 ff.

[2] D. R. Bates and D. A. Williams, Proc. Phys. Soc. (London) **83**, 425 (1964).

[3] D. C. Lorents and W. Aberth, Phys. Rev. **139**, A1017 (1965).

[4] E. Everhart, Phys. Rev. **132**, 2083 (1963).

[5] (a) C. Lehmann and G. Leibfried, Z. Physik **172**, 465 (1962); (b) G. Leibfried and T. Plesser, *ibid.* **187**, 411 (1965); (c) G. Leibfried, *Bestrahlungseffekte in Festkörpern* (Teubner, Stüttgart, Germany, 1965), p. 37.

[6] F. T. Smith, J. Chem. Phys. **42**, 2419 (1965).

quantities directly measured in scattering experiments, whose results are usually obtained as measured intensities or currents as a function of energy and scattering angle θ. For this reason it is important to convert the series expansions from an explicit dependence on the impact parameter b to a form in which the only explicit variables appearing are pairs of observable parameters such as (E,θ), (E,τ), or (E,φ) where $\varphi=\pi-\theta$. The latter pair of variables is particularly useful in the backscattering situation.

The practical need for a backscattering expansion has only recently been brought home to us. Naturally, in most experiments the decline in intensities at large angles in the laboratory system precludes direct measurement of backscattering phenomena. However, the recent observation of an interference effect in the differential scattering of diatomic systems involving identical nuclei makes it possible to deduce information on the backscattering from the secondary oscillations at intermediate angles approaching forward scattering.[7] For this reason we expect the backward impact expansion to have immediate usefulness almost as great as that of the forward expansion.

We have confined our attention here to the expansion of purely classical functions, primarily the scattering angle, the impact parameter, the differential cross section, and the classical action A. As Ford and Wheeler have pointed out,[8] a great many interference effects of a quantum-mechanical nature can actually be calculated extremely well through the use of classical approximations, provided one introduces a classical scattering amplitude of the form

$$f(E,\theta)=\sigma(E,\theta)^{1/2}e^{iA(E,\theta)/\hbar}. \tag{1}$$

This procedure has proven highly convenient and valuable in calculations of $He^{+}+He$ scattering,[9,10] and in the empirical analysis of data from a number of other systems such as $He^{+}+Ne$, $He^{+}+Ar$, $Ar^{+}+Ar$, $Li^{+}+He$, etc.[11]

In addition to presenting the expansions in question and their derivations, one of our aims in this paper is to test their value in some representative calculations. We have done this using some fairly realistic potentials which we have previously used to approximate the potentials for $He^{+}+He$ scattering.[9] Obviously the expansions are not really necessary when calculating the scattering parameters from the potentials since the exact calculations of the integrals in question are almost trivial. However, we believe the expansions will obtain their greatest value in the analysis of experimental data and in the endeavor to extract information about the interactions from such data. As a matter of fact, the leading terms in these expansions can be used most effectively in simplifying the inversion procedures that can be used to deduce experimental potentials. We have therefore devoted a section to these simplified inversion procedures.

We have limited our attention here to spherically symmetric potential scattering. Obviously generalizations can be sought in several directions for use with more complicated interactions. Furthermore, it is interesting to speculate about the possible quantal extension of what is clearly a valuable technique in the classical approximation.

B. THE SCATTERING FUNCTIONS

It is the task of scattering theory to compute from an assumed interaction, such as the potential $V(r)$, observable functions such as the scattering cross section σ in their dependence on the experimental variables, especially the energy E and the angle of scattering θ. Because it is conserved in the spherically symmetric interaction, the angular momentum L, together with its close relative the impact parameter b, plays an important part in mediating the connection between $V(r)$ and $\sigma(E,\theta)$, even though L and b are seldom if ever directly observable. The usual procedure for deducing σ is first to obtain the deflection function $\Theta(E,b)$ (whose absolute value is the scattering angle θ), invert this function to obtain $b(E,\theta)$, and then compute the cross section by the formula

$$\sin\theta\sigma(E,\theta)=\tfrac{1}{2}|\partial b^2/\partial\theta|_E. \tag{2}$$

Of great importance also are the action $A(E,\Theta)$ and the phase $\Delta(E,L)$, which are connected with each other by the formula

$$A(E,\Theta)=\Delta(E,L)-L\Theta. \tag{3}$$

Not only are these generators of the other scattering functions,

$$L(E,\Theta)=b[2\mu E]^{1/2}=-(\partial A/\partial\Theta)_E, \tag{3a}$$

$$\Theta(E,L)=(\partial\Delta/\partial L)_E, \tag{3b}$$

but the action A plays a controlling part both in the fine structure of rainbow scattering and in the elastic scattering of symmetric systems such as $H^{+}+H$ or $He^{+}+He$, because of its appearance in the scattering amplitude $f(E,\theta)$ of Eq. (1). Also important is the collision lifetime Q:

$$Q(E,L)=Q(E,\Theta)=(\partial A/\partial E)_\Theta. \tag{4}$$

In a classical computation the scattering functions are first arrived at as functions of the two parameters E and b, expressed as integrals over the potential $V(r)$. The lower limit of these integrals is the classical turning

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[7] W. Aberth, D. C. Lorents, R. P. Marchi, and F. T. Smith, Phys. Rev. Letters 14, 776 (1965).
[8] K. W. Ford and J. A. Wheeler, Ann. Phys. (N.Y.) 7, 259 (1959).
[9] R. P. Marchi and F. T. Smith, Phys. Rev. 139, A1025 (1965).
[10] F. T. Smith, D. C. Lorents, W. Aberth, and R. P. Marchi, Phys. Rev. Letters 15, 742 (1965).
[11] W. Aberth and D. C. Lorents, Phys. Rev. 144, 109 (1966); work reported at Fourth International Conference on Physics of Electronic and Atomic Collisions, Quebec, 1965 (unpublished).

point $r_0(E,b)$, the largest root of the equation

$$\frac{V(r_0)}{E}+\frac{b^2}{r_0^2}=1. \tag{5}$$

The most important integral forms of these functions are

$$\Theta(E,b)=\pi-2b\int_{r_0}^{\infty}\left[1-\frac{V(r)}{E}-\frac{b^2}{r^2}\right]^{-1/2}\frac{dr}{r^2}$$
$$=-b\int_{r_0}^{\infty}\left(\frac{r}{E}\frac{dV}{dr}\right)\left(1-\frac{V(r)}{E}\right)^{-1}\times\left[1-\frac{V(r)}{E}-\frac{b^2}{r^2}\right]^{-1/2}\frac{dr}{r^2}, \tag{6}$$

$$\frac{\Delta(E,b)}{(2\mu E)^{1/2}}=2\lim_{R\to\infty}\left\{\int_{r_0}^{R}\left[1-\frac{V(r)}{E}-\frac{b^2}{r^2}\right]^{1/2}dr-\int_{b}^{R}\left[1-\frac{b^2}{r^2}\right]^{1/2}dr\right\}$$
$$=\int_{r_0}^{\infty}\left(\frac{r}{E}\frac{dV}{dr}\right)\left(1-\frac{V(r)}{E}\right)^{-1}\left[1-\frac{V(r)}{E}-\frac{b^2}{r^2}\right]^{1/2}dr, \tag{7}$$

$$\frac{A(E,b)}{(2\mu E)^{1/2}}=2\lim_{R\to\infty}\left\{\int_{r_0}^{R}\left(1-\frac{V(r)}{E}\right)\times\left[1-\frac{V(r)}{E}-\frac{b^2}{r^2}\right]^{-1/2}dr-R\right\}$$
$$=\int_{r_0}^{\infty}\left(\frac{r}{E}\frac{dV}{dr}\right)\left[1-\frac{V(r)}{E}-\frac{b^2}{r^2}\right]^{-1/2}dr. \tag{8}$$

The common pattern that runs through Eqs. (6)–(8) is brought out even more clearly if we note that

$$2b\int_{b}^{\infty}\left[1-\frac{b^2}{r^2}\right]^{-1/2}\frac{dr}{r^2}=\pi, \tag{6a}$$

$$\int_{b}^{R}\left[1-\frac{b^2}{r^2}\right]^{-1/2}dr=(R^2-b^2)^{1/2}\to R \text{ as } R\to\infty. \tag{8a}$$

The initial form given in each of Eqs. (6)–(8) is the fundamental expression that is encountered initially in the derivation, while the final form (derived in Ref. 6) is a rapidly convergent one suitable for computation; the second form is valid only if $V(r)$ vanishes faster than r^{-2} at large r.

C. THE IMPACT EXPANSIONS

1. Expansion Parameters

Among the many possible expansions that could be used to simplify the scattering functions in various specific situations, there are two that have a particularly simple and natural origin. If we examine the deflection function $\Theta(E,b)$ at a fixed energy, we observe that there are two particularly simple limits: The region of large impact parameter b corresponds to small values of the scattering angle $\theta=|\Theta|$, and when, as in the collision of two atoms or ions, the potential has a repulsive singularity at small r, we find Θ approaching π linearly as $b\to 0$. We therefore seek expansions adapted to these two regions $b\to\infty$ and $b\to 0$. The integrals with which we must deal depend on the turning point r_0, and Eq. (5) shows that this quantity is also simplified in these two limits [provided that $V(r)$ vanishes rapidly at large r], so that $r_0(E,b)$ approaches b as $b\to\infty$, and as $b\to 0$ it approaches the root $r_{00}(E)$ of the equation

$$V(r_{00})=E. \tag{9}$$

Because of the rapid fall of $V(r)$ at large r, we can be assured that the following inequalities must hold through the region of integration in these two limits:

$$b\to\infty,\quad \frac{|V(r)|}{E}\ll\frac{b^2}{r^2}\leq 1 \quad\text{for}\quad r\geq r_0(E,b)\approx b; \tag{10a}$$

$$b\to 0,\quad \frac{b^2}{r^2}\ll 1 \quad\text{for}\quad r\geq r_0(E,b)\approx r_{00}(E). \tag{10b}$$

We shall exploit these two inequalities in deriving the expansions appropriate to these two limits. Thus it comes about that forward scattering ($\Theta\to 0$, $b\to\infty$) calls for an expansion in powers of

$$\epsilon=E^{-1}, \tag{11}$$

while backwardscattering ($\Theta\to\pi$, $b\to 0$) calls for an expansion in powers of b^2.

2. Lagrange's Expansion

The expansion formulas we are seeking can be obtained by a variety of methods, and our results were achieved first through the tedious manipulation of series illustrated in an earlier paper.[6] Because we are often dealing with functions defined implicitly, the direct application of Taylor's expansion may not be feasible. In such a case, however, the tedium can be eliminated by the use of Lagrange's expansion, which is the natural inverse to the Taylor procedure.[12] Though it dates from 1770, the Lagrange procedure is still not widely used, but renewed attention has recently been devoted to its formalism and consequences.[13]

[12] See, for example, (a) E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, Cambridge, England, 1958), 4th ed., p. 133; or (b) H. and B. S. Jeffreys, *Methods of Mathematical Physics* (Cambridge University Press, Cambridge, England, 1956), 3rd ed., p. 382.

[13] P. A. Sturrock, J. Math. Phys. **1**, 405 (1960); K. G. Dedrick and E. L. Chu, Arch. Ratl. Mech. Anal. **16**, 385 (1964).

The Lagrange problem is to express a function $f(y)$ in terms of a new variable x that is defined implicitly in its turn as another function of y:

$$x=g(y)=y-\zeta(y), \tag{12}$$

so that

$$dx/dy=g'(y)=1-\zeta'(y). \tag{12a}$$

Lagrange showed that, when y is sufficiently close to x, $f(y)$ can be written as the expansion

$$f(y)=\sum_{n=0}^{\infty}\frac{1}{n!}\frac{d^n}{dx^n}[\zeta^n(x)f(x)g'(x)]. \tag{13}$$

An alternative form, given by Darboux, is obtained by setting

$$h(u)=f(u)g'(u) \tag{14}$$

on both sides of (13):

$$f(y)=\frac{h(y)}{g'(y)}=\sum_{n=0}^{\infty}\frac{1}{n!}\frac{d^n}{dx^n}[\zeta^n(x)h(x)]. \tag{15}$$

It is the latter form that we shall generally have occasion to employ.

3. The Forward Expansion

Let us consider the first integral appearing in Eq. (6) for the deflection function Θ. If we introduce a new variable y such that

$$y=r^2,\quad 2dr/r=dy/y,\quad y_0=r_0^2, \tag{16}$$

and a second new variable x such that

$$x=r^2(1-V(r)/E),\quad x_0=b^2, \tag{17}$$

the integral in question can be rewritten in the form

$$\pi-\Theta=b\int_{y_0}^{\infty}\frac{dy}{y[x-b^2]^{1/2}}=b\int_{b^2}^{\infty}\frac{(dy/dx)dx}{y[x-b^2]^{1/2}}. \tag{18}$$

Clearly we can also write (6a) in the form

$$\pi=b\int_{b^2}^{\infty}\frac{dx}{x[x-b^2]^{1/2}}. \tag{18a}$$

If we now identify y and x with the corresponding variables of Eq. (12), we see that

$$\zeta(y)=\epsilon yV(y^{1/2}). \tag{19}$$

In order to replace the function $y^{-1}dy/dx$ in the last integral of (18) with an explicit function of x alone, we need merely set

$$1/y=h(y) \tag{20}$$

and use Lagrange's expansion in the form (15)

$$f(y)=\frac{1}{y}\frac{dy}{dx}=\sum_{n=0}^{\infty}\frac{\epsilon^n}{n!}\frac{d^n}{dx^n}[x^{n-1}V^n(x^{1/2})]. \tag{21}$$

Comparing (18) and (18a) we see that it is convenient to write

$$F(x)=\frac{1}{y}\frac{dy}{dx}-\frac{1}{x}=\sum_{n=0}^{\infty}\epsilon^{n+1}F_n(x), \tag{22}$$

where

$$F_n(x)=\frac{1}{(n+1)!}\frac{d^{n+1}}{dx^{n+1}}[x^nV^{n+1}(x^{1/2})]. \tag{23}$$

Using these expressions and multiplying through by E, we obtain a series expansion for the reduced deflection function

$$\tau(E,b)=E\Theta(E,b)=-b\int_{b^2}^{\infty}\frac{F(x)dx}{[x-b^2]^{1/2}}=\sum_{n=0}^{\infty}\epsilon^n\tau_n(b), \tag{24}$$

where

$$\tau_n(b)=-b\int_{b^2}^{\infty}\frac{F_n(x)dx}{[x-b^2]^{1/2}}. \tag{25}$$

The transformations of the classical phase Δ and the action A follow precisely the same pattern, the phase being given by

$$\frac{\Delta(E,b)}{(2\mu E)^{1/2}}=\int_{b^2}^{\infty}F(x)[x-b^2]^{1/2}dx, \tag{26}$$

while the action, in reduced form, is

$$\alpha(E,b)=\left(\frac{E}{2\mu}\right)^{1/2}A(E,b)=E\int_{b^2}^{\infty}\frac{xF(x)dx}{[x-b^2]^{1/2}}$$
$$=\sum_{n=0}^{\infty}\epsilon^n\alpha_n(b), \tag{27}$$

where

$$\alpha_n(b)=\int_{b^2}^{\infty}\frac{xF_n(x)dx}{[x-b^2]^{1/2}}. \tag{28}$$

The lifetime Q can be found by simple differentiation, by (4), and its expansion need not be written out explicitly here.

One limitation on our procedure is exposed by Eqs. (18) and (12a), from which we see that we must avoid the situation where $g'(y)$ may vanish. This is equivalent to the vanishing of

$$E-V(r)-\tfrac{1}{2}r(dV/dr), \tag{29}$$

something that can only occur if $V(r)$ has an attractive part, and then only for sufficiently small values of E. Often this difficulty can be circumvented by breaking the integral into two or more parts.

4. The Backward Expansion

In the region of backscattering, where Θ is close to π, it is convenient to use a new angular variable,

$$\varphi(E,b)=\pi-\Theta(E,b)=2b\int_{r_0}^{\infty}\frac{dr}{r^2\left[1-\dfrac{V(r)}{E}-\dfrac{b^2}{r^2}\right]^{1/2}}. \qquad (30)$$

We now introduce the potential itself as the new variable of integration,

$$y=V(r), \qquad (31)$$

so that

$$\varphi(E,b)=-2bE^{1/2}\int_0^{V(r_0)}\frac{\dfrac{dr}{dy}dy}{r^2(y)\left[E-y-\dfrac{Eb^2}{r^2(y)}\right]^{1/2}}. \qquad (32)$$

Equation (32) must be modified if the potential is not purely repulsive but has an attractive minimum where dV/dr vanishes. In that case we can break the function $r(y)$ into two branches,

$$\begin{aligned} &r_<(y) \quad \text{for} \quad r<r_{\min}, \quad V_{\min}\leq y\leq\infty; \\ &r_>(y) \quad \text{for} \quad r>r_{\min}, \quad V_{\min}\leq y\leq 0. \end{aligned} \qquad (32a)$$

The integral then falls into two portions, with the respective limits shown in (32a).

We now proceed to introduce a second variable,

$$x=V+Eb^2/r^2=y+Eb^2/r^2(y), \qquad (33)$$

thus transforming (32) to

$$\varphi(E,b)=-2bE^{1/2}\int_0^E\left(\frac{1}{r^2(y)}\frac{dr}{dy}\right)\frac{dy}{dx}\frac{dx}{[E-x]^{1/2}}. \qquad (34)$$

We can identify $\zeta(y)$ by comparing (33) and (12),

$$\zeta(y)=-b^2E/r^2(y), \qquad (35)$$

and apply the Lagrange expansion (15) by taking

$$h(y)=\frac{1}{r^2(y)}\frac{dr}{dy}. \qquad (36)$$

The expanded function can be written

$$G(x)=h(y)\frac{dy}{dx}=\sum_{n=0}^{\infty}(b^2E)^nG_n(x), \qquad (37)$$

where we have, setting $x=V$ again,

$$G_n(V)=\frac{(-)^{n+1}}{(2n+1)n!}\frac{d^{n+1}}{dV^{n+1}}[r^{-(2n+1)}(V)]. \qquad (38)$$

The backscattering angle is then

$$\begin{aligned}\varphi(E,b)&=-2bE^{1/2}\int_0^E G(V)\frac{dV}{[E-V]^{1/2}}\\ &=\sum_{n=0}^{\infty}b^{2n+1}\varphi_n(E),\end{aligned} \qquad (39)$$

where

$$\varphi_n(E)=-2E^{n+1/2}\int_0^E G_n(V)\frac{dV}{[E-V]^{1/2}}. \qquad (40)$$

If we start with the final integral form in Eq. (8) and make the same transformations, the expansion of the action A takes a still simpler course:

$$\begin{aligned}\frac{A(E,b)}{(2\mu)^{1/2}}&=-\int_0^E r(y)\frac{dy}{dx}\frac{dx}{[E-x]^{1/2}}\\ &=-\int_0^E H(x)\frac{dx}{[E-x]^{1/2}}\\ &=(2\mu)^{-1/2}\sum_{n=0}^{\infty}b^{2n}A_n(E),\end{aligned} \qquad (41)$$

where

$$H(x)=\sum_{n=0}^{\infty}b^{2n}E^nH_n(x), \qquad (42)$$

$$H_n(x)=\frac{(-)^n}{n!}\frac{d^n}{dx^n}[r^{-2n+1}(x)], \qquad (42a)$$

and

$$\frac{A_n(E)}{(2\mu)^{1/2}}=-E^n\int_0^{\infty}H_n(V)\frac{dV}{[E-V]^{1/2}}. \qquad (43)$$

D. ELIMINATION OF b

In the previous section we have seen how to express the various scattering parameters such as Θ, A, and σ as functions of the two variables E and b and have derived two expansion formulas for these functions. The variable b has the greatest importance in these expansions—but since it cannot be directly measured, it must be replaced by an observable variable, usually the scattering angle, for the purposes of experimental comparison. Since the details of the procedure are different in the two expansions, we shall continue to treat the two cases separately.

1. Forward Expansion

We shall here work entirely with the reduced variables, especially $\tau(E,b)$ [Eq. (24)] and $\alpha(E,b)$ [Eq. (27)]. In order to eliminate b we first must invert (24) to find the expansion

$$b(E,\tau)=\sum_{n=0}^{\infty}\epsilon^nb_n(\tau). \qquad (44)$$

Assuming that $b(\epsilon,\tau)$ has a Taylor expansion in ϵ, we can identify

$$b_n(\tau)=\frac{1}{n!}\left(\frac{\partial^n b(\epsilon,\tau)}{\partial\epsilon^n}\right)_{\epsilon=0}, \tag{45}$$

and evaluate the partial derivatives in terms of the known partials of $\tau(\epsilon,b)$ from (24). Necessarily, $b_0(\tau)=b(0,\tau)$ is the inverse of $\tau(0,b)=\tau_0(b)$, satisfying the equation

$$\tau=\tau_0(b_0(\tau)). \tag{46}$$

The next two terms are

$$b_1(\tau)=\frac{-\tau_1(b_0(\tau))}{\tau_0'(b_0(\tau))}, \tag{47}$$

$$b_2(\tau)=-\frac{1}{\tau_0'(b_0(\tau))}[2\tau_2(b_0(\tau))+2b_1(\tau)\tau_1'(b_0(\tau))+b_1^2(\tau)\tau_0''(b_0(\tau))]. \tag{47a}$$

The existence of (44) as a Taylor series requires that $\tau_0(b)$ have an inverse and that $\tau_0'(b_0(\tau))$ not vanish. These conditions are satisfied by most physically realistic interactions except possibly at isolated points b_r, where $\tau_0'(b_r)=0$. These are just the locations of rainbow scattering, where the classical cross section has a singularity and where, in addition, quantal effects are especially important. To establish the domain of convergence of (44) is clearly more difficult; it will depend in general both on the interaction $V(r)$ and on the value of τ. We can now insert (44) in α to get

$$a(E,\tau)=\alpha(E,b(E,\tau))=\sum_{n=0}^{\infty}\epsilon^n a_n(\tau), \tag{48}$$

where

$$a_0(\tau)=\alpha_0(b_0(\tau)) \tag{49}$$

and

$$a_1(\tau)=\alpha_1(b_0(\tau))+\alpha_0'(b_0(\tau))b_1(\tau). \tag{49a}$$

To complete the set of formulas commonly needed we can write the reduced classical cross section as

$$\rho(\tau,\epsilon)=\theta\sigma(E,\theta)\sin\theta=\tfrac{1}{2}\tau\left|\frac{\partial b^2}{\partial\tau}\right|_{\epsilon}=\rho_0(\tau)+\epsilon\rho_1(\tau)+\cdots. \tag{50}$$

If we assume, for definiteness, the signs appropriate to a simple repulsive potential, we find, using (44), that

$$s_0(\tau)=-b_0(\tau)/\tau_0'(b_0(\tau)). \tag{51}$$

and

$$s_1(\tau)=\left[\frac{-b\tau_1\tau_0''}{(\tau_0')^3}+\frac{b\tau_1'}{(\tau_0')^2}+\frac{\tau_1}{(\tau_0')^2}\right]_{b_0(\tau)}. \tag{51a}$$

The derivatives of τ_n and α_n with respect to b that are needed in Eqs. (47) to (51) can be obtained directly from Eqs. (25) and (28). Explicit forms that are readily integrable are given in the Appendix.

2. Backward Expansion

Here the appropriate angular variable is neither τ nor Θ but $\varphi(E,b)$, which is given as an expansion by Eq. (38a). In this case the expansion is simply a power series in b, so the inversion to obtain the function

$$b=\beta(E,\varphi)=\sum_{n=0}^{\infty}\varphi^{2n+1}\beta_n(E) \tag{52}$$

is straightforward. The first term, in particular, gives us

$$\frac{1}{\beta_0(E)}=\varphi_0(E)=-2E^{1/2}\int_0^E r^{-2}(V)\frac{dr}{dV}[E-V]^{-1/2}dV. \tag{52a}$$

The next term gives

$$\beta_1(E)=-\frac{\varphi_1(E)}{\varphi_0(E)}\beta_0^3(E)=-\frac{\varphi_1(E)}{\varphi_0^4(E)}, \tag{52b}$$

where

$$\varphi_1(E)=2E^{3/2}\int_0^E\frac{d}{dV}\left[r^{-4}(V)\frac{dr}{dV}\right]\frac{dV}{[E-V]^{1/2}}. \tag{52c}$$

By inserting (52) into (43) we obtain the action as

$$A(E,\beta(E,\varphi))=\mathcal{A}(E,\varphi)=\sum_{n=0}^{\infty}\varphi^{2n}\mathcal{A}_n(E). \tag{53}$$

The first term is easily seen to be

$$\mathcal{A}_0(E)=A_0(E)=-(2\mu)^{1/2}\int_0^E\frac{r(V)dV}{[E-V]^{1/2}}. \tag{53a}$$

For the higher terms we can use an identity derived from (3a),

$$b=(2\mu E)^{-1/2}\frac{\partial A}{\partial\varphi}=\left(\frac{2}{\mu E}\right)^{1/2}\sum_{n=0}^{\infty}(n+1)\varphi^{2n+1}\mathcal{A}_{n+1}(E), \tag{54}$$

with the result that

$$(n+1)\mathcal{A}_{n+1}(E)=(\mu E/2)^{1/2}\beta_n(E). \tag{54a}$$

Without evaluating any further integrals we can obtain the leading term in the classical cross section:

$$\sigma(E,\varphi)=\frac{1}{2\sin\varphi}\left|\frac{\partial b^2}{\partial\varphi}\right|=\sum_{n=0}^{\infty}\varphi^{2n}\sigma_n(E), \tag{55}$$

where we find immediately, by using (52) and expanding

$1/\sin\varphi$ itself, that

$$\sigma_0(E)=2\beta_0^2(E)=\frac{2}{\varphi_0^2(E)} \qquad (55a)$$

and

$$\sigma_1(E)=8\beta_0(E)\beta_1(E)+\tfrac{1}{3}\beta_0^2(E)=\frac{1}{3\varphi_0^2(E)}-\frac{8\varphi_1(E)}{\varphi_0^5(E)}. \qquad (55b)$$

Thus we verify that the classical cross section goes to a finite limit in backscattering.

E. THE INVERSION PROBLEM

1. Treatment of Experimental Data

The problem of deducing the interaction from scattering data has provoked a very considerable literature. In the classical limit, with a spherically symmetric potential, Firsov showed how the potential function could be extracted from differential scattering data at a fixed energy.[14,15] This elegant method, which is broadly equivalent to some other treatments of the same problem,[16] will form the basis for our discussion here.

Ideally, if experimental scattering data were of absolute accuracy and if it were available over the full range of angle from 0 to π (in the center-of-mass system) at a single energy E, there would be no problem in extracting the potential by Firsov's method—provided we are dealing with a monotonic repulsive interaction. Practically, we are obliged to deal with a limited angular range of data, of limited accuracy—but we can extend the domain accessible to measurement greatly in another dimension by varying the energy E. There is therefore much to be gained by combining all the data from a wide range of energies in a single inversion procedure, instead of being restricted to the limited and incomplete sets of data available at each separate energy.

Because of the extremely rapid falloff of the intensity of experimental scattered currents as θ becomes large, in practical cases the cross section $\sigma(E,\theta)$ is often known only for relatively small angles in the forward direction. In that event it is natural to express the data in terms of the reduced variables suggested by the forward impact expansion, namely the reduced center-of-mass scattering angle $\tau=E\theta$ and the reduced center-of-mass cross section $\rho(E,\tau)=\theta\sin\theta\sigma(E,\theta)$. This variable has at least two advantages: uncertainties in the energy E are not introduced into ρ (though they cannot be avoided in τ) and the steepness of fall with which $\sigma(E,\tau)$ is afflicted at small τ is greatly ameliorated.

Calculations using several potential functions have shown us that the higher terms in the series (57), namely, $\rho_1(\tau)$, $\rho_2(\tau)$, etc., are functions that usually if not always decline rapidly as $\tau\to 0$, unlike $\rho_0(\tau)$. Consequently a plot of the functions $\rho(E,\tau)$ versus τ at several values of E reveals a set of curves that follow the asymptote $\rho_0(\tau)$ at small τ and then peel away from it at higher τ successively as E increases. Each curve $\rho(E,\tau)$ terminates at $\tau=E\pi$ because its range of θ ends there. In a number of cases where simple potential scattering can be expected to dominate, the experimental data when plotted as $\rho(E,\tau)$ versus τ on a single plot show a similar tendency to follow a single asymptote at small τ and then peel away as τ and E increase. Consequently it is possible to delineate the asymptotic function $\rho_0(\tau)$ directly. In some cases the definition of this function can be improved by plotting $\rho(\tau,\epsilon)$ versus $\epsilon=E^{-1}$ for each value of τ, and reading $\rho_0(\tau)$ as the intercept in an extrapolation to $\epsilon=0$; with less accuracy it is also possible to estimate $\rho_1(\tau)$ from the slope of such a plot. In this way it is often possible to fix $\rho_0(\tau)$ experimentally over a range of τ that is enormous compared to the range accessible at any single energy E by itself. This function $\rho_0(\tau)$ can now be inverted to obtain the potential.

2. The Forward Inversion

The first step in the Firsov inversion procedure is to obtain the relation between the impact parameter b and the scattering angle—or, in our case, between b and τ. This is done by integrating the equation

$$-\tfrac{1}{2}(db_0^2/d\tau)=s_0(\tau)=\tau^{-1}\rho_0(\tau). \qquad (56)$$

The result,

$$b_0^2(\tau)=2\int_\tau^\infty \frac{\rho_0(t)}{t}dt, \qquad (57)$$

assumes that we can extrapolate the declining integrand to infinity; alternatively, we can content ourselves with obtaining a lower bound for b_0:

$$b_0^2(\tau)>b_0^2(\tau,\tau^*)=2\int_\tau^{\tau^*} \frac{\rho_0(t)}{t}dt. \qquad (58)$$

Inverting these relationships, and noting that τ is a monotonic decreasing function of b [at least if $V(r)$ is pure repulsive], we can obtain $\tau_0(b)$ as the inverse of (57), or $\tau_0(b,\tau^*)$ as a lower bound to $\tau_0(b)$, obtained by inverting (58):

$$\tau_0(b)>\tau_0(b,\tau^*). \qquad (59)$$

From higher terms in the series (50) we might also obtain estimates of $b_1(\tau)$, $b_2(\tau)$, etc., from which $\tau_1(b)$, etc., could be obtained by an argument like (47).

The inversion to obtain $\tau_0(b)$ can be properly carried out only if b is a single-valued function of τ. For a monotonic repulsive potential $V(r)$ this is always the case; for a potential with an attractive well $b(\tau)$ is single-valued as long as τ exceeds the reduced rainbow angle τ_r, and b is smaller than some upper limit b_r. Even with an attractive potential, then, it is possible to find

[14] O. B. Firsov, Zh. Eksperim. i Teor. Fiz. 24, 279 (1953).
[15] G. H. Lane and E. Everhart, Phys. Rev. 120, 2064 (1960).
[16] J. B. Keller, I. Kay, and J. Shmoys, Phys. Rev. 102, 557 (1956).

a considerable range in τ and b within which we can unambiguously establish a good lower bound, Eq. (59), to the function $\tau_0(b)$. In this range of τ and b the scattering is dominated by the inner repulsive core of the potential $V(r)$.

Having obtained an estimate of one or more of the functions $\tau_n(b)$ over some finite (and, we may hope, extensive) range of b, the task of obtaining the potential becomes that of solving Eq. (25) for the function $F_n(x)$ in the integrand.

The tool that is required for the solution of this problem is Dirichlet's formula for changing the order of integration in certain double integrals.[17] We do not need the most general form of this theorem, but write down here a special case:

$$\int_a^c dy \int_y^c \frac{f(x,y)dx}{(x-y)^{1/2}(y-a)^{1/2}} = \int_a^c dx \int_a^x \frac{f(x,y)dy}{(x-y)^{1/2}(y-a)^{1/2}}. \quad (60)$$

When $f(x,y)=f(x)$ is independent of y it follows that the double integral can be converted to a single integral:

$$\int_a^c dy \int_y^c \frac{f(x)dx}{(x-y)^{1/2}(y-a)^{1/2}} = \int_a^c dx f(x) \int_a^x \frac{dy}{(x-y)^{1/2}(y-a)^{1/2}} = \pi \int_a^c f(x)dx. \quad (61)$$

In order to exploit (61) we create the following transform of $\tau_n(b)$:

$$W_n(r) = \frac{2}{\pi} \int_r^\infty \frac{\tau_n(b)db}{(b^2-r^2)^{1/2}}. \quad (62)$$

Inserting the right-hand side of (25) into (62) and applying (61) we find immediately that

$$W_n(r) = -\int_{r^2}^\infty F_n(x)dx = \frac{1}{(n+1)!} \frac{d^n}{d(r^2)^n} [r^{2n} V^{n+1}(r)]. \quad (63)$$

In particular,

$$W_0(r) = V(r). \quad (63a)$$

This procedure is intimately related to Firsov's, which consists in obtaining the deflection function $\Theta(E,b)$ at a fixed energy E, constructing the transform $W(E,s)$, and evaluating it:

$$W(E,s) = \frac{2E}{\pi} \int_s^\infty \frac{\Theta(E,b)db}{(b^2-s^2)^{1/2}} = -E \int_{s^2}^\infty F(x)dx = 2E \ln[r(E,s)/s]. \quad (64)$$

From this one immediately finds $s(E,r)$, which leads to $V(r)$ because of Eq. (17):

$$s^2(E,r) = r^2[1 - V(r)/E]. \quad (64a)$$

In some cases of scattering in symmetric systems, it is possible to obtain experimental information about the action $A(E,\theta)$, or about the difference δA between the actions for scattering in two different molecular states. The resulting information is best analyzed experimentally through the reduced variable

$$a(E,\tau) = (E/2\mu)^{1/2} A(E,\theta), \quad (65)$$

from which the limiting function $a_0(\tau)$ [and sometimes higher functions $a_n(\tau)$] can be estimated. Because of Eq. (3a), we can differentiate to find

$$b(E,\tau) = -\partial a(E,\tau)/\partial\tau, \quad b_n(\tau) = -da_n(\tau)/d\tau, \quad (66)$$

which can be inverted to yield the functions $\tau_n(b)$. The remainder of the inversion procedure is identical with what has gone before.

In the development of Eq. (62) we have ignored the embarrassing fact that the integrations needed to construct $W_n(r)$ must be carried out to infinity in b, while the functions $\tau_n(b)$ can at best be considered known only out to some finite limit R. In that case it is necessary to use a judicious extrapolation of the integrand in order to perform the inversion successfully. This problem arises in any application of Firsov's method, and the large range of b (or τ) made available by the reduced coordinate system makes a more reliable extrapolation possible than in other methods. On the other hand, if the integrals of (62) are carried only to a finite upper limit the result will be to underestimate $W_n(r)$, which enables us to establish a firm lower (or upper) bound for the functions sought. As an example, let us consider the case of $W_0(r)$, recognizing furthermore that we often will know only the lower bound given by (59) for the function $\tau_0(b)$. We can then write

$$W_0(r,b_{\max}) = \frac{2}{\pi} \int_r^{b_{\max}} \frac{\tau_0(b,\tau^*)db}{(b^2-r^2)^{1/2}} < \frac{2}{\pi} \int_r^{b_{\max}} \frac{\tau_0(b)db}{(b^2-r^2)^{1/2}} < W_0(r) = V(r). \quad (67)$$

Here $b_{\max}$ is the largest value of b found in the integration of (58), and so corresponds to $\tau_{\min}$, the smallest value of τ in the measured range, while τ^* is the upper limit of this range.

[17] Reference 12a, p. 77.

3. Analysis of Interference Data

In practical cases where interference patterns are measured in forward scattering it is often impossible to deduce the action $A(E,\theta)$ associated with scattering in a single state. Instead, the patterns observed represent the interference between two or more scattering amplitudes of the form of Eq. (1), each with its own action $A_i(E,\theta)$ derivable from its own potential $V_i(r)$. The oscillating part of the observed cross section,

$$\sigma(E,\theta)=\tfrac{1}{4}|f_1(E,\theta)+f_2(E,\theta)|^2, \tag{68}$$

is of the form

$$\cos[2\pi N(E,\tau)], \tag{68a}$$

where

$$N(E,\tau)=[A_1(E,\tau)-A_2(E,\tau)]/h. \tag{69}$$

By following the oscillations as E is varied over a wide range, it is possible to determine N absolutely and not merely modulo π. As we saw in Eqs. (27) and (65), the proper reduced action variable is A multiplied by a velocity, so the experimental values of $N(E,\tau)$ are best handled by plotting the reduced variable

$$\delta a(E,\tau)=(E/2\mu)^{1/2}hN(E,\tau) \tag{69a}$$

against τ. There results a series of curves at different values of E peeling away from the common asymptote $\delta a_0(\tau)$, the first term in the series

$$\delta a(E,\tau)=\sum_{n=0}^{\infty}\epsilon^n\delta a_n(\tau). \tag{69b}$$

The precision with which the oscillations of an interference pattern can be located means that the function $\delta a_0(\tau)$ [and possibly higher functions $\delta a_n(\tau)$] may contain much more information than is available in the measured amplitudes of the cross section (the envelopes of the oscillating pattern, for instance). It is therefore important to exploit $\delta a_0(\tau)$ fully in extracting information about the interactions. As Everhart[4] and Russek[18] have earlier noted, $\delta a_0(\tau)$ is closely connected with the difference potential $\delta V(r)$ and provides much information about it.

Since $\delta a_0(\tau)$ represents the difference between two functions arising from two different potentials, we cannot proceed directly as in Eq. (65a) to obtain a relationship between τ and a single impact parameter. However, if we assume momentarily that we know something about the individual functions $a_0^1(\tau)$ and $a_0^2(\tau)$ whose difference is $\delta a_0(\tau)$ and whose average is $\bar{a}_0(\tau)$,

$$\bar{a}_0(\tau)=\tfrac{1}{2}[a_0^1(\tau)+a_0^2(\tau)],\quad \delta a_0(\tau)=a_0^1(\tau)-a_0^2(\tau), \tag{70}$$

we see that an average impact parameter can be derived,

$$\bar{b}_0(\tau)=-d\bar{a}_0/d\tau, \tag{70a}$$

from which in turn an inverse function can be obtained,

$$\bar{\tau}_0(b). \tag{70b}$$

This gives the average reduced scattering angle as a function of a single impact parameter. Following the notation of previous sections, and assuming that any difference function δf_0 is smaller than the associated average function $\bar{f}_0$ so that Taylor series expansions in δf_0 are allowed, we can now formally define the function $\delta\alpha_0(b)$ and deduce:

$$\begin{aligned}\delta\alpha_0(b)&=a_0^1[\bar{\tau}_0(b)+\tfrac{1}{2}\delta\tau_0(b)]-a_0^2[\bar{\tau}_1(b)-\tfrac{1}{2}\delta\tau_0(b)]\\&=\delta a_0(\bar{\tau}_0(b))+(d\bar{a}_0/d\tau)_{\bar{\tau}_0(b)}\delta\tau_0(b)+\cdots.\end{aligned} \tag{71}$$

Using (3a) we thus find, to first order in the difference functions,

$$\delta a_0(\bar{\tau}_0(b))=\delta\alpha_0(b)+b\delta\tau_0(b). \tag{72}$$

The purpose of this tedious manipulation was to connect the observed function $\delta a_0(\tau)$ with the potentials, which can be written as the average $\bar{V}$ and the difference δV.

By Eqs. (23), (25), and (28) we see that the functions $\alpha_0{}^i$ and $\tau_0{}^i$ are linear in the potentials, so that the right-hand side of (72) is a functional of $\delta V(r)$ alone:

$$\begin{aligned}\delta\alpha_0(b)+b\delta\tau_0(b)&=\int_{b^2}^{\infty}(x-b^2)^{1/2}\delta F_0(x)dx\\&=-\frac{1}{2}\int_{b^2}^{\infty}\frac{\delta V(x^{1/2})}{(x-b^2)^{1/2}}dx.\end{aligned} \tag{73}$$

We know the function on the left-hand side of (72) as a function of τ; to convert it to a function of b, we need to know $\bar{\tau}_0(b)$, which depends only on the average potential $\bar{V}(r)$. Depending on circumstances, we may know $\bar{V}(r)$ well enough theoretically to make a reasonable calculation of $\bar{\tau}_0(b)$, or we may be able to evaluate the latter function experimentally from the average behavior of the cross section $\sigma(E,\tau)$. One way or another, we can now assume we know the left-hand side of (72) as a function of b, which we can equate with (73).

The ground has now been prepared for the final step of the inversion procedure, which we accomplish by constructing the transform $I_0(r)$ and applying the Dirichlet integration (61):

$$\begin{aligned}I_0(r)&=\frac{2}{\pi}\int_{r^2}^{\infty}\frac{\delta a_0[\bar{\tau}(b)]db^2}{(b^2-r^2)^{1/2}}\\&=-\int_{r^2}^{\infty}\delta V(x^{1/2})dx.\end{aligned} \tag{74}$$

The difference potential is obtained by differentiating

$$\delta V(r)=dI_0(r)/dr^2. \tag{74a}$$

[18] F. P. Ziemba and A. Russek, Phys. Rev. 115, 922 (1959).

4. The Backscattering Inversion

Where backscattering data are available, the inversion problem is considerably simpler than in the forward-scattering limit. By extrapolating the cross section $\sigma(E,\varphi)$ or the action $\mathcal{A}(E,\varphi)$ to $\varphi=0$ we can obtain the functions $\sigma_n(E)$, $\mathcal{A}_n(E)$, and from the $\sigma_n(E)$ it is easy to deduce the $\varphi_n(E)$ by (55a). If the inversion is carried out from the functions $\varphi_n(E)$ no intermediate calculations involving b need be made.

If we know one of the functions $\varphi_n(E)$, we construct the transform

$$M_n(U)=\frac{1}{2\pi}\int_0^U \frac{\varphi_n(E)dE}{E^{n+1/2}[U-E]^{1/2}}, \qquad (75)$$

insert (40) and apply (61), from which we find

$$M_n(U)=-\int_0^U G_n(V)dV$$

$$=\frac{(-)^n}{(2n+1)n!}\frac{d^n}{dU^n}[r^{-(2n+1)}(U)]. \qquad (75a)$$

In particular,

$$M_0(U)=1/r(U). \qquad (75b)$$

Similarly from the $A_n(E)$ of Eq. (43) we can construct

$$N_n(U)=\frac{1}{\pi(2\mu)^{1/2}}\int_0^U \frac{A_n(E)dE}{E^n[U-E]^{1/2}}, \qquad (76)$$

from which we find

$$N_0(U)=-\int_0^U H_0(V)dV=-\int_0^U r(V)dV \qquad (76a)$$

and

$$N_n(U)=-\int_0^U H_n(V)dV=\frac{(-)^{n+1}}{n!}\frac{d^{n-1}}{dV^{n-1}}[r^{-2n+1}(V)] \quad \text{for } n\neq 0. \qquad (76b)$$

The backscattering inversion is intimately related to Hoyt's inversion procedure,[19] which formed the basis for Firsov's work and which is in turn related to the Rydberg-Klein-Rees method for deducing potentials from vibrational spectra. After integrating the cross section at fixed energy to obtain the relation between backscattering angle and angular momentum,

$$L^2(E,\varphi)=\frac{E}{2\mu}\int_0^\varphi \sigma(E,\varphi')d\varphi', \qquad (77)$$

one finds the function $\Phi(E,L)$, creates the transform $M(U,L)$, and evaluates it:

$$M(U,L)=\frac{1}{2\pi}\int_0^U \frac{\Phi(E,L)dE}{(U-E)^{1/2}}=-L(2\mu)^{-1/2}\int_0^U G(x)dx$$

$$=\frac{L}{(2\mu)^{1/2}r_0(U,L)}, \qquad (78)$$

where r_0 is the classical turning point for motion with the energy U and angular momentum L. From $r_0(U,L)$ the potential $V(r)$ can immediately be found.

F. EXAMPLES

1. The Screened Coulomb Potential

The exponentially screened Coulomb potential is one of the most useful approximations to the interactions in ion-atom scattering. Using it, potential parameters have been deduced by Lane and Everhart[15] from experiments on a number of scattering systems. Classical scattering cross sections have been computed exactly for this potential, and the small-angle reduced cross section has also been obtained. Lehmann and Leibfried[5] have given the first few terms in the forward expansion for the scattering angle. We can usefully supplement these results with the initial terms of expansions for the reduced action and the reduced cross section.

If the screened Coulomb potential is written

$$V(r)=(Bc/r)e^{-r/c}, \qquad (79)$$

it is convenient to express all the scattering parameters and functions in dimensionless form:

$$\beta=b/c=\sum_n \epsilon^n\beta_n(\tau), \qquad (80)$$

$$\epsilon=B/E, \qquad (81)$$

$$\tau=E\theta/B=\theta/\epsilon=\sum_n \epsilon^n\tau_n(\beta), \qquad (82)$$

$$\alpha=\left(\frac{E}{2\mu}\right)^{1/2}\frac{A(E,b)}{Bc}=\alpha(\epsilon,\beta)=a(\epsilon,\tau)=\sum_n \epsilon^n a_n(\tau), \qquad (83)$$

$$\rho=\frac{\theta\sin\theta\sigma(E,\theta)}{c^2}=\rho(\epsilon,\tau)=\sum_n \epsilon^n\rho_n(\tau). \qquad (84)$$

Lehmann and Leibfried give the first 3 terms of (82):

$$\tau_0(\beta)=K_1(\beta),$$
$$\tau_1(\beta)=-K_1(2\beta),$$
$$\tau_2(\beta)=\frac{9}{8}\left\{\left[1-\frac{2}{9\beta^2}\right]K_1(3\beta)-\frac{1}{\beta}K_0(3\beta)\right\}. \qquad (82a)$$

The first term in the expansion of $\beta(\tau,\epsilon)$ is identically the inverse of $\tau_0(\beta)$, i.e., the function $\beta_0(\tau)$ satisfying the equation

$$\tau=K_1(\beta_0). \qquad (80a)$$

[19] F. C. Hoyt, Phys. Rev. 55, 664 (1939).

For brevity, whenever we write β_0 hereafter we shall imply just this function $\beta_0(\tau)$. Thus, the function $\beta_1(\tau)$ is

$$\beta_1(\tau)=\frac{-\beta_0 K_1(2\beta_0)}{\beta_0 K_0(\beta_0)+K_1(\beta_0)}. \tag{80b}$$

The first two terms of (84) are given by

$$\rho_0(\tau)=\frac{\beta_0^2 K_1(\beta_0)}{\beta_0 K_0(\beta_0)+K_1(\beta_0)} \tag{84a}$$

and

$$\rho_1(\tau)/\rho_0(\tau)=\psi_1(\tau)=\frac{1}{\beta_0 K_0(\beta_0)+K_1(\beta_0)}$$
$$\times\{2\beta_0 K_0(2\beta_0)-K_1(2\beta_0)[1+(1+\beta_0^{-2})\rho_0(\tau)]\}. \tag{84b}$$

To express the reduced action we obtain first the functions

$$\alpha_0(\beta)=-[K_0(\beta)+\beta K_1(\beta)],$$
$$\alpha_1(\beta)=\tfrac{1}{2}[K_0(2\beta)+2\beta K_1(2\beta)], \tag{85}$$

and then the final result,

$$a_0(\tau)=-[K_0(\beta_0)+\beta_0 K_1(\beta_0)], \tag{83a}$$

$$a_1(\tau)=\tfrac{1}{2}K_0(2\beta_0). \tag{83b}$$

In Table I we present the result of an evaluation of the functions (80a), (83a), (84a), and (84b). In addition we can find limiting expressions valid at large and small τ by using the expansion formulas for the Bessel functions. When β is small and τ is large, we find

$$\rho_0(\tau)=\tau^{-2}-\tau^{-4}[2\ln(2\tau)-0.6554]+\cdots, \tag{86}$$

$$\beta_0(\tau)=\tau^{-1}-\tau^{-3}[\tfrac{1}{2}\ln(2\tau)-0.0386]+\cdots. \tag{86a}$$

The first term of (86) shows the characteristic Coulomb behavior of the reduced cross section, a special case of Eq. (58), and the higher terms show the incipient deviation due to the exponential screening. At large β, where τ is small, we can use the asymptotic expansions to obtain the equations

$$\rho_0(\beta)=\beta-\tfrac{1}{2}-\frac{53}{32\beta}\cdots, \tag{87}$$

$$\tau_0(\beta)=(\pi/2\beta)^{1/2}e^{-\beta}\left[1+\frac{3}{8\beta}-\frac{12}{128\beta^2}\cdots\right], \tag{87a}$$

which can be inverted to get the expressions

$$\beta_0(\rho)=\rho+\tfrac{1}{2}+\frac{53}{32\rho}\cdots, \tag{87b}$$

$$\tau_0(\rho)=e^{-\rho}\left(\frac{\pi}{2e\rho}\right)^{1/2}\left[1-\frac{49}{32\rho}-\frac{2545}{2048\rho^2}\cdots\right]. \tag{87c}$$

TABLE I. Reduced scattering functions: screened Coulomb potential.

τ	ρ_0	β	ψ_1	a_0	Z_0
		0.00			0.5000
5.000×10^{1}	3.995×10^{-4}	0.02	-9.931×10^{-1}	5.003×10^{1}	0.4821
2.492	1.592×10^{-3}	0.04	−9.776	2.506	0.4646
1.656	3.563	0.06	−9.566	1.674	0.4491
1.238	6.296	0.08	−9.321	1.259	0.4347
9.855×10^{0}	9.757	0.10	−9.045	1.010	0.4212
7.020	1.880×10^{-2}	0.14	−8.452	7.255×10^{0}	0.3967
4.776	3.726	0.20	−7.519	5.127	0.3643
3.058	7.924	0.30	−6.018	3.468	0.3190
2.060	1.449×10^{-1}	0.42	−4.482	2.509	0.2745
1.430	2.366	0.56	−3.083	1.895	0.2316
1.009	3.559	0.72	−1.941	1.469	0.1908
7.164×10^{-1}	5.023	0.90	−1.082	1.155	0.1523
4.932	6.940	1.12	-4.468×10^{-2}	8.917×10^{-1}	0.1124
3.403	9.123	1.36	-6.765×10^{-3}	6.901	0.0775
1.981	1.271×10^{0}	1.74	1.804×10^{-2}	4.720	0.0264
9.982×10^{-2}	1.775	2.26	2.561	2.877	−0.0280
4.990	2.323	2.82	1.847	1.706	−0.0764
1.980	3.098	3.60	1.066	8.285×10^{-2}	−0.1321
9.938×10^{-3}	3.695	4.20	6.492×10^{-3}	4.743	−0.1697
4.943	4.317	4.82	3.761	2.662	−0.2039
4.048	4.490	5.00	3.203	2.250	−0.2134
1.993	5.133	5.64	1.777	1.236	−0.2441
1.345	5.496	6.00	1.265	8.805×10^{-3}	−0.2614
9.904×10^{-4}	5.780	6.28	9.743×10^{-4}	6.763	
7.000	6.093	6.60	7.204	5.004	−0.2869
4.546	6.494	7.00	4.921	3.427	−0.3035
2.652	6.996	7.50	2.867	2.134	−0.3231
1.554	7.500	8.00	1.876	1.327	−0.3423
9.120×10^{-5}	7.991	8.50	1.157	8.246×10^{-4}	−0.3596
5.364	8.493	9.00	7.110×10^{-5}	5.115	−0.3767
3.160	8.993	9.50	4.363	3.174	−0.3933
1.865	9.493	10.00	2.674	1.964	−0.4029
1.102	9.993	10.50			

We have included in Table I one further quantity which will prove of some value in later applications. It is a dimensionless parameter characterizing the motion in τ of a feature that depends on the energy in such a way that the classical turning point r_0 remains fixed. If we define

$$Z(\epsilon,r_0)=\tau^{-2}(\partial\tau/\partial\epsilon)_{r_0} \tag{88}$$

and expand in powers of ϵ, the first term is

$$Z_0(\beta)=\tau_0^{-2}(\beta)\left[\tau_1(\beta)-\tfrac{1}{2}\beta\frac{V(\beta)}{B}\frac{d\tau_0(\beta)}{d\beta}\right], \tag{88a}$$

where we may insert $\beta\cong r_0/c$. This parameter is of use in connection with the detailed study of curve-crossing perturbations whose effect is concentrated near a fixed value of the classical turning point r_0.[10]

The data in Table I can be used to construct the two-term expansion of $\rho(\epsilon,\tau)$, Eq. (84b), for various values of ϵ. We have carried out this evaluation in a number of cases for which exact calculations were made by Everhart, Stone, and Carbone.[20] Qualitatively, their

[20] E. Everhart, G. Stone, and R. J. Carbone, Phys. Rev. 99, 1287 (1955).

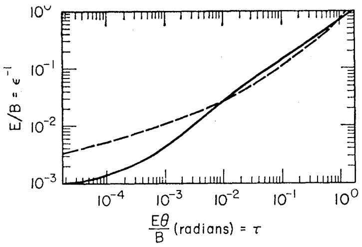

FIG. 1. Convergence behavior for the screened Coulomb potential. The forward-scattering approximation converges in the region to the left of the solid line. The backward-scattering expansion converges in the region to the right of the dashed line.

results parallel the prediction of (84b) and Table I, showing that the correction $\rho_1(\tau)=\rho_0(\tau)\psi_1(\tau)$ is positive at small τ and negative at large τ. Taking as an example the scattering at 36°, in the range $0.1\leq\epsilon\leq 10$ the maximum deviation between $\rho_0(\tau)$ and the exact $\rho(\tau,\epsilon)$ is about 17%; when the second term $\epsilon\rho_1(\tau)$ is included this deviation is reduced to less than about 3% in all cases.

Because of the awkard series inversions that are involved in the calculation, it will probably be quite difficult to obtain general convergence criteria for series like (83) and (84). However, Leibfried and Plesser[5] have developed such criteria for the forward and backward expansions of the function $\tau(\epsilon,\beta)$. They give a plot showing the domains of convergence of the two expansions in the (ϵ,β) plane. By using the exact classical integration to evaluate $\tau(\epsilon,\beta)$, we have mapped these domains in the (ϵ,τ) plane, Fig. 1. Even though the convergence properties of each series may be different, for lack of a better criterion we may look to Fig. 1 for some warning about the regions where our expansions should be treated with suspicion.

2. The Simple Power Law

If the potential has the form

$$V/B=(c/r)^{\mu}, \tag{89}$$

the reduced scattering functions can be put in form of Eqs. (80) to (84). Lehmann and Leibfried[5] have shown that the reduced scattering angle (82) involves the functions

$$\tau_n(\beta)=(-)^n\beta^{-\mu(n+1)}\frac{\Gamma[\frac{1}{2}(n+1)\mu+\frac{1}{2}]\Gamma[\frac{1}{2}]}{\Gamma[n+2]\Gamma[\frac{1}{2}(n+1)\mu-n]}$$
$$=(-)^n\beta^{-\mu(n+1)}C_n(\mu). \tag{90}$$

Similarly we find

$$\alpha_n(\beta)=(-)^{n+1}\mu(n+1)C_n(\mu)\beta^{-[\mu(n+1)-1]}. \tag{91}$$

The first two terms of the cross section then are given by

$$\rho_0(\tau)=\mu^{-1}[C_0(\mu)/\tau]^{2/n}, \tag{92}$$

$$\psi_1(\tau)=\frac{\rho_1(\tau)}{\rho_0(\tau)}=\frac{\mu-2}{\mu}\frac{C_1(\mu)}{C_0^2(\mu)}\tau, \tag{92a}$$

and the higher terms ψ_n are proportional to τ^n, so that we can write

$$\rho(\tau,\epsilon)/\rho_0(\tau)=1+\sum_{n=1}^{\infty}\theta^n D_n(\mu); \tag{92b}$$

it is significant that this quantity is actually independent of ϵ. The parameter Z_0 is independent of τ:

$$Z_0(\mu)=\frac{\mu}{2\pi^{1/2}}\frac{\Gamma(\frac{1}{2}\mu)}{\Gamma(\frac{1}{2}(\mu+1))}\times\left[1-\frac{\Gamma(\mu+\frac{1}{2})\Gamma(\frac{1}{2}\mu)}{\mu\Gamma(\mu-1)\Gamma(\frac{1}{2}(\mu+1))}\right]; \tag{93}$$

as μ increases from 1, $Z_0(\mu)$ decreases from $\frac{1}{2}$, becoming negative for $\mu\gtrsim 3$.

3. A Numerical Example

While some of the common analytic potentials lead to readily integrable expansions for the forward-scattering expansion, this is much less true for the backward expansion. Here the Coulomb potential is an exception, but the expansions are not very valuable in that case since they can be immediately summed to get the well-known Rutherford formulas. In order to test the backward expansion, we have carried out the integrations numerically for the first two terms of both the forward and the backward expansions, using two fairly realistic potentials, namely, the *gerade* and *ungerade* potentials we have used earlier in the analysis of scattering in the system He^++He.[9] We have carried out the comparisons for three energies, namely, 15, 50, and 300 eV, for which we had already made an exact classical computation. Figure 2 shows the comparison for the classical action $a(\tau)$ at 300 eV. The results are similar at 50 and 15 eV, the principal conclusions being that the two-term ap-

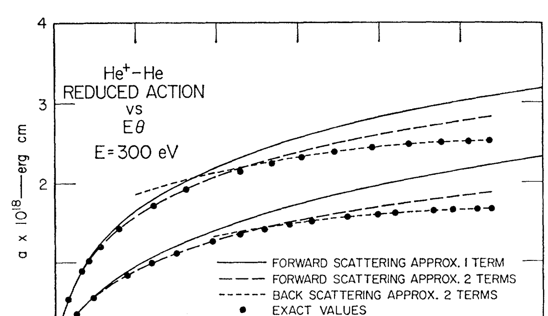

FIG. 2. The reduced action computed by various approximations for the He^+-He potential at 300 eV. The upper set of curves are from the gerade potential and the lower set from the ungerade potential.

proximation nowhere deviates from the exact results by more than $2\frac{1}{2}\%$ and that the crossover point where the backward expansion becomes more reliable than the forward one occurs in all cases at about 90°.

In view of the attractiveness of using just the first term of the forward expansion in the inversion to obtain potentials from experiments, it is important to take note of the range in θ, at each energy, over which we can rely on a one-term expression. If we can tolerate at 10% error in $a_0(\tau)$ as an estimate of $a(\epsilon,\tau)$, the one-term expression $a_0(\tau)$ can safely be used out to angles of about 45° in all the cases tested. However, in the *ungerade* case at 15 eV this permitted range has also a lower bound at about 25° (about twice the rainbow angle), below which the effects of the attractive well make the approximation unreliable.

G. APPLICATIONS

This paper has been concerned with the development and justification of certain expansions which can be used as tools for the analysis and interpretation of data from differential scattering experiments. We intend to make use of these tools in forthcoming publications. Here we shall briefly outline some of the applications we have in mind.

In the presentation of data from the usual scattering experiments in which forward scattering is measured, there are great advantages to using the reduced scattering angle $\tau = E\theta$ and cross section $\rho = \theta \sin\theta\sigma(\theta)$. Indeed as differential-scattering experiments become more common, we suspect that it will soon become desirable to adopt a standard method of presentation of their results and we urge our colleagues in this field to consider this set of variables for that purpose. In an analysis which we are now completing of differential scattering in the systems $He^+ + Ne$ and $He^+ + Ar$ this coordinate system allows a uniform presentation and compilation of the scattering data obtained by Aberth and Lorents[11] along with that obtained by Fuls, Jones, Ziemba, and Everhart,[21] ranging in laboratory energies from 10 eV to 100 keV and ranging over a span of more than 10^5 in the reduced scattering angle. Both because the resulting curves are not so steep as the cross section σ itself and because of the close connection between τ and the classical turning point, this coordinate system reveals several features that are obscured by the presentation of cross-section data in its original form.

In conducting further analysis of the experiments on $He^+ + He$, we expect to exploit the backward-scattering expansion in connection with the nuclear symmetry oscillations in the interference pattern. The interference peaks also give information on the relative phases of the scattering amplitudes and their analysis requires the employment of the expansions for the reduced action as well as the reduced cross section. Using these reduced data we expect to be able to employ the inversion procedures we have described here to extract the potentials from the scattering data alone.

The exponentially screened Coulomb potential is the simplest analytical form that can be used to represent the interaction over a very wide range of internuclear distances. In the cases of $He^+ + Ne$ and $He^+ + Ar$ we have found that the reduced cross section fits the screened Coulomb form quite well over a very large span of the reduced angle. As a result, it is possible also to associate a unique value of the impact parameter b with each value of the reduced angle τ. We are thus able to locate various features of the interactions such as crossing points entirely from the empirical data provided by the scattering.

Note added in proof. Dr. Frank Chilton has kindly called our attention to the connection between the variables (ρ,τ) of the forward impact expansion and the variables usually employed in the analysis of elastic scattering at very high energies. In that case, the independent variable is taken as the 4-momentum transfer squared, t; with equal masses and in the limit of small angle θ and high relative kinetic energy E, this is related to τ^2:

$$-t = 4p^2_{\text{rel}}c^2 \sin^2\theta/2 \to p^2_{\text{rel}}c^2\theta^2 = E(E+2\mu c^2)\theta^2 \to E^2\theta^2 = \tau^2. \quad (94)$$

In elastic scattering at high energies it is found experimentally that the function

$$d\sigma_{\text{el}}/dt = \sigma_{\text{el}} A e^{At}. \quad (95)$$

For all known examples, σ_{el} is independent of energy and A may be either independent of energy or have a slight energy dependence. This fact appears to be a consequence of an expansion theorem, since we have in the limit

$$\frac{d\sigma_{\text{el}}}{dt} \to \frac{\rho(\tau,E)}{2\tau^2} \to \frac{\rho_0(\tau)}{2\tau^2} + \frac{\rho_1(\tau)}{2\tau^2 E} \cdots. \quad (96)$$

It would appear to be useful to seek the proper generalization of the small-angle expansion to the case of classical relativistic scattering.

APPENDIX A

The integrals needed in evaluating the functions of Eqs. (47) to (51) can be written in various forms. A version convenient for quadrature by various methods including Gauss-Mehler is given here. It must be remembered that $V = V(x^{1/2})$.

$$\tau_0(b) = -b \int_{b^2}^{\infty} \frac{dV}{dx} \frac{dx}{(x-b^2)^{1/2}}, \quad (A1)$$

[21] E. N. Fuls, P. R. Jones, F. P. Ziemba, and E. Everhart, Phys. Rev. **107**, 704 (1957).

$$\alpha_0(b)=\int_{b^2}^{\infty}\frac{dV}{dx}\frac{xdx}{(x-b^2)^{1/2}}, \quad \text{(A2)}$$

$$\tau_0'(b)=-b^{-1}\alpha_0'(b)=2\int_{b^2}^{\infty}\frac{d^2V}{dx^2}(x-2b^2)\frac{dx}{(x-b^2)^{1/2}}, \quad \text{(A3)}$$

$$\tau_0''(b)=4b\int_{b^2}^{\infty}\frac{d^3V}{dx^3}(3x-4b^2)\frac{dx}{(x-b^2)^{1/2}}, \quad \text{(A4)}$$

$$\tau_1(b)=\frac{b}{2}\int_{b^2}^{\infty}\frac{d^2V^2}{dx^2}(3x-4b^2)\frac{dx}{(x-b^2)^{1/2}}, \quad \text{(A5)}$$

$$\alpha_1(b)=-\frac{1}{3}\int_{b^2}^{\infty}\frac{d^2V^2}{dx^2}(x^2+4xb^2-8b^4)\frac{dx}{(x-b^2)^{1/2}}, \quad \text{(A6)}$$

$$\tau_1'(b)=-\int_{b^2}^{\infty}\frac{d^3V^2}{dx^3}(x^2-8xb^2+8b^4)\frac{dx}{(x-b^2)^{1/2}}. \quad \text{(A7)}$$

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Approach to the N-Body Problem with Hard-Sphere Interaction Applied to the Collision Domains of Three Bodies*

G. Sandri and A. H. Kritz
Aeronautical Research Associates of Princeton, Incorporated, Princeton, New Jersey
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We present a simple numerical method for determining the phase-space domains that correspond to a chain of successive collisions among N hard spheres. The method is applied to the three-body problem, and it is shown to yield with ease results that are difficult to obtain analytically. The exact phase-space domains corresponding to the allowed collision chains among three spheres are described in full detail for the coplanar case.

I. INTRODUCTION

Considerable attention has been given recently to the density dependence of gaseous transport coefficients.[1–6] The transport coefficients are of considerable physical importance since they fulfill a basic role in determining the macroscopic distributions of density, temperature, and flow velocity. For a gas in which only two-body interactions are operative, the transport coefficients satisfy "Maxwell's law"[7]; namely, the transport coefficients are density-independent. Density dependence of the transport coefficients results when three-body interactions are included.

Three-body interactions are essential to describe transport properties in two types of gases, gases which are "dense" ($p\geq 5$ atm, $T=300°$K) and gases in which chemical transmutations occur. The understanding of dense monatomic gases requires knowledge of the bulk viscosity coefficient. This transport coefficient as deduced from the Boltzmann equation vanishes identically for monatomic gases, since this equation includes only binary collisions. With regard to reacting gases, one can readily verify that even the simplest association-dissociation reaction requires a three-body collision as a consequence of energy and momentum balance.

The recent interest in the density dependence of transport properties was triggered by the discovery[8] in 1961 that Bogoliubov's method[9] for systematizing the kinetic theory yields divergent results for all nonequilibrium density-dependent effects in neutral gases. Moreover, Bogoliubov's method, which is of sufficient scope to describe ionized gases, yields divergent results for the plasma properties when calculations are extended beyond the lowest order in the plasma parameter $(n\lambda_D{}^3)^{-1}$.

Bogoliubov's technique yields formally the effects of n-body collisions on the transport coefficients. But, by giving this formal solution, Bogoliubov imposes an asymptotic behavior on the transport properties ("functional assumption") which, in view of the convergence difficulties, contradicts three-body dynamics.

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