CLASSICAL AND QUANTAL SCATTERING
I THE CLASSICAL ACTION*

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ABSTRACT

Classical scattering is based on the action $A - S_0$, the action over the actual trajectory and S_0 is over the equivalent without interaction. For 2-body spherical potential scattering $A = \Delta(L,E) - L\Theta$, where Θ is the deflection angle and Δ is the classical phase, the classical limit of $2\hbar\delta_l(E)$. A new, rapidly convergent expression is given for $\Delta(L,E)$. From this is derived a convergent expansion in $1/E$ valid for fixed $L \neq 0$, and an equivalent form in $1/L$ valid for fixed E. The lowest term in $1/L$ agrees with Massey and Mohr, and higher terms are evaluated.

A. INTRODUCTION

Atomic scattering theory is securely based in quantum mechanics. Just as properly, many problems are best treated, to a very good approximation, by classical methods. The quantal justification of this procedure is well understood[1,2], but the profound and intimate connection between the quantal and classical formulations has not always been sufficiently recognized.

All the formulas of classical scattering can be derived from a classical action A that can be defined for any collision.[3] For spherical symmetry this is closely related to the classical phase $\Delta(L,E)$, the limit of the quantal phase shift in the form $2\hbar\delta_l(E)$. Using the action A it is natural to define the classical scattering amplitude by $F(\Theta,E) = \sigma_{cl}^{1/2} e^{iA/\hbar}$. These definitions will be justified and discussed in Section B.

In order to exploit the parallel further, I intend[4] to show the quantal scattering amplitude can be summed so that the classical result is the leading term and the major quantal corrections can be computed directly and easily. Naturally, the simplest example on which to work out this program

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is 2-body isotropic potential scattering. In order to pave the way for that, Section C of this paper includes a brief restatement of the relevant classical expressions from that case. They can be put into a form that may be new and has some merits of rapid convergence and simplicity. The resulting expressions make it easy to obtain expansions in $1/E$ valid at fixed non-zero L and in $1/L$ valid at fixed E. These results have their own value independent of their use in II, and some examples will be worked out.

B. CLASSICAL ACTION AND SCATTERING AMPLITUDE

If the classical trajectory is known for a scattering event, the corresponding action is

$$S = \int \mathbf{p} \cdot \mathbf{dq} \quad . \tag{1}$$

The integral diverges because of the tail at large r where the interaction usually vanishes, so it is natural to subtract the standard action for the equivalent collision without interaction,

$$S_0 = \int \mathbf{p}_0 \cdot \mathbf{dq}_0 \tag{2}$$

The result of the subtraction is the collision action

$$A = S - S_0 \quad . \tag{3}$$

Obviously, if the collision is inelastic S_0 must be taken in two parts: an incoming part matching the initial trajectory and taken up to the point of closest approach, and an outgoing part matching the final trajectory and beginning at the point of closest approach of the comparison trajectory. Further, this definition of A fails to converge for the coulomb interaction, so the argument is limited to forces of shorter range $[e.g., \lim_{r \to \infty} r^2 V(r) = 0]$.

When the collision is governed by a simple isotropic 2-body potential $V(r)$, the actions S and S_0 can be written in terms of radial and azimuthal components:

$$S = \int p_r dr + L \int_0^{\pi - \Theta} d\theta \quad , \tag{4}$$

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$$S_0 = \int p_{r,0} dr + L \int_0^{\pi} d\theta , \qquad (5)$$

where Θ is the deflection angle of the actual trajectory (Θ is not necessarily positive). We then get

$$A = \Delta(E,L) - L\Theta , \qquad (6)$$

where

$$\Delta(E,L) = \int p_r dr - \int p_{r,0} dr \qquad (7)$$

can be called the classical phase since it represents the limit of the quantal phase shift $\delta_l(E)$ in the sense

$$\Delta(E,L) = \lim_{h \to 0} 2\hbar\delta_l(E); \quad \left(l + \frac{1}{2}\right)\hbar \to L . \qquad (8)$$

It is well known that the classical scattering angle Θ, differential cross section σ, and collision lifetime Q depend simply on $\Delta(L,E)$:

$$\Theta = \frac{\partial \Delta}{\partial L} = \Theta(L,E), \qquad (9)$$

$$\sigma = \frac{\pi}{2\mu E} \left| \frac{\partial(L^2)}{\partial\Theta} \right| = \frac{\pi L}{\mu E} \left| \frac{\partial^2 \Delta}{\partial L^2} \right|^{-1} , \qquad (10)$$

$$Q = \frac{\partial \Delta}{\partial E} . \qquad (11)$$

Inverting Eq. (9) we find

$$L = L(E,\Theta) . \qquad (12)$$

As a consequence of Eqs. (9) and (6) we can assert that

$$A = A(E,\Theta) , \quad \frac{\partial A}{\partial L} = 0 . \qquad (13)$$

It is natural to pursue the implication of Eq. (8) by defining the classical limit of the scattering matrix **S**.

$$\mathbf{S}_{cl} = e^{i\Delta(L,E)/\hbar} \ .$$ (14)

This construct is very reminiscent of the classical wave function,

$$\psi_{cl} = e^{iS/\hbar} \ ,$$ (15)

where S is the classical action.[5] A form of ψ_{cl} is the basis of Feynman's treatment of quantum mechanics,[6] and ψ_{cl} has recently been used to good effect by Motz.[7] Expressions like (15) go back to Schrödinger's demonstration of the relation between his equation and the Hamilton-Jacobi equation, and the same form is encountered in the WKB approximation to the wave function.

It is therefore no suprise that $\Delta(L,E)/2\hbar$ is identical to the lowest order WKB approximation to the phase shift $\delta_l(E)$. However, in order to see clearly the structure of the physics underlying these expressions, it seems to me of great importance to look upon $\Delta(L,E)$ as an important classical quantity in its own right, and not to submerge it from view under the time-honored but demeaning label of "WKB phase shift."

It remains to define the classical limit of the scattering amplitude. It is helpful first to write the quantal amplitude formally as

$$f(E,\theta) = e^{iA_{qu}/\hbar} \ ,$$ (16)

where A_{qu} is expanded in powers of $\hbar$:

$$A_{qu} = A + \hbar A_1 + \hbar^2 A_2 \ldots,$$ (17)

A being the classical term of Eq. (6). The simplest classical analog of (16) is

$$F_0 = e^{iA/\hbar} \ ,$$ (18)

but it is obviously preferable to seek a form such that

$$|F|^2 = \sigma(E,\boldsymbol{\theta}) \ .$$ (19)

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One is therefore led to look at the next term in the expansion (17), since (19) would be satisfied if

$$\text{Im}(A_1) = \frac{1}{2} \ln \sigma_{cl} \quad .$$
(20)

We then find that

$$F_1(E,\Theta) = \sigma^{\frac{1}{2}} e^{i[(A/\hbar)+\alpha]} \quad ,$$
(21)

where

$$\alpha = \text{Re}(A_1) \quad .$$
(22)

Applying the considerations of semiclassical scattering theory,[2] α can be shown to depend on $\Delta(L,E)$:

$$\alpha = \frac{5\pi}{4} + \frac{\pi}{2} \left(\frac{\Theta}{|\Theta|}\right) + \frac{\pi}{4} \left(\frac{\Delta''}{|\Delta''|}\right) \quad ,$$
(23)

where $\Delta'' = \partial^2\Delta/\partial L^2$. Since F_1 does not include any terms of higher than *zeroth* order in $\hbar$, I shall term it simply the classical scattering amplitude. (When the distinction must be made, F_0 can be called the primitive, and F_1 the refined, classical amplitude.) When there is a single term of this form, observations are always confined to the cross section given by (19) which is purely classical. Semiclassical scattering appears in its most primitive form when 2 or more terms of the form (21) are added, which results in nonclassical interference effects in the square of the sum.

It should be pointed out that the expansion of A in powers of $\hbar$, Eq. (17), is suggestive only and probably does not represent a convergent series mathematically. This is just like the situation encountered in the well-known breakdown of the WKB expansion of the wave function in the neighborhood of a classical turning-point. This deficiency in the wave function can be remedied by the use of different approximating functions in the connection region, and one of the purposes of the following paper, II, is to show what kind of corrections are needed to improve the scattering amplitude. In general the amplitude will not appear as an analytic function of $\hbar$ near $\hbar = 0$, and the same is true of related quantities such as the phase shift, the collision lifetime, or the density of states. For this

reason, power series expansions may not be at all appropriate for studying quantal corrections to the classical transport coefficients or virial coefficients. This phenomenon is quite general, and has been found to occur also in connection with the Thomas-Fermi formula for the particle density in a fermion system.[8]

Despite this failure of the power series expansion, the lowest order term obtained in a formal expansion like (17) usually does give a very good approximation for most regions of the variables involved. For example, the WKB wave function is usually very satisfactory far away from the classical turning points. Similarly, the classical scattering amplitude is usually very good (for large enough energies) except for θ close to 0 and π or near a rainbow angle, and the classical phase shifts and collision lifetimes are very good except for energies close to the region of orbiting or near resonances of an attractive potential.[9]

C. THE CLASSICAL PHASE $\Delta(L,E)$

1. INTEGRAL FORMULAS

In this section I shall derive some formulas for the classical phase $\Delta(L,E)$ and its derivatives. $\Delta(L,E)$ can be cast into several alternative forms:

$$\Delta(L,E) = L\pi - 2p_\infty r_0 + 2 \int_{r_0}^{\infty} [p(r) - p_\infty] \, dr \tag{24}$$

$$= 2 \lim_{R \to \infty} \left\{ \int_{r_0}^{R} p(r) \, dr - \int_{b}^{R} p_0(r) \, dr \right\} \tag{24a}$$

$$= 2 \lim_{R \to \infty} \left\{ \int_{r_0}^{R} p(r) \, dr - \int_{b_1(R)}^{R} p_1(R,r) \, dr \right\} \tag{24b}$$

$$= \int_{r_0}^{\infty} p(r) \, \frac{r \dfrac{dV}{dr}}{E - V(r)} \, dr \quad . \tag{24c}$$

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Here the p's are radial momenta,

$$p^2(r) = 2\mu[E - V(r)] - \frac{L^2}{r^2} \quad , \tag{25}$$

$$p_0^2(r) = 2\mu E - \frac{L^2}{r^2} \quad , \tag{25a}$$

$$p_1^2(R,r) = 2\mu[E - V(R)] - \frac{L^2}{r^2} \tag{25b}$$

$$p_\infty^2 = 2\mu E, \quad p_R^2 = 2\mu[E - V(R)] \quad , \tag{25c}$$

and the turning points r_0, b, and $b_1(R) = b_1$ are defined by

$$L = r_0\{2\mu[E - V(r_0)]\}^{\frac{1}{2}} = bp_\infty = b_1(R)p_R \quad . \tag{26}$$

The connection between the Eqs. (24) and (24c) depends on the evaluation of the integral

$$F(R) = \int_b^R p_0(R)dr = p_\infty R \left(1 - \frac{b^2}{R^2}\right)^{\frac{1}{2}} - L\frac{\pi}{2} + L \sin^{-1}\frac{b}{R}$$

$$= p_\infty R - L\frac{\pi}{2} + O\left(\frac{b}{R}\right) \dots \tag{27}$$

and its replacement by a function with the same limiting behavior,

$$F'(R) = \int_{b_1}^R p_1(R,r)dr$$

$$= p_R\left[1 - \frac{b_1^2(R)}{R^2}\right]^{\frac{1}{2}} - L\frac{\pi}{2} + L \sin^{-1}\left[\frac{b_1(R)}{R}\right]$$

$$= L \int_1^{Rp_R/L} \frac{(x^2 - 1)^{\frac{1}{2}}}{x} dx \quad . \tag{28}$$

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The final connection with Eq. (24c) comes about because

$$F'(r_0) = 0,$$

$$\frac{dF'(r)}{dr} = p(r)\left(1 - \mu r \frac{dV}{dr}\{2\mu[E - V(r)]\}^{-1}\right) \quad . \tag{29}$$

The first form of Eq. (24) is the familiar one. The second shows how the phase shift is composed of the difference between two simple action integrals, one over the radial motion on the actual trajectory and another over the radial motion on a comparison trajectory with vanishing inter-action. In the third form the comparison trajectory is taken as force-free inside R, but with the constant potential $V'(r \leq R) = V(R)$. The last form shows the contribution to the phase shift from different regions of the trajectory, displaying explicitly the dependence on the radial force $- (dV/dr)$; this form has the computational advantage of converging rapidly at large r if the interaction is of short range.

The classical deflection function is well known to be a derivative of Δ:

$$\Theta(L,E) = \left(\frac{\partial \Delta}{\partial L}\right)_E = \pi - 2L \int_{r_0}^{\infty} \frac{dr}{r^2 p(r)} \tag{30}$$

$$= 2L \int_{b}^{\infty} \frac{dr}{r^2 p_0(r)} - 2L \int_{r_0}^{\infty} \frac{dr}{r^2 p(r)} \tag{30a}$$

$$= 2 \lim_{R \to \infty} \left\{ L \int_{b_1}^{R} \frac{dr}{r^2 p_1(R,r)} - L \int_{r_0}^{R} \frac{dr}{r^2 p(r)} \right\} \tag{30b}$$

$$= - L \int_{r_0}^{\infty} \frac{r \frac{dV}{dr}}{E - V(r)} \frac{dr}{r^2 p(r)} \tag{30c}$$

The last form shows the dependence of Θ on the radial force. It is equiv-alent to a form used by Firsov[10] in the study of the inverse problem, the

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deduction of the potential from the classical deflection. Since it converges more rapidly than the first form at large r, it is also useful for the direct problem. The classical collision lifetime is also a derivative of Δ:

$$Q(L,E) = \left(\frac{\partial \Delta}{\partial E}\right)_L - 2\mu \int_{r_0}^{\infty} [p^{-1}(r) - p_{\infty}^{-1}]\,dr - 2\mu r_0 p_{\infty}^{-1} \tag{31}$$

$$= 2\lim_{R\to\infty}\left\{\mu \int_{r_0}^{R} \frac{dr}{p(r)} - \mu \int_{b}^{R} \frac{dr}{p_0(r)}\right\} \tag{31a}$$

$$= 2\lim_{R\to\infty}\left\{\mu \int_{r_0}^{R} \frac{dr}{p(r)} - \mu \int_{b_1(R)}^{R} \frac{dr}{p_1(R,r)}\right\} \tag{31b}$$

$$= \mu \int_{r_0}^{\infty} \frac{\left(-\dfrac{dV}{dr}\right)[E - V(r) - L^2\mu r^2]}{[E - V(r)]^2 p(r)}\,dr \quad . \tag{31c}$$

The last form converges rapidly, and displays conveniently the analytical behavior of Q.

It is useful to introduce another form of these equations depending on reduced variables:

$$\rho = \frac{r}{r_0}, \quad U(r_0\rho) = \frac{V(r)}{E}$$

$$\left(\frac{L^2}{2\mu E r_0^2}\right) = 1 - U(r_0) \quad . \tag{32}$$

With these we can write:

$$\Delta(L,E) = [2\mu E]^{1/2} r_0 \int_{1}^{\infty} \frac{r_0 U'(r_0\rho)}{1 - U(r_0\rho)}\{[1 - U(r_0\rho)]\rho^2 - [1 - U(r_0)]\}^{1/2}\,d\rho \quad , \tag{33}$$

$$\Theta(L,E) = \pi - 2[1 - U(r_0)]^{\frac{1}{2}} \int_1^\infty \frac{d\rho}{\rho\{[1 - U(r_0\rho)]\rho^2 - [1 - U(r_0)]\}^{\frac{1}{2}}}$$

(34)

$$= -[1 - U(r_0)]^{\frac{1}{2}} \int_1^\infty \frac{r_0 U'(r_0\rho)}{1 - U(r_0\rho)} \{[1 - U(r_0\rho)]\rho^2 - [1 - U(r_0)]\}^{-\frac{1}{2}} d\rho \ ,$$

(34a)

$$Q(L,E) = -\left(\frac{\mu}{2E}\right)^{\frac{1}{2}} r_0 \int_1^\infty \frac{r_0 U'(r_0\rho)\{[1 - U(r_0 p)]\rho^2 - 2[1 - U(r_0)]\} d\rho}{[1 - U(r_0\rho)]^2 \{[1 - U(r_0\rho)]\rho^2 - [1 - U(r_0)]\}^{\frac{1}{2}}} \ .$$

(35)

Higher derivatives of Δ with respect to L can be obtained by differentiating with respect to r_0 and using

$$\left(\frac{\partial r_0}{\partial L}\right)_E = \frac{L r_0}{L^2 - \mu E r_0^3 U'(r_0)} = \left(\frac{2}{\mu E}\right)^{\frac{1}{2}} \frac{[1 - U(r_0)]^{\frac{1}{2}}}{2[1 - U(r_0)] - r_0 U'(r_0)} \ .$$ (36)

For evaluating the classical cross section we need the next derivative; differentiating Eq. (34) we get:

$$\Gamma(L,E) = \frac{\partial \Theta}{\partial L} = \frac{\partial^2 \Delta}{\partial L^2}$$

$$= \frac{2(2\mu E r_0^2)^{-\frac{1}{2}}}{2[1 - U(r_0)] - r_0 U'(r_0)} \int_1^\infty \frac{r_0\{U'(r_0)[1 - U(r_0\rho)] - \rho U'(r_0\rho)[1 - U(r_0)]\}}{\{[1 - U(r_0\rho)]\rho^2 - [1 - U(r_0)]\}^{3/2}} d\rho \ .$$

(37)

An alternative form, involving the second derivative of U, would be obtained by starting from Eq. (34a).

2. Expansions in $1/E$ and $1/L$

In the limit of high energy or high L these expressions for Δ and its derivatives are conveniently evaluated by expansion in powers of U and its derivatives, which is equivalent to expansion in powers of $1/E$. The expansion for Δ converges for all $L > 0$ and all $E > 0$ if the potential is entirely repulsive; for an attractive potential convergence is assured for all L if $E > |V_{min}|$, and for any E provided L is large enough that $|U(r_0\rho)| < 1$ for all $\rho > 1$. The term $1 - U(r_0\rho)^{-1}$ is expanded in powers of U, and the square root is expanded after writing it as

$$(\rho^2 - 1)^{\frac{1}{2}}[1 - U(r_0\rho) + G(r_0,\rho)(\rho^2 - 1)^{-1}]^{\frac{1}{2}} \quad , \tag{38}$$

where

$$G(r_0,\rho) = U(r_0) - U(r_0\rho) \quad . \tag{39}$$

For the expansion coefficients we can use the identity

$$\begin{pmatrix} 1/2 \\ k,l \end{pmatrix} = \frac{1/2!}{(1/2 - k - l)!\,k!\,l!} = (-)^{k+l}\frac{(k+l-3/2)!}{(-3/2)!\,k!\,l!} = (-)^{k+l}\begin{pmatrix} k+l-3/2 \\ k,l \end{pmatrix}. \tag{40}$$

The integrand then involves terms $G^l(r_0,\rho)U^{m+k}(r_0\rho)$, and for $l \neq 0$ it is useful to substitute for $U(r_0\rho)$ from (39). We then have

$$\frac{\Delta(L,E)}{(2\mu E)^{\frac{1}{2}}r_0} = \sum_{m,k=0}^{\infty}\begin{pmatrix} 1/2 \\ k \end{pmatrix}(-)^k\int_1^{\infty}(\rho^2 - 1)^{\frac{1}{2}}U^{m+k}(r_0\rho)\frac{\partial U(r_0\rho)}{\partial(\rho^2)}d(\rho^2)$$

$$+ \sum_{m,k=0}^{\infty}\sum_{l=1}^{\infty}\sum_{p=0}^{m+k}\begin{pmatrix} 1/2 \\ k,l \end{pmatrix}\begin{pmatrix} m+k \\ p \end{pmatrix}(-)^{k+p+1}U^{m+k-p}(r_0)\int_1^{\infty}(\rho^2-1)^{\frac{1}{2}-l}G^{l+p}(r_0,\rho)\frac{\partial G}{\partial(\rho^2)}d(\rho^2) \quad . \tag{41}$$

After an integration by parts $\Delta(L,E)$ can be expressed in a form free of derivatives of the potential,

$$\frac{\Delta(L,E)}{(2\mu E)^{\frac{1}{2}}r_0} = \sum_{m,k=0}^{\infty} \binom{1/2}{k}(-)^{k+1}\frac{1/2}{m+k+1}\int_1^{\infty}(\rho^2-1)^{-\frac{1}{2}}U^{m+k+1}(r_0\rho)d(\rho^2)$$

$$+ \sum_{m,k=0}^{\infty}\sum_{l=1}^{\infty}\sum_{p=0}^{m+k}\binom{1/2}{k,l}(-)^{k+p+1}\frac{l+1/2}{p+l+1}U^{m+k-p}(r_0)\int_1^{\infty}(\rho^2-1)^{-(l+\frac{1}{2})}G^{l+p+1}(r_0,\rho)d(\rho^2) \quad .$$

(42)

From this, differentiation with respect to L will give Θ, Γ, etc. These contain successively higher derivatives of U with respect to r, which cannot be eliminated by further integration by parts. Thus, the nth derivative $\partial^n\Delta/\partial L^n$ includes in its leading term an integral over $\partial^n U/\partial\rho^n$, weighted near the turning point by the factor $(\rho^2-1)^{-\frac{1}{2}}$.

An alternative form for Δ, particularly useful when U is a differentiable function, is obtained by a different integration by parts, followed by considerable manipulation (see Appendix). In the end one needs the coefficients

$$f(q,l,t) = \frac{(-)^{q+t+1}}{(t+1)}\frac{(q-1/2)!}{(l-1/2)!(q-t)!(q-l)!(t+l-q)!} \quad , \quad (43)$$

and the integrals

$$J_{l,t}[U(r_0\rho)] = \int_1^{\infty}(\rho^2-1)^{-\frac{1}{2}}\frac{\partial^l U^{t+1}(r_0\rho)}{\partial(\rho^2)^l}d\left(\frac{\rho^2}{2}\right) \quad . \quad (44)$$

The final form of Δ is then

$$\frac{\Delta(L,E)}{(2\mu E)^{\frac{1}{2}}r_0} = \sum_{q=0}^{\infty}\sum_{l,t=0}^{q}f(q,l,t)U^{q-t}(r_0)J_{l,t}[U(r_0\rho)] \quad . \quad (45)$$

It is also useful to have the alternative form

$$\frac{\Delta(L,E)}{L} = \sum_{p=0}^{\infty}\sum_{l,t=0}^{p}g(p,l,t)U^{p-t}(r_0)J_{l,t}[U(r_0\rho)] \quad , \quad (46)$$

where

$$g(p,l,t) = \sum_k \binom{k - 1/2}{k} f(p - k,l,t) \quad . \tag{47}$$

The expansions given in Eqs. (42), (45), and (46) are series in E^{-1} in which L appears implicitly in each term through the functional dependence between L and r_0, and thus $U(r_0)$ and $U(r_0\rho)$. For many purposes it is useful to make this dependence explicit in the form of an expansion—there are actually two expansions, one valid for small L and the other for large. Both can be obtained by a single procedure.

Let us write

$$r_0^2 = x^2 + c \quad , \tag{48}$$

and expand $U(r_0)$ and $U(r_0\rho)$:

$$U(r_0) = \sum_j \frac{c^j}{j!} \left[\frac{d^j U(r_0)}{d(r_0^2)^j} \right]_x = \sum_j \frac{c^j}{j!} U_x^{(j)} \quad , \tag{49}$$

$$U(r_0\rho) = \sum_j \frac{c^j}{j!} \left[\frac{\partial^j U(r_0\rho)}{\partial(r_0^2)^j} \right]_x = \sum_j \frac{c^j \rho^{2j}}{j! r_0^{2j}} \frac{\partial^j U(x\rho)}{\partial(\rho^2)^j} \quad . \tag{50}$$

When L is small we can expand the turning point r_0 about $x = y$, the turning point for $L = 0$:

$$U(y) = 1 \quad ; \tag{51}$$

when L is large we can expand r_0 about the impact parameter b. In either case, we need the dependence of c on L or b. This is obtained from the relation

$$b^2 = r_0^2 [1 - U(r_0)] = (x^2 + c)[1 - U(r_0)] \tag{52}$$

Using Eq. (49) (note its convention defining $U_x^{(j)}$!), this can be converted to the form

$$c = \gamma_0 + \sum_{j=2}^{\infty} \gamma_j c^j \quad , \tag{53}$$

where

$$\gamma_0 = \frac{b^2 - x^2(1 - U_x)}{1 - U_x - x^2 U_x^{(1)}}$$

and

$$\gamma_j = \frac{1}{1 - U_x - x^2 U_x^{(1)}} \left[\frac{U_x^{(j-1)}}{(j-1)!} + \frac{x^2 U_x^{(j)}}{j!} \right] \quad . \tag{54}$$

As long as γ_0 and c are small, iteration of (53) gives

$$c = \gamma_0 + \gamma_2 \gamma_0^2 + (\gamma_3 + 2\gamma_2^2)\gamma_0^3 + (\gamma_4 + 2\gamma_2\gamma_3 + \gamma_2^3)\gamma_0^4 \dots . \tag{55}$$

The coefficients γ simplify in the 2 cases of interest:

a) L near 0: $\quad \gamma_0 = -\dfrac{b^2}{y^2 U_y^{(1)}} \quad ,$

$$\gamma_j = \frac{-1}{y^2 U_y^{(1)}} \left[\frac{U_y^{(j-1)}}{(j-1)!} - \frac{y^2 U_y^{(j)}}{j!} \right] \quad , \tag{56}$$

b) L large: $\quad \gamma_0 = \dfrac{b^2 U_b}{1 - U_b - b^2 U_b^{(1)}} \quad ,$

$$\gamma_j = \frac{1}{1 - U_b - b^2 U_b^{(1)}} \left[\frac{U_b^{(j-1)}}{(j-1)!} - \frac{y^2 U_b^{(j)}}{j!} \right] . \tag{57}$$

In case (a) the expansion is in ascending powers of b^2 or L^2. In case (b), as long as $r^3 U(r) \to 0$ for $r \to \infty$, the expansion is in descending powers of b or L, and is in fact an asymptotic expansion. The same is true when c is inserted in (49) and (50) and these in turn in Eq. (45) or (46). In case (a), in the limit $L = 0$, we finally get a result that could be obtained much more easily by expanding Eq. (31c) directly after setting $L = 0$.

3. AN EXAMPLE: THE POTENTIAL r^{-n}

The evaluation of the integrals in (42) and (44) can be carried out analytically if U has a simple functional form. For a simple power law of the form r^{-n}, we encounter the integrals

$$I(n) = \int_1^\infty (\rho^2 - 1)^{-\frac{1}{2}} \rho^{-n} \rho \, d\rho = \frac{n-3}{n-2} I(n-2) \quad ,$$

$$I(3) = 1 \quad , \quad I(2) = \frac{\pi}{2} \quad . \tag{58}$$

With

$$U = \pm \frac{4\epsilon}{E} \left(\frac{\sigma}{r_0 \rho} \right)^n \quad , \tag{59}$$

the phase can be expressed as a series in inverse powers of b, the impact parameter:

$$\pm \frac{E\Delta(L,E)}{4\epsilon L} = \Phi(\beta) = \sum_{k=0}^\infty \alpha_k(n) \beta^{-n(k+1)}$$

where

$$\beta = \frac{b}{\sigma} \left(\frac{E}{\epsilon} \right)^{1/2} \quad .$$

The first few coefficients $\alpha_k(n)$ are given here for the cases $n = 4, 6, 12$:

$$n = 4, \quad \alpha_0 = -I(4) = -0.785398,$$

$$\alpha_1 = \frac{3}{2} I(8) = +0.736309,$$

$$\alpha_2 = -I(4) - \frac{10}{3} I(12) = -2.07394;$$

$$n = 6, \quad \alpha_0 = -I(6) = -0.589048,$$

$$\alpha_1 = \frac{5}{2} I(12) = +0.966405$$

$$\alpha_2 = -\frac{21}{2} I(6) - \frac{28}{3} I(18) = -9.06407;$$

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$$n = 12, \quad \alpha_0 = -I(12) = -0.386562,$$

$$\alpha_1 = \frac{11}{2} I(24) = 1.45302,$$

$$\alpha_2 = -3I(12) - \frac{136}{3} I(36) = -10.82755.$$

The first term α_0 is just the one obtained by Massey and Mohr.[11]

The value of the higher terms in extending the applicable range of the analytical formula to smaller impact parameters is illustrated in Table I with the repulsive r^{-12} potential as the example. In the table we also give exact values of the function $\Phi(b/\sigma) = E\Delta(L,E)/4\epsilon L$ for a wide range of values of β to supplement Hirschfelder's table[12] where the deflection angle $\partial\Delta/\partial L$ may be found. The tabulated values were obtained by evaluation of the integral, Eq. (24c), for $\Delta(L,E)$ by Gauss-Mehler quadrature.[13] The first few values given by the expansion in Table I illustrate the asymptotic nature of the series, the higher terms diverging.

Table I

$\Phi(b/\sigma) = E_\Delta(L,E)/4\epsilon L$ AS A FUNCTION OF $\beta = (b/\sigma)(E/\epsilon)^{1/2}$
FOR $n = 12$: EXACT CALCULATION AND ASYMPTOTIC EXPANSION

β	Φ(exact)	β	Φ(exact)	Φ(expansion) 3 Terms	2 Terms	1 Term
0.06	−32.331	1.00	−0.13476			
0.08	−23.405	1.05	−9.7202 $\times 10^{-2}$			
0.10	−18.099	1.10	−6.8663 $\times 10^{-2}$			
0.15	−11.099	1.15	−4.7543 $\times 10^{-2}$	−9.2189 $\times 10^{-2}$	−2.1491 $\times 10^{-2}$	−7.2251 $\times 10^{-2}$
0.20	− 7.6338	1.20	−3.2353 $\times 10^{-2}$	−4.0354 $\times 10^{-2}$	−2.5078 $\times 10^{-2}$	−4.3356 $\times 10^{-2}$
0.25	− 5.5790	1.25	−2.1731 $\times 10^{-2}$	−2.3256 $\times 10^{-2}$	−1.9742 $\times 10^{-2}$	−2.6604 $\times 10^{-2}$
0.30	− 4.2281	1.30	−1.4483 $\times 10^{-2}$	−1.4771 $\times 10^{-2}$	−1.3915 $\times 10^{-2}$	−1.6592 $\times 10^{-2}$
0.35	− 3.2796	1.35	−9.6276 $\times 10^{-3}$	−9.687 $\times 10^{-3}$	−9.467 $\times 10^{-3}$	−1.0549 $\times 10^{-2}$
0.40	− 2.5826	1.40	−6.4127 $\times 10^{-3}$	−6.4257 $\times 10^{-3}$	−6.3663 $\times 10^{-3}$	−6.8184 $\times 10^{-3}$
0.45	− 2.0534	1.45	−4.2941 $\times 10^{-3}$	−4.2972 $\times 10^{-3}$	−4.2804 $\times 10^{-3}$	−4.4751 $\times 10^{-3}$
0.50	− 1.6419	1.50	−2.8972 $\times 10^{-3}$	−2.8981 $\times 10^{-3}$	−2.8931 $\times 10^{-3}$	−2.9794 $\times 10^{-3}$
0.55	− 1.3160	1.55	−1.9722 $\times 10^{-3}$	−1.9724 $\times 10^{-3}$	−1.9709 $\times 10^{-3}$	−2.0102 $\times 10^{-3}$
0.60	− 1.0546	1.60	−1.3554 $\times 10^{-3}$	−1.3555 $\times 10^{-3}$	−1.3550 $\times 10^{-3}$	−1.3733 $\times 10^{-3}$
0.65	− 0.84292	1.70	−6.5926 $\times 10^{-4}$	−6.5926 $\times 10^{-4}$	−6.5921 $\times 10^{-4}$	−6.6349 $\times 10^{-4}$
0.70	− 0.67043	1.80	−3.3308 $\times 10^{-4}$	−3.3307 $\times 10^{-4}$	−3.3306 $\times 10^{-4}$	−3.3415 $\times 10^{-4}$
0.75	− 0.52945	1.90	−1.7436 $\times 10^{-4}$		−1.7435 $\times 10^{-4}$	−1.7465 $\times 10^{-4}$
0.80	− 0.41421	2.00	−9.4289 $\times 10^{-5}$		−9.4288 $\times 10^{-5}$	−9.4375 $\times 10^{-5}$
0.85	− 0.32027	2.50	−6.4850 $\times 10^{-6}$		−6.4850 $\times 10^{-6}$	−6.4854 $\times 10^{-6}$
0.90	− 0.24416	3.50	−1.1439 $\times 10^{-7}$			−1.14394 $\times 10^{-7}$
0.95	− 0.18309	5.00	−1.5834 $\times 10^{-9}$			−1.58336 $\times 10^{-9}$

NOTE: For $\beta = 1.15$, 1.20, and 1.25 the best approximation is given by the value underlined, showing the asymptotic nature of the expansion. For larger β, further terms would give a more exact result.

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APPENDIX

To obtain Eq. (45), the second type of integral in Eq. (41) is trans-
formed by successive integrations by parts so that

$$\int_1^\infty (\rho^2 - 1)^{-(l-\frac{1}{2})} \frac{\partial G^{p+l+1}}{\partial(\rho^2)} d(\rho^2) = \frac{\left(-\frac{1}{2}\right)!}{\left(l - \frac{3}{2}\right)!} \int_1^\infty (\rho^2 - 1)^{-\frac{1}{2}} \frac{\partial^l G^{p+l+1}(r_0,\rho)}{\partial(\rho^2)^\rho} d(\rho^2) \quad .$$

(A-1)

Equation (39) is then substituted for G. The resulting cluster of co-
efficients can be reduced by successive application of various identities
among the binomial coefficients, including the following:

$$(-)^k \binom{m}{k} = \binom{1-m}{k} \quad , \qquad (A-2)$$

$$\sum_j \binom{M-m}{n-j} \binom{m}{j} = \binom{M}{n} \quad , \qquad (A-3)$$

$$\sum_{s=m}^n \binom{s}{m} = \binom{n+1}{m+1} \quad . \qquad (A-4)$$

In the end it is found that the terms arising from both the first integral
in Eq. (41) [which is treated as in Eq. (42)], and from the other integrals
(with $l \neq 0$), are special cases of the same general formula, even though
the routes to them are different.

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