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The classical limit of quantum mechanical Coulomb scattering

E G Peter Rowe
Department of Mathematical Sciences, University of Durham, Durham DH1 3LE, UK

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Abstract. The exact solution of the Coulomb scattering problem in non-relativistic quantum mechanics has been known for many decades. Here its asymptotic form as $\hbar \to 0$, for constant energy and through all space, is discussed and shown to reproduce exactly the classical action surfaces and classical orbits for a statistical beam undergoing classical Coulomb scattering.

1. Introduction

The WKBJ approximation in quantum mechanics leads to fairly definite expectations about the classical ($\hbar \to 0$) limit of the quantum mechanical treatment of Coulomb scattering. Yet the limit seems not to have been worked out.

If in the Schrödinger equation for a particle scattering in a potential V,

$$-(\hbar^2/2m)\nabla^2\Psi + V\Psi = E\Psi$$

we substitute

$$\Psi = R \exp(\mathrm{i}S/\hbar)$$

with real R and S, we get the conservation equation

$$\nabla \cdot [R^2\nabla S] = 0$$

and an equation which formally would reduce to the Hamilton-Jacobi equation in the limit $\hbar \to 0$:

$$\frac{1}{2m}(\nabla S)^2 + V - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} = E.$$

Because R and S depend on $\hbar$, the limit is not as simple as the formal argument suggests, but nonetheless the expectation is aroused that the asymptotic form for Ψ as $\hbar \to 0$ will have the structure

$$\Psi \sim (\rho_{\text{classical}})^{1/2} \exp(\mathrm{i}S_{\text{classical}}/\hbar).$$

A rigorous discussion of such limits is given by Truman (1976) for the case when V is sufficiently smooth.

The exact solution of the Schrödinger equation for Coulomb scattering is well known (Temple (1928), or, for a more extended description, Mott and Massey (1965)). The solution involves the confluent hypergeometric function $F(a, b, z)$, or, equivalently, Whittaker's function $M_{\kappa,m}(z)$. Such functions of three variables have many facets, and when the standard reference works were being written in the 1950s the theory of their asymptotic forms was far from complete.

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The asymptotic form of Whittaker's function required for the Coulomb problem is discussed below and it results in the following asymptotic form for Ψ:

$$\Psi(\boldsymbol{x}) \sim \mathrm{e}^{\mathrm{i}\phi}[(\rho_{\mathrm{in}}(\boldsymbol{x}))^{1/2}\exp(\mathrm{i}S_{\mathrm{in}}(\boldsymbol{x})/\hbar) - \mathrm{i}(\rho_{\mathrm{out}}(\boldsymbol{x}))^{1/2}\exp(\mathrm{i}\, S_{\mathrm{out}}(\boldsymbol{x})/\hbar)].$$

This is the asymptotic form for all $\boldsymbol{x}$ (except on the positive Z axis) as $\hbar \to 0$. It must be sharply distinguished from the commonly quoted asymptotic form for fixed $\hbar$ as $|\boldsymbol{x}| \to \infty$. The functions ρ_{in} and ρ_{out} are the classical densities for the incoming and outgoing statistical beams; S_{in} and S_{out} are the classical action functions for the orbits of the same statistical ensemble. The $\boldsymbol{x}$ -independent phase ϕ appears because of the from-our-point-of-view-unnatural standard phase in the usual solution.

Classical limits help us to understand quantum mechanics better. Questions such as 'what physical reality does the Schrödinger equation describe?' are still actively debated. Does Ψ describe the scattering of a single particle or an ensemble? In the $\hbar \to 0$ limit the classical reality to which the quantum mechanical treatment limits is a statistical ensemble of individual single-particle scattering orbits. The quantum mechanical probability becomes a statistical probability for an ensemble of classical orbits with the same initial velocity $v_0\boldsymbol{k}$ and uniform density on the initial plane $z = -\infty$. To put it no more strongly, the simplest interpretation of the quantum mechanical formalism when $\hbar \neq 0$ which agrees with the required interpretation in the $\hbar \to 0$ limit is the statistical interpretation (Ballentine 1970).

The actual details of the transition from quantum mechanics to classical mechanics are of interest too. For example, the classical description of the scattering of a (statistical) beam involves two sets of fields throughout space. Every point in space has one incoming orbit and one outgoing orbit (the Z axis excepted) passing through it (see figure 1). Yet the quantum mechanical wavefunction Ψ is single-valued in space. How are these two formalisms to be reconciled?

A few words are said about the reconciliation of classical mechanics and quantum mechanics in the concluding section of this paper. In preparation for it and for the asymptotic form of quantum mechanics, the classical ensemble is described in the section immediately below.

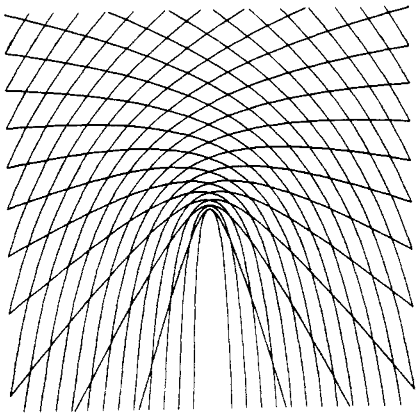

Figure 1. A family of orbits for attractive classical Coulomb scattering. All the particles have the same energy and initial velocity but differ in their impact parameters. The scattering charge is fixed at the centre. The figure is a superposition of two sheets of a surface on which the velocity field is single-valued.

It should be mentioned also that asymptotic forms for quantum mechanical scattering wavefunctions have emerged in work originally directed towards understanding gravitational scattering on black holes (see DeWitt-Morette and Nelson 1984, DeWitt-Morette and Tian-Rong Zhang 1983, DeWitt-Morette *et al* 1983, Nelson 1983, Handler and Matzner 1980).

2. Classical Coulomb scattering

The relevant formulae of non-relativistic classical Coulomb scattering can be derived very simply, so for completeness sake and to avoid ambiguity in the notation this will be done here.

We first consider the orbit of a point charge q of mass m scattering against an infinitely heavy target charge Q fixed at the origin $\mathbf{0}$. In the first instance the whole process will be presumed to take place in the YZ plane. The projectile q enters at $z=-\infty$ with impact parameter $y=B$ (positive or negative) and initial velocity $\boldsymbol{v}=v_0\boldsymbol{k}$.

The initial values of the conserved vectors

$$\boldsymbol{L}=\boldsymbol{x}\times m\dot{\boldsymbol{x}} \tag{2.1}$$

and

$$\boldsymbol{C}=\dot{\boldsymbol{x}}\times\boldsymbol{L}+qQ\boldsymbol{x}/r \tag{2.2}$$

are

$$\boldsymbol{L}_0=mv_0B\boldsymbol{i} \tag{2.3}$$

and

$$\boldsymbol{C}_0=mv_0^2(B\boldsymbol{j}-A\boldsymbol{k}) \tag{2.4}$$

where

$$A\equiv qQ/mv_0^2. \tag{2.5}$$

To be definite we consider only attractive scattering, so

$$A<0. \tag{2.6}$$

The equation for the orbits can be deduced from

$$\dot{\boldsymbol{x}}(t)\cdot\boldsymbol{C}_0=\dot{\boldsymbol{x}}(t)\cdot\boldsymbol{C}(t). \tag{2.7}$$

This may be written in the form

$$B\dot{y}-A\dot{z}=A\frac{\dot{\boldsymbol{x}}\cdot\boldsymbol{x}}{r}=A\dot{r}$$

after which integration with respect to t gives

$$B(y-B)=A(r+z). \tag{2.8}$$

We may now consider the whole family of orbits for particles with the same initial velocity $v_0\boldsymbol{k}$ but whose initial positions $z=-\infty$, $y=B$ have different impact parameters. These orbits are given by (2.8) for all real values of B. Each of the orbits crosses the positive Z axis (at $z=-B^2/2A$) and it is convenient to call the parts before the crossing *incoming* and the parts after the crossing *outgoing*. The family of orbits is illustrated in figure 1.

Solving equation (2.8) for B gives the impact parameters of the two orbits, one incoming and one outgoing, that pass through a given point:

$$B_\pm = \tfrac{1}{2}y\{1 \pm [1 - 4A/(r-z)]^{1/2}\}. \tag{2.9}$$

Since B_+ has the same sign as y, this case is incoming (recall that we are assuming $A < 0$); since B_- has the opposite sign from y, this case is outgoing.

All the incoming orbits determine a velocity field $\boldsymbol{v}_{\text{in}}$ throughout the plane (except the Z axis), and the outgoing orbits similarly determine another field $\boldsymbol{v}_{\text{out}}$. In each case the velocity at a point is just the velocity of a particle whose orbit passes through the point. We can obtain the velocity for a particle on an orbit with impact parameter B from

$$\boldsymbol{i} \times \boldsymbol{C}_0 = \boldsymbol{i} \times \boldsymbol{C}(t). \tag{2.10}$$

This gives (writing $\boldsymbol{v}$ for $\dot{\boldsymbol{x}}$)

$$\boldsymbol{v} = v_0\boldsymbol{k} + \frac{v_0 A}{B}\frac{1}{r}[(r+z)\boldsymbol{j} - y\boldsymbol{k}]. \tag{2.11}$$

We get $\boldsymbol{v}_{\text{in}}$ by replacing B with the expression B_+ from (2.9), and we get $\boldsymbol{v}_{\text{out}}$ by replacing B with the expression B_-.

Writing $\xi \equiv r - z$, $\boldsymbol{\nabla}\xi = \hat{\boldsymbol{x}} - \boldsymbol{k}$, we find

$$\boldsymbol{v}_{\text{in}} = v_0\boldsymbol{k} + v_0\tfrac{1}{2}[1 - (1 - 4A/\xi)^{1/2}]\boldsymbol{\nabla}\xi \tag{2.12}$$

and

$$\boldsymbol{v}_{\text{out}} = v_0\boldsymbol{k} + v_0\tfrac{1}{2}[1 + (1 - 4A/\xi)^{1/2}]\boldsymbol{\nabla}\xi. \tag{2.13}$$

The action S is a scalar field whose gradient gives the momentum field

$$m\boldsymbol{v} = \boldsymbol{\nabla}S. \tag{2.14}$$

From (2.12) and (2.13) we get S_{in} and S_{out} by simple integration. It is convenient to fix the arbitary constants so that both actions vanish at the origin, where $z = \xi = 0$. Then

$$S_{\text{in}} = mv_0\left[z + \tfrac{1}{2}\xi - \tfrac{1}{2}[\xi(\xi - 4A)]^{1/2} + A\log\left(\frac{\xi - 2A + [\xi(\xi-4A)]^{1/2}}{-2A}\right)\right] \tag{2.15}$$

$$S_{\text{out}} = mv_0\left[z + \tfrac{1}{2}\xi + \tfrac{1}{2}[\xi(\xi - 4A)]^{1/2} - A\log\left(\frac{\xi - 2A + [\xi(\xi-4A)]^{1/2}}{-2A}\right)\right]. \tag{2.16}$$

Formulae (2.15) and (2.16) were derived by Gordon (1928) in a slightly different shape. Their asymptotic forms for $\xi \to \infty$ are more familiar:

$$S_{\text{in}} \sim mv_0[z + A\log(r - z)] \tag{2.17}$$

$$S_{\text{out}} \sim mv_0[r - A\log(r - z)]. \tag{2.18}$$

We can formulate the whole dynamical system in a simpler single-valued way by working on a two-sheeted Riemann-like surface consisting of two copies of the YZ plane each cut along the positive Z axis, an in-sheet and an out-sheet. Along the positive Z axis, the $y \geqslant 0$ edge of the in-sheet is smoothly joined to the $y \leqslant 0$ edge of the out-sheet, and vice versa.

On the two-sheeted surface there is just one orbit of the form (2.8) through each point, the impact parameter being given by (2.9) with B_+ on the in-sheet and B_- on the out-sheet. The velocity fields (2.12) and (2.13) can be united to form a single-valued continuous vector field $\boldsymbol{v}$ on the surface. Similarly, S_{in} and S_{out} can be united to form a single-valued scalar field S on the surface. The orbits and the velocity field $\boldsymbol{v}$ are orthogonal at each point to the surfaces of constant action S.

We can define action waves on the surface by

$$S(\boldsymbol{x}) - Et = 0 \tag{2.19}$$

where the energy $E = \frac{1}{2}mv_0^2$. As time passes from $-\infty$ to $+\infty$, the surfaces of constant action determined by (2.19) propagate like a wavefront which begins at $z = -\infty$ on the in-sheet as a distorted plane wave, and emerges on the out-sheet as a distorted spherical wave. These surfaces are illustrated in figure 2.

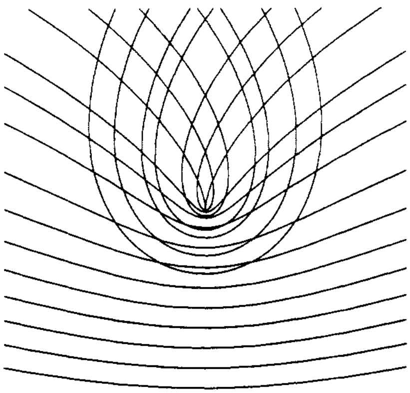

Figure 2. Surfaces of constant action determine progressive action waves (see equation (2.19)). At $t = -\infty$ they begin as distorted plane waves at the bottom of the figure. After encountering the scattering centre they emerge as distorted spherical waves. The two sheets of the surface on which the action is single-valued have been superposed.

Using the family of orbits described above we can define a continuous time-independent flow of particles by a current density

$$\boldsymbol{j}(\boldsymbol{x}) = \sigma(\boldsymbol{x})\boldsymbol{v}(\boldsymbol{x}). \tag{2.20}$$

Here, $\sigma(\boldsymbol{x})$ is the particle density in the plane (for the generalisation to 3-space, the symbol ρ will be used for the density). We define $\sigma(\boldsymbol{x})$ by the initial condition $\sigma(z = -\infty) = 1$ and the requirement that $\boldsymbol{j}(\boldsymbol{x})$ be conserved, $\nabla \cdot \boldsymbol{j} = 0$.

The current (2.20) describes a continuous statistical aggregation of particle motions, not a real beam. Each particle follows an orbit determined by its interaction with the scattering charge Q alone.

To calculate $\sigma(\boldsymbol{x})$ we consider two nearby orbits with impact parameters B and $B + \delta B$, $\delta B > 0$. At $(y = B, z = -\infty)$ the number of particles flowing across a perpendicular line between the two orbits is $\delta B v_0$ per unit time since we are assuming $\sigma(z = -\infty) = 1$. To conserve $\boldsymbol{j}$ this must equal $|\delta \boldsymbol{N}| v\sigma$ at any other point (y, z) on the B orbit, where $\delta \boldsymbol{N} = \delta y \boldsymbol{j} + \delta z \boldsymbol{k}$ is the perpendicular displacement to the second orbit, and the speed v is given by

$$\frac{v}{v_0} = \left(1 - \frac{2A}{r}\right)^{1/2} \qquad \text{(energy conservation).}$$

Using (2.11) for the direction of the B orbit, and (2.8) applied to both orbits, we find

$$\sigma(x) = \frac{|B|}{|y-2B|}. \tag{2.21}$$

By inserting one or the other of the expressions (2.9) for B, we get from (2.21) the density on both the in-sheet and the out-sheet. The density given by (2.21) is finite everywhere, a fact which is obvious from figure 1.

As a last step in specifying the classical Coulomb system to which the quantum mechanical treatment limits, we rotate everything about the Z axis, that is, we impose axial symmetry consistent with the above description in the YZ plane. Equations (2.12)–(2.19) require no change to be interpreted in 3-space. The two-sheeted surface on which $\boldsymbol{v}$ and S are single-valued becomes a pair of copies of three-dimensional space communicating through the positive Z axis.

Equations (2.20) and (2.21) require slight alteration. In place of (2.20),

$$\boldsymbol{j}(\boldsymbol{x}) = \rho(\boldsymbol{x})\boldsymbol{v}(\boldsymbol{x}) \tag{2.22}$$

and ρ is determined by particle conservation and the initial condition $\rho(z=-\infty)=1$. Instead of the perpendicular lines in the calculation of $\sigma(x)$ we must work with two annuli of areas $2\pi|B|\delta B$ and $2\pi|y|\,|\delta N|$. The argument is otherwise the same and we obtain

$$\rho(\boldsymbol{x}) = \frac{|B|^2}{|y|\,|y-2B|}. \tag{2.23}$$

This density diverges on the positive Z axis because every orbit in the whole 3-space crosses it.

Substituting from (2.9) in (2.23) we obtain the densities for the in-space and the out-space:

$$\rho_{\text{in}}(\boldsymbol{x}) = \tfrac{1}{4}[(1-4A/\xi)^{1/2}+1]^2 \frac{1}{(1-4A/\xi)^{1/2}} \tag{2.24}$$

$$\rho_{\text{out}}(\boldsymbol{x}) = \tfrac{1}{4}[(1-4A/\xi)^{1/2}-1]^2 \frac{1}{(1-4A/\xi)^{1/2}}. \tag{2.25}$$

As $\xi\to\infty$, the asymptotic forms of these densities are

$$\rho_{\text{in}} \sim 1 \tag{2.26}$$

$$\rho_{\text{out}} \sim \frac{A^2}{\xi^2} = \frac{1}{r^2}\frac{(qQ/mv_0^2)^2}{4\sin^4\theta/2}. \tag{2.27}$$

The asymptotic form for ρ_{out} is equivalent to Rutherford's formula for the Coulomb scattering cross section.

We shall see in the next section that the physical system to which the quantum mechanical version of Coulomb scattering tends as $\hbar\to 0$ is the time-independent statistical ensemble of single-particle scattering motions described above. Its density is given through all space by ρ_{in} and ρ_{out} in equations (2.24) and (2.25); its velocity field is given by $\boldsymbol{v}_{\text{in}}$ and $\boldsymbol{v}_{\text{out}}$ of (2.12) and (2.13). The velocity fields are perpendicular to the surfaces of constant action S_{in} and S_{out} of equations (2.15) and (2.16).

3. Classical limit of quantum mechanical Coulomb scattering

The Schrödinger equation for the scattering problem of the previous section is

$$-\frac{\hbar^2}{2m}\nabla^2\Psi+\frac{qQ}{r}\Psi=E\Psi=\tfrac{1}{2}mv_0^2\Psi. \tag{3.1}$$

For the case of an incoming (distorted) plane wave representing particles travelling initially with velocity $v_0\boldsymbol{k}$, the exact solution Ψ is known. It is described in most books on quantum mechanics, for example, Messiah (1961).

The wavefunction is usually normalised and standardised with reference to its asymptotic form for large $\xi=r-z$. For scattering on a short-range potential this asymptotic form, as $|\boldsymbol{x}|\to\infty$, would be just

$$\exp(\mathrm{i}kz)+(f/r)\exp(\mathrm{i}kr) \tag{3.2}$$

where

$$k\equiv mv_0/\hbar. \tag{3.3}$$

The otherwise arbitrary constant in Ψ is chosen to make its asymptotic form, as $\xi\to\infty$, correspond as closely as possible to (3.2).

Our present interest is in a completely different asymptotic form: the form of Ψ for any finite $\boldsymbol{x}$, constant q, Q, m, v_0, as $\hbar\to 0$ (or, equivalently, $k\to\infty$). We will call this the classical limit, even though it is not a limit function that is obtained (even when $qQ=0$ the wavefunction $\mathrm{e}^{\mathrm{i}kz}$ has no limit function as $k\to\infty$).

Since Ψ is known exactly, all that is needed is the asymptotic form of this known function as $k\to\infty$. But the required case does not appear in the standard references, so the work below is directed towards finding it *ab initio*. This will be done in the manner of Erdélyi and Swanson (1957) from the differential equation itself rather than from an integral representation of the solution (see also Olver 1974, Skovgaard 1966).

With the notation (2.5) and (3.3), equation (3.1) may be rewritten

$$\nabla^2\Psi+k^2[1-2A/r]\Psi=0. \tag{3.4}$$

The known solution has the form

$$\Psi=C(k)\,\mathrm{e}^{\mathrm{i}kz}f(\xi) \tag{3.5}$$

where $C(k)$ is a normalisation-standardisation constant (it will be brought in explicitly below).

Substituting (3.5) in (3.4) shows that

$$\xi f''(\xi)+(1-\mathrm{i}k\xi)f'(\xi)-k^2Af(\xi)=0. \tag{3.6}$$

The only acceptable solution is the standard one given in terms of the confluent hypergeometric function (see, for example, Erdélyi 1953)

$$f(\xi)=F(-\mathrm{i}kA,1,\mathrm{i}k\xi). \tag{3.7}$$

The function $F(a,b,z)$ is entire; near $z=0$ it behaves like

$$F(a,b,z)=1+(a/b)z+\dots \tag{3.8}$$

and it satisfies

$$zF''+(b-z)F'-aF=0. \tag{3.9}$$

Once $f(\xi)$ has been specified exactly it allows us to quote the conventional value of the constant $C(k)$

$$C(k)=\Gamma(1+\mathrm{i}kA)\exp(-\tfrac{1}{2}\pi kA) \tag{3.10}$$

(see Messiah 1961). Its asymptotic form for large, real, positive k and real $A<0$ can easily be found from Stirling's formula:

$$C(k)\sim(2\pi|kA|)^{1/2}\exp(-\mathrm{i}\pi/4)\exp[\mathrm{i}kA(\log|kA|-1)]. \tag{3.11}$$

The problem is to find the asymptotic form of (3.7). When using the differential equation method, the most efficient strategy seems to be to eliminate the first derivative. Introducing Whittaker's function accomplishes this:

$$M_{\kappa,0}(z)\equiv z^{1/2}\,\mathrm{e}^{-z/2}F(a,1,z) \tag{3.12}$$

where $\kappa\equiv\frac{1}{2}-a$ in general, and for our case

$$\kappa=\tfrac{1}{2}+\mathrm{i}kA. \tag{3.13}$$

The differential equation for $M_{\kappa,0}(z)$ is

$$M''_{\kappa,0}+\left(-\frac{1}{4}+\frac{\kappa}{z}+\frac{\frac{1}{4}}{z^2}\right)M_{\kappa,0}=0 \tag{3.14}$$

and its behaviour near $z=0$ is given by

$$M_{\kappa,0}=z^{1/2}(1-\kappa z+\ldots). \tag{3.15}$$

From (3.7) and (3.12),

$$f(\xi)\equiv(\mathrm{i}k\xi)^{-1/2}\exp(\mathrm{i}k\xi/2)g(\xi) \tag{3.16}$$

where

$$g(\xi)=M_{\kappa,0}(\mathrm{i}k\xi) \tag{3.17}$$

with κ given by (3.13). From (3.14), the differential equation satisfied by $g(\xi)$ is

$$g''(\xi)+\left[k^2\left(\frac{1}{4}-\frac{\kappa/\mathrm{i}k}{\xi}\right)+\frac{\frac{1}{4}}{\xi^2}\right]g(\xi)=0. \tag{3.18}$$

From (3.15), its behaviour near $\xi=0$ is

$$g(\xi)=(\mathrm{i}k\xi)^{1/2}(1-\kappa\mathrm{i}k\xi+\ldots). \tag{3.19}$$

We need the asymptotic form, as $k\to\infty$, of the solution of (3.18) for real $\xi\geqslant 0$ whose behaviour near $\xi=0$ is given by (3.19).

As a final step to neaten up (3.18) we put

$$D\equiv-\frac{4\kappa}{\mathrm{i}k}=-4A+\frac{2\mathrm{i}}{k}\equiv D_0+\frac{2\mathrm{i}}{k} \tag{3.20}$$

and note that

$$D_0=\mathrm{Re}\,D>0 \qquad \mathrm{Im}\,D>0.$$

Equation (3.18) now becomes

$$g''(\xi)+\left[\frac{k^2}{4}(1+D/\xi)+\frac{\frac{1}{4}}{\xi^2}\right]g(\xi)=0. \tag{3.21}$$

This equation is singular at $\xi = 0$, but the coefficient of k^2 does not vanish on the positive ξ axis (or near it) so there are no transition points on this axis. We can then hope to find a uniform approximation for the whole positive axis. Erdélyi and Swanson (1957) treated an equation like (3.21) but with real D. Although $\operatorname{Im} D \to 0$ as $k \to \infty$, its effect is nonetheless very great.

We follow the procedure of Erdélyi and Swanson without attempting to maintain their rigour.

The main idea is to compare (3.21) with a differential equation related to Bessel's equation. Suppose $y(z)$ satisfies Bessel's equation of order p:

$$y''(z) + (1/z)y'(z) + (1 - p^2/z^2)y(z) = 0. \tag{3.22}$$

With $\psi(\xi)$ to be chosen presently, we put

$$U(\xi) = (\psi/\psi')^{1/2} y(k\psi). \tag{3.23}$$

Then $U(\xi)$ satisfies

$$U'' + U\left[k^2\psi'^2 + \left(\frac{1}{4} - p^2\right)\frac{\psi'^2}{\psi^2} + \frac{1}{2}\frac{\psi'''}{\psi'} - \frac{3}{4}\frac{\psi''^2}{\psi'^2}\right] = 0. \tag{3.24}$$

To increase the similarity between (3.21) and (3.24) we choose

$$\psi'^2 = \tfrac{1}{4}(1 + D/\xi). \tag{3.25}$$

With $\psi(0) = 0$, we then have

$$2\psi(\xi) = \int_0^\xi d\xi (1 + D/\xi)^{1/2}$$

$$= [\xi(\xi + D)]^{1/2} + \tfrac{1}{2}D \log\left(\frac{2\xi + D + 2[\xi(\xi + D)]^{1/2}}{D}\right) \tag{3.26}$$

in which the square roots with positive real part are intended, and the principal value of the log. Using the behaviour of ψ near $\xi = 0$,

$$\psi(\xi) \sim (D\xi)^{1/2} \qquad \psi'(\xi) \sim \tfrac{1}{2}(D/\xi)^{1/2} \qquad \text{etc} \tag{3.27}$$

one can check that the choice $p = 0$ in (3.24) means its ξ^{-2} singularity has the same coefficient as the one in (3.21).

Near $z = 0$, $J_0(z) \sim 1$; so, having chosen $p = 0$, and bearing in mind (3.27), if we use the solution of Bessel's equation which is regular at the origin and whose normalisation is given by

$$y(z) = (\mathrm{i}k/2)^{1/2} J_0(z) \tag{3.28}$$

then $U(\xi)$ determined by (3.23) will have the same behaviour near $\xi = 0$ as $g(\xi)$ exhibits in (3.19).

We have been led finally to

$$U(\xi) = \left(\frac{\mathrm{i}k}{2}\right)^{1/2} \left(\frac{\psi}{\psi'}\right)^{1/2} J_0(k\psi) \tag{3.29}$$

a function which has the same behaviour near $\xi = 0$ as $g(\xi)$ and which satisfies a differential equation very similar to (3.21). We omit a pure mathematical proof that $U(\xi)$ gives the asymptotic form of $g(\xi)$ as $k \to \infty$. In the similar cases that they deal with, Erdélyi and Swanson (1957) use a Green function scheme of successive approximations to incorporate the differences between the two differential equations and they find that the asymptotic form of U gives the asymptotic form of g:

$$g(\xi) \sim U(\xi) \qquad \text{as } k \to \infty. \tag{3.30}$$

The asymptotic form of the Bessel function $J_0(z)$ as $|z| \to \infty$ is (Erdélyi 1953)

$$J_0(z) \sim \left(\frac{2}{\pi z}\right)^{1/2} \cos\left(z - \frac{\pi}{4}\right) \tag{3.31}$$

so, from (3.29) and (3.30), for $\xi > 0$, as $k \to \infty$,

$$g(\xi) \sim \left(\frac{\mathrm{i}}{\pi \psi'}\right)^{1/2} \cos\left(k\psi - \frac{\pi}{4}\right). \tag{3.32}$$

We need the real and imaginary parts of $k\psi$ for use in (3.32). From (3.20) and with a slightly more elaborate notation in (3.26),

$$\begin{aligned} \psi(\xi, D) &= \frac{D}{2} \int_0^{\xi/D} \mathrm{d}y \left(1 + \frac{1}{y}\right)^{1/2} \\ &= \psi(\xi, D_0) + \frac{2\mathrm{i}}{k} \frac{\partial \psi}{\partial D}\bigg|_{D=D_0} + \ldots \\ &= \psi(\xi, D_0) + \frac{\mathrm{i}}{k} \log\left(\frac{\xi + [\xi(\xi + D_0)]^{1/2}}{(\xi D_0)^{1/2}}\right) + \ldots \\ &= \psi_0 + \frac{\mathrm{i}}{k} \log\left(-\frac{\xi}{4A}\right)^{1/2} \left[1 + \left(1 - \frac{4A}{\xi}\right)^{1/2}\right] + \ldots \end{aligned} \tag{3.33}$$

where

$$\psi_0 = \tfrac{1}{2}[\xi(\xi - 4A)]^{1/2} - A \log\left(\frac{\xi - 2A + [\xi(\xi - 4A)]^{1/2}}{-2A}\right). \tag{3.34}$$

Substituting (3.33) in (3.32) gives

$$\begin{aligned} g(\xi) \sim \frac{1}{(2\pi)^{1/2}} \frac{[\xi/(-4A)]^{1/2}}{(1 - 4A/\xi)^{1/4}} \{&[(1 - 4A/\xi)^{1/2} - 1] \exp(\mathrm{i}k\psi_0) \\ &+ \mathrm{i}[(1 - 4A/\xi)^{1/2} + 1] \exp(-\mathrm{i}k\psi_0)\} \end{aligned} \tag{3.35}$$

and then bringing in the extra factors from (3.16) produces

$$\begin{aligned} f(\xi) \sim \frac{1}{(\mathrm{i}2\pi|kA|)^{1/2}(1 - 4A/\xi)^{1/4}} \tfrac{1}{2}\{&[(1 - 4A/\xi)^{1/2} - 1] \exp[\mathrm{i}k(\xi + 2\psi_0)/2] \\ &+ \mathrm{i}[(1 - 4A/\xi)^{1/2} + 1] \exp[\mathrm{i}k(\xi - 2\psi_0)/2]\}. \end{aligned} \tag{3.36}$$

This is the required asymptotic form for the function in (3.7).

Referring to the expressions for the classical densities in (2.24) and (2.25), we may write the asymptotic form of $f(\xi)$ more briefly:

$$f(\xi) \sim \frac{1}{(\mathrm{i}2\pi|kA|)^{1/2}} \{(\rho_{\mathrm{out}})^{1/2} \exp[\mathrm{i}k(\xi + 2\psi_0)/2] + \mathrm{i}(\rho_{\mathrm{in}})^{1/2} \exp[\mathrm{i}k(\xi - 2\psi_0)/2]\}. \tag{3.37}$$

At last, from (3.5) and (3.11), we get the asymptotic form for the wavefunction

$$\Psi \sim \exp[\mathrm{i}kA(\log|kA|-1)]\{(\rho_{\mathrm{in}})^{1/2}\exp[\mathrm{i}k(z+\xi/2-\psi_0)] \\ -\mathrm{i}(\rho_{\mathrm{out}})^{1/2}\exp[\mathrm{i}k(z+\xi/2+\psi_0)]\}. \tag{3.38}$$

Comparing the exponentials in (3.38) with (2.15) and (2.16), we see that

$$\Psi \sim \exp[\mathrm{i}kA(\log|kA|-1)][(\rho_{\mathrm{in}})^{1/2}\exp(\mathrm{i}\,S_{\mathrm{in}}/\hbar)-\mathrm{i}(\rho_{\mathrm{out}})^{1/2}\exp(\mathrm{i}\,S_{\mathrm{out}}/\hbar)]. \tag{3.39}$$

This is the final expression for the asymptotic form, as $k\to\infty$ ($\hbar\to 0$), for the Coulomb wavefunction. It applies through the whole of space, except the positive Z axis (where ρ_{in} and ρ_{out} diverge).

The 'peculiar' phase factor in (3.39) arises because the conventional standardisation (3.10) was chosen to make the $\xi\to\infty$ asymptotic form of the in-term as neat as possible. If we look again at the $\xi\to\infty$ asymptotic forms of $S_{\mathrm{in}}/\hbar$ and $S_{\mathrm{out}}/\hbar$ but carry the expansion one term further than in (2.17) and (2.18) we find

$$S_{\mathrm{in}}/\hbar \underset{(\xi\to\infty)}{\sim} k[z+A(1+\log\xi-\log|A|)] \tag{3.40}$$

$$S_{\mathrm{out}}/\hbar \underset{(\xi\to\infty)}{\sim} k[r+A(-1-\log\xi+\log|A|)]. \tag{3.41}$$

Then, from (3.39) we can write the asymptotic form as $\xi\to\infty$ of the asymptotic form as $k\to\infty$ of the wavefunction. We get (using (2.27) and (2.26) also)

$$\Psi \underset{\substack{k\to\infty\\ \xi\to\infty}}{\sim} \left(\exp[\mathrm{i}k(z+A\log k\xi)]-\frac{\mathrm{i}|A|}{\xi}\exp[2\mathrm{i}kA(\log|kA|-1)]\exp[\mathrm{i}k(r-A\log kr)]\right). \tag{3.42}$$

This is the usually quoted $\xi\to\infty$ asymptotic form of the Coulomb wavefunction but with the factor

$$\Gamma(1+\mathrm{i}kA)/\Gamma(1-\mathrm{i}kA)$$

replaced by its $k\to\infty$ form $(-\mathrm{i})\exp[2\mathrm{i}kA(\log|kA|-1)]$.

4. Conclusions

From the asymptotic ($\hbar\to 0$) form (3.39) one gets the asymptotic form of the quantum mechanical position probability density

$$|\Psi|^2 \sim \rho_{\mathrm{in}}+\rho_{\mathrm{out}}+2(\rho_{\mathrm{in}}\rho_{\mathrm{out}})^{1/2}\sin[(S_{\mathrm{out}}-S_{\mathrm{in}})/\hbar]$$

If this is interpreted as a distribution, so that it appears only under an integral sign with a smooth test function, then in the limit $\hbar\to 0$ it is equivalent to

$$\lim_{\hbar\to 0}|\Psi|^2=\rho_{\mathrm{in}}+\rho_{\mathrm{out}}. \tag{4.1}$$

The quantum mechanical probability density limits to the sum of the classical in- and out-densities for the statistical flow described in § 2.

In time-independent quantum mechanical scattering theory a rather artificial argument is used to separate the two pieces corresponding to ρ_{in} and ρ_{out}, and to justify the neglect of the interference term.

With the same understanding that it is to be interpreted as a distribution, the quantum mechanical current density has the limit

$$\lim_{\hbar\to 0}\frac{-\mathrm{i}\Psi^*\hbar\nabla\Psi}{m}=\frac{\nabla S_{\mathrm{in}}}{m}\rho_{\mathrm{in}}+\frac{\nabla S_{\mathrm{out}}}{m}\rho_{\mathrm{out}}=\boldsymbol{v}_{\mathrm{in}}\rho_{\mathrm{in}}+\boldsymbol{v}_{\mathrm{out}}\rho_{\mathrm{out}}. \tag{4.2}$$

At each point in space this is the total current for the classical flow.

In order to extract out of the quantum mechanical asymptotic form something corresponding to time development in the classical flow, one may show how the action waves (2.19) of the classical theory emerge from the quantum mechanical theory. The action waves do not, of course, travel with the speed of the particles in their orbits but they do display a time ordering for the whole system of orbits and in particular this allows a distinction to be made between the velocity $\boldsymbol{v}_{\mathrm{in}}$ and $\boldsymbol{v}_{\mathrm{out}}$ at any point in space.

The asymptotic form for the time-dependent wavefunction for a scattering energy eigenstate is given by

$$\exp(-\mathrm{i}\phi)\Psi(\boldsymbol{x},t)\sim\{(\rho_{\mathrm{in}})^{1/2}\exp[\mathrm{i}(S_{\mathrm{in}}-Et)/\hbar]-\mathrm{i}(\rho_{\mathrm{out}})^{1/2}\exp[\mathrm{i}(S_{\mathrm{out}}-Et)/\hbar]\}. \tag{4.3}$$

(The phase factor, which is constant in spacetime but variable with respect to $\hbar$, has been put on the left to simplify the structure on the right.)

The relation (4.3) is an asymptotic form of a function of $\hbar$, as $\hbar\to 0$, with the spacetime point a parameter. The behaviour of the right-hand side, as a function of $\hbar$ but for fixed $\boldsymbol{x}$, t, is completely different when one or other exponent vanishes (they can only vanish together on the Z axis) from the general behaviour when neither vanishes. Hence the set of points in spacetime for which either

$$S_{\mathrm{in}}(\boldsymbol{x})-Et=0 \tag{4.4}$$

or

$$S_{\mathrm{out}}(\boldsymbol{x})-Et=0 \tag{4.5}$$

can be determined. For fixed t the spatial points satisfying either of these equations give the action surfaces illustrated in figure 2 and represented by equation (2.19). For $t<0$ only (4.4) can be satisfied, but for $t>0$ both equations can be satisfied—at differential spatial points. One can see clearly the different character of the cases $t<0$ and $t>0$ in figure 2, where the transitional curve, $S_{\mathrm{in}}=0$, exhibits a cusp. If the curves for $t>0$ are described as seagulls, the wings are formed from the points satisfying (4.4) and the bodies by (4.5). The sections meet on the Z axis and the union is a representation of (2.19).

From the action waves the complete set of particle orbits, which are everywhere orthogonal to the surfaces of constant action, can be recovered.

Although the time-independent quantum mechanical wavefunction is single-valued in space, the action wave (2.19), derived from it by the above procedure meets every spatial point twice. It is this fact that provides the reconciliation between single-valued quantum mechanics and the two velocity fields of classical mechanics.

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