

Semiclassical approximation of the radial equation with two-dimensional potentials

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Received 24 April 1973

Abstract. The radial equation for scattering from a cylindrically symmetrical potential is examined, because two-dimensional scattering arises in high-energy electron diffraction from crystals. Particular attention is paid to the case of s waves, where there is a *centripetal* attractive potential for free particles. After showing that the Langer transformation, which leads to correct semiclassical wavefunctions for all other cases in two and three dimensions, fails for s waves, we apply the method of comparison equations, which enables us to express the phase shifts and bound state conditions in a simple form valid for all angular momenta. We test the theory for s waves by comparison with exactly-calculated energy levels.

1. Introduction

The properties of wavefunctions, energy levels, etc, in a cylindrically symmetric field of force do not seem to have been studied very much, probably because of the lack of experimental motivation. However, recent investigations (Berry 1971, Berry and Ozorio de Almeida 1972) of the theory underlying high-energy electron microscopy of metal foils have drawn attention to two-dimensional systems. Briefly, the reason for this is that a fast electron (kinetic energy ~ 1 MeV) does not respond to all the details of the force field inside the metal, but only to the *average* potential along its direction of motion; this is true in both classical and quantum mechanics (Lindhard 1965, Berry 1971). For certain crystal orientations (the so-called 'cross-grating' case) the strings of atoms constituting the metal average to cylinders, along the axes of which the potential has a logarithmic singularity arising from the Coulomb field of the atomic nuclei. The observed diffraction from the foil depends on the 'two-dimensional band structure' of this array of cylinders, so that it is necessary to study the phaseshifts, bound states, etc, of an individual cylinder. This work has led to problems in the interpretation and approximation of radial wavefunctions which we present here as they may be of wider interest.

The wave equation for a particle of mass m and energy E moving in two dimensions in a cylindrically symmetrical potential $V(R)$ is

$$\nabla^2 \chi(R, \theta) + \frac{1}{\epsilon^2} (E - V(R)) \chi(R, \theta) = 0, \quad (1)$$

where R, θ are the usual plane polar coordinates and ϵ^2 is the 'semiclassical parameter'

$\hbar^2/2m$. Separation of variables leads to

$$\chi(R, \theta) = \sum_{l=-\infty}^{\infty} a_l e^{i l \theta} \frac{\psi_l(R)}{R^{1/2}}, \quad (2)$$

where the reduced radial wavefunction $\psi_l(R)$ satisfies

$$\frac{d^2 \psi_l(R)}{dR^2} + \frac{1}{\epsilon^2} [E - V(R) - \epsilon^2(l^2 - \frac{1}{4})/R^2] \psi_l(R) = 0, \quad (3)$$

l being the angular momentum quantum number. We assume that the potential $V(R)$ is regular, so that any singularity at the origin satisfies

$$R^2 V(R) \xrightarrow{R \rightarrow 0} 0. \quad (4)$$

The radial equation (3) differs from its three-dimensional analogue only in the appearance of $l^2 - \frac{1}{4}$ instead of the more familiar $l(l+1)$. The case of s waves ($l = 0$) is unique: It is the only instance where a radial equation acquires a *centripetal potential well* instead of the usual centrifugal barrier, and this will obviously need special treatment. For the higher partial waves, on the other hand, we expect that it should be easy to adapt familiar three-dimensional methods for calculating bound-state energies and scattering phaseshifts.

In § 2 we examine the behaviour of (3) for free particles, concentrating on the case of s waves. In § 3 we attempt to find semiclassical approximations (Berry and Mount 1972) for $\psi_l(R)$ by using the modified WKB technique developed by Langer (1937) to deal with the singularity of the centrifugal potential at the origin. We find that the method fails for s waves and in § 4 we deal with this delicate case by using the 'method of comparison equations' (Miller and Good 1953, Dingle 1956). Finally, in § 5, we give general approximate formulae for the energy levels and phaseshifts of equation (3), and compare the first few s wave bound states in a logarithmic potential with the exactly-calculated values.

2. The free particle

We study this case not only because the radial equation (3) can be solved exactly when $V(R)$ is zero, but also because even in the presence of a potential the situation near the origin is dominated by the free-particle term $(l^2 - \frac{1}{4})/R^2$, due to our assumption of regularity (equation (4)). The general free-particle solution of (3) can be expressed in terms of standard Bessel functions (Abramowitz and Stegun 1964), as

$$\begin{aligned} \psi_l(R) &= AR^{1/2} J_l \left(\frac{E^{1/2} R}{\epsilon} \right) + BR^{1/2} Y_l \left(\frac{E^{1/2} R}{\epsilon} \right) & (E > 0) \\ &= CR^{1/2} I_l \left(\frac{(-E)^{1/2} R}{\epsilon} \right) + DR^{1/2} K_l \left(\frac{(-E)^{1/2} R}{\epsilon} \right) & (E < 0) \end{aligned} \quad (5)$$

where A , B , C and D are constants.

The square-integrability condition on $\chi(R, \theta)$ (equation (2)) in any finite region (which is necessary in order to exclude solutions corresponding to an infinite number of

particles in the region), requires that

$$\int_0^R dR' \psi_i^2(R') \xrightarrow{R \rightarrow 0} 0, \quad \frac{\psi_i^2(R)}{R} \xrightarrow{R \rightarrow \infty} \text{bounded.} \quad (6)$$

When l is nonzero the first condition demands that B is zero if $E > 0$, and that D is zero if $E < 0$, while the second condition demands only that C is zero if $E < 0$. Thus there are, as expected, no bound states, and the free states take the simple form

$$R^{1/2} J_l \left(\frac{E^{1/2} R}{\epsilon} \right).$$

When l is zero, (6) no longer requires B and D to vanish (although C must still be zero), so that the function

$$\psi_0(R) = DR^{1/2} K_0 \left(\frac{(-E)^{1/2} R}{\epsilon} \right) \quad (7)$$

appears to correspond to a normalizable s wave bound state with arbitrary negative energy, possessing no nodes in the centripetal potential well $-\epsilon^2/4R^2$! But this solution (as well as the positive-energy solution with $B \neq 0$) can be excluded on physical grounds because (i) the solution (7) will not permit the consistent calculation of expectation values of operators† and (ii) the solution does not appear as a limiting case when we consider a set of finite potential wells of the form

$$\begin{aligned} V(R) &= -\frac{\epsilon^2}{4R^2} & R > \Delta R \\ &= -\frac{\epsilon^2}{4(\Delta R)^2} & R < \Delta R \end{aligned} \quad (8)$$

and let $\Delta R \rightarrow 0$.

When the potential $V(R)$ is not zero, $\psi_l(R)$ still takes the form (5) (with $C = 0$) as $R \rightarrow \infty$. For positive energies the values of A and B define two-dimensional phaseshifts η_l from the relation

$$\begin{aligned} \psi_l(R) \underset{(R > R_c)}{=} & \cos \eta_l R^{1/2} J_l \left(\frac{E^{1/2} R}{\epsilon} \right) - \sin \eta_l R^{1/2} Y_l \left(\frac{E^{1/2} R}{\epsilon} \right) \\ & \xrightarrow{R \rightarrow \infty} \text{constant} \times \cos \left(\frac{E^{1/2} R}{\epsilon} - \left(l + \frac{1}{2} \right) \frac{\pi}{2} + \eta_l \right), \end{aligned} \quad (9)$$

where R_c is the range of $V(R)$, and the two-dimensional scattering amplitude is

$$F(\theta) = \frac{(2\hbar/\pi)^{1/2}}{(2mE)^{1/4}} \sum_{l=-\infty}^{\infty} e^{i\eta_l} \sin \eta_l e^{i l \theta}. \quad (10)$$

The ‘scattering width’—analogous to the three-dimensional cross section—is simply $|F(\theta)|^2$.

† Consider for example the kinetic energy operator $p^2/2m$. Its expectation value for a state $|\chi\rangle$ may be written either as $\langle \chi | (p^2/2m) | \chi \rangle$ or as $(\langle \chi | p) \cdot (p | \chi \rangle) / 2m$. For these two expressions to have the same value, we must have $\psi(R) R^{1/2} \partial / \partial R (\psi(R) / R^{1/2}) \xrightarrow{R \rightarrow 0} 0$, and this condition is violated by (7). (Similarly arguments exclude the solution $\exp\{(-E)^{1/2} r / \epsilon\}$ in three dimensions.)

3. WKB approximations and the Langer transformation

Under semiclassical conditions ϵ is small, and the most obvious procedure is to approximate (3) by the WKB method. This leads to

$$\psi_l(R) \simeq \psi_l^{\text{WKB}}(R) = (Q_0(R))^{-1/2} \exp\left(\pm \frac{i}{\epsilon} \phi_0(R_0, R)\right), \quad (11)$$

where

$$Q_0^2(R) \equiv E - V(R) - \frac{\epsilon^2(l^2 - \frac{1}{4})}{R^2}, \quad (12)$$

and

$$\phi_0(R_0, R) \equiv \int_{R_0}^R dR Q_0(R), \quad (13)$$

R_0 being any fixed point, usually a zero of $Q_0(R)$ —a 'turning point'.

It is well known, however (Berry and Mount 1972), that this procedure fails because ψ_l^{WKB} is not a valid approximation at the origin. To see this we follow Langer (1937) and note that ψ_l^{WKB} satisfies

$$\frac{d^2 \psi_l^{\text{WKB}}}{dR^2} + \frac{1}{\epsilon^2} (Q_0^2(R) - \epsilon^2 W_0(R)) \psi_l^{\text{WKB}} = 0, \quad (14)$$

where

$$W_0(R) = \frac{3(Q_0'(R))^2}{4Q_0^2(R)} - \frac{Q_0''(R)}{2Q_0(R)}. \quad (15)$$

The semiclassical approximation is the first term of an asymptotic expansion in powers of ϵ , and (14) will be equivalent to (3), ie ψ_l^{WKB} will be a good approximation to ψ_l , provided the following conditions are satisfied:

- (a) If $Q_0^2(R)$ is bounded and not zero, $W_0(R)$ must be bounded.
- (b) If $Q_0^2(R)$ diverges, $\epsilon^2 W_0(R)/Q_0^2(R)$ must be negligible.
- (c) If $Q_0^2(R)$ vanishes, $W_0(R)$ must vanish also.

Along most of the real axis, case (a) applies, and the WKB method may be used. At a simple turning point, case (c) is violated and the WKB method fails. In the present case $Q_0^2(R)$ diverges at the origin (equation (12)) and case (b) applies; it is easy to show that, for all $V(R)$ satisfying (4),

$$\frac{\epsilon^2 W_0(R)}{Q_0^2(R)} \xrightarrow{R \rightarrow 0} \frac{1}{4l^2 - 1}, \quad (16)$$

which is certainly not negligible for the small values of l frequently considered.

Langer overcomes this difficulty in three-dimensional cases by making the transformation

$$R \equiv e^x, \quad \psi_l(R) \equiv e^{x/2} u_l(x), \quad (17)$$

where the domain of the new variable x is the whole real axis. Applied to the two-dimensional equation (3), this gives

$$\frac{d^2 u_l(x)}{dx^2} + \frac{1}{\epsilon^2} q^2(x) u_l(x) = 0, \quad (18)$$

where

$$q^2(x) = e^{2x}(E - V(e^x)) - \epsilon^2 l^2. \tag{19}$$

The WKB method will apply under the same conditions as follow equation (15), with $q^2(x)$ replacing $Q_0^2(R)$, and

$$w(x) \equiv \frac{3(q'(x))^2}{4q^2(x)} - \frac{q''(x)}{2q(x)} \tag{20}$$

replacing $W_0(R)$. At the origin of R , ie as $x \rightarrow -\infty$, we have $q^2(x) \rightarrow -\epsilon^2 l^2$, so that for nonzero l case (a) applies, and, since $w(x) \rightarrow 0$ for regular potentials, the condition is satisfied.

The approximate solution of (3) for this case is given by the WKB approximation to (18), namely

$$\begin{aligned} \psi_l(R) &\simeq \psi_l^{\text{(Langer WKB)}} = \frac{e^{x/2}}{(q(x))^{1/2}} \exp\left(\pm \frac{i}{\epsilon} \int_{x_0}^x q(x) dx\right) \\ &= (Q_1(R))^{-1/2} \exp\left(\pm \frac{i}{\epsilon} \phi_1(R)\right), \quad (l \neq 0) \end{aligned} \tag{21}$$

where

$$\begin{aligned} Q_1^2(R) &\equiv e^{-2x} q^2(x) = E - V(R) - \frac{\epsilon^2 l^2}{R^2} \\ \phi_1(R_0, R) &\equiv \int_{x_0}^x dx q(x) = \int_{R_0}^R dR Q_1(R). \end{aligned} \tag{22}$$

Thus the effect of the Langer transformation is to replace $l^2 - \frac{1}{4}$ by l^2 in ψ_l^{WKB} as given by (11); this is precisely analogous to replacing $l(l+1)$ by $(l+\frac{1}{2})^2$ in three-dimensional cases (Berry and Mount 1972).

However, the Langer method fails completely for s waves. When l is zero, $q^2(x) \rightarrow 0$ as $x \rightarrow -\infty$, so that case (c) applies; $w(x)$ does not vanish, but tends to a constant characteristic of $V(R)$. For the attractive logarithmic case of physical interest, where, near the origin

$$V(R) = a \ln R, \tag{23}$$

we have

$$w(x) \xrightarrow{x \rightarrow -\infty} \frac{1}{4}. \tag{24}$$

Thus condition (c) is violated, and we must seek a different approximate method to deal with s waves near the origin.

To understand what has gone wrong, we use the potential (23) as an example, and notice that $q^2(x)$ (equation (19)) can be written in the form

$$q^2(x) = -bx e^{2x} - \epsilon^2 l^2, \tag{25}$$

where the origin of x has been displaced by $-E/a$, and

$$b \equiv a e^{2E/a}. \tag{26}$$

With this form for $q^2(x)$, the Langer-transformed equation (18) resembles a one-dimensional Schrödinger equation with 'energy' $-\epsilon^2 l^2$ and 'potential' $bx e^{2x}$ (figure 1). For

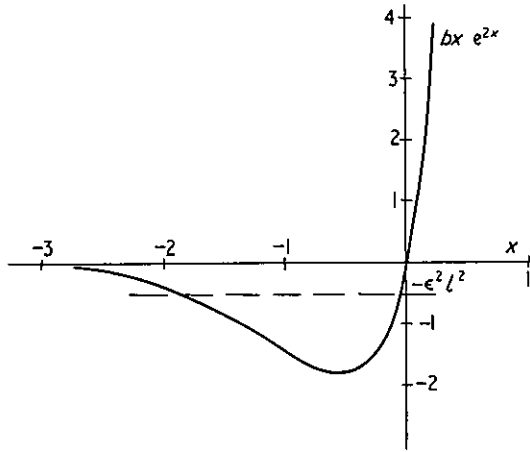


Figure 1. 'Potential energy' diagram corresponding to equation (18) with attractive logarithmic potential ($b = 10$).

nonzero l the point $x = -\infty$ lies in an ordinary 'classically forbidden region' dominated by the centrifugal repulsion, while for s waves the point $x = -\infty$ lies just on the boundary between free and bound states, since the Langer transformation neatly eliminates the centripetal well. For $l = 0$, (18) has the exact limiting solution

$$u_0(x) \xrightarrow{x \rightarrow -\infty} Ax + B. \tag{27}$$

For the corresponding $\psi_0(R)$ to be an acceptable wavefunction near the origin (cf footnote after equation (7)), A must vanish. This, together with boundedness of $\psi_0(R)$ as R or $x \rightarrow +\infty$, imposes a discrete spectrum on b and hence on E . The WKB approximation to (18) does not behave like (27), however, but like

$$u_0^{\text{WKB}}(x) = \frac{e^{-x/2}}{(-bx)^{1/4}} \sin\left(\frac{1}{\epsilon} \int_{-\infty}^x dx' q(x') + \alpha\right) \tag{28}$$

$$\xrightarrow{x \rightarrow -\infty} \frac{e^{x/2}}{\epsilon} (-bx)^{1/4} \cos \alpha + \frac{e^{-x/2}}{(-bx)^{1/4}} \sin \alpha, \tag{29}$$

where α is a phase angle which must be set equal to zero for an acceptable solution. This incorrect form arises because the 'turning point' at $x = -\infty$ has not been treated properly, and we shall see in § 5 that (28) leads to totally false numerical values for eigenvalues.

4. The comparison equation method for s waves

To deal with this delicate case we map the unknown solution $u_0(x)$ of the Langer-transformed equation (18) onto the known solution $U_0(X)$ of

$$\frac{d^2 U_0(X)}{dX^2} + \frac{1}{\epsilon^2} Q^2(X) U_0(X) = 0, \tag{30}$$

where $Q(X)$ is a simple function resembling $q(x)$. The simplest approximate mapping

procedure can easily be shown (Miller and Good 1953) to yield

$$u_0(x) \simeq u_0^{\text{comp eq}}(x) = \left(\frac{dX(x)}{dx} \right)^{-1/2} U_0(X(x)), \tag{31}$$

where $X(x)$ is defined by

$$\int_{-\infty}^{X(x)} dX Q(X) = \int_{-\infty}^x dx q(x). \tag{32}$$

The approximate solution satisfies

$$\frac{d^2 u_0^{\text{comp eq}}(x)}{dx^2} + \frac{1}{\epsilon^2} (q^2(x) - \epsilon^2 w_1(x)) u_0^{\text{comp eq}}(x) = 0, \tag{33}$$

where

$$w_1(x) = \frac{3}{4} \left(\frac{X''}{X'} \right)^2 - \frac{1}{2} \frac{X'''}{X'}, \tag{34}$$

and $u_0^{\text{comp eq}}(x)$ will be a good approximation under the conditions following equation (15).

The WKB method, which fails for s waves, corresponds to taking $Q(X)$ as constant; $w_1(x)$ is then equal to $w(x)$ (equation (20)), and we have seen that case (c) applies, and the condition is violated. It is evident by inspection of (19) or (25) that a better approximation will be obtained by taking

$$Q(X) = \beta e^{2X} \tag{35}$$

for s waves (β is an arbitrary constant). The exact solution of equation (30) which behaves properly as $X \rightarrow -\infty$ (cf equation (27) and following) is

$$U_0(X) = J_0 \left(\frac{1}{\epsilon} \sqrt{\beta} e^X \right). \tag{36}$$

Transforming back to the original variables via equations (31), (17) and (22) gives, for the s wave reduced radial wavefunction:

$$\psi_0(R) \simeq \psi_0^{\text{comp eq}}(R) = \left(\frac{\phi_1(0, R)}{Q_1(R)} \right)^{1/2} J_0 \left(\frac{1}{\epsilon} \phi_1(0, R) \right). \tag{37}$$

Is this solution valid near the origin? Only if $w_1(x) \rightarrow 0$ as $x \rightarrow -\infty$, since we are dealing with case (c), but from (34) it can be shown that

$$w_1(x) \xrightarrow{x \rightarrow -\infty} \left(\frac{R(E - V(R))^{1/2}}{\int_0^R dR' (E - V(R'))^{1/2}} \right)^{1/2} R \frac{d}{dR} R \frac{d}{dR} \left(\frac{\int_0^R dR' (E - V(R'))^{1/2}}{R(E - V(R))^{1/2}} \right)^{1/2}, \tag{38}$$

which is zero for all regular potentials, repulsive as well as attractive.

5. Phaseshifts and bound states

We have found that near the origin the solution (21) holds if $l \neq 0$, and (37) holds for s waves. These solutions break down, of course, when any turning points of equation (18) for nonzero R ($x > -\infty$) are reached, since the condition for case (c) (following equation (15)) is violated. Let R_1 be a turning point which is a simple zero of $Q_1^2(R)$ (equation (22)), and which therefore separates a classically allowed region $Q_1^2(R) > 0$ from a forbidden

region $Q_1^2(R) < 0$; standard theory (Berry and Mount 1972) then leads to the 'connection formula'

$$[Q_1^2(R) < 0] \exp \frac{(-|\phi_1(R_1, R)|/\epsilon)}{2|Q_1(R)|^{1/2}} \leftarrow \psi_l(R) \rightarrow \frac{\cos(\phi_1(R_1, R)/\epsilon - \pi/4)}{|Q_1(R)|^{1/2}} [Q_1^2(R) > 0]. \quad (39)$$

The disposition of turning points, which determines how this formula must be applied, is different if $E \geq 0$ and if l is zero or not, and we deal with these cases in turn.

5.1. Phaseshifts: ($E > 0$)

When l is not zero there must be an odd number of simple turning points, since the origin is in the forbidden region dominated by centrifugal repulsion, and the region $R \rightarrow \infty$ is classically allowed. For cases where there is just one turning point at R_1 we can use (39) directly, since the appropriate Langer solution (21) grows exponentially away from $R = 0$, ie it decays away from R_1 towards R_0 . Thus we have

$$\psi_l(R) \underset{(R \gg R_c)}{\approx} \frac{\cos[(1/\epsilon)\phi_1(R_1, R) - \pi/4]}{(Q_1(R))^{1/2}} \\ \xrightarrow{R \rightarrow \infty} E^{-1/4} \cos \left(\frac{RE^{1/2}}{\epsilon} + \frac{1}{\epsilon} \int_{R_1}^{\infty} (Q_1(R) - E^{1/2}) dR - \frac{R_1 E^{1/2}}{\epsilon} - \frac{\pi}{4} \right) \quad (l \neq 0). \quad (40)$$

(Cases of three or more turning points involve resonance behaviour (Berry and Mount 1972).)

For the s wave case we must use (37); there are no turning points for $R > 0$, so that no connection formula is required, and we obtain the asymptotic behaviour directly from (37) as

$$\psi_0(R) \xrightarrow{R \rightarrow \infty} \text{constant} \times \frac{\cos[(1/\epsilon)\phi_1(0, R) - \pi/4]}{(Q_1(R))^{1/2}}. \quad (41)$$

This has precisely the same form as (40) since $R = 0$ is a turning point of the Langer-transformed equation (18) on which our treatment is based.

Comparison with (9) gives the phaseshift

$$\eta_l = \frac{1}{\epsilon} \left(\int_{R_1}^{\infty} dR (Q_1(R) - E^{1/2}) - R_1 E^{1/2} \right) + \frac{l\pi}{2} \quad (42)$$

valid for all l . If we had used the incorrect WKB expression (21) for $l = 0$, we would have found a value for η_0 which was too small by $\pi/4$.

5.2. Bound states: ($E < 0$)

When l is not zero there must be an even number of simple turning points, since $R \rightarrow \infty$ is now classically forbidden. We consider the commonest case of two turning points, at R_1 and R_2 ($R_2 > R_1$). Then (39) must be used twice, to connect the wave (21) across R_1 into

the potential well between R_1 and R_2 , and to connect the wave which must decay exponentially at $R \rightarrow \infty$ across R_2 into the potential well. The two expressions for the wave in the potential well must be the same (Berry and Mount 1972), so that

$$\cos\left(\frac{1}{\epsilon}\phi_1(R_1, R) - \frac{\pi}{4}\right) = \pm \cos\left(\frac{1}{\epsilon}\phi_1(R, R_2) - \frac{\pi}{4}\right), \tag{43}$$

that is,

$$\frac{1}{\epsilon}\phi_1(R_1, R_2) = (n - \frac{1}{2})\pi, \tag{44}$$

which for $n = 1, 2, 3, \dots$ gives the eigenvalues E for each partial wave l .

For s waves there is only one finite turning point of (18), at R_2 , since $R_1 = 0$ (cf figure 1). Taking the asymptotic form of (18) and using (39), we find precisely the condition (44), which therefore holds for all l . To test the theory for s waves, we have computed the exact eigenvalues b_n (using the well-known Milne method of numerical integration) for a logarithmic potential (equation (18), with $q^2(x)$ given by (25) and $l = 0$). Then (cf equation (22)),

$$\frac{1}{\epsilon}\phi_1(R_1, R_2) = b_n^{1/2} \int_{-\infty}^0 dx (-x)^{1/2} e^x = \frac{1}{2}(\pi b_n)^{1/2} \tag{45}$$

which is compared with the value $(n - \frac{1}{2})\pi$ predicted by (44) in table 1. To show that our analysis is more than a pedagogic exercise we also show in the last column the values of $(n - \frac{1}{4})\pi$ which would have occurred in the eigenvalue condition if the wavefunction (21) had been incorrectly used for s waves.

Table 1. Comparison of exact phase ϕ of bound states in a logarithmic potential with comparison equation approximation $((n - \frac{1}{2})\pi)$ and Langer-type WKB approximation $((n - \frac{1}{4})\pi)$

n	$\phi(R_1, R_2)$	$(n - \frac{1}{2})\pi$	$(n - \frac{1}{4})\pi$
1	1.50	1.57	2.36
2	4.67	4.71	5.50
3	7.82	7.85	8.64
4	10.96	10.99	11.78

Summing up, we find that the Langer transformation is useful for two-dimensional radial equations, but that for s waves further analysis, employing the method of comparison equations, is required to elucidate the form of wavefunctions near the origin. A pleasing consequence of the analysis is that the equations for phaseshifts (42) and bound states (44) take the same form for all l .

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