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A uniform asymptotic approximation of the 3D scattering wavefunction for a central potential: a new Ansatz

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Abstract
A uniform asymptotic approximation of the 3D scattering wavefunction for a central potential is obtained by using a new Ansatz on the form of a solution. This Ansatz employs the regular reduced radial wavefunction of zero orbital angular momentum, generated by the problem itself, rather than a standard special function. The uniform asymptotic approximation of the 3D scattering wavefunction allows finding of the scattering amplitude without using the partial wave expansion. The method is applied to the scattering by a pure Coulomb potential. In contrast to the uniform asymptotic approximation of the 3D Coulomb wavefunction, based on the Airy function that breaks down at the caustic $\xi = 0$, the uniform asymptotic approximation obtained in this paper is valid over the whole range of the variables. It is shown that the uniform asymptotic approximation of the 3D Coulomb scattering wavefunction obtained through the new Ansatz is the same expression as that of the Gordon solution written in the form obtained by the present authors of a previous paper.

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1. Introduction

The knowledge in physics of molecules, atoms and nuclei can be obtained by the study of quantum collision processes. In order to solve the scattering problem for a central potential, the most frequently used method is the partial wave expansion of the solution [1–3]. However, it is well known that even for problems that have been solved, unfortunately this solution is too complicated to be used in practical applications. Moreover, the partial wave expansion does not emphasize the functional dependence of the wavefunction nor the scattering amplitude on the potential parameters, which is necessary if one desires to analyze the formula in order to obtain a description of what is happening during the collision. Because of this, considerable effort has been devoted to the study of approximate solution methods. The method of the Wentzel–Kramers–Brillouin (WKB) approximation is applied in almost all branches of physics, from tides and earthquakes, optics to ionospheric theory and quantum mechanics.

The 3D WKB approximation is the main approximation used in the study of the scattering processes. This is a non-uniform asymptotic approximation, obtained by taking a small parameter: the Planck constant $\hbar$ [4].

The advantage of the 3D WKB approximation is its high precision. The main merit of the 3D WKB approximation is that it is a 'doubly asymptotic expansion' [5, 6]. This is an approximation that has asymptotic character not only for small $\hbar$, but also with respect to large $|\vec{r}|$. The remainder of this approximation is small both for small $\hbar$ and large $|\vec{r}|$. The knowledge of this doubly asymptotic approximation is extremely helpful. This allows us to describe the solutions in a unique fashion and to select the scattering solution that satisfies the radiation condition at infinity.

The main shortcoming of the WKB approximation is that it becomes infinite on certain surfaces, called caustics. Caustics are the higher dimensional analog for partial differential equations of the turning points of the WKB theory for ordinary differential equations. The problem of caustic fields is topical in the scattering of light and particles (e.g. rainbow phenomena in optics, in atomic and nuclear physics), in the wave propagation (e.g. radio and microwave antenna, problems of eigenmodes and waves in cavities and waveguides), etc. Caustics as physical objects have been analyzed by Kravtsov [7].

In order to overcome the above-mentioned shortcoming of the WKB approximation, a different approximation that is uniformly valid in a region containing one or more caustics is necessary. The asymptotic representation of the solution is greatly simplified if one uses a uniform asymptotic approximation. The Stokes phenomenon is obviated, and the solution is represented by a single form over the entire range of variables [5, 6]. Thus, a uniform asymptotic approximation provides a smooth transition across a caustic. Kravtsov [8] and Ludwig [9] derived the uniform asymptotic approximation of the solution in a region containing the simplest caustics. They have represented the solution of the problem in terms of the solution of a 'related' or 'comparison' equation, by a method introduced and developed by Langer [10]. The method of the 'comparison' equation has been discussed in detail by Olver [11]. Applications of the comparison equation method to the wave theory are given in [12].

In the case of the smooth convex caustic, the Airy function equation has been taken as a comparison equation [8, 9]. In other terms, the solution has been represented as a linear combination of the Airy function and its derivative. In the vicinity of the caustics, the wavefunction has a smooth transition between oscillatory and exponentially damped behavior, with large values on the caustic itself. The term of the solution which involves the derivative of the Airy function is relatively small near the caustics, but prominent away from caustics. This term makes the uniform expansion possible [9, 13]. Away from the caustic, the solution reduces to the 3D WKB approximation.

The uniform asymptotic approximations have been used in a large variety of problems, each problem imposing the type of special functions to be employed. The generalized Bessel and Hankel functions, Airy function, Weber functions, Fresnel integral functions have been used by Ludwig [14], Lewis, Bleinstein and Ludwig [15], Matkowsky [16], Kravtsov [17], Lewis and Boersma [18], Smith [19], Zauderer[20], Shen and Keller [21], Shen [22], Keller and Ahluwalia [23] in order to give the asymptotic solution for phenomena such as the scattering by a general convex obstacle, creeping waves, gallery modes, edge diffraction, trapped waves, surface waves on fluid, wave propagation in a rotating ocean. More references to the uniform asymptotic approximation can be found in the books [13, 24–26].

While specific problems have been solved by the uniform asymptotic approximation method, a general theory for the 3D scattering problem has not been given, in contrast to the 1D case where there is the theory for the turning points problem [5, 6]. There is no general method to determine the appropriate uniform expansion for any given problem. Catastrophe theory [13] paved the way for a general theory of uniform asymptotics based on standard integrals. However, there is no general method for determining the appropriate 'Ansatz' about the form of the solution *a priori*. The method of the uniform asymptotic approximation has some characteristic difficulties [27]. An accurate guess ('Ansatz') for the form of the solution is necessary, otherwise singularities will occur in some undetermined coefficients. Another difficulty of the uniform asymptotic approximation is that the labor involved increases sharply as the complexity of the problem increases [27].

The success of the uniform asymptotic expansions is connected with the principle of parsimony formulated by Ludwig [28]: it is important not to take too many terms in the expansion (usually not more than one term), and it is important not to include more complications in the asymptotics than are absolutely necessary. This parsimony principle makes the method of the uniform asymptotic expansion easy to apply and makes it insensitive to the fine features of the structure under consideration.

In the present work, a uniform asymptotic expansion with one term of the 3D wavefunction describing the scattering process of a spinless particle by a central potential is obtained. In the study of the scattering process, the uniform asymptotic approximation of the wavefunction is very important because its asymptotic at $r \to \infty$ allows us to obtain the explicit expression of the scattering amplitude, emphasizing the dependence on the potential parameters. This paper is based on a new Ansatz. Instead of using the standard special functions (Airy, Bessel, Weber, etc) as solutions of the comparison equation, a function generated by the problem itself is used. The special function used in this work is the regular reduced radial wavefunction of zero orbital angular momentum. The uniform asymptotic approximation of the 3D scattering wavefunction allows finding the scattering amplitude without using the partial waves expansion. In this way, the convergence difficulties related to the scattering amplitude expansion in Legendre polynomials are obviated [29]. The method is applied to a pure Coulomb potential. The more general case of a short-range plus Coulomb potential will be presented in a separate paper. In [30], a uniform asymptotic approximation of the Coulomb wavefunction based on the Airy function was given. This approximation is valid in the region of the caustic $\xi = 4\eta/k$, but fails at the caustic $\xi = 0$, where $\xi = r(1 - \cos\theta)$ is a parabolic coordinate. In contrast, the uniform asymptotic approximation obtained in this paper is valid over the whole range of the variables, including the caustic $\xi = 0$.

This paper is organized as follows. In section 2, a uniform asymptotic approximation for the 3D scattering wavefunction by a central potential is deduced by using a new Ansatz. The special function of the approximation is the regular reduced radial wavefunction of zero angular momentum. In section 3, the 3D uniform asymptotic approximation of the Coulomb scattering wavefunction is obtained. The 3D WKB asymptotic approximation is deduced for the Coulomb potential in order to identify and analyze the caustics of this problem. This allows us to choose the appropriate comparison equation in order to obtain the 3D uniform asymptotic approximation, according to the criteria to be fulfilled by the comparison equation method presented in appendix A. The uniform asymptotic approximation of the 3D Coulomb scattering wavefunction is obtained by using the new Ansatz on the form of a solution. The uniform asymptotic approximate wavefunction is in fact the exact Gordon solution expressed in the form obtained by Grama, Grama and Zamfirescu in a previous paper [30]. This demonstrates the accuracy of the guess (Ansatz) of the solution.

2. Uniform asymptotic approximation of the 3D scattering wavefunction for a central potential. New Ansatz

We consider the scattering of a spinless particle by a potential $U(\vec{r})$ that decreases at infinity. The wavefunction Ψ that describes the scattering process satisfies the Schrödinger equation

$$\Delta\Psi + (k^2 - V(\vec{r}))\Psi = 0, \tag{1}$$

with $k^2 = \frac{2m}{\hbar^2}E$, $V(\vec{r}) = \frac{2m}{\hbar^2}U(\vec{r})$. Ψ is a regular function in $\mathbf{R}^3$ and

$$\Psi = \text{plane wave} + \phi(r), \tag{2}$$

where $\phi(r)$ satisfies the radiation condition at infinity. If $V(\vec{r})$ is a short-range potential, i.e. $\lim_{r\to\infty} V(\vec{r}) \sim \mathcal{O}(r^{-\epsilon})$, $\epsilon > 2$, then the radiation condition is [31]

$$\lim_{r\to\infty} (\partial\phi/\partial r - \mathrm{i}k\phi) = 0. \tag{3}$$

If $V(\vec{r})$ is a long-range potential, i.e. $\lim_{r\to\infty} V(\vec{r}) \sim \mathcal{O}(r^{-\epsilon})$, $\epsilon < 2$, then the radiation condition is 'non-spherical' [32, 33],

$$\lim_{r\to\infty} (\nabla\phi - \mathrm{i}k\nabla S\phi) = 0, \tag{4}$$

where S satisfies the eikonal equation

$$(\nabla S)^2 = 1 - \frac{V(\vec{r})}{k^2}. \tag{5}$$

We shall find the asymptotic solution of (1) for small Plank constant $\hbar$. Instead of working in (1) with small $\hbar$ a large parameter λ is introduced. In other words, the asymptotic solution for large λ of the following equation will be obtained:

$$\Delta\Psi + \lambda^2(k^2 - V(\vec{r}))\Psi = 0. \tag{6}$$

In the final expression of the wavefunction, the parameter λ will be put $\lambda = 1$. Let us consider the 3D WKB approximation of the solution for the scattering by a central potential $V(r)$. In order to obtain the 3D WKB approximation for Ψ, we look for a solution of (6) for large λ of the form [4, 34]

$$\Psi = A(\vec{r})\,\mathrm{e}^{\mathrm{i}\lambda S(\vec{r})}. \tag{7}$$

Substituting (7) into (6) and by grouping the like-power terms, the following equations are obtained:

$$(\nabla S)^2 = k^2 - V(r) \quad \text{eikonal equation}, \tag{8}$$

$$2\nabla A\nabla S + A\Delta S = 0 \quad \text{transport equation}. \tag{9}$$

By solving (8) and (9) the eikonal $S(\vec{r})$ and the amplitude $A(\vec{r})$ are obtained, i.e. the 3D WKB approximation is obtained.

Our problem is to determine a uniform asymptotic approximation of the 3D solution of the Schrödinger equation which describes the scattering by a central potential $V(r)$. Taking into account the characteristic difficulties of a uniform asymptotic approximation mentioned in section 1, we introduce a new initial guess ('new Ansatz'). We start from the idea that the special function used in the form of a solution must be generated by the problem itself, rather than using standard special functions (Airy, Bessel, Weber, etc). Let us consider the partial waves expansion of the wavefunction $\Psi(\vec{r})$ which describes the scattering

$$\Psi(\vec{r}) = \sum_{l=0}^{\infty} C_l \frac{R_l(r)}{r} P_l(\cos\theta), \tag{10}$$

where $R_l(r)$ are the regular reduced radial wavefunctions and $P_l(\cos\theta)$ are the Legendre polynomials. Let us take the WKB approximation of both parts of (10). Then the singularities of the WKB approximations of the regular reduced radial wavefunctions at the turning points and the singularities must be somehow reflected in the singularities of the 3D WKB approximation of $\Psi(\vec{r})$ at caustics. This leads us to the new Ansatz, namely we take as the special function which occurs in the uniform approximation of the solution $\Psi(\vec{r})$ the regular reduced radial wave function of zero orbital angular momentum $R_0(r)$. In other words, we take the form

$$\Psi(\vec{r}) = \mathrm{e}^{\mathrm{i}\lambda\omega(\vec{r})}\left\{g(\vec{r})R_0(\rho(\vec{r})) - \frac{\mathrm{i}}{\lambda}h(\vec{r})R_0'(\rho(\vec{r}))\right\}. \tag{11}$$

Here, R_0 is the regular solution of the second-order ordinary differential equation

$$\frac{\mathrm{d}^2 R_0}{\mathrm{d}\rho^2} + \lambda^2 P(\rho)R_0 = 0, \tag{12}$$

where

$$P(\rho) = 1 - \frac{1}{k^2}V(\rho/k). \tag{13}$$

In order to obtain the uniform asymptotic approximation, the functions $\omega(\vec{r})$, $\rho(\vec{r})$, $g(\vec{r})$, and $h(\vec{r})$ have to be determined.

In appendix B, it is shown that the functions $\omega(\vec{r})$, $\rho(\vec{r})$, $g(\vec{r})$ and $h(\vec{r})$ can be expressed in terms of new functions $\mathcal{S}_\pm$, $\mathcal{A}_\pm$ in the following way:

$$\omega = \frac{1}{2}(\mathcal{S}_+ + \mathcal{S}_-), \tag{14}$$

$$\int^\rho P^{1/2}(t)\,\mathrm{d}t = \frac{1}{2}(\mathcal{S}_+ - \mathcal{S}_-), \tag{15}$$

$$g = \frac{1}{2}P^{1/4}(\mathcal{A}_+ + \mathcal{A}_-), \tag{16}$$

$$h = \frac{1}{2}P^{-1/4}(\mathcal{A}_+ - \mathcal{A}_-), \tag{17}$$

where $\mathcal{S}_\pm$ and $\mathcal{A}_\pm$ satisfy the generalized eikonal equations and generalized transport equations, respectively,

$$(\nabla\mathcal{S}_\pm)^2 = k^2 - V(r), \tag{18}$$

$$2\nabla\mathcal{S}_\pm\nabla\mathcal{A}_\pm + \mathcal{A}_\pm\Delta\mathcal{S}_\pm = 0. \tag{19}$$

In order to find the uniform asymptotic approximation of the scattering solution of the Schrödinger equation (1) for a central potential $V(r)$ using the new Ansatz, the generalized eikonal and transport equations (18) and (19) have to be solved, then their solutions $\mathcal{S}_\pm$, $\mathcal{A}_\pm$ used to determine the functions $\omega(\vec{r})$, $\rho(\vec{r})$, $g(\vec{r})$ and $h(\vec{r})$, according to (14)–(17). With the functions $\omega(\vec{r})$, $\rho(\vec{r})$, $g(\vec{r})$ and $h(\vec{r})$ the uniform asymptotic approximation of the solution of (1) is constructed in the form given by (11). The new Ansatz (11) uses the regular reduced radial wavefunction of zero orbital angular momentum R_0 and its derivative, rather than standard special functions. In this way, the pattern of the caustics of the 3D WKB approximation is the same as the pattern of the caustics of the regular radial wavefunctions. Indeed, the signature of the caustics of the radial wave equation (turning points and singularities) is preserved by the caustics of the 3D problem because the comparison function $R_0(\rho(\vec{r}))$ satisfies the zero angular radial equation written in the variable $\rho(\vec{r})$. Moreover, the new Ansatz ensures the correct behavior at infinity, i.e. the wavefunction satisfies the radiation condition at infinity. The uniform asymptotic approximation must be multiplied by a constant that is determined from the condition to have an incident wave of unit amplitude. The uniform asymptotic approach obviates the shortcomings of the partial wave expansion that consist in the impossibility to bring into prominence the dependence of the wavefunction on the potential parameters and the poor convergence of the expansion for large k. Instead of the series of the partial wave expansion, a closed-form expression for the wavefunction is obtained. The asymptotics at $r \to \infty$ of the uniform asymptotic approximation of the scattering wavefunction leads to the explicit expression of the scattering amplitude, emphasizing the dependence on the potential parameters.

3. Uniform asymptotic approximation for the 3D Coulomb scattering wavefunction based on a new Ansatz

In the following, we will obtain the uniform asymptotic approximation of the 3D scattering wavefunction in the case of the pure Coulomb potential acting between two charged particles using the new Ansatz. First, we will obtain the 3D WKB asymptotic approximation. This approximation has been given in [35] by using parabolic coordinates; see also [36–38]. However, in order to make the paper self-consistent we will give a short deduction of the approximation. This 3D WKB approximation is necessary in order to identify and analyze the caustics of the problem. This allows us to choose an appropriate comparison equation (see appendix A). The analysis of the caustics characteristics shows that the new introduced Ansatz is suited for the present problem. Moreover, in order to find the uniform asymptotic approximation, the solutions of the eikonal and transport equations that occur in obtaining the 3D WKB approximation are needed.

We start with the eikonal equation for the Coulomb potential $V(r) = 2c/r$, where $c = \eta k$. Here $\eta = Z_1 Z_2 e^2 m/\hbar^2 k$ is the Sommerfeld parameter:

$$(\nabla S)^2 = k^2 - \frac{2c}{r}. \tag{20}$$

For $c = 0$ the solutions of this equation are kz and kr that correspond to a plane wave and an outgoing wave, respectively. For $c \neq 0$ we look for a solution of the form

$$S = k(r + W). \tag{21}$$

By introducing S given by (21) in (20) the following equation for W is obtained:

$$(\nabla W)^2 + 2\frac{\partial W}{\partial r} = -\frac{2c}{k^2 r}. \tag{22}$$

We are looking for a similitude variable $t(r, \theta)$, where (r, θ) are two spherical coordinates. In other words we take $W = \Phi(t(r, \theta))$. It results in

$$\Phi'^2(t) r (\nabla t)^2 + 2\Phi'(t) r \frac{\partial t}{\partial r} = -\frac{2c}{k^2}. \tag{23}$$

The similitude variable $t(r, \theta)$ exists if $r(\nabla t)^2$ and $r\frac{\partial t}{\partial r}$ are functions of t. In other words, $t(r, \theta)$ must satisfy the system of equations

$$\frac{J(r(\nabla t)^2, t)}{J(r, \theta)} = 0, \tag{24}$$

$$\frac{J(r\partial t/\partial r, t)}{J(r, \theta)} = 0, \tag{25}$$

where $J(f, g)/J(r, \theta)$ is the Jacobian of functions f and g. By introducing the expressions of the Jacobians in (24) and (25) one obtains

$$\frac{\partial}{\partial r}\left[r\left(\frac{\partial t}{\partial r}\right)^2 + \frac{1}{r}\left(\frac{\partial t}{\partial \theta}\right)^2\right]\frac{\partial t}{\partial \theta} - \frac{\partial}{\partial \theta}\left[r\left(\frac{\partial t}{\partial r}\right)^2 + \frac{1}{r}\left(\frac{\partial t}{\partial \theta}\right)^2\right]\frac{\partial t}{\partial r} = 0 \tag{26}$$

$$\frac{\partial}{\partial r}\left(r\frac{\partial t}{\partial r}\right)\frac{\partial t}{\partial \theta} - \frac{\partial}{\partial \theta}\left(r\frac{\partial t}{\partial r}\right)\frac{\partial t}{\partial r} = 0. \tag{27}$$

We are looking for a solution of the form

$$t = f(r)u(\theta). \tag{28}$$

From (27) the result is that the solution is

$$t = ru(\theta), \tag{29}$$

where $u(\theta)$ is an arbitrary function. By introducing $t = ru(\theta)$ in (26) the result is that $u(\theta)$ satisfies the equation

$$\frac{u'}{u} = \frac{(u^2 + u'^2)'}{u^2 + u'^2}, \tag{30}$$

whose solution is

$$u(\theta) = 1 - \cos\theta. \tag{31}$$

It results in

$$t = r(1 - \cos\theta). \tag{32}$$

Equation (23) becomes

$$\Phi'^2(t) + \Phi'(t) + \frac{c}{k^2 t} = 0, \tag{33}$$

with the solutions

$$\Phi(t) = \frac{1}{2}\left(-t \pm \int^t \sqrt{1 - \frac{4c}{k^2 u}}\,\mathrm{d}u\right). \tag{34}$$

Let us consider the parabolic coordinates (ξ, ζ, ϕ), where $\xi = r(1 - \cos\theta)$, $\zeta = r(1 + \cos\theta)$ and ϕ is the azimuthal angle. We observe that $t = \xi = r(1 - \cos\theta)$. In this way, the solutions for the eikonal equation for the Coulomb potential is obtained

$$S_\pm = k\left[r + \frac{1}{2}\left(-\xi \pm \int^\xi \sqrt{1 - \frac{4c}{k^2 u}}\,\mathrm{d}u\right)\right], \tag{35}$$

or

$$S_\pm = \frac{k}{2}\left(\zeta \pm \int^\xi \sqrt{1 - \frac{4c}{k^2 u}}\,\mathrm{d}u\right). \tag{36}$$

Taking $c = 0$ in the above expression the solutions kz and kr are obtained. Let us solve the transport equation

$$2\nabla A_\pm \nabla S_\pm + A_\pm \Delta S_\pm = 0. \tag{37}$$

By using (36) the equation for A_+ in terms of parabolic coordinates is obtained,

$$2\xi w(\xi)\frac{\partial A_+}{\partial \xi} + 2\zeta\frac{\partial A_+}{\partial \zeta} + [1 + \xi w'(\xi) + w(\xi)]A_+ = 0, \tag{38}$$

where

$$w(\xi) = \sqrt{1 - \frac{4c}{k^2\xi}}. \tag{39}$$

By introducing the variable $w(\xi)$ instead of ξ in (38) the following equation for A_+ is obtained,

$$(1-w^2)\frac{\partial A_+}{\partial w} + 2\zeta\frac{\partial A_+}{\partial \zeta} + \frac{(1+w)^2}{2w}A_+ = 0, \tag{40}$$

whose solution is

$$A_+ = \frac{1-w}{2w^{1/2}}. \tag{41}$$

In the same way we find

$$A_- = \frac{1+w}{2w^{1/2}}. \tag{42}$$

In this way we have obtained the 3D WKB asymptotic approximations for two solutions

$$\Psi_{\text{in}} \sim A_-\,\mathrm{e}^{\mathrm{i}S_-}, \tag{43}$$

$$\Psi_{\text{out}} \sim A_+\,\mathrm{e}^{\mathrm{i}S_+}. \tag{44}$$

For $c = 0$ we have $w = 1$, so that $A_- = 1$, $A_+ = 0$, $S_- = kz$, $S_+ = kr$. It results in $\Psi_{\text{in}} = \mathrm{e}^{\mathrm{i}kz}$, $\Psi_{\text{out}} = 0$. For $c \neq 0$ the function Ψ_{in} is the Coulomb-distorted plane wavefunction and Ψ_{out} is the Coulomb-distorted outgoing wavefunction.

Taking into account the WKB that is a doubly asymptotic approximation we may take the asymptotics for $r \to \infty$ of Ψ_{in} and Ψ_{out}. By calculating the integral in (36) and by introducing the result in equations (43) and (44) one obtains

$$\Psi_{\text{in}} \underset{r\to\infty}{\sim} \mathrm{e}^{\mathrm{i}(kz+\eta\ln k\xi)}, \tag{45}$$

$$\Psi_{\text{out}} \underset{r\to\infty}{\sim} -\frac{\eta}{k(1-\cos\theta)}\frac{\mathrm{e}^{\mathrm{i}(kr-\eta\ln k\xi)}}{r}. \tag{46}$$

Note that from (46) the Rutherford scattering amplitude results up to a constant

$$a_c \sim K\frac{\eta}{2k\sin^2\theta/2}, \qquad \theta \neq 0. \tag{47}$$

The constant K in the above equation cannot be determined in the WKB approximation. From (39), (41) and (42) one can see that if $\xi = \frac{4\eta}{k}$ or $\xi = 0$, then $A_\pm \to \infty$ and the 3D WKB approximation breaks down. In other words, the 3D WKB approximation has caustics at $\xi = 0$ and $\xi = \frac{4\eta}{k}$. The 3D WKB approximation of the Coulomb scattering wavefunction fails at the caustics, because the amplitudes $A_\pm$ become infinite there. The caustic represented by the surface of the paraboloid $\xi = \frac{4\eta}{k}$ separates the classically forbidden region $\left(0 < \xi < \frac{4\eta}{k}\right)$ from the classically allowed region $\left(\xi > \frac{4\eta}{k}\right)$. The caustic $\xi = 0$ is the Oz axis. The axial caustic (Oz axis) is characteristic to the solution of scattering problems that do not depend on the azimuthal angle [7, 13]. Although the 3D WKB approximation of the wavefunction is singular at the caustics, the actual wavefunction is finite there.

In order to overcome the mentioned shortcoming of the 3D WKB approximation, a uniform asymptotic approximation, valid near and away from the caustics, is necessary. The uniform asymptotic approximation reduces to the 3D WKB approximation away from the caustics and remains finite at the caustics. We are looking for a uniform asymptotic approximation for the 3D Coulomb scattering wavefunction based on the new Ansatz of the form

$$\Psi \sim \mathrm{e}^{\mathrm{i}\lambda\omega(\vec{r})}\left\{g(\vec{r})R_0(\rho(\vec{r})) - \frac{\mathrm{i}}{\lambda}h(\vec{r})R_0'(\rho(\vec{r}))\right\}, \tag{48}$$

where R_0 is the regular solution of the reduced radial equation for zero angular momentum

$$\frac{\mathrm{d}^2R_0}{\mathrm{d}\rho^2} + \lambda^2\left(1 - \frac{2\eta}{\rho}\right)R_0 = 0. \tag{49}$$

In order to determine the functions $\omega(\vec{r})$, $\rho(\vec{r})$, $g(\vec{r})$ and $h(\vec{r})$ we need the solutions $\mathcal{S}_\pm$ and $\mathcal{A}_\pm$ of the generalized eikonal and transport equations (18) and (19). Taking into account that equations (18) and (19) for $\mathcal{S}_\pm$ and $\mathcal{A}_\pm$ are identical to equations (8) and (9) for $S_\pm$ and $A_\pm$ it results in $\mathcal{S}_\pm = \mathrm{S}_\pm$, $\mathcal{A}_\pm = \mathrm{A}_\pm$. Consequently we determine $\omega(\vec{r})$, $\rho(\vec{r})$, $g(\vec{r})$ and $h(\vec{r})$ by using $S_\pm$ and $A_\pm$ given by equations (36), (41) and (42). By introducing the functions $S_\pm$ and $A_\pm$ in equations (14)–(17) the functions $\omega = \frac{k}{2}\zeta$, $\rho = \frac{k}{2}\xi$, $g = \frac{1}{2}$ and $h = -\frac{1}{2}$ are obtained. In this way, the uniform asymptotic approximation of the 3D Coulomb scattering wavefunction is obtained up to a constant factor,

$$\Psi \sim \frac{1}{2}\mathrm{e}^{\frac{\mathrm{i}}{2}k\zeta}\left\{R_0\left(\frac{1}{2}k\xi\right) + \mathrm{i}\mathrm{R}_0'\left(\frac{1}{2}k\xi\right)\right\}, \tag{50}$$

where $R_0\left(\frac{1}{2}k\xi\right) = F_0\left(\frac{1}{2}k\xi\right)$ is the regular Coulomb wavefunction for zero angular momentum [39], i.e. $F_0(\rho)$ is the regular solution of the differential equation

$$\frac{\mathrm{d}^2F_0}{\mathrm{d}\rho^2} + \left(1 - \frac{2\eta}{\rho}\right)F_0 = 0. \tag{51}$$

We have seen that one of the caustics is the convex surface of the paraboloid $\xi = 4\eta/k$ having Oz as the axis of symmetry and the focus in the origin. This caustic separates the classically forbidden region $\left(0 < \xi < \frac{4\eta}{k}\right)$ from the classically allowed region $\left(\xi > \frac{4\eta}{k}\right)$. The classical trajectories of the charged particles scattered by the Coulomb potential are situated in the last region and are tangent to the caustic surface [35, 36, 38].

We consider the uniform asymptotic approximation of the Coulomb scattering obtained above:

$$\Psi \sim \frac{1}{2}\,\mathrm{e}^{\mathrm{i}\omega}\{F_0(\rho) + \mathrm{i}\mathrm{F}_0'(\rho)\}. \tag{52}$$

We will show that through the WKB approximation of this function we will obtain a linear combination of the 3D WKB approximations of the Coulomb-distorted plane wave and Coulomb-distorted outgoing wavefunction obtained above. The 1D WKB approximation of the Coulomb function and its derivative valid for $\rho > 2\eta$ [39] is

$$F_0(\rho) \sim g^{-1/4}\sin(\phi + \pi/4), \tag{53}$$

$$F_0'(\rho) \sim g^{1/4}\cos(\phi + \pi/4), \tag{54}$$

where

$$\phi = \int_{2\eta}^{\rho}\sqrt{1 - \frac{2\eta}{u}}\,\mathrm{d}u, \qquad g = 1 - \frac{2\eta}{\rho}. \tag{55}$$

By introducing (53) and (54) in (52) it results in

$$\Psi \sim \frac{\mathrm{i}}{4}\,\mathrm{e}^{\mathrm{i}\omega}[(g^{1/4} - g^{-1/4})\,\mathrm{e}^{\mathrm{i}(\phi+\pi/4)} + (g^{1/4} + g^{-1/4})\,\mathrm{e}^{-\mathrm{i}(\phi+\pi/4)}]. \tag{56}$$

By using $\omega = k\zeta/2$ and $\rho = k\xi/2$ one obtains

$$\Psi \sim \frac{\mathrm{i}}{4}(-A_+\mathrm{e}^{\mathrm{i}S_+}\,\mathrm{e}^{\mathrm{i}\pi/4} + A_-\mathrm{e}^{\mathrm{i}S_-}\,\mathrm{e}^{-\mathrm{i}\pi/4}). \tag{57}$$

The result is that by taking the WKB approximation of the uniform asymptotic approximation for $\xi > \frac{4\eta}{k}$ a linear combination of the 3D WKB approximations of the Coulomb-distorted plane wave and Coulomb-distorted outgoing wave is obtained (see (43) and (44)), in other words we see that away from caustic the uniform asymptotic approximation of the 3D Coulomb scattering wavefunction passes into the 3D WKB approximation.

In order to have an incident Coulomb-distorted plane wave of unit amplitude, the uniform asymptotic approximation (52) must be multiplied by a constant. In order to determine this constant, we need the asymptotic approximation for large argument of the Coulomb wavefunction F_0 and of its derivative.

Wheeler [40] has applied the phase-amplitude method to Coulomb wavefunctions $F_0(\rho)$ and $G_0(\rho)$, writing

$$F_0(\rho) = A_0(\rho)\sin\phi_0(\rho), \tag{58}$$

$$G_0(\rho) = A_0(\rho)\cos\phi_0(\rho). \tag{59}$$

The two terms asymptotic approximation for large ρ of A_0 and ϕ_0 is [40]

$$A_0 = 1 + \frac{\eta}{2\rho}, \tag{60}$$

$$\phi_0 = \rho - \eta\ln 2\rho + \sigma_0, \tag{61}$$

where $\sigma_0 = arg\Gamma(1 + \mathrm{i}\eta)$ (see also[39]).

The Wronskian of the approximations of F_0 and G_0 is unit, as it should be, since the Wronskian of the exact solutions is unit. This is an important merit of these approximations and taking the multiplicative constant in front of the uniform asymptotic approximation equal to $2\mathrm{i}\mathrm{e}^{\mathrm{i}\sigma_0}$ we find

$$\Psi \sim \mathrm{e}^{\mathrm{i}(kz+\eta\ln k\xi)} - \frac{\eta\Gamma(1+\mathrm{i}\eta)}{k\Gamma(1-\mathrm{i}\eta)}\frac{\mathrm{e}^{\mathrm{i}(kr-\eta\ln k\xi)}}{\xi}. \tag{62}$$

From this relation, the well-known Coulomb scattering amplitude can be deduced:

$$f_c(\theta) = -\frac{\eta}{2k\sin^2\theta/2}\frac{\Gamma(1+\mathrm{i}\eta)}{\Gamma(1-\mathrm{i}\eta)}\,\mathrm{e}^{-\mathrm{i}\eta\ln\sin^2\theta/2}, \qquad \theta \neq 0. \tag{63}$$

In this way, the uniform asymptotic approximation obtained by using the new Ansatz is

$$\Psi = \mathrm{e}^{\mathrm{i}\sigma_0}\,\mathrm{e}^{\frac{\mathrm{i}}{2}k\zeta}\left[F'\left(\frac{1}{2}k\xi\right) - \mathrm{i}F_0\left(\frac{1}{2}k\xi\right)\right], \tag{64}$$

where ξ and ζ are the parabolic coordinates. This asymptotic approximation is valid on the whole range of the variables, including the caustics $\xi = 0$ and $\xi = 4\eta/k$. In [30] a uniform asymptotic approximation of the 3D Coulomb scattering wavefunction has been obtained by using an Ansatz based on the Airy function. Although this approximation is valid at the paraboloid caustic $\xi = 4\eta/k$, it breaks down at the caustic $\xi = 0$ (Oz axis).

The uniform asymptotic approximation (64) coincides with the Gordon solution of the Coulomb scattering problem. Indeed, in [30] we expressed the Gordon solution in terms of the Coulomb wavefunction F_0 and its derivative by using some recurrence relations of the Whittaker functions. In other words, the new Ansatz based on the regular reduced radial wavefunction of zero orbital angular momentum provides a uniform asymptotic approximation of the scattering wavefunction that in the case of the Coulomb potential is the exact solution.

4. Conclusions

In this paper, a uniform asymptotic approximation, based on a new Ansatz, is obtained for the scattering wavefunction in the case of an arbitrary central potential $V(r)$. The new Ansatz is introduced by using a function generated by the scattering problem, rather than by using a standard special function. This function, generated by the problem itself, is the regular reduced radial wavefunction of zero orbital angular momentum. By expressing the 3D uniform asymptotic approximation in terms of this function we are sure that the WKB approximation of this uniform asymptotic approximation has the same structure of caustics as the caustics of the studied 3D scattering problem. In other words, this ensures that the proper Ansatz has been chosen, as discussed in appendix A. The uniform asymptotic approximation of the scattering wavefunction for an arbitrary central potential led to an explicit expression of the scattering amplitude, emphasizing the dependence on the potential parameters.

The method is applied to the scattering by a pure Coulomb potential. The 3D WKB approximation of the Coulomb scattering wavefunction has two caustics: a paraboloid $\xi = 4\eta/k$ and the Oz axis ($\xi = 0$), where $\xi = r(1 - \cos\theta)$ is a parabolic coordinate. By using the new Ansatz based on the regular reduced radial wavefunction of zero orbital angular momentum a uniform asymptotic approximation valid on the whole range of the variables is obtained. It obviates the shortcoming of the uniform asymptotic approximation based on the Airy function [30] that is valid on the caustic $\xi = 4\eta/k$, but is singular at the axial caustic Oz. The uniform asymptotic approximation of the Coulomb wavefunction obtained in this paper is in fact the Gordon solution of the Coulomb scattering problem expressed in terms of the Coulomb wavefunction $F_0(\rho)$ and its derivative, as has been obtained in [30]. Being valid on the whole range of the variables, the obtained uniform asymptotic approximation allows us to get the scattering amplitude by using its asymptotics at $r \to \infty$. By using the Coulomb wavefunction $F_0(\rho)$ as a solution of the comparison equation the configuration of the exceptional points (turning point and singular point), which are essential for the uniform asymptotic approximation, has been preserved.

Appendix A

In the following, a short description of the method of the comparison equation is given. This method is used in order to obtain the uniform asymptotic expansion for large parameter of the solution of the ordinary second-order linear differential equation. Let us consider the differential equation

$$\frac{\mathrm{d}^2 y(x,\lambda)}{\mathrm{d}x^2} + \lambda^2 p(x,\lambda) y(x,\lambda) = 0. \tag{A.1}$$

We are looking for a uniform asymptotic expansion of $y(x,\lambda)$ for large λ. Let $w(z,\lambda)$ be the solution of the equation (the comparison equation)

$$\frac{\mathrm{d}^2 w(z,\lambda)}{\mathrm{d}z^2} + \lambda^2 q(z,\lambda) w(z,\lambda) = 0. \tag{A.2}$$

We consider the asymptotic expansion of $y(x,\lambda)$ for large λ

$$y(x,\lambda) = A(x,\lambda) w(z,\lambda) + \frac{1}{\lambda} B(x,\lambda) \frac{\mathrm{d}w(z,\lambda)}{\mathrm{d}z}, \tag{A.3}$$

where $A(x,\lambda)$ and $B(x,\lambda)$ are expanded in inverse powers of λ. The comparison equation (A.2) is chosen so that it had the same configuration of turning points and singularities as the initial equation (A.1). If there is a turning point of first order, the comparison equation is the Airy function equation. If there are two turning points of first order or one of second order, then the comparison equation is the Weber differential equation. Lynn and Keller [41] have extended the method of the comparison equation for equations having an arbitrary finite number of turning points of any order. In [42–44], the authors have obtained uniform asymptotic approximations of Coulomb wavefunctions $F_L(\rho)$ and $G_L(\rho)$ for large η by using the comparison equation method. We restrict ourselves to $L = 0$. The Coulomb wavefunction equation for $L = 0$ is

$$\frac{\mathrm{d}^2 F_0}{\mathrm{d}\rho^2} + \left(1 - \frac{2\eta}{\rho}\right) F_0 = 0. \tag{A.4}$$

This differential equation has two exceptional points: $\rho = 0$ and $\rho = 2\eta$ that are a regular singular point and a turning point, respectively. The above-mentioned authors have obtained two uniform asymptotic approximations of $F_0(\rho)$ and $G_0(\rho)$ using two comparison equations: the Airy equation and the Bessel equation. The uniform approximation using Airy functions is valid for $\rho > 2\eta$. The uniform asymptotic approximation using Bessel functions is valid for $\rho < 2\eta$ (for details see [42–44]). In order to obtain a uniform asymptotic approximation valid on the whole interval $\rho \in [0, \infty)$, a comparison differential equation should be used which has a turning point and a regular singular point. A uniform asymptotic approximation for a second-order linear differential equation having a simple pole and a turning point was obtained by Dunster [45]. The turning point and the singularity may become close. The comparison equation used by Dunster was the Whittaker functions equation. In other words, in the case of the Coulomb wavefunction equation the comparison equation that gives the uniform asymptotic approximation on the whole interval $[0, \infty)$ is the Coulomb wavefunction equation, i.e. the uniform asymptotic approximation is the Coulomb wavefunction itself.

Appendix B

We look for the asymptotic solution for large λ of the Schrödinger equation

$$\Delta\Psi + \lambda^2(k^2 - V(\vec{r}))\Psi = 0. \tag{B.1}$$

A new Ansatz is used, namely we take as the special function which occurs in the uniform approximation of the solution $\Psi(\vec{r})$ the regular reduced radial wavefunction of zero orbital angular momentum $R_0(r)$. In other words, we take the form

$$\Psi(\vec{r}) = \mathrm{e}^{\mathrm{i}\lambda\omega(\vec{r})} \left\{ g(\vec{r}) R_0(\rho(\vec{r})) - \frac{\mathrm{i}}{\lambda} h(\vec{r}) R_0'(\rho(\vec{r})) \right\}. \tag{B.2}$$

Here, R_0 is the regular solution of the second-order ordinary differential equation

$$\frac{\mathrm{d}^2 R_0}{\mathrm{d}\rho^2} + \lambda^2 P(\rho) R_0 = 0, \tag{B.3}$$

where

$$P(\rho) = 1 - \frac{1}{k^2} V(\rho/k). \tag{B.4}$$

In order to obtain the uniform asymptotic approximation, the functions $\omega(\vec{r})$, $\rho(\vec{r})$, $g(\vec{r})$ and $h(\vec{r})$ have to be determined. By substituting (B.2) into the Schrödinger equation (B.1) and by using (B.3) $R_0''(\rho)$ is eliminated. Then the coefficients that multiply $R_0(\rho)$ and $R_0'(\rho)$ in the Schrödinger equation are separately equated to zero. In this way two equations are obtained. By collecting in these equations the coefficients with the same power of λ the following system of equations for $\omega(\vec{r})$, $\rho(\vec{r})$, $g(\vec{r})$ and $h(\vec{r})$ one obtains

$$(\nabla\omega)^2 + P(\rho)(\nabla\rho)^2 = k^2 - V(r), \tag{B.5}$$

$$\nabla\omega\nabla\rho = 0, \tag{B.6}$$

$$2\nabla\omega\nabla g + \Delta\rho P h + 2\nabla\rho\nabla h P + g\Delta\omega + (\nabla\rho)^2 P' h = 0, \tag{B.7}$$

$$2\nabla g\nabla\rho + h\Delta\omega + g\Delta\rho + 2\nabla\omega\nabla h = 0. \tag{B.8}$$

In order to obtain the functions $\rho(\vec{r})$ and $\omega(\vec{r})$, the new functions $\mathcal{S}_\pm(\vec{r})$ defined as

$$\mathcal{S}_\pm(\vec{r}) = \omega(\vec{r}) \pm \int^{\rho(\vec{r})} P^{1/2}(t)\mathrm{d}t \tag{B.9}$$

are introduced. By adding equation (B.5) to equation (B.6) multiplied by $2P^{1/2}(\rho)$ one obtains

$$(\nabla\omega + P^{1/2}\nabla\rho)^2 = k^2 - V(r). \tag{B.10}$$

Similarly, by subtracting from (B.5) equation (B.6) multiplied by $2P^{1/2}(\rho)$ one obtains

$$(\nabla\omega - P^{1/2}\nabla\rho)^2 = k^2 - V(r). \tag{B.11}$$

Taking into account the definition (B.9) of $S_\pm$ this results in that equations (B.10) and (B.11) can be written as

$$(\nabla\mathcal{S}_\pm)^2 = k^2 - V(r), \tag{B.12}$$

which represents the generalized eikonal equation.

In order to obtain the functions $g(\vec{r})$ and $h(\vec{r})$, the new functions $\mathcal{A}_\pm(\vec{r})$ defined as

$$\mathcal{A}_\pm(\vec{r}) = P^{-1/4}(\rho)[g(\vec{r}) \pm P^{1/2}(\rho)h(\vec{r})] \tag{B.13}$$

are introduced. By adding equation (B.8) multiplied by $P^{1/4}$ to equation (B.7) multiplied by $P^{-1/4}$ and taking into account the definitions of $\mathcal{S}_+$ and $\mathcal{A}_+$ one obtains

$$2\nabla\mathcal{S}_+\nabla\mathcal{A}_+ + \mathcal{A}_+\Delta\mathcal{S}_+ = 0. \tag{B.14}$$

Similarly by subtracting equation (B.8) multiplied by $P^{1/4}$ from equation (B.7) multiplied by $P^{-1/4}$ and taking into account the definitions of $\mathcal{S}_-$ and $\mathcal{A}_-$ one obtains

$$2\nabla\mathcal{S}_-\nabla\mathcal{A}_- + \mathcal{A}_-\Delta\mathcal{S}_- = 0. \tag{B.15}$$

Equations (B.14) and (B.15) represent the generalized transport equation.

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