New method for calculating the phase shifts of the radial wave function in scattering by a spherically symmetric potential

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The equation $\psi'' + \varkappa^2 \psi = 0$ for the radial part of the wave function can be reduced to a first-order differential equation (stable and nonsingular at the turning point) for the phase shifts. The boundary conditions at this point are specified analytically and directly in the form of an asymptotic series. For the Lennard-Jones potential the proposed method of calculation of the phase shifts is compared with the WKB method.

1. INTRODUCTION

As is well known, the asymptotic behavior of a wave scattered by a spherically symmetric potential $V(r)$ can be specified by the phase shifts of the radial function (see, e.g., Ref. 1). With the exception of the small number of cases that can be solved exactly, to calculate the phase shifts one uses the WKB method (see Ref. 2 and Ref. 3, p. 163). This involves representing the solution of the Schrödinger equation in the form of a sum of two functions—analogs of the incident wave and the reflected wave. This makes it possible to reduce the wave equation to a system of two first-order equations, which, far from the turning point r_0, is solved by the method of successive approximations. In the neighborhood of $r = r_0$ this technique is inapplicable, since the equations of the system have singularities at this point, and the incident and reflected waves are indistinguishable there. At the same time, analysis of the solution near the turning point is necessary, since it is precisely in this interval that the form of the solution changes and a substantial phase shift arises. Therefore, to investigate the solution in such cases one has to use other methods (Ref. 2 and Ref. 3, p. 195), which basically reduce to solving an approximate equation in the neighborhood of $r = r_0$ and then matching the resulting solutions in a region suitable for this. Thus, the presence of singularities in the system of equations used in the WKB method gives rise to appreciable complications and additional errors in the calculation of the phase shifts.

Many papers devoted to improving the WKB method and to widening its region of applicability have been published recently.[4–6]

In the present paper, we propose for a solution of the radial wave equation with one turning point a representation in the form of a sum of two functions that makes it possible to obtain for the phase shifts an everywhere-exact ordinary first-order differential equation without singularities at the turning point. This representation removes the need to investigate the equation in the classically inaccessible region and makes it possible to specify boundary conditions directly at the point $r = r_0$, thereby avoiding the need to invoke special methods of analysis of the solutions near the singularities. To specify the initial conditions, the wave function is expanded at the turning point in an asymptotic series in the dimensionless parameter

$$a = \left\{ r_0^3 \frac{dq^2}{dr}(r_0) \right\}^{1/5}, \quad q^2 = k^2 - \frac{2mV}{\hbar^2} - \frac{l(l+1)}{r^2}.$$

By considering truncations of this series of different lengths, we obtain different approximations to the magnitude of the phase shift. The expansion is performed analytically, i.e., there exist explicit formulas that express the first, second, ..., nth approximations of the boundary condition in terms of an integral characteristic and derivatives at the point r_0 of the function q^2. Therefore, to calculate the next approximation there is no need (as there is in the WKB method) to calculate the previous ones. The two functions of which the wave function is composed are also interpreted as analogs of the incident wave and the reflected wave. The equations relating the "amplitudes" do not have singularities at the turning point. This makes it possible to distinguish the incident wave and reflected wave in the entire classically accessible region and to take account of the influence of the reflected wave in the calculation of the phase shift.

The proposed method can be used not only for the calculation of phase shifts in scattering but also in other problems that involve solving a wave equation with one turning point.

The natural question arises as to why, with the present-day level of computational techniques, one should solve approximate equations rather than find the exact solution by numerical methods. Exact solution is inconvenient for the following reasons. First, if the potential has a singularity at the origin, in the classically inaccessible region the derivatives take on large values, and this greatly complicates both the programming and the computations. Second, exact solution is more unwieldy, since it is directed toward obtaining superfluous information: First, the wave function is found, and only then are the phase shifts found. In problems that require multiple calculation of phase shifts (e.g., the calculation of a cross section), these factors lead to appreciable complication.

Below, we describe the basic equation, the boundary conditions for it, and the results of a numerical calculation. The exact mathematical formulations necessary to justify the proposed approximate solution are given in the Appendix.

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2. THE BASIC EQUATION, ITS PROPERTIES, AND ITS BOUNDARY CONDITIONS

The problem of scattering by a centrally symmetric potential can be reduced in the standard way to a one-dimensional equation for the radial part of the wave function:

$$d^2\varphi/dr^2+q^2(r)\varphi=0.$$

For convenience, we change to dimensionless variables:

$$z=r/r_0, \quad \psi(z)=\varphi(r_0z), \quad \varkappa^2(z)=r_0^2q^2(r_0z).$$

Then

$$d^2\psi/dz^2+\varkappa^2(z)\psi=0 \tag{1}$$

and the turning point is $z=1$. We shall denote the eikonal by S, and seek the solution of Eq. (1) in the form

$$\psi(z)=A(z)\sin S+B(z)\cos S, \quad S=\int_1^z \varkappa(\tau)\,d\tau. \tag{2}$$

We require the amplitudes $A(z)$ and $B(z)$ to obey the conditions

$$A'\sin S+B'\cos S=0, \tag{3}$$

$$(\varkappa A)'\sin S-(\varkappa B)'\cos S=0, \tag{4}$$

which can be interpreted as the analog of the Fresnel formulas for reflection from the boundary of two media. By direct substitution one can convince oneself that the function $\psi(z)$ given by formula (2) satisfies Eq. (1) if $A(z)$ and $B(z)$ are solutions of the system of equations (3), (4). Expressing A' and B' from the system (3), (4), we obtain

$$\begin{aligned} A' &= \frac{\varkappa'}{2\varkappa}\sin(2S)B-\frac{\varkappa'}{\varkappa}\cos^2(S)A, \\ B' &= \frac{\varkappa'}{2\varkappa}\sin(2S)A-\frac{\varkappa'}{\varkappa}\sin^2(S)B. \end{aligned} \tag{5}$$

At the turning point ($\varkappa 0$) this system has a singularity [the coefficient $(\varkappa'/\varkappa)\cos^2S$] that arises for the following reasons. The solution $\psi(z)=A(z)\sin S+B(z)\cos S$ of Eq. (1) is a smooth function. At the turning point its second derivative is equal to zero, while its first (as shown by the examples of Airy functions or Bessel functions) does not vanish, generally speaking. At the same time, the first derivative of the function $\sin S\propto S\propto\varkappa(z-1)$ is equal to zero while the second is not defined at all, and the singularity of the amplitude $A(z)\propto\varkappa^{-1}$ plays the role of canceling the anomalous character of the behavior of the eikonal in the neighborhood of the point $z=1$. The coefficient $B(z)$, on the other hand, has to be smooth at this point, in order not to spoil the smoothness of $\psi(z)$.

The above qualitative considerations can be partly illustrated by the following example. We introduce the modified amplitude $\tilde{A}(z)=f(z)A(z)$ and define the phase shift by $\delta=\arctan(\tilde{A}/B)$, so that the solution takes the form

$$\psi(z)=\frac{B(z)}{\cos\delta}\left[\frac{1}{f(z)}\sin\delta\sin S+\cos\delta\cos S\right],$$

and the quantity δ no longer has the meaning of an additive correction to the eikonal if $f\neq 1$.

The factor $f(z)$ must be chosen in such a way that the equation for the function δ is nonsingular and stable against small changes of the boundary conditions.

From the system (5) we find

$$\begin{aligned} \tilde{A}' &= \left(\frac{f'}{f}-\frac{\varkappa'}{\varkappa}\cos^2S\right)\tilde{A}+\frac{\varkappa'}{\varkappa}f\sin(2S)B, \\ B' &= \frac{\varkappa'}{2\varkappa f}\sin(2S)\tilde{A}-\frac{\varkappa'}{\varkappa}\sin^2(S)B. \end{aligned} \tag{6}$$

For the ratio $\xi=\tilde{A}/B$ we obtain, in the usual way, the Ricatti equation

$$\xi'=\frac{\varkappa'}{2\varkappa}\sin 2S\left[f-\frac{\xi^2}{f}\right]+\left(\frac{f'}{f}-\frac{\varkappa'}{\varkappa}\cos 2S\right)\xi,$$

which is easily transformed into an equation for the phase shift δ:

$$\begin{aligned} \delta' &= \frac{\varkappa'}{2\varkappa}\sin 2S\left[f-\left(f+\frac{1}{f}\right)\sin^2\delta\right] \\ &\quad +\frac{1}{2}\left(\frac{f'}{f}-\frac{\varkappa'}{\varkappa}\cos 2S\right)\sin 2\delta. \end{aligned} \tag{7}$$

It is possible to find several functions $f(z)$ that make it possible to fulfill the regularity requirement, e.g., $f'/f=\varkappa'/\varkappa$, $f'/f=(\varkappa'/\varkappa)\cos^2S$, $f'/f=(\varkappa'/\varkappa)\cos 2S$. But stability requires that variant for which the last bracket of Eq. (7) vanishes. Therefore, we set

$$\frac{f'}{f}=\frac{\varkappa'}{\varkappa}\cos 2S, \quad f=\exp\left\{-\int_z^\infty\frac{\varkappa'(\tau)}{\varkappa(\tau)}\cos 2S(\tau)\,d\tau\right\}. \tag{8}$$

Equations (6) and (7) now take the form

$$\tilde{A}'=-\frac{\varkappa'}{\varkappa}\sin^2(S)\tilde{A}+\frac{\varkappa'}{2\varkappa}f\sin(2S)B, \tag{9}$$

$$B'=\frac{\varkappa'}{2\varkappa f}\sin(2S)\tilde{A}-\frac{\varkappa'}{\varkappa}\sin^2(S)B,$$

$$\delta'=\frac{\varkappa'}{2\varkappa}\sin 2S\left[f-\left(f+\frac{1}{f}\right)\sin^2\delta\right]. \tag{10}$$

Since for $z\to 1$ we have

$$S\propto(z-1)^{3/2}\propto\varkappa^3, \quad f\propto(z-1)^{1/2}\propto\varkappa, \quad \varkappa'\propto\varkappa^{-1},$$

Eqs. (9), (10) do not have a singularity at the turning point. Moreover, $\lim f(z)=1$ as $z\to\infty$, and therefore the phase shift

$$\eta_l=\lim_{z\to\infty}[S-kr_0z+(l+1)\pi/2-\delta(\infty)].$$

Thus, for the function $\delta(z)$, which asymptotically determines the phase shift, we obtain an ordinary first-order differential equation without singularities.

We shall denote by $\varkappa_0^2$ the effective potential normalized by the condition $d\varkappa_0^2/dz=1$, and consider the family of functions $\varkappa=a\varkappa_0$. An investigation of Eq. (10) has shown that, for any coefficient $\varkappa_0$, for sufficiently large values of the parameter a the equation is stable against small changes of the boundary conditions. This means that, for any two solutions $\delta_1(z)$ and $\delta_2(z)$ of the equation, the following inequality is valid:

$$|\delta_1(z)-\delta_2(z)|\leqslant|\delta_1(1)-\delta_2(1)|+T(a,\varkappa_0)\sup_{z\geqslant 1}|\delta_1(z)-\delta_2(z)|,$$

with

$$T(a, \varkappa_0)<1 \qquad (11)$$

for $a > a_0(\varkappa_0)$. Consequently,

$$\sup_{z>1} |\delta_1(z)-\delta_2(z)| \leqslant |\delta_1(1)-\delta_2(1)|/[1-T(a, \varkappa_0)].$$

In the Appendix we give an exact formulation of this statement, and all the necessary bounds. We note that the bounds are, of course, overestimates, and, as shown by numerical examples, the region of stability of Eq. (10) is actually significantly wider than that determined by the inequality (11).

In order to specify the boundary conditions at the point $z = 1$, we expand the solution $\psi(z)$ in the neighborhood of this point in a series in powers of the variable $\tilde{z} = z - 1$ and in an asymptotic series in the large parameter $a = [(d\varkappa^2/dz)(1)]^{1/2}$. We set

$$g_a = \lim_{\tilde{z}\to 0} f^{-1}(z)\tilde{z}^{1/3}a^{1/3} = a^{1/3}\varkappa_0(\infty)\exp\left\{-2\int_1^\infty \frac{\varkappa_0'(\tau)}{\varkappa_0(\tau)}\sin^2 S(\tau)\,d\tau\right\}.$$

The values g_a and g_a^{-1} have uniform upper bounds with respect to the parameter a (see the Appendix).

Using the representation (2) and the system (9), we obtain

$$\psi(z) = \bar{A}(\tilde{z})\sin S + B(\tilde{z})\cos S = B(1) + \bar{A}(1)a^{2/3}g_a\tilde{z} + O(\tilde{z}^3). \qquad (12)$$

We now make use of the asymptotic expansion proposed by Olver (Ref. 7 and Ref. 3, p. 195):

$$\psi(z) = \sum_{i=0}^\infty A_i(\tilde{z})a^{-i}w(a^{2/3}\xi) + \sum_{i=0}^\infty B_i(\tilde{z})a^{-i-1/3}w'(a^{2/3}\xi),$$

$$\xi = \left(\frac{3S}{2a}\right)^{2/3}, \quad A_{-1}=0, \quad B_{-1}=0, \qquad (13)$$

$$A_i = -\frac{1}{(\xi')^{1/2}}\int_0^{\tilde{z}} \frac{B_{i-1}(\tau)\,d\tau}{(\xi'(\tau))^{1/2}},$$

$$B_i = -\frac{1}{2(\xi\xi')^{1/2}}\int_0^{\tilde{z}} \frac{A_{i-1}''(\tau)\,d\tau}{(\xi\xi')^{1/2}},$$

where the function $w(x)$ satisfies the equation $w''(x) + xw(x) = 0$. In the same paper, Olver proved that the expansion (13) converges asymptotically to the solution $\psi(z)$ uniformly in $\tilde{z}$. Despite the complicated definitions of the functions A_i and B_i, their values and the values of their derivatives at the origin can be calculated analytically in terms of derivatives of the effective potential $\varkappa_0^2(z)$. For example,

$$\frac{A_0'(0)}{A_0(0)} = -0.1\frac{d^2\varkappa_0^2}{dz^2}(1),$$

$$\frac{B_1(0)}{A_0(0)} = -\frac{1}{14}\frac{d^3\varkappa_0^2}{dz^3}(1) + \frac{9}{25}\frac{d^2\varkappa_0^2}{dz^2}(1).$$

Analogous formulas can be obtained for any index i.

Using the known expansion (see Ref. 8, p. 264)

$$w(x) = c_1 + c_2(x) + O(x^3), \quad x \ll 1;$$

$$c_1 = 0.355028, \; c_2 = 0.258819,$$

we obtain from (12) and (13) the initial conditions for the system (6):

$$\bar{A}(1) = \frac{1}{g_a}\left(c_2A_0(0) + c_1\sum_{i=0}^\infty A_i'(0)a^{-i-1/3} + c_2\sum_{i=1}^\infty B_i'(0)a^{-i-1}\right),$$

$$B(1) = A_0(0)c_1 + \sum_{i=1}^\infty B_i(0)a^{-i-1/3}c_2.$$

Consequently,

$$\operatorname{tg}\delta(1) = \frac{\bar{A}(1)}{B(1)} = \frac{1}{g_a}\left[c_2A_0(0) + c_1\sum_{i=0}^\infty A_i'(0)a^{-i-1/3} + c_2\sum_{i=1}^\infty B_i'(0)a^{-i-1}\right] \times\left[A_0(0)c_1 + \sum_{i=1}^\infty B_i(0)a^{-i-1/3}c_2\right]^{-1}.$$

This is the desired initial condition for δ. We give the formulas for the first three approximations:

$$\operatorname{tg}\delta(1) = c_2/c_1g_a,$$

$$\operatorname{tg}\delta(1) = \frac{1}{g_a}\left(\frac{c_2}{c_1} + \frac{A_0'(0)}{A_0(0)}a^{-2/3}\right) = \frac{1}{g_a}\left(\frac{c_2}{c_1} - 0.1\frac{d^2\varkappa_0^2}{dz^2}(1)a^{-2/3}\right),$$

$$\operatorname{tg}\delta(1) = \frac{1}{g_a}\left\{\frac{c_2}{c_1} - 0.1\frac{d^2\varkappa_0^2}{dz^2}(1)a^{-2/3} + \frac{c_2^2}{c_1^2}\left(\frac{9}{35}\left[\frac{d^2\varkappa_0^2}{2dz^2}(1)\right]^2 - \frac{1}{14}\frac{d^3\varkappa_0^2}{dz^3}(1)\right)a^{-4/3}\right\}.$$

It can be shown that, for the family of effective potentials

$$\varkappa_l^2 = k^2r_l^2 - r_l^2V(r_lz) - \frac{l(l+1)}{z^2},$$

where r_l is the corresponding turning point, the family of normalized potentials

$$\varkappa_{0l}^2 = \frac{\varkappa_l^2}{a_l^2} = \frac{\varkappa_l^2}{2l(l+1) - r_l^3V'(r_lz)}$$

converges uniformly on any interval (a, ∞) $(a > 0)$ to the function $\eta^2 = \frac{1}{2}(1 - 1/z^2)$ as $l \to \infty$.

In the case when $V(r)$ is an analytic function in the region containing $(0, \infty)$ it follows from this that all the derivatives $d^n\varkappa_{0l}^2/dz^n$ converge uniformly to the corresponding derivatives $d^n\eta^2/dz^n$. Since the initial conditions $\tan\delta(1)$ and the parameter $T(a_l, \varkappa_{0l})$ are entirely determined by derivatives of the function $\varkappa_{0l}^2$, we obtain

$$|T(a_l, \varkappa_l) - T(\sqrt{l(l+1)}, \eta)| \to 0, \quad l \to \infty,$$

and the k th approximation to the initial conditions $\tan\delta(1)$ for the potential $\varkappa_l^2$ converges to the k th approximation to $\tan\delta(1)$ for the potential $l(l+1)\eta_l^2$.

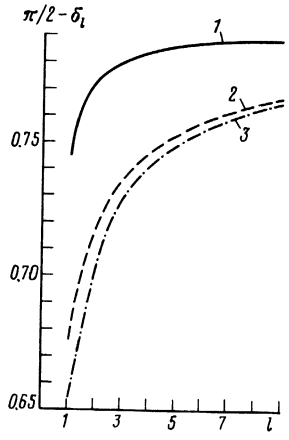

FIG. 1. Values of δ_l for Bessel functions [the potential $\varkappa^2 = l(l+1)(1-z^{-2})$]. Curve 1 is the first approximation to the solution of Eq. (10), curve 2 is the second approximation to the solution of Eq. (10), and curve 3 gives the true values.

3. RESULTS OF THE NUMERICAL CALCULATIONS

To check the efficiency of the proposed method, we have used it to calculate the phase shifts $\delta_l = \lim(z - l\pi/2 - S)$ for $z \to \infty$ for the Bessel functions $z^{1/2}J_{l+1/2}(z)$, which are the exact solution of Eq. (1) with the potential $\varkappa^2 = l(l+1)(1-z^{-2})$.

Here, as before, S denotes the eikonal $S = \int_1^z \varkappa d\tau$ [i.e., in it we have not replaced $l(l+1)$ by $(l+1/2)^2$]. As is well known, in this case the relation

$$\delta_l = [l + {}^1/_2 - \sqrt{l(l+1)}]\pi/2 + \pi/4$$

is valid.

The results of the calculation are shown in Fig. 1. We give the values Δ_l of the errors for different values of the parameter l (as percentages of the true value):

l	1	2	3	4
Δ_l	3.9	2.13	0.96	0.67

For comparison with the WKB method, we have calculated the phase shifts δ_l (in units of $\pi\sigma^2$):

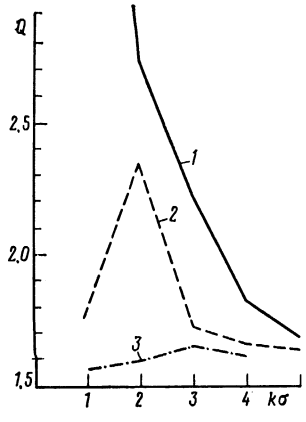

FIG. 2. Dependence of the cross section Q on the parameter $k\sigma$ for the Lennard-Jones potential with $\Lambda = 3.08$: 1—calculations by the WKB method; 2—solutions of Eq. (10); 3—the true values.

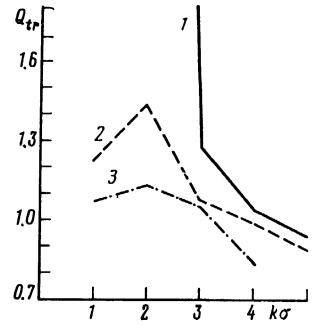

FIG. 3. Dependence of the transport cross section Q_{tr} on the parameter $k\sigma$ for the Lennard-Jones potential with $\Lambda = 3.08$: 1—calculated by the WKB method; 2—solution of Eq. (10); 3—the true values.

$$Q = \frac{4}{(k\sigma)^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l$$

and the transport cross sections

$$Q_{tr} = \frac{4}{(k\sigma)^2}\sum_{l=1}^{\infty} l\sin^2(\delta_l - \delta_{l-1})$$

for scattering by a Lennard-Jones potential. It was assumed that, in Eq. (1),

$$\varkappa^2 = k^2 r_0^2 - 16\pi^2\Lambda^{-2}[(\sigma/r_0)^{12}z^{-12} - (\sigma/r_0)^6 z^{-6}].$$

The parameter $\Lambda^2 = h^2/2\mu\sigma^2\varepsilon$, where μ is the reduced mass, ε is the depth of the potential well, and σ is the root of the potential, characterizes the interaction of the colliding particles. The bigger its value, the more strongly pronounced are the quantum effects. The calculations were performed for the values $\Lambda = 3.08$ (^{3}He–He^3 collision) and $\Lambda = 0.562$ (Hg–H_2). The exact values of the phase shifts were taken from the literature (Ref. 9, p. 860, and Ref. 10). The values of the phase shifts in the WKB method were calculated by the Langer method [i.e., the eikonal was calculated with $l(l+1)$ replaced by $(l+1/2)^2$]. The value $\Lambda = 3.08$ does not fall in the region of applicability defined by the inequality (11). The results of the calculations for this value of the parameter Λ are given in Figs. 2 and 3 and in the table. It should be noted that for $k\sigma = 1.2$ the parameter $a^{2/3}$, which, for a successful calculation, should be large, is in fact small: $a^{2/3}_{\min} = 2.0$ (see the table). This explains the large magnitude of the error at these points. The parameter value $\Lambda = 0.562$ lies on the boundary of the region of stability of Eq. (10). Figures 4 and 5 and the table display the results of the calculations in this case. The smallest value of the parameter $a^{2/3}$ here is always greater than eight. It should be noted that the small magnitude of the error in the calculation of the cross section by the WKB method for $k\sigma = 3$ is explained not by the accuracy of the method but by the mutual cancellation of two errors in the phase shifts: $\delta_3 = 2.77$ (the true value is $\delta_3 = 2.68$), and $\delta_4 = 0.220$ (the true value is $\delta_4 = 0.145$).

In all the calculations cited, the third approximation in the proposed method was compared with the first approximation in the WKB method. This was done to demonstrate the following fact. Since, for any approximation, the boundary conditions are specified analytically, and Eq. (10) is ex-

TABLE I. Errors in the calculations of the phase, cross sections and transport cross sections for two values of Λ.

$k\sigma$	Cross section,%		Transport cross section, %		Average error in the phase, rad		Smallest value of $a^{2/3}$
	WKB	Equation (10)	WKB	Equation (10)	WKB	Equation (10)	
			Λ=3.08				
1	496	12	571	20	0.46	0	2.0
2	74	47	85	27	0.14	0.05	2.0
3	34	5	22	1	0.19	0.03	2.7
4	15	3	27	13	–	–	3.4
			Λ=0.562				
3	2.3	10	42.9	6.8	0.067	0.017	
5	4.9	2.9	6	1	0.084	0.013	
7	4.3	0	12.1	2.5	0.088	0.007	

Note: Since the true values of the phases are known only to the second decimal place, all quantities are given to this accuracy.

act everywhere, we can obtain any approximation (in this case, the third) from the first sweep, whereas the first iteration of the WKB method gives only the first approximation. Thus, in numerical calculations what we compare is not the same approximation obtained by different methods, but quantities obtained as a result of one iteration of each of them. The calculations given show that where the WKB method in the first approximation is not sufficiently accurate the proposed method gives a better result, since it permits one to calculate any approximation (in the given case, the third) from the very first sweep.

CONCLUSION

In the paper we have proposed the following method of approximate solution of a radial wave equation with one turning point $r = r_0$. The desired function $\psi(z)$ $(z = r/r_0)$ is represented in the form [see formulas (2) and (8)]

$$\psi(z) = f^{-1}\tilde{A}(z)\sin S + B(z)\cos S$$

in such a way that the amplitudes $\tilde{A}$ and B and the function $\delta = \arctan(\tilde{A}/B)$ do not have singularities at the turning point $z = 1$. The function δ determines the phase shift asymptotically as $z \to \infty$ and obeys Eq. (10).

This equation is stable for large values of the parameter

$$a = \left[\frac{d\varkappa^2}{dz}(1)\right]^{1/2} = \frac{\varkappa}{\varkappa_0}$$

and does not have singularities at the turning point; this makes it possible to specify the boundary conditions $\delta(1)$ directly at this point. The boundary conditions are represented by an asymptotic series of the form

$$\operatorname{tg}\delta(1) = \sum_{i=0}^{\infty} p_i a^{-2i/3},$$

in which the coefficients p_i are expressed analytically in terms of integral and differential characteristics of the effective potential $\varkappa_0^2$, i.e., do not depend on a. To calculate the nth approximation it is not necessary (as it is in the WKB

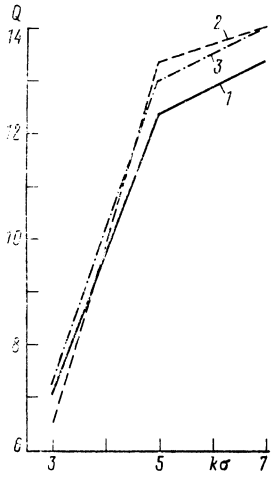

FIG. 4. Dependence of the cross section Q on the parameter $k\sigma$ for the Lennard-Jones potential with $\Lambda = 0.562$: 1—calculated by the WKB method; 2—solution of Eq. (10); 3—the true values.

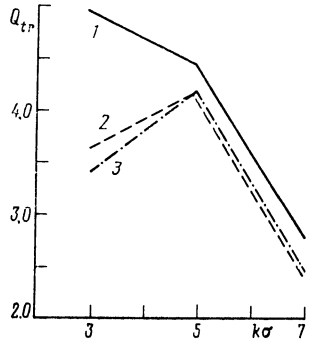

FIG. 5. Dependence of the transport cross section Q_{tr} on the parameter $k\sigma$ for the Lennard-Jones potential with $\Lambda = 0.562$: 1—calculated by the WKB method; 2—solution of Eq. (10); 3—the true values.

method) to calculate the previous approximations. In view of this, in those cases in which the first approximation of the WKB method is not sufficiently accurate, it makes sense to employ the proposed method, and this is confirmed by the above examples of numerical comparison of these two methods. We note that the proposed method is much simpler than exact numerical solution of the wave equation, since it does not involve analysis of the solution in the classically inaccessible region.

APPENDIX

Here we show under what conditions Eq. (10) will certainly be stable against small changes of the boundary conditions. Let $\varkappa_0^2$ be the effective potential, normalized by the condition

$$\frac{d\varkappa_0^2}{dz}=(1), \quad t=\int_1^z \varkappa_0 dz, \quad \varkappa_0=t^{1/3}\eta(t^{2/3}), \quad \varkappa=a\varkappa_0.$$

We choose a certain number $h(0<h<\pi)$, and introduce the following notation:

$$c_1=\sup_{z>z(h)}\left|\frac{1}{\varkappa}\frac{d\varkappa}{dt}\right|=\sup_{z>z(h)}\left|\frac{\varkappa'}{\varkappa^2}\right|,$$

$$c_2=\int_h^\infty\left|\frac{d}{dt}\left(\frac{1}{\varkappa}\frac{d\varkappa}{dt}\right)\right|dt,$$

$$p_1=\sup_{t<h}\left|\frac{\eta'}{\eta}\right|=\sup_{t<h}\left|\frac{3}{2\varkappa^2}\frac{d\varkappa}{dz}t^{1/3}-\frac{t^{-2/3}}{2}\right|,$$

$$p_2=\sup_{t<h}\left|\left(\frac{\eta'}{\eta}\right)'\right|.$$

For definiteness and for simplicity of the formulas, we set $h=2$. Below, we give the results of straightforward, but laborious and unwieldy, estimates, from which it can be seen how and by what parameters the stability of Eq. (10) is determined.

1. The function

$$f_\varkappa=\exp\left\{-\int_z^\infty\frac{\varkappa'}{\varkappa}\cos 2S\right\}=\exp\left\{-\int_{t(z)}^\infty\frac{d\varkappa_0}{dt}\frac{1}{\varkappa_0}\cos 2at\,dt\right\}$$

possesses the following properties: For $t(z)>h/2a$,

$$f_\varkappa(z)\leqslant 1.15A(a,\varkappa_0); \tag{A1}$$

$$f_\varkappa^{-1}(z)\leqslant 1.07A(a,\varkappa_0); \tag{A2}$$

$$|f_\varkappa(z)+f_\varkappa^{-1}(z)|\leqslant 2.02A(a,\varkappa_0); \tag{A3}$$

$$|f_\varkappa(z)-f_\varkappa^{-1}(z)|\leqslant 0.3A(a,\varkappa_0); \tag{A4}$$

$$g_a=\lim_{z\to 1}f_\varkappa(z)a^{-1/3}(z-1)^{-1/2}\leqslant 1.4\exp\{p_1/a^{2/3}\}A(a,\varkappa_0); \tag{A5}$$

$$g_a^{-1}=\lim_{z\to 1}f_\varkappa^{-1}(z)a^{1/3}(z-1)^{1/2}\leqslant 1.1\exp\{p_1/a^{2/3}\}A(a,\varkappa_0). \tag{A6}$$

Here,

$$(a,\varkappa_0)=\exp\left\{\frac{c_1+c_2}{2a}+\frac{1}{3}\operatorname{ci}(4a)+\frac{2}{3}p_1a^{-2/3}+\frac{p_2}{a}0.83\right\}.$$

We note that $A(a,\varkappa_0)\sim 1+O(p_1/a^{2/3})$.

2. If in Eq. (10) the effective potential $\varkappa=a\varkappa_0$, and $\delta_1(z)$ and $\delta_2(z)$ are two solutions of this equation, then

$$|\delta_1(z)-\delta_2(z)|\leqslant|\delta_1(1)-\delta_2(1)|+T(a,\varkappa_0)\sup_{z>1}|\delta_1(z)-\delta_2(z)|,$$

where

$$\begin{aligned}T(a,\varkappa_0)=&A(a,\varkappa_0)\{0.44+0.12A(a,\varkappa_0)\\&+a^{-2/3}p_1(0.78+0.39A(a,\varkappa_0)\\&+a^{-1}(0.87p_2+0.13p_1^2+1.8A(a,\varkappa_0)p_1^2)\}\\&+\frac{c_1+c_2}{a}\exp\left\{\frac{c_1+c_2}{2a}\right\}.\end{aligned}$$

It is obvious that, for all sufficiently large $a>a_0(\varkappa_0)$, the quantity $T(a,\varkappa_0)<1$, and it is this inequality that determines the region in which Eq. (10) is stable.

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