SOVIET PHYSICS

USPEKHI

A Translation of Uspekhi Fizicheskikh Nauk

SOVIET PHYSICS USPEKHI (Russian Vol. 92, Nos. 1 and 2) NOVEMBER-DECEMBER 1967

530.145

THE PHASE-FUNCTION METHOD IN QUANTUM MECHANICS

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Usp. Fiz. Nauk 92, 3—26 (May, 1967)

1. INTRODUCTION

THERE is a continually broadening range of applications of quantum mechanics to problems of modern physics, chemistry, and technology. Moreover, with the construction of fast electronic computers the problem of finding the most effective algorithms for solving quantum-mechanical problems has become urgent. Therefore it is of interest to a wide circle of specialists to become acquainted with a new approach to the formulation and solution of problems in quantum mechanics, which differs from the standard method of solution of the Schrödinger equation. This approach has been intensively developed in recent years (1963—1966) and has not yet been reflected in textbooks or monographs. All of the material is contained in a number of journal articles.[1-42] The present article is a brief review* of the main equations and results derived in the new method, which is called the phase-function method.

The mathematical foundation of the method is a fact well known in the theory of differential equations, that a linear homogeneous equation of the second order, such as the Schrödinger equation, can be reduced to a nonlinear equation of the first order—the Riccati equation. The physical content of this approach is that a function which satisfies the Riccati equation (a phase function) has at each point the meaning of the phase shift (in comparison with the case of free motion) of the wave function for scattering by the potential cut off at that point. Accordingly, the problem reduces to the direct determination of the desired scattering phase shift. At the same time it turns out that a knowledge of the phase function is sufficient for the complete determination of the wave function. One can also introduce functions corresponding to other observable quantities, such as, for example, the partial scattering amplitudes, whose poles correspond to the energies of bound states. The phase-function method* (PFM), originally developed for the case of scattering by a spherically symmetrical potential, was subsequently extended to more general cases: scattering in the field of noncentral forces, many-channel scattering, relativistic equations, and so on. Evidently any problem of quantum mechanics, whether of scattering or of bound states, can be formulated and solved in terms of phase functions.

Advantages of the new method are:

1) The intuitive physical meaning of the phase function, which at each point is the phase of the scattering by the corresponding part of the potential; this enables us in the process of the solution to see the effect of the action of different regions of the potential.

*This review includes papers published up to May, 1966.

*This term, which reflects the functional character of the important quantity, seems to us preferable to the expression "phase method" which is sometimes used. At the same time it must be pointed out that the term PFM is a very restricted one, because the method in question is applied not only to the calculation of phase shifts, but also to the calculation of other scattering parameters, for example the scattering length, and also of the energies of bound states.

2) The monotonic, not oscillating, character of the PF, which allows us to make numerical calculations with great accuracy and makes it easier to estimate the error of a computation.

3) The fact that the equation studied is a first-order equation, albeit a nonlinear one. On one hand this decreases the number of operations (and consequently also the time) in calculations with electronic computers, and on the other hand it makes it possible to use a number of known results of the theory of differential equations.

4) As is shown in the present article, the PFM leads to the construction of new algorithms for the exact calculation of various scattering parameters (phases, scattering lengths, effective radii, and so on) and of the energies of bound states, and also to new approximate methods of calculation.

5. The PFM allows us to derive well known general theorems in a simple way: the analytical properties of scattering amplitudes, the number of bound states in the field of a given potential, and so on.

The material to be expounded falls into several sections. In Sec. 2 we derive the equations for the phase functions corresponding to nonrelativistic and relativistic potential scattering, and describe a new method for calculating the energies of bound states. The important case of low-energy scattering and the calculation of such parameters as the scattering length, the effective radius, etc., are considered in Sec. 3. Section 4 contains an exposition of approximate methods of solving the equations for the PF. In Sec. 5 we analyze in the framework of the PFM some general questions of the theory of potential scattering. In the concluding section there is a brief discussion of the possibilities of further development and application of the phase-function method.

We shall make frequent use of the following notation* for the Riccati-Bessel functions of real and imaginary argument and the Riccati-Hankel functions:

$$\left.\begin{aligned} j_l(x) &\equiv \sqrt{\frac{\pi x}{2}}\, J_{l+1/2}(x), \quad n_l(x) \equiv \sqrt{\frac{\pi x}{2}}\, N_{l+1/2}(x),\\ i_l(x) &\equiv \sqrt{\frac{\pi x}{2}}\, I_{l+1/2}(x) = (-i)^{l+1} j_l(ix),\\ k_l(x) &\equiv \sqrt{\frac{\pi x}{2}}\, K_{l+1/2}(x) = \frac{\pi}{2} i^{l+1} h_l^{(1)}(ix),\\ h_l^{(1)}(x) &\equiv \sqrt{\frac{\pi x}{2}}\, H^{(1)}_{l+1/2}(x) = j_l(x) + i n_l(x),\\ h_l^{(2)}(x) &\equiv \sqrt{\frac{\pi x}{2}}\, H^{(2)}_{l+1/2}(x) = j_l(x) - i n_l(x). \end{aligned}\right\} \quad (1.1)$$

These functions can be expressed in a simple way in terms of trigonometric and monomial functions, for example

$$\left.\begin{aligned} j_0(x) &= \sin x, & n_0(x) &= -\cos x,\\ j_1(x) &= \frac{1}{x}\sin x - \cos x, & n_1(x) &= -\frac{1}{x}\cos x - \sin x. \end{aligned}\right\} \quad (1.2)$$

For $l > 1$ the functions $j_l(x)$ and $n_l(x)$ can be obtained from (1.2) by means of the recurrence relations

$$z_{l+1}(x) = \frac{2l}{x} z_l(x) - z_{l-1}(x), \qquad l = 1, 2, 3, \ldots \quad (1.3)$$

We note also the behavior of $j_l(x)$ and $n_l(x)$ for large and small values of the argument:

$$j_l(x) \to \sin\left(x - \frac{l\pi}{2}\right), \quad n_l(x) \to -\cos\left(x - \frac{l\pi}{2}\right), \quad x \to \infty, \quad (1.4)$$

$$j_l(x) \to \frac{x^{l+1}}{(2l+1)!!}, \quad n_l(x) \to -\frac{(2l-1)!!}{x^l}, \quad x \to 0. \quad (1.5)$$

2. THE EQUATIONS FOR THE PHASE FUNCTIONS

In this section we give the exact equations for the phase functions, which are very convenient in practical numerical computations. The most important cases of potential scattering are considered.

2.1 Central Potential

Let us consider the case of elastic scattering by a central potential, or the somewhat more general case of elastic scattering by an arbitrary potential which does not lead to mixing of partial waves with different orbital angular momenta l, i.e., the case of a one-channel reaction. Then the Schrödinger equation for the radial wave function $u_l(r)$ is of the form*

$$u_l'' + \left[k^2 - \frac{l(l+1)}{r^2} - V(\eta)\right] u_l = 0. \quad (2.1)$$

The functions $j_l(kr)$ and $n_l(kr)$ are two independent solutions of the free equation (2.1) ($V \equiv 0$).

We introduce two new functions $\delta_l(r)$ and $A_l(r)$ by setting

$$u_l(r) = A_l(r)\,[\cos\delta_l(r)\, j_l(kr) - \sin\delta_l(r)\, n_l(kr)]. \quad (2.2)$$

This expression (2.2) still does not allow us to determine both new functions uniquely.

We require in addition that the derivative of the wave function at each point be given by

$$u_l'(r) = A_l(r)\,[\cos\delta_l(r)\, j_l'(kr) - \sin\delta_l(r)\, n_l'(kr)]. \quad (2.3)$$

This is equivalent to a supplementary condition for $A_l(r)$ and $\delta_l(r)$:

$$A_l'[\cos\delta_l j_l - \sin\delta_l n_l] - \delta_l' A_l[\sin\delta_l j_l + \cos\delta_l n_l] = 0. \quad (2.4)$$

The conditions (2.3), (2.4) are obvious for $r \to \infty$ if we desire that at large distances, where $V(r) \to 0$, the functions $\delta_l(r)$ and $A_l(r)$ approach constant values, namely the scattering phase shift and the normaliza-

*The symbols $j_l(x)$ and $n_l(x)$ are often used to denote spherical Bessel functions, which differ from the definitions (1.1) by a factor x^{-1}. To simplify the form of the expressions we have decided to avoid the more complicated notations.

*Here and everywhere in what follows, unless explicitly stated, we set $\hbar = 2m = 1$. Primes indicate differentiations with respect to r.

tion constant of the wave function. The meaning of these same conditions for finite values of r can be explained in the following way. We assume that the potential has a finite range R, so that V(r) = 0 for r > R. Then in the region r > R the functions $\delta_l(r)$ and $A_l(r)$ must also take constant values $\delta_l(R)$ and $A_l(R)$, corresponding to the phase shift and normalization of the wave function for scattering by the potential V(r) cut off to zero at the point r = R. Then it is easy to see that the relation (2.3) corresponds to the condition of continuity of the derivative of the wave function at the point r = R. Consequently the supplementary condition (2.4) imposed on $\delta_l(r)$ and $A_l(r)$ corresponds to a definite choice of the physical meaning of these functions.

It follows from (2.1), (2.2), and (2.4) that the functions $\delta_l(r)$ and $A_l(r)$ satisfy first-order equations. Furthermore the equation for $\delta_l(r)$ turns out to be independent of $A_l(r)$:

$$\delta_l'(r) = -\frac{1}{k} V(r)[\cos\delta_l(r) j_l(kr) - \sin\delta_l(r) n_l(kr)]^2, \quad \delta_l(0) = 0. \tag{2.5}$$

As was noted above and as follows directly from (2.2) and (2.5), the value of the function $\delta_l(r)$ at any point r = R is the phase shift for the scattering at the potential V(r) θ(R − r) cut off at this point. Therefore the initial condition $\delta_l(0) = 0$ corresponds to the actual absence of any potential if R = 0 (Fig. 1); the function $\delta_l(r)$ is called the phase function (PF).

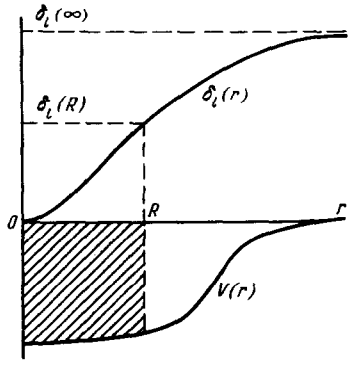

FIG. 1. Nature of the behavior of the phase function for an attractive potential.

Equation (2.5) has been derived in papers by Drukarev,[2] Bergmann,[3] Olsson,[4] Kynch,[5] Spruch,[7] and Calogero.[8] The equation for the PF takes an especially simple form for $l = 0$:

$$\delta_0'(r) = -\frac{1}{k} V(r) \sin^2[kr + \delta_0(r)], \qquad \delta_0(0) = 0. \tag{2.6}$$

The equation for the function $A_l(r)$, which is naturally called the amplitude function, is linear:

$$A_l' = -\frac{1}{k} A_l V [\cos\delta_l j_l - \sin\delta_l n_l][\sin\delta_l j_l + \cos\delta_l n_l] \tag{2.7}$$

and when the solution of (2.5) is known it can be integrated in explicit form

$$A_l(r) = \exp\left\{-\frac{1}{k}\int_{r_0}^{r} dr' V(r')[\cos\delta_l(r') j_l(kr') - \sin\delta_l(r') n_l(kr')][\sin\delta_l(r') j_l(kr') + \cos\delta_l(r') n_l(kr')]\right\}. \tag{2.8}$$

Here the normalization assumed for the amplitude function is $A_l(r_0) = 1$, where r_0 is as yet an arbitrary point.

Because of the singular behavior of the functions $n_l(kr)$ for $l > 0$, in practical cases Eq. (2.5) must be integrated from a point $r = \epsilon > 0$. The initial condition for the PF is then determined by the behavior of the potential at small distances and can be obtained directly from Eq. (2.5) when it is written in integral form

$$\delta_l(r) = -\frac{1}{k}\int_0^r V(r')[\cos\delta_l(r') j_l(kr') - \sin\delta_l(r') n_l(kr')]^2 dr'. \tag{2.9}$$

There are three possible cases. In the first the potential is nonsingular or weakly singular, i.e.,

$$r^2 V(r) \to 0, \qquad r \to 0. \tag{2.10}$$

Then, using (1.5) we can easily verify that

$$\delta_l(\varepsilon) \to -\frac{1}{k[(2l+1)!!]^2}\int_0^{\varepsilon} V(r) r^{2l+2} dr, \qquad \varepsilon \to 0. \tag{2.11}$$

For example, for

$$V(r) \to V_0 r^p [1 + O(r^s)], \quad p > -2, \quad s > 0, \tag{2.12}$$

we have

$$\delta_l(\varepsilon) = -\frac{V_0 (k\varepsilon)^{2l+1}\varepsilon^{2+p}}{(2l+3+p)[(2l+1)!!]^2}[1 + O(\varepsilon^m)],$$
$$m = \min(s, 2, 2+p). \tag{2.13}$$

The various correction terms arise from the corrections to the potential (m = s), from the expansion of the function $j_l(kr)$ (m = 2), and from inclusion of the term $\delta_l(r) n_l(kr)$ (m = 2 + p). In the case of a nonsingular or weakly singular potential the normalization of the amplitude function is entirely arbitrary. In particular, we can set $r_0 = 0$ in (2.8), so that $A_l(0) = 1$.

The second possible case is that of a strongly singular repulsive potential

$$r^2 V(r) \to +\infty, \qquad r \to 0. \tag{2.14}$$

It is not hard to verify that in this case

$$\delta_l(\varepsilon) = -\frac{(k\varepsilon)^{2l+1}}{(2l+1)!!\,(2l-1)!!}\left[1 - \frac{2l+1}{\varepsilon V^{1/2}(\varepsilon)}\right]. \tag{2.15}$$

The first term in (2.15) is the phase shift in the scattering by a hard sphere of radius ϵ ($k\epsilon \ll 1$). This corresponds to the fact that at the very smallest distances the potential barrier becomes very large. In this case the amplitude function can be normalized to

unity only for finite r_0. For $r \to 0$ the function $A_l(r)$ becomes exponentially small:

$$A_l(r) \to \exp\left[-\int_r^{r_0} dr' V^{1/2}(r')\right], \quad r \to 0. \qquad (2.16)$$

A special case of a strongly singular potential is a hard repulsive core of finite radius r_0:

$$V(r) = +\infty, \quad 0 \leqslant r < r_0. \qquad (2.17)$$

The initial condition at $r = r_0$ for the phase function is then given by the relation

$$\delta_l(r) = \operatorname{arctg} \frac{j_l(kr)}{n_l(kr)}, \quad 0 \leqslant r \leqslant r_0. \qquad (2.18)$$

The amplitude function is discontinuous

$$\begin{aligned} &A_l(r) = 0, \quad 0 \leqslant r < r_0, \\ &A_l(r_0) = 1. \end{aligned} \qquad (2.19)$$

The third case is the intermediate one:

$$r^2 V(r) \to \text{const} = \beta > -(l+1/2)^2, \quad r \to 0. \qquad (2.20)$$

The restriction on the quantity β arises from the condition that there be no falling into the center for an attractive potential ($\beta < 0$). The analysis then shows that for $r \to 0$

$$\delta_l(r) \to -q_l \frac{(kr)^{2l+1}}{(2l+1)!!\,(2l-1)!!}, \quad A_l(r) \to \text{const} \cdot r^{\frac{\beta(1-q_l)}{2l+1}}. \qquad (2.21)$$

Here we use the notation

$$q_l = 1 + \frac{(2l+1)^2}{2\beta} - \frac{(2l+1)^2}{2\beta}\sqrt{1 + \frac{4\beta}{(2l+1)^2}}, \quad -1 < q_l < 1. \qquad (2.22)$$

In spite of the fact that the amplitude function $A_l(r)$ is singular in the case of an attractive potential, the restriction $\beta > -(l + 1/2)^2$ assures that the square of the wave function (2.2) is integrable.

Accordingly, the problem of determining the scattering phase shift for a potential V(r) reduces to the integration of Eq. (2.5) and the finding of the asymptotic value of the PF, $\delta_l(\infty)$.

The main advantages of this approach have already been pointed out in the introduction. We here add only that by starting from (2.5) we can also get new equations for such quantities as, for example, the tangent of the phase shift, $t_l(r) = \tan \delta_l(r)$:

$$t_l'(r) = -\frac{1}{k} V(r) [j_l(kr) - t_l(r) n_l(kr)]^2, \quad t_l(0) = 0, \qquad (2.23)$$

or for the partial scattering amplitude $f_l(r) = e^{i\delta_l(r)} \sin \delta_l(r)$:

$$f_l'(r) = -\frac{1}{k} V(r) [j_l(kr) + i f_l(r) h_l^{(1)}(kr)]^2, \quad f_l(0) = 0, \qquad (2.24)$$

or for the S-matrix element $S_l = e^{2i\delta_l} = 1 + 2if_l$:

$$S_l'(r) = -\frac{i}{2k} V(r) [h_l^{(2)}(kr) + S_l(r) h_l^{(1)}(kr)]^2, \quad S_l(0) = 1. \qquad (2.25)$$

Equation (2.23), unlike (2.5), can be used for numerical computations only under the condition $\delta_l(r) < \pi/2$ in the entire range of integration. If a resonance is possible in the scattering by any of the sequence of cut-off potentials $V(r)\,\theta(R - r)$—i.e., if $\delta_l(R) = \pi/2$—we can change over in the region $r \approx R$ to an equation analogous to (2.23) for the inverse quantity, namely for the function $\cot \delta_l(r)$. In papers by Franchetti,[6] Calogero,[8] Dashen,[15] and Calogero and Ravenhall[18] other versions of the basic equation (2.5) are given.

It has so far been tacitly assumed that the potential V(r) falls off more rapidly than $O(r^{-1})$ for $r \to \infty$. Equation (2.5) can be easily extended, however, to the case in which there is a Coulomb interaction: $V(r) + 2k\eta/r$. As has been shown by Olsson,[4] Kynch,[5] Babikov,[17] Kalogero and Ravenhall,[18] and Tietz,[33] for this case one must in all expressions, beginning with (2.2), carry out a replacement of the Ricatti-Bessel functions by Coulomb functions:

$$j_l(kr) \to F_l(kr, \eta), \quad n_l(kr) \to -G_l(kr, \eta). \qquad (2.26)$$

The equation for the PF then takes the form

$$\delta_l'(r, \eta) = -\frac{1}{k} V(r) [\cos \delta_l(r, \eta) F_l(kr, \eta) + \sin \delta_l(r, \eta) G_l(kr, \eta)]^2, \quad \delta_l(0, \eta) = 0. \qquad (2.27)$$

We note that the asymptotic form of the wave function is now

$$u_l \approx \sin\left(kr - \eta \ln 2kr - \frac{\pi l}{2} + \sigma_l + \delta_l\right), \quad r \to \infty, \qquad (2.28)$$

where $\sigma_l = \arg \Gamma(l + 1 + i\eta)$, is the phase shift for pure Coulomb scattering.

As an illustration of the behavior of the PF there are shown in Fig. 2, taken from[8], five curves, which are the solutions of Eq. (2.6) for a rectangular well of depth $V(r) = -V_0 = -9$ and radius R = 2 for five values of k. As can be seen from the figure, for sufficiently small k there are sharp changes of the value of $\delta_0(r, k)$ near the points $r_1 = \pi/6$ and $r_2 = \pi/2$, which are the radii of the potential well at which it is possible for a bound state to appear with zero binding energy. It is not hard to derive from (2.6) the following estimate of the interval Δr_i around the point r_i in which an in-

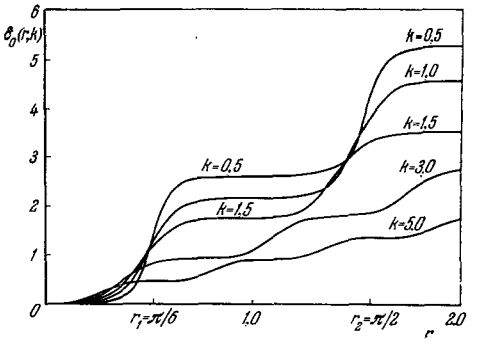

FIG. 2. The phase function for a rectangular potential well, for various values of k.

crease of the phase by the amount π occurs for small k:

$$\Delta r_i \approx \frac{k\pi}{V(r_i)}. \tag{2.29}$$

In the limiting case k = 0, for any l and for an arbitrary potential, the PF becomes a step function (N is the number of bound states with angular momentum l):

$$\delta_l(r, 0) = \pi \sum_{i=1}^{N} \theta(r - r_i). \tag{2.30}$$

This relation (2.30) is the well known Levinson theorem.

2.2 Tensor Potential. Many-channel Scattering

The PFM can be extended to the case of a noncentral tensor interaction and many-channel inelastic scattering. An important case of a two-channel reaction is the elastic scattering interaction of two particles having spin $\frac{1}{2}$ (for example, nucleons), when the tensor interaction is taken into account. In the triplet spin state the tensor forces $T_J(r)$ mix the partial waves which for a given total angular momentum J of the system correspond to different orbital angular momenta $L = J \mp 1$. The equations for the corresponding radial wave functions $u_J(r)$ and $w_J(r)$ are coupled:

$$\begin{aligned} u_J'' + \left[k^2 - \frac{J(J-1)}{r^2} - V_{J,J-1}\right] u_J - T_J w_J &= 0, \\ w_J'' + \left[k^2 - \frac{(J+2)(J+1)}{r^2} - V_{J,J+1}\right] w_J - T_J u_J &= 0. \end{aligned} \tag{2.31}$$

The coupling of the equations (2.31) decidedly complicates the calculation of the scattering parameters, which are now two phase shifts and a mixing parameter. The point is that for small r one of the two linearly independent solutions of the system (2.31) is very much larger than the other. Therefore it is difficult to "extract" the slowly increasing solution against the background of the first solution. The PFM enables us to derive for three functions which correspond to the three scattering parameters a simple system of first-order equations which is free from this disadvantage. It is well known that a different parametrization of the scattering matrix is possible with a tensor potential. The equations of the PFM for various representations of the parameters have been derived in papers by Kynch,[5] Babikov,[17,26] and Cox and Perlmutter.[34]

Here we shall consider only the equations for the functions $\bar{\delta}_{J,J-1}(r)$, $\delta_{J,J+1}(r)$, and $\bar{\epsilon}_J(r)$, which correspond to the Stapp parametrization, that most used in nuclear physics. As in the case of the central potential, these functions have the meaning of the scattering parameters for potentials $V_{J,J-1}(r)$, $V_{J,J+1}(r)$, and $T_J(r)$, cut off at the point r.

It is convenient to introduce an abbreviated notation by setting

$$\begin{aligned} P_{J,L}(r) &\equiv \cos\bar{\delta}_{J,L}(r)\, j_L(kr) - \sin\bar{\delta}_{J,L}(r)\, n_L(kr), \\ Q_{J,L}(r) &\equiv \sin\bar{\delta}_{J,L}(r)\, j_L(kr) + \cos\bar{\delta}_{J,L}(r)\, n_L(kr). \end{aligned} \tag{2.32}$$

The desired system of equations is then[17,26]

$$\left.\begin{aligned} \bar{\delta}'_{J,J-1} &= -\frac{1}{k\cos 2\bar{\varepsilon}_J}\,[V_{J,J-1}(\cos^4\bar{\varepsilon}_J P^2_{J,J-1} - \sin^4\bar{\varepsilon}_J Q^2_{J,J-1}) \\ &\quad - V_{J,J+1}\sin^2\bar{\varepsilon}_J\cos^2\bar{\varepsilon}_J\,(P^2_{J,J+1} - Q^2_{J,J+1}) \\ &\quad - 2T_J\sin\bar{\varepsilon}_J\cos\bar{\varepsilon}_J\,(\cos^2\bar{\varepsilon}_J P_{J,J-1}Q_{J,J+1} \\ &\quad - \sin^2\bar{\varepsilon}_J P_{J,J+1}Q_{J,J-1})], \quad \bar{\delta}^2_{J,J-1}(0) = 0, \\ \bar{\delta}'_{J,J+1} &= -\frac{1}{k\cos 2\bar{\varepsilon}_J}\,[V_{J,J+1}(\cos^4\bar{\varepsilon}_J P^2_{J,J+1} - \sin^4\bar{\varepsilon}_J Q_{J,J+1}) \\ &\quad - V_{J,J-1}\sin^2\bar{\varepsilon}_J\cos^2\bar{\varepsilon}_J\,(P^2_{J,J-1} - Q^2_{J,J-1}) \\ &\quad - 2T_J\sin\bar{\varepsilon}_J\cos\bar{\varepsilon}_J\,(\cos^2\bar{\varepsilon}_J P_{J,J+1}Q_{J,J-1} \\ &\quad - \sin^2\bar{\varepsilon}_J P_{J,J-1}Q_{J,J+1})], \quad \bar{\delta}_{J,J+1}(0) = 0, \\ \bar{\varepsilon}'_J &= -\frac{1}{k}\,[T_J(\cos^2\bar{\varepsilon}_J P_{J,J-1}P_{J,J+1} + \sin^2\bar{\varepsilon}_J Q_{J,J-1}Q_{J,J+1}) \\ &\quad - V_{J,J-1}\sin\bar{\varepsilon}_J\cos\bar{\varepsilon}_J P_{J,J-1}Q_{J,J-1} \\ &\quad - V_{J,J+1}\sin\bar{\varepsilon}_J\cos\bar{\varepsilon}_J P_{J,J+1}Q_{J,J+1}], \quad \bar{\varepsilon}_J(0) = 0. \end{aligned}\right\} \tag{2.33}$$

These equations are a generalization of (2.5). It is easy to see that when the tensor potential is turned off ($T_J \equiv 0$) the mixing parameter becomes identically zero ($\bar{\epsilon}_J \equiv 0$) and the system (2.33) breaks up into two independent equations for the partial waves with $L = J - 1$ and $L = J + 1$. A Coulomb potential can be included by using the substitution (2.26) in the equations. Systems of equations analogous to (2.33) can be derived[26] for the parametric functions in other representations, for example the Blatt-Biedenharn and McHale-Thaler representations.

The values of the phase functions for small r are determined by the behavior of the potentials for $r \to 0$, and can be found directly from an analysis of the equations (2.33). Let us consider some of the most important cases. Suppose that for $r \to 0$

$$\begin{aligned} V_{J,J-1}(r) &\to V^0_{J,J-1} r^p, \quad V_{J,J+1}(r) \to V^0_{J,J+1} r^p, \\ T_J(r) &\to T^0_J r^p, \quad p > -2. \end{aligned} \tag{2.34}$$

Then

$$\left.\begin{aligned} \bar{\delta}_{J,J-1}(r) &\to -\frac{V^0_{J,J-1} k^{2J-1} r^{2J+1+p}}{(2J+1+p)\,[(2J-1)!!]^2}, \\ \bar{\delta}_{J,J+1}(r) &\to -\frac{V^0_{J,J+1} k^{2J+3} r^{2J+5+p}}{(2J+5+p)\,[(2J+3)!!]^2}, \\ \bar{\varepsilon}_J(r) &\to -\frac{T^0_J k^{2J+1} r^{2J+3+p}}{(2J+3+p)\,(2J-1)!!\,(2J+3)!!}. \end{aligned}\right\} \tag{2.35}$$

For repulsive singular potentials

$$r^2 V_{J,J-1}(r) \to +\infty, \quad r^2 V_{J,J+1}(r) \to +\infty, \quad r \to 0, \tag{2.36}$$

we have

$$\left.\begin{aligned} &\bar{\delta}_{J,J-1}(r) \to -\frac{(kr)^{2J-1}}{(2J-1)!!\,(2J-3)!!}, \quad \bar{\delta}_{J,J+1}(r) \to \\ &-\frac{(kr)^{2J+3}}{(2J+3)!!\,(2J+1)!!}, \quad \bar{\varepsilon}_J(r) \to -\frac{k^{2J+1}}{(2J-3)!!\,(2J+1)!!} \\ &\times \int_0^r dr'\,(r')^{2J}\,\frac{T_J(r')}{V^{1/2}_{J,J-1}(r')\,V^{1/2}_{J,J+1}(r')} \\ &\times \exp\left\{-\int_{r'}^{r} dr''\,[V^{1/2}_{J,J-1}(r'') + V^{1/2}_{J,J+1}(r'')]\right\}. \end{aligned}\right\} \tag{2.37}$$

Accordingly, the mixing parameter is exponentially small. For a hard core of finite radius r_0

$$\left.\begin{aligned} \bar{\delta}_{J,J-1}(r) &= \operatorname{arctg}\frac{j_{J-1}(kr)}{n_{J-1}(kr)}, && 0\leqslant r\leqslant r_0,\\ \bar{\delta}_{J,J+1}(r) &= \operatorname{arctg}\frac{j_{J+1}(kr)}{n_{J+1}(kr)}, && 0\leqslant r\leqslant r_0,\\ \bar{\varepsilon}_J(r) &= 0, && 0\leqslant r\leqslant r_0. \end{aligned}\right\} \quad (2.38)$$

To take a Coulomb potential into account one must make the replacement (2.26) in all these expressions.

As an example we show in Fig. 3 the results of integrating (2.33) for the phase shifts of $^3P_2$ and $^3F_2$ and the mixing parameter $\bar{\epsilon}_2$ for nucleon-nucleon scattering with the well known Hamada-Johnston potential with a hard core ($r_0 = 0.343$). The solid and dashed curves correspond to energy values E = 320 MeV (k = 2.78) and E = 180 MeV (k = 2.08). Because of the short range of the potential all of the functions quickly take their constant asymptotic values. The sharp breaks in the curves for $\bar{\delta}_{2,1}(r)$ correspond to the change of sign of the potential $V_{J,J-1}(r)$ at the point $r = r_0$.

The PFM for more general cases of many-channel scattering, including inelastic scattering, has been developed in papers by Kynch,[5] Zemach,[20] Degasperis,[24] and Cox.[35] The various parametric functions are found by solving a system of $\frac{1}{2}n(n+1)$ nonlinear first-order equations of the form of (2.33); here n is the number of channels. The amplitude functions satisfy a system of n linear equations; unlike the equation for the case of a central potential, these cannot be integrated in quadratures. Accordingly, in the many-channel case the problem of finding the scattering parameters reduces to the solution of a Cauchy problem with initial conditions, which is much more convenient than solving a system of Schrödinger equations and constructing from the solutions linear combinations which satisfy given boundary conditions.

Sometimes one includes besides the elastic-scattering channel only one reaction channel which describes

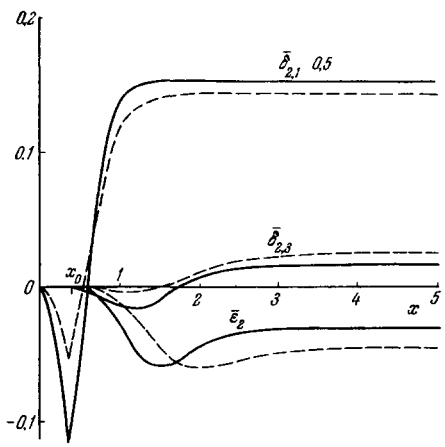

FIG. 3. Phase shifts and mixing parameter for nucleon-nucleon scattering in the $^3P_2$ and $^3F_2$ states for the Hamada-Johnston potential, as functions of $x = \mu_\pi r$.

all of the inelastic scattering and absorption. In the so-called optical model inclusion of the inelastic-scattering channel corresponds to a complex term added to the potential in the elastic-scattering channel. The parameters that describe the scattering in this case are the S-matrix elements or scattering coefficients S_l. By means of Eq. (2.25) the PFM can be used easily in the optical model of nuclear reactions.[28] This eliminates all of the problems associated with the normalization of the wave functions, which cause difficulties in the standard methods of calculating cross sections in the optical model. We also point out that owing to the simple and intuitive physical meaning of the phase functions it is very convenient to use the PFM to study such a problem as, for example, the surface or volume character of the absorption in a nucleus. Moreover, one can obtain additional information in the process of integrating the equations for the phase functions.

In the problems considered above, in which the angular variables can be completely separated, one uses a representation diagonal in the angular momentum. In the general case of a noncentral potential $V(r, \theta, \varphi)$, however, an expansion is partial waves is useless, although the total scattering amplitude $f(\theta, \varphi)$ exists. So far no equation equivalent to the equation (2.5) for the PF has been obtained for this case. The equation for the function $f_r(\theta, \varphi)$ given in[7] and used in[21] is incorrect owing to the use of an incorrect wave function.

2.3 Velocity-dependent Potential. Scattering of Relativistic Particles

In a number of problems of nuclear and atomic physics one has to deal with an effective potential depending on the velocity:

$$V_{\text{eff}}(r) = V(r) + \frac{1}{2}[\mathbf{p}^2 W(r) + W(r)\mathbf{p}^2]. \quad (2.39)$$

The Schrödinger equation for the radial wave function is then of the form

$$(1+W)u_l'' + W'u_l' + \left[k^2 - \frac{l(l+1)}{r^2}(1+W) - V + \frac{1}{2}W''\right]u_l = 0. \quad (2.40)$$

According to the PFM we can obtain the following equations for the phase and amplitude functions defined by the relations (2.2) and (2.3):

$$(1+W)\delta_l' = -\frac{1}{k}\left[\left(V + k^2W - \frac{1}{2}W''\right)P_l + W'R_l\right]P_l, \qquad \delta_l(0) = 0, \quad (2.41)$$

$$(1+W)A_l' = -\frac{1}{k}A_l\left[\left(V + k^2W - \frac{1}{2}W''\right)P_l - W'R_l\right]Q_l, \qquad A_l(r_0) = 1. \quad (2.42)$$

Along with the notations (2.32) we have here used the expression

$$R_l(r) \equiv \cos\delta_l(r)\, j_l'(kr) - \sin\delta_l(r)\, n_l'(kr). \quad (2.43)$$

The solution of the linear equation (2.42) can be expressed in quadratures, in a form like (2.8). As before, the initial conditions in concrete problems must be found from Eq. (2.41) by means of a series expansion. Equation (2.41) was derived by McKellar and May,[39] who also considered potentials of the form $\mathbf{p}W(r)\mathbf{p}$. They showed that in this case the study of the phase function is useful in comparing the effects of the action of various velocity-dependent potentials.

In a paper by Calogero[19] the PFM was extended to the case of a nonlocal central potential. Here the PF satisfies an integro-differential equation whose solution can be found by an iterative method.

The potential scattering of relativistic particles can also be treated with the PFM. For charged particles with zero spin the relativistic Schrödinger equation is ($\hbar = 1$)

$$\Delta\psi + [(E - e\varphi)^2 c^{-2} - (mc^2 + V)^2 c^{-2}]\psi = 0. \quad (2.44)$$

Here $e\varphi(\mathbf{r})$ and $V(\mathbf{r})$ are respectively the electrostatic and the static scalar potentials. It can be shown that if the potentials are spherically symmetric the equations for the phase and amplitude functions are given by (2.5) and (2.8) if in these equations we set

$$2m = 1, \quad k = \sqrt{E^2 c^{-2} - \tfrac{1}{4} c^2},$$
$$V_{\text{eff}} = V + 2Ec^{-2} e\varphi + c^{-2} V^2 - c^{-2} (e\varphi)^2. \quad (2.45)$$

If the potential $V_{\text{eff}}(r)$ contains a term which falls off like $O(r^{-1})$ for $r \to \infty$, we must separate out from it an effective Coulomb interaction corresponding to this term and rewrite the equations in terms of the Coulomb functions [Eq. (2.26)].

The extension of the PFM to the Dirac equation has been made in papers by Kynch,[5] Calogero,[10] and Calogero and Ravenhall.[18] These authors considered the scattering of a Dirac particle by a central electrostatic* potential $e\varphi(r)$. If there is also a static scalar potential the Dirac equation is of the form ($\hbar = c = 1$)

$$[E - e\varphi + \boldsymbol{\alpha}\mathbf{p} + \beta(m + V)]\psi = 0. \quad (2.46)$$

Owing to the spin-orbit coupling, for a given total angular momentum j there are two possible values $l = j \pm 1/2$ of the orbital angular momentum; for example for $j = 1/2$ there are states $s_{1/2}$ and $p_{1/2}$. Accordingly the scattering of the j-th partial wave is described by two phase shifts $\delta_{j \pm 1/2}$. Using the notations (2.32), we can write the equations for the phase and amplitude functions in the form

$$\delta'_{j \pm 1/2}(r) = -\lambda^{-1}[\dot{V}(r) + e\varphi(r)] P^2_{j \pm 1/2,\, j \pm 1/2}(r) + \lambda [V(r) - e\varphi(r)] P^2_{j \pm 1/2,\, j \mp 1/2}(r),$$
$$\delta_{j \pm 1/2}(0) = 0, \quad (2.47)$$

$$A'_{j \pm 1/2}(r) = \exp\left\{ -\lambda^{-1} \int_{r_0}^{r} dr' [V(r') + e\varphi(r')] P_{j \pm 1/2,\, j \pm 1/2}(r') Q_{j \pm 1/2,\, j \pm 1/2}(r') + \lambda \int_{r_0}^{r} dr' [V(r') - e\varphi(r')] P_{j \pm 1/2,\, j \mp 1/2}(r') Q_{j \pm 1/2,\, j \mp 1/2}(r') \right\}. \quad (2.48)$$

Here $\lambda = [(E - m)/(E + m)]^{1/2}$, $k = (E^2 - m^2)^{1/2}$, so that in the nonrelativistic limit $\lambda = k/2m$ and these equations go over into (2.5) and (2.8). In the ultrarelativistic case $\lambda = 1$.

Equations (2.47) and (2.48) are valid for potentials which fall off sufficiently rapidly at infinity. If there is an unscreened Coulomb potential, one must proceed in a way analogous to that described above for the scattering of a scalar particle.

2.4 The Energies of Bound States

Although the PFM is obviously best fitted for scattering problems, Kynch[5] and Calogero[8] have shown that the problem of eigenvalues can also be formulated in the framework of this method.

For bound states $k = i\kappa$ ($\kappa > 0$) and the asymptotic form of the solution of the Schrödinger equation (2.1) is

$$u_l(r) \approx \text{const} \cdot [e^{-\kappa r} - (-1)^l \tilde{S}_l^{-1}(\infty, \kappa) e^{\kappa r}], \quad r \to \infty. \quad (2.49)$$

Therefore a necessary condition for the vanishing of the wave function at large distances and the right asymptotic behavior is that the S-matrix element $\tilde{S}_l(\infty, \kappa) \equiv S_l(\infty, i\kappa)$ have a pole at a definite value of κ, so that

$$\tilde{S}_l^{-1}(\kappa, r) e^{2\kappa r} \to 0, \qquad r \to \infty. \quad (2.50)$$

The condition (2.50) is the basis of the treatment of bound-state problems by the PFM. The real function $\tilde{S}_l(\kappa, r)$ satisfies a real equation which follows from (2.25),

$$\tilde{S}'_l(\kappa, r) = (-1)^l \frac{2}{\kappa} V(r) \left\{ i_l(\kappa r) + \frac{(-1)^{l+1}}{\pi} [\tilde{S}_l(\kappa, r) - 1] k_l(\kappa r) \right\}^2, \quad \tilde{S}_l(0, \kappa) = 1. \quad (2.51)$$

It can be seen from (2.51) that in the case of a bound state, for $r \to \infty$, when $k_l(\kappa r) \to (\pi/2) e^{-\kappa r}$,

$$\tilde{S}_l^{-1}(\kappa, r) \approx \frac{(-1)^l}{2\kappa} \int_r^{\infty} e^{-2\kappa r'} V(r'), \qquad r \to \infty. \quad (2.52)$$

Accordingly, the condition (2.50) is in fact satisfied.

Using Eq. (2.51) and the analogous equation for the inverse quantity $\tilde{S}_l^{-1}(\kappa, r)$, one can determine by numerical methods the energies $E_n = -\kappa_n^2$ of the bound states in a given potential. Let us consider a potential of finite range R. The required values κ_n are those for which $\tilde{S}_l^{-1}(R, \kappa_n) = 0$. Figure 4, taken from[8], shows the behavior for various values of κ of the functions $\tilde{Y}_l(\kappa, r)$ and $\tilde{Y}_l^{-1}(\kappa, r)$, which are simply related to $\tilde{S}_l(\kappa, r)$,

$$\tilde{Y}_l(\kappa, r) = \frac{\tilde{S}_l(\kappa, r) k_l(\kappa r)}{k_l(\kappa r) + \pi (-1)^l i_l(\kappa r)}, \quad (2.53)$$

*We emphasize that, contrary to the abstract of [10], the results derived in that paper are really for an electrostatic potential, not a true scalar potential.

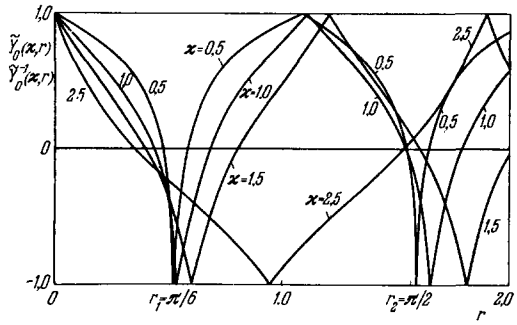

FIG. 4. The functions $\tilde{Y}_0(\kappa, r)$ and $\tilde{Y}_0^{-1}(\kappa, r)$ for a rectangular potential well, for various values of κ.

for S scattering ($l = 0$) by a rectangular well of depth $V_0 = 9$ and radius $R = 2$. The points of intersection of the curves of $\tilde{Y}_0^{-1}(\kappa, r)$ with the axis of abscissas correspond to poles of the S matrix and show the widths of the well for which there is a level $E = -\kappa^2$. For $\kappa = 0$ this occurs at the points $r_1 = \pi/6$ and $r_2 = \pi/2$ (see Fig. 2). As can be seen from Fig. 4, in a well of width $R = 2$ there are two bound states, the first with an energy a little larger than -2.25 ($\kappa \approx 1.5$) and the second with an energy a little smaller than -6.25 ($\kappa \approx 2.5$). An analogous argument can be carried out for an arbitrary potential $V(r)$, by cutting it off at sufficiently large distances. As can be seen from Fig. 4, with increase of r the intervals between the points r_i at which $\tilde{Y}_0^{-1}[r_i(\kappa), \kappa] = 0$ become larger. Therefore the accuracy of the determination of the bound-state energies also increases.

This method can also be used to determine the parameters of a potential which has bound states with given binding energies.

3. LOW-ENERGY SCATTERING

We present exact equations for the calculation of parameters of low-energy scattering such as the scattering length, the effective radius, and so on.

3.1 Short-range Central Potential

Suppose $V(r)$ is a short-range potential, i.e., suppose it decreases at least exponentially for $r \to \infty$. Then, as is well known, the scattering phase shift $\delta_l(k)$, and consequently also $\tan \delta_l(k)$, are odd functions of k which are regular at the point $k = 0$. In this case the quantity $k^{-1} \tan \delta_l(k)$ can be expanded in a power series in k^2, whose first coefficients completely determine the scattering at low energies. A PFM for the calculation of these coefficients has been given in papers by Kynch,[5] Levy and Keller,[11] and Dashen.[12]

Representing the function $\tan \delta_l(r, k)$ in the form of a series

$$\operatorname{tg} \delta_l(r, k) = -\frac{k^{2l+1}}{(2l+1)!!\,(2l-1)!!} \sum_{n=0}^{\infty} k^{2n} a_{ln}(r) \qquad (3.1)$$

and using the well known expansions of the functions $j_l(kr)$ and $n_l(kr)$, we can get from (2.23) a system of recurrence equations for the coefficients $a_{ln}(r)$. The first equation is nonlinear, and all of the rest are linear; for example,

$$a'_{l0} = \frac{1}{2l+1} V (r^{l+1} - r^{-l} a_{l0})^2, \qquad a_{l0}(0) = 0,$$
$$a'_{l1} = -\frac{1}{2l+1} r^{-l} V (r^{l+1} - r^{-l} a_{l0}) \left(2a_{l1} + \frac{r^2}{2l-1} a_{l0} + \frac{r^{2l+3}}{2l+3} \right),$$
$$a_{l1}(0) = 0. \qquad (3.2)$$

In the case $l = 0$ the equations take a particularly simple form:

$$\left.\begin{aligned} a'_{00} &= V (r - a_{00})^2, \quad a_{00}(0) = 0, \\ a'_{01} &= -2V (r - a_{00}) a_{01} - r^2 V \left(a_{00} - \frac{4}{3} r a_{00} + \frac{1}{3} r^2 \right), \quad a_{01}(0) = 0, \\ a'_{02} &= -2V (r - a_{00}) a_{02} + V \left(a_{01}^2 - 2r^2 a_{00} a_{01} + \frac{4}{3} r^3 a_{01} \right. \\ &\quad \left. + \frac{1}{3} r^4 a_{00}^2 - \frac{4}{15} r^5 a_{00} + \frac{2}{45} r^6 \right), \quad a_{02}(0) = 0. \end{aligned}\right\} \qquad (3.3)$$

The initial conditions for Eqs. (3.2), (3.3) in the case of singular potentials can be easily found from the conditions (2.13), (2.15), (2.18), and (2.21). The functions a_{0n} are connected in a simple way with the parameters of the effective-range theory—the scattering length a_0, the effective range r_e, the shape parameter P, and so on, which are defined by the expansion

$$k \operatorname{ctg} \delta_0 = -\frac{1}{a_0} + \frac{1}{2} r_e k^2 - P r_e^3 k^4 + O(k^6). \qquad (3.4)$$

It is not hard to verify that

$$\left.\begin{aligned} a_0 &= \lim_{r \to \infty} a_{00}(r), \qquad r_e = \lim_{r \to \infty} \frac{2a_{01}(r)}{a_{00}^2(r)}, \\ P &= \lim_{r \to \infty} \frac{1}{8} \frac{a_{00}^3(r)}{a_{01}^3(r)} [a_{01}^2(r) - a_{00}(r) a_{02}(r)]. \end{aligned}\right\} \qquad (3.5)$$

For finite values of r the relations (3.5) define the functions $a_0(r)$, $r_e(r)$, and $P(r)$ which correspond to the scattering parameters for the cut-off potential $V(r') \theta(r - r')$.

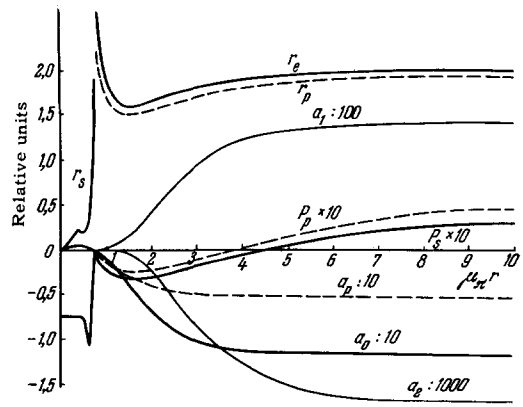

FIG. 5. Solutions of Eqs. (3.3) and the parameters a_0, r_e, P_s for singlet $^1S_0$ neutron-proton scattering with the Hamada-Johnston potential, as functions of $x = \mu_\pi r$. The dashed curves show the scattering length, effective range, and shape parameter for $^1S_0$ proton-proton scattering.

The equations (3.3) are very convenient for numerical calculations. As an example, in Fig. 5 the solid lines show the solutions of (3.3) and the calculated[27] parametric functions $a_0(r)$, $r_e(r)$, $P(r)$ for $^1S_0$ neutron-proton scattering with the Hamada-Johnston potential. It can be seen from the figure that the effective range r_e goes to infinity at the point where the scattering length $a_0(r)$ is zero.

The calculation of the scattering length for a velocity-dependent potential has been considered by KcKellar and May.[39]

3.2 Long-range Central Potential

In the case of a long-range potential, for example one decreasing according to a power law, the phase function $\delta_l(r, k)$ is no longer analytic at the point $k = 0$; it has logarithmic and fractional-power singularities. Therefore the expansion (3.1) takes a more complicated form, including terms of the types $k^m \ln k$ and $k^{m/n}$. The PFM for the determination of the coefficients in this case has been developed by Levy and Keller.[11] They treated potentials having the asymptotic form $O(r^{-\nu})$ with $\nu > 3$. The extremely important case of a short-range potential together with a Coulomb potential, for which $\delta_l(k)$ has an essential singularity for $k = 0$, has been treated in[17-27].

The parameters for low-energy S scattering are then defined by the expansion

$$2\pi\eta\,(e^{2\pi\eta}-1)\,k\operatorname{ctg}\delta_0 + R^{-1}h(\eta) = -\frac{1}{a_p}+\frac{1}{2}r_p k^2 - P_p r_p^3 k^4 + \ldots \tag{3.6}$$

Here $R = \hbar^2/2mz_1z_2e^2$, $\eta = (2kR)^{-1}$, and $h(\eta)$ is a known function. As is shown in[17,27], for the calculation of the parameters a_p, r_p, P_p it is necessary to solve a system of equations analogous to (3.3). For example, the equation that holds for the scattering length $a_p(r)$ is

$$a_p'(r) = V(r)\,[rL_1(r/R) - a_p(r)\,H(r/R)]^2, \qquad a_p(0)=0. \tag{3.7}$$

The notations here are: $L_1(r/R) = (r/R)^{1/2}I_1[2(r/R)^{1/2}]$, $H_1(r/R) = 2(r/R)^{1/2}K_1[2(r/R)^{1/2}]$, where $I_1(x)$ and $K_1(x)$ are the Bessel functions of imaginary argument. The results of calculations[27] of $a_p(r)$, $r_p(r)$, and $P_p(r)$ for $^1S_0$ proton-proton scattering with the Hamada-Johnston potential are shown as dashed curves in Fig. 5. The calculations showed that the PFM, which allows us to take the Coulomb interaction into account exactly in nuclear scattering, is very convenient for numerical calculations.

3.3 Tensor Potential

The exact theory of the effective range for scattering by a tensor potential has been developed in the PFM in[26,27]. In the case of a short-range potential the expansions used are

$$\left.\begin{aligned}
\operatorname{tg}\bar\delta_{J,J-1}(r,k) &= -\frac{k^{2J-1}}{(2J-1)!!\,(2J-3)!!}\sum_{n=0}^{\infty}k^{2n}A_{Jn}(r),\\
\bar\varepsilon_J(r,k) &= -\frac{k^{2J+1}}{(2J+1)!!\,(2J-3)!!}\sum_{n=0}^{\infty}k^{2n}B_{Jn}(r),\\
\operatorname{tg}\bar\delta_{J,J+1}(r,k) &= -\frac{k^{2J+3}}{(2J+3)!!\,(2J+1)!!}\sum_{n=0}^{\infty}k^{2n}C_{Jn}(r).
\end{aligned}\right\} \tag{3.8}$$

From Eq. (2.33) there follow systems of coupled equations for each value of n. In particular, the equations for the first (n = 0) coefficients of the expansions (3.8) are

$$\left.\begin{aligned}
A'_{J0} &= \frac{1}{2J-1}V_{J,J-1}(r^J - A_{J0}r^{-J+1})^2 - 2T_J(r^J - A_{J0}r^{-J+1})\\
&\quad\times B_{J0}r^{-J-1} + (2J-1)V_{J,J+1}B_{J0}^2r^{-2J-2},\\
B'_{J0} &= \frac{1}{(2J-1)(2J+3)}T_J(r^J - A_{J0}r^{-J+1})(r^{J+2} - C_{J0}r^{-J-1})\\
&\quad + T_JB_{J0}^2r^{-2J} - \frac{1}{2J-1}V_{J,J-1}(r^J - A_{J0}r^{-J+1})B_{J0}r^{-J+1}\\
&\quad - \frac{1}{2J+3}V_{J,J+1}(r^{J+2} - C_{J0}r^{-J-1})B_{J0}r^{-J-1},\\
C'_{J0} &= \frac{1}{2J+3}V_{J,J+1}(r^{J+2} - C_{J0}r^{-J-1})^2 - 2T_J(r^{J+2} - C_{J0}r^{-J-1})\\
&\quad\times B_{J0}r^{-J+1} + (2J+3)V_{J,J-1}B_{J0}^2r^{-2J+2}.
\end{aligned}\right\} \tag{3.9}$$

In this case the scattering length for the $^3S_1$ state is the quantity $A_{1,0}(r)$. The relations (3.5) connect the other parameters for low-energy $^3S_1$ scattering with the other coefficients $A_{Jn}(r)$.

3.4 Regularization of the Equations in the Presence of Bound States

All of the equations given above for the coefficients of the low-energy expansions of the scattering phase shifts are valid only if the potential does not contain any bound states. Otherwise at some point r_1, at which the potential $V(r)\,\theta(r_1 - r)$ has a level with zero binding energy, the first coefficient $a_{l0}(r_1)$ and all the other $a_{ln}(r_1)$ become infinite. For $l = 0$ this corresponds to the well known fact that the scattering length is unbounded for resonance scattering at a level with zero binding energy.

In such cases it is necessary to reformulate Eqs. (3.2), (3.3), (3.7), and (3.9) in such a way that all of the quantities contained in them become finite. The first nonlinear equation is regularized if we set[5,12] $a_{l0}(r) = \tan\alpha_l(r)$. The equation for the function $\alpha_l(r)$ is

$$\alpha_l'(r) = \frac{1}{2l+1}V(r)\,[r^{l+1}\cos\alpha_l(r) - r^{-l}\sin\alpha_l(r)]^2, \alpha_l(0)=0. \tag{3.10}$$

For a tensor potential the regularization of (3.9) is achieved in an analogous way.[17,26]

The linear equations for the other coefficients $a_{ln}(r)$ in the case of a central potential, and the equations for the coefficients $A_{ln}(r)$, $B_{ln}(r)$, $C_{ln}(r)$ in the case of a tensor potential, can be regularized by

separating off the divergent terms.[17,27] In particular, this can be achieved by defining new functions which are the coefficients of negative powers of $\cos\alpha_l(r)$. For example, setting $a_{01}(r) = \beta_{01}(r)\cos^{-2}\alpha_0(r)$, we get an equation for the determination of $\beta_{01}(r)$ which contains no divergent terms

$$\beta'_{01} = -2\beta_{01}V(r\cos\alpha_0 - \sin\alpha_0)(\cos\alpha_0 + r\sin\alpha_0) - \frac{1}{3}r^2V(r^2\cos^2\alpha_0 - 4r\sin\alpha_0\cos\alpha_0 + 3\sin^2\alpha_0), \quad \beta_{01}(0) = 0. \tag{3.11}$$

The effective range is then $r_e(r) = 2\beta_{01}(r)/\sin^2\alpha_0(r)$. The equations for the case of a tensor potential can be regularized in an analogous way.

It is simplest, however, to use along with the system of equations for the functions $a_{ln}(r)$ a system for the inverse quantities $b_{ln}(r) = a^{-1}_{ln}(r)$, which can be obtained easily from (3.2), (3.3). In the range of r where $|a_{l0}(r)| > 1$, one is to change over to the integration of the system of equations for the functions $b_{ln}(r)$, and conversely, where $|b_{l0}(r)| > 1$ one can return to the first system.

4. APPROXIMATE METHODS

The phase-function method enables us to obtain besides the well known approximate methods a number of new approximate formulas for the calculation of phase shifts and other scattering parameters.

4.1 The Born and Modified-Born Approximations

As is well known, the Born approximation is applicable when $\operatorname{tg}\delta_l(k) \ll 1$. Therefore it is convenient to start with Eq. (2.23). Neglecting terms containing $\operatorname{tg}\delta_l(r, k)$ in the right member, we get the first term of the Born series

$$\operatorname{tg}\delta_l(r, k) = -\frac{1}{k}\int_0^r V(r')\,j_l^2(kr')\,dr'. \tag{4.1}$$

Substituting the value (4.1) in the right member of (2.23), we can find the next term of the Born approximation. Repeating this procedure, we get the whole perturbation-theory series.

We can, however, perform a partial summation of the perturbation-theory series if in (2.23) we keep the term linear in $\operatorname{tg}\delta_l(r)$ and solve the resulting equation exactly. We then get[8]

$$\operatorname{tg}\delta_l(r) = -\frac{1}{k}\int_0^r dr'V(r')\,j_l^2(kr') \times \exp\left\{\frac{2}{k}\int_{r'}^r dr''V(r'')\,j_l(kr'')\,n_l(kr'')\right\}. \tag{4.2}$$

The expression (4.2) is the first term of the modified-Born approximation. Substituting (4.2) in the term in (2.23) which is quadratic in $\operatorname{tg}\delta_l(r)$, and again solving a linear equation, we can get a new modified-perturbation-theory series.

Analogous approximate formulas are obtained for the partial scattering amplitude and the element of the S matrix if we start from Eqs. (2.24) and (2.25). A very detailed treatment of $S_l(r)$ with this sort of method has been made by Klar, Krüger, and Flügge.[41,42]

In the case of low-energy scattering the respective values given by the Born and modified-Born approximations for the scattering length defined by the first equation in (3.3) are[12]

$$a_0(r) = \int_0^r V(r')\,r'^2\,dr', \tag{4.3}$$

$$a_0(r) = \int_0^r dr'V(r')\,r'^2\exp\left[-2\int_{r'}^r r''V(r'')\,dr''\right]. \tag{4.4}$$

It is natural to suppose that the modified-perturbation-theory series will give a better approximation to the phase shift or the scattering length than the ordinary Born expansion, and will converge faster. This can be verified by means of Fig. 6, which shows the behavior of the exact solution for $a_0(r)$ and of the approximate solutions obtained from (4.3) and (4.4), for the case of the potential barrier $V(r) = \theta(2 - r)$.[12] The conclusion is the same if we compare the expansions of the expressions (4.3) and (4.4) with the expansion in terms of the coupling strength.[42] A number of approximate formulas for the special case of a singular potential have been derived by Calogero,[22,36] Calogero and Cassandro,[25] and Dombey.[37] It is not hard to make an analogous treatment for the more complicated cases in which there is a Coulomb potential or tensor forces, and for the case of relativistic scattering.

Instead of the basic functions $j_l(kr)$ and $n_l(kr)$ corresponding to free motion or the functions $F_l(kr, \eta)$ $G_l(kr, \eta)$ for the Coulomb potential, we may obviously choose any other system of functions corresponding to some part $V_1(r)$ of the potential. The approximate calculation of scattering phase shifts by using the remaining part $V(r) - V_1(r)$ of the potential then corresponds to the well known method of distorted waves in the theory of nuclear scattering.

Finally, let us consider the limiting case of large energies. In the nonrelativistic case this means

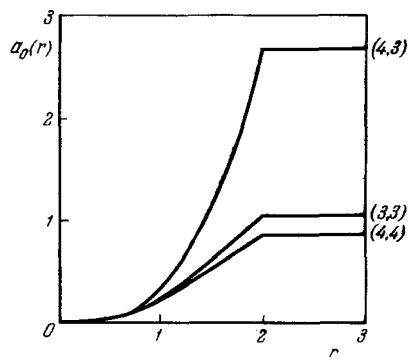

FIG. 6. The exact solution of Eq. (3.3) for the scattering length for a rectangular barrier, and the approximate solutions corresponding to Eqs. (4.3) and (4.4).

$k \to \infty$. It is not hard to see, by using the asymptotic expressions (1.4) for the Riccati-Bessel functions, that

$$\operatorname{tg}\delta_l(k) \to -\frac{m}{\hbar^2 k}\int_0^\infty V(r)\,dr \to 0. \qquad (4.5)$$

In the ultrarelativistic case, both for the scattering of bosons described by the Klein-Gordon equation (2.44) and for the scattering of Dirac particles, Eq. (2.47), a scalar potential makes a vanishingly small contribution (4.5) to the phase shift, as compared with a finite contribution from the fourth component of the vector potential, in particular, from the electrostatic potential ($l = j \pm 1/2$)

$$\operatorname{tg}\delta_l(k) \to -\frac{1}{\hbar c}\int_0^\infty e\varphi(r)\,dr, \qquad k \to \infty. \qquad (4.6)$$

The result (4.6) is due to the fact that the effective interaction (2.45) of a relativistic particle with the vector potential increases in proportion to the energy.

Equations (4.5) and (4.6) are of course valid only for nonsingular potentials. In other cases one must deal separately with a range of distances $r \lesssim 1/k$ near the origin, where the expansions (1.5) are legitimate. Then it can be shown[22] that the phase shift increases with the energy, but not faster than the first power of k. In the case of large energies one can also start from the modified Born approximation for the functions $S_l(r, k)$, sum all of the partial amplitudes, and obtain an analytic expression[42] for the total scattering amplitude $f(\theta)$.

4.2 The Quasiclassical Approximation

It has been shown in a paper by Dashen[15] that the PFM can be used to derive well known formulas of the quasiclassical approximation, under the condition

$$\frac{d}{dr}\ln\sqrt{E-\frac{\hbar^2 l(l+1)}{r^2}-V(r)} \ll 1. \qquad (4.7)$$

It is interesting to study the behavior of the phase shift δ_l of a given partial wave as a function of $\hbar$ for $\hbar \to 0$. Let us consider the case $l = 0$. We separate out the dependence on $\hbar$ explicitly and set $2m = E = 1$. Then Eq. (2.6) takes the form

$$\delta_0'(r, \hbar) = -\frac{1}{\hbar}V(r)\sin^2\left[\frac{r}{\hbar}+\delta_0(r, \hbar)\right], \quad \delta_0(0, \hbar) = 0. \qquad (4.8)$$

We note that the phases, which are odd functions of $k = \hbar^{-1}$, are odd functions of $\hbar$. Accordingly the phase shift $\delta_0(r, \hbar)$ can be looked for in the form of the expansion

$$\delta_0(r, \hbar) = \hbar^{-1}\alpha_0(r) + \hbar\alpha_1(r) + \hbar^3\alpha_2(r) + \ldots \qquad (4.9)$$

It can then be shown that for a potential regular at the point $r = 0$ the first two coefficients are given by

$$\alpha_0(\infty) = -\frac{1}{2}\int_0^\infty V(r)\,dr, \qquad (4.10)$$

$$\alpha_1(\infty) = -\frac{V'(0)}{[2-V(0)]^3}\exp\left[-\frac{V(0)}{2-V(0)}\right]. \qquad (4.11)$$

The expansion (4.9) is not the quasiclassical expansion, since the quantity fixed is l, and not the angular momentum $\hbar l$, which has a classical limit. It is of interest from the mathematical point of view. The expression (4.11) shows that the coefficients of the expansion of the phase shift in powers of the parameter $\hbar$ contain essential singularities with respect to the strength of the interaction. A similar result can be proved for the expansions of the phase shifts for $l > 0$.

4.3 Variational Methods

As has been shown by Spruch,[7] Calogero,[8,9,13,16] and Tietz,[38] new variational principles for the scattering phase shifts can be formulated in the framework of the PFM. In particular, it is found that the tangent of the phase shift is the stationary value of a functional[9]

$$\operatorname{tg}\delta_l(k) = \operatorname*{Stat}_{y_l}\left\{-\frac{1}{k}\int_0^\infty drV(r)\left[j_l(kr)-y_l(r)\,n_l(kr)\right]^2 \times \exp\left[\frac{2}{k}\int_r^\infty dr'V(r')\,n_l(kr')\left(j_l(kr')-y_l(r')\,n_l(kr')\right)\right]\right\} \qquad (4.12)$$

for variations of the function $y_l(r)$. The expression (4.12) can serve as the starting point for the derivation of approximate values of $\operatorname{tg}\delta_l(k)$. Knowing the potential V(r), owing to the intuitive meaning of the PF one can make a very accurate choice of the initial form of the test function $y_l(r)$. For example, by taking the test function $y_l(r) = 0$, we get the modified Born approximation (4.2).

If the potential is everywhere of the same sign, i.e., attractive or repulsive, variational principles[16] can be formulated for the maximum or the minimum of the functional (4.12). In this case the variational principle allows us to calculate an upper or lower limit on the phase shifts and their derivatives with respect to energy and angular momentum. Naturally analogous variational principles can be derived for Eqs. (2.24) and (2.25), for the calculation of the parameters for low-energy scattering, and for calculating the energies of bound states. Unlike the standard methods, the variational principles for the Riccati equation make it possible not only confidently to find a class of test functions, but also to estimate the sign and magnitude of the resulting error.

5. SOME GENERAL QUESTIONS OF THE THEORY OF POTENTIAL SCATTERING

By means of the phase-function method one can derive more simply and intuitively than usual not only well known theorems but also a number of new results in the theory of potential scattering. We shall demonstrate this with a number of examples.

5.1 Analytic Properties of the Partial Scattering Amplitudes

In papers by Calogero[14] and by Chadan and Guennegues[23] the PFM has been applied to the study of the analytic properties of partial scattering amplitudes. It has been shown[23] that Eq. (2.24) is very convenient for the direct analysis of the singularities of the partial amplitudes in the complex planes of the energy and the angular momentum. There is then no need to use such auxiliary quantities as the Yost functions. In[14] and[23] derivations have been found for all of the theorems of Regge and other authors on the meromorphic property of the scattering amplitudes in the region Re $l \leq -1/2$, their analytic behavior for $l \to \infty$, the complex regions of localization of the poles of the amplitudes, the kinematic cut which begins at k = 0, and possible dynamic cuts in the complex plane of the energy.

Another example of the application of the PFM to general problems of the theory is the study of the question of the convergence of the peratization method. This method has been proposed as a tool for work with nonrenormalizable field theories. Its analog in the nonrelativistic theory of potential scattering is the statement that the scattering phase shifts for a potential V(r) which is strongly singular at r = 0 can be obtained as the limiting values of the phase shifts for a regularized potential, in particular a potential $V(r)\,\theta(r-\epsilon)$ cut off at small distances, for $\epsilon \to 0$. When, for example, one considers the equation for the scattering length, Eq. (3.3), it can be shown that its solution $a_0(\infty, \epsilon, g)$ for the potential $V = g^2 r^{-4}\,\theta(r-\epsilon)$ is

$$a_0(\infty, \varepsilon, g) = g \operatorname{th}(g/\varepsilon), \qquad g > 0. \tag{5.1}$$

Accordingly, although the radius of convergence of the perturbation-theory series is equal to ϵ and goes to zero for $\epsilon \to 0$, $\lim a_0(\epsilon)$ exists and its value is $a_0 = g$ for the regularized potential.

5.2 The Number of Bound States in a Given Potential

Calogero has shown[30-32] that the phase-function method allows us to get new estimates of the number n of bound states in a given potential and to find simple conditions which determine a class of potentials which have at least one bound state with each of the angular momenta $l \leq L$. For this purpose one looks for poles of the solutions of the Riccati equation (3.2) for the function $a_{l_0}(r)$, which, as we have noted, correspond to bound states with zero binding energy. Under the condition that the potential V(r) is everywhere attractive, the number of poles determines the number of bound states. The results of the analysis are as follows[30]: an upper limit for nonsingular potentials is

$$n_l \leq n_0 \leq \frac{2}{\pi} \int_0^\infty dr\, |V(r)|^{1/2}, \qquad V'(r) \geq 0, \tag{5.2}$$

and a lower limit is

$$n_l \geqslant \left\{ \frac{1}{2} + \frac{1}{\pi} \int_0^\infty dr \min\left[q\,(qr)^{2l},\ -\frac{V(r)}{q}(qr)^{-2l} \right] \right\}. \tag{5.3}$$

Here $\{\}$ denotes the integer part of the expression, and min [A, B] has the value A for $A \leq B$ and the value B for $B \leq A$. The quantity q is an arbitrary constant with the dimension of inverse length. It follows from the conditions (5.2) and (5.3) that if g is the coupling constant of the potential the number of bound states cannot increase with g more rapidly than as the square root—i.e., asymptotically

$$n_l \sim \sqrt{g}\,. \tag{5.4}$$

As for the condition that there be bound states with $l \leq L$ contained in the potential V(r), it is of the form[31]

$$\int_0^\infty \frac{d(qr)\,|V(r)|}{(qr)^{2L} q^2 + (qr)^{-2L}\,|V(r)|} > 1. \tag{5.5}$$

For S states (L = 0), for example, this condition is satisfied by the Hulthén class of potentials

$$V(r) = -\frac{(1+\varepsilon)\,q^2}{e^{qr}-1}, \tag{5.6}$$

where $\epsilon > 0$, $q > 0$ are arbitrary constants.

As was already pointed out in Sdc. 2, the PFM gives an intuitive interpretation of Levinson's theorem on the connection between the scattering phase shift at zero energy and the number of bound states.[8]

5.3 The Inverse Problem of Scattering

The equations for the phase function [Eq. (2.5)] and for the other scattering parameters can be used to find potentials which lead to a given value of a parameter. For example, let the value of the scattering length be known to be A_0. Then, fixing on an arbitrary form of the function $a_0(r)$ which satisfies the boundary conditions* $a_0(0) = 0$, $a_0(\infty) = A_0$, we find from (3.3)

$$V(r) = \frac{a_0'(r)}{[r - a_0(r)]^2}. \tag{5.7}$$

For example, if

$$a_0(r) = A_0 r\,(r + A_0)^{-1},$$

then $V(r) = A_0^2 r^{-4}$.

The equations of the PFM also give the possibility of a new formulation of the problem of finding the potential V(r) if the dependence of a given phase $\delta_l(k)$ on the energy $E = k^2$ is known in the entire range $0 \leq k < \infty$. Let us write Eq. (2.23) in the form

$$\int_0^\infty V(r)\,K_l(r, k)\,dr = T_l(k). \tag{5.8}$$

Here $T_l(k) = k \tan \delta_l(k)$ is a known function, and the kernel of the integral equation,

*It is also necessary that for small r the derivative $a_0'(r)$ satisfy the conditions $-1 < a_0'(r) < 1$, which follows from (2.18) and (2.21).

$$K_l(r, k) = [j_l(kr) - t_l(r, k)\, n_l(r, k)]^2 \geq 0 \qquad (5.9)$$

is a functional of V(r). Equation (5.8) is the starting point of an iteration process for the determination of V(r), if we regard it as a Fredholm equation of the first kind with a known kernel. As the first step, having chosen a test function $V^{(0)}(r)$, we can determine from (2.23) an initial value $t^{(0)}(r, k)$ for the tangent of the phase shift, and substitute it in the kernel (5.9). With the resulting kernel $K^{(0)}(r, k)$ we solve Eq. (5.8) and find the next approximation for the potential, $V^{(1)}(r)$. Repeating this procedure a sufficient number of times, we arrive at the desired solution V(r). We can expect good convergence of the iteration process if the first approximation $V^{(0)}(r)$ is well chosen.

We note also that the PFM is very convenient in models of the type of the model with boundary conditions, in which the action of the unknown inner part of the potential is replaced by definite boundary conditions for the scattering phase shifts. These boundary conditions are then the initial conditions for Eqs. (2.5), (2.23), and so on.

6. CONCLUSION

As has been pointed out earlier, the new formalism of quantum mechanics described here has a number of advantages over the standard method of solving the Schrödinger equation. This is true of the numerical methods for calculating phase shifts and other scattering parameters and also of its use for general problems of the theory of potential scattering. The PFM is very convenient for the solution of problems of nuclear[29] and atomic[40] physics.

The exposition has been arranged so as on one hand to show the starting points of the method, and on the other hand to give the main equations and results in a form suitable for direct practical use. All more complicated or specialized questions have been dealt with very briefly, in view of the fact that the details are contained in the original papers.

It must be emphasized that a number of problems still await their solutions. For example, as yet no analog to the equation for the phase function has been constructed for the total scattering amplitude for an arbitrary potential. It would be interesting to treat in the framework of the PFM problems of three or more bodies, as well as the two-body problem. There has also been no study from this point of view of the case of a time-dependent potential.

In conclusion we note that a series of papers by Calogero, beginning with a major article,[8] has contributed greatly to the development of the PFM.

Note added in proof. Professor F. Calogero has informed us that his book devoted to the phase-function method will soon be published by Academic Press, Inc., New York.

[1] P. M. Morse and W. P. Allis, Phys. Rev. 44, 269 (1933).

[2] G. F. Drukarev, JETP 19, 247 (1949). G. F. Drukarev, Teoriya stolknoveniĭ élektronov s atomami (Theory of Collisions of Electrons with Atoms), Moscow, Fizmatgiz, 1963, page 37.

[3] O. Bergmann, Acta Phys. Austriaca 4, 62 (1950).

[4] P. O. Olsson, Ark. Fys. 4, 217 (1952).

[5] G. I. Kynch, Proc. Phys. Soc. A65, 83, 94 (1952).

[6] S. Franchetti, Nuovo Cimento 6, 601 (1957).

[7] L. Spruch, in "Lectures in Theoretical Physics", vol. 4, ed. W. E. Brittin, B. W. Downs and I. Downs, Intern. Publ. Inc., N. Y., 1962.

[8] F. Calogero, Nuovo Cimento 27, 261 (1963).

[9] F. Calogero, Nuovo Cimento 27, 947 (1963).

[10] F. Calogero, Nuovo Cimento 27, 1007 (1963).

[11] B. R. Levy and J. B. Keller, J. Math. Phys. 4, 54 (1963).

[12] R. F. Dashen, J. Math. Phys. 4, 338 (1963).

[13] F. Calogero, J. Math. Phys. 4, 427 (1963).

[14] F. Calogero, Nuovo Cimento 28, 66 (1963).

[15] R. F. Dashen, Nuovo Cimento 28, 229 (1963).

[16] F. Calogero, Nuovo Cimento 28, 320 (1963).

[17] V. V. Babikov, Nekotorye metody vychisleniya parametrov potentsial'-nogo rasseyaniya (Some Methods for Calculating the Parameters of Potential Scattering), OIYaI, R-1728, Dubna, 1964.

[18] F. Calogero and D. G. Ravenhall, Nuovo Cimento 32, 1755 (1964).

[19] F. Calogero, Nuovo Cimento 33, 352 (1964).

[20] Ch. Zemach, Nuovo Cimento 33, 939 (1964).

[21] T. F. O'Malley, Phys. Rev. 134, A1188 (1964).

[22] F. Calogero, Phys. Rev. 135, B693 (1964).

[23] K. Chadan and J. Y. Guennegues, Nuovo Cimento 34, 665 (1964).

[24] A. Degasperis, Nuovo Cimento 34, 1667 (1964).

[25] F. Calogero and M. Cassandro, Nuovo Cimento 34, 1712 (1964).

[26] V. V. Babikov, YaF 1, 360 (1965), Soviet JNP 1, 261 (1965).

[27] V. V. Babikov, YaF 1, 793 (1965), Soviet JNP 1, 567 (1965).

[28] V. V. Babikov, YaF 1, 984 (1965), Soviet JNP 1, 701 (1965).

[29] V. V. Babikov, Materialy Soveshchaniya po matematicheckim metodam resheniya zadach yadernoĭ fiziki (Proceedings of Conference on Mathematical Methods for Solving Problems of Nuclear Physics), OIYaI, 2005, Dubna, 1965, page 28.

[30] F. Calogero, Commun. Math. Phys. 1, 80 (1965).

[31] F. Calogero, J. Math. Phys. 6, 161, 1105 (1965).

[32] F. Calogero, Nuovo Cimento 36, 199 (1965).

[33] T. Tietz, Nuovo Cimento 35, 308 (1965).

[34] J. R. Cox and A. Perlmutter, Nuovo Cimento 37, 76 (1965).

[35] J. R. Cox, Nuovo Cimento 37, 474 (1965).

[36] F. Calogero, Nuovo Cimento 37, 756 (1965).

[37] N. Dombey, Nuovo Cimento 37, 1743 (1965).
[38] T. Tietz, Nuovo Cimento 37, 1774 (1965).
[39] B. H. J. McKellar and R. M. May, Nucl. Phys. 65, 289 (1965).
[40] T. F. O'Malley, Phys. Rev. 137, A1668 (1965).
[41] H. Klar and H. Krüger, Z. Phys. 191, 409 (1966).
[42] S. Flügge, H. Klar, and H. Krüger, Z. Phys. 191, 417 (1966).

Translated by W. H. Furry