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Integral equations and scattering solutions for a square-well potential

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s-wave scattering solutions of the Schrödinger equation with an arbitrary central local potential are considered. Green's functions and integral equations are derived for scattering solutions subject to a variety of boundary conditions. Exact solutions are obtained for the case of a finite spherical square-well potential, and properties of these solutions are discussed.

I. INTRODUCTION

Whitten and McCormick¹ have emphasized the desirability of introducing the Green's function as early as possible in the physics curriculum. Using the variation of parameters method they have provided an excellent introduction to this topic. Recently this method has been extended by Byrd,² who has derived formulas for the Green's function corresponding to one- and two-point boundary conditions. In the present work we show that the Green's function method can be easily applied to convert the radial Schrödinger equation (a second-order differential equation) into an integral equation whose solution satisfies the imposed boundary conditions. We then consider the specific boundary conditions which lead to the integral equations for the regular, Jost and physical s-wave scattering solutions.3 Exact solutions to these integral equations are obtained for an attractive square-well potential. In most quantum-mechanics text books,4 the square-well potential is solved only to the extent that an expression for the phase shift is deduced. This is done by matching solutions at the edge of the potential. Scattering solutions such as the regular solution, the Jost solutions, and the physical wave solutions are rarely mentioned. A discussion of even one of these solutions is not common. Using the Green's function approach these solutions are obtained without any matching and the phase shift follows by examining the asymptotic behavior of any of these solutions. In addition, relationships between the various solutions and expressions for the T and S matrices are easily obtained. This introduction to the derivation of these important scattering solutions will also provide some insights regarding the boundary conditions.

In Sec. II we derive the proper Green's functions and set up the integral equations for the different solutions. In Sec. III we obtain exact solutions to the integral equations for a square-well potential. In Sec. IV we study the asymptotic forms of the solutions. Throughout this work we assume positive energy (E > 0) and zero orbital angular momentum (I = 0).

II. BOUNDARY CONDITIONS AND INTEGRAL EQUATIONS

As mentioned earlier, Byrd² has extended the work of Whitten and McCormick¹ to obtain specific formulas for the Green's function for one- and two-point boundary conditions. In this section we review his formulas and derive integral equations for the regular, Jost and physical solutions³ for a central local potential V(r).

Following Byrd,² a particular solution $u_p(r)$ of the equation

$$u''(r) + p(r)u'(r) + q(r)u(r) = R(r), \tag{1}$$

may be expressed for a single-point (r_0) initial condition as

$$u_p(r) = \int_{r_0}^r G_S(r, r') R(r') dr'$$
 (2a)

and for two-point (a and b) boundary conditions as

$$u_p(r) = \int_a^b G_T(r, r') R(r') dr', \qquad (2b)$$

where the subscripts S and T refer to single- and two-point conditions. The Green's functions $G_S(r,r')$ and $G_T(r,r')$ are obtained by using two different methods. If $u_1(r)$ and $u_2(r)$ are any two linearly independent solutions of the homogeneous equation associated with Eq. (1), then

$$G_S(r,r') = \frac{u_1(r')u_2(r) - u_1(r)u_2(r')}{W},$$
 (3)

where W is the Wronskian of $u_1(r)$ and $u_2(r)$, and is independent of r.

The complete solution to Eq. (1) may be written

$$u(r) = Au_1(r) + Bu_2(r) + u_p(r).$$
 (4)

The initial boundary condition is imposed on u(r) to determine the constants A and B.

For the two-point boundary conditions,

$$G_T(r,r') = \begin{cases} u_1(r')u_2(r)/W, & a \le r' \le r \\ u_1(r)u_2(r')/W, & r \le r' \le b. \end{cases}$$
 (5)

In this case, however, any two linearly independent solutions (of the homogeneous equation) will not do. If the boundary conditions at a and b are written

$$C_1u(a) + D_1u'(a) = U_a.$$

and

$$C_2 u(b) + D_2 u'(b) = U_b \tag{6}$$

[this form of boundary condition is referred to as unmixed (in a and b)] then u_1 and u_2 are to be selected to satisfy similar equations, namely

$$C_1 u_1(a) + D_1 u_1'(a) = 0,$$

and

$$C_2 u_2(b) + D_2 u_2'(b) = 0.$$
 (7)

The general solution is again of the form (4), with the proviso that u_1 and u_2 satisfy Eq. (7) and that A and B are selected to satisfy the boundary conditions (6).

We illustrate an application of the above results by

considering various solutions to the differential equation

$$u''(r) + k^2 u(r) = v(r)u(r), \tag{8}$$

This equation, which is a special case of Eq. (1) with p =0 and $q = k^2$, is the Schrödinger equation for the zero orbital angular momentum radial wave function.5 The square of the wave number is proportional to the center of mass energy, that is, $k^2\hbar^2 = 2\mu E$ and $v(r) = (2\mu/\hbar^2)V(r)$, where V(r) is the potential energy and μ is the reduced mass.

A. Regular solution $\varphi(k,r)$

The regular solution is defined as the solution of Eq. (8) that satisfies the following conditions³ at the origin,

$$\varphi(k,0) = 0 \text{ and } \varphi'(k,0) = 1. \tag{9}$$

The two linearly independent homogeneous solutions can be taken as $u_1(r) = \sin kr$ and $u_2(r) = \cos kr$. Then using Eq. (3) we find

$$G_S(r,r') = k^{-1}\sin k(r-r').$$
 (10)

Finally imposing conditions (9) on the form (4) we get

$$\varphi(k,r) = k^{-1} \sin kr$$

$$+ k^{-1} \int_0^r \sin k(r - r') v(r') \varphi(k, r') dr'.$$
 (11)

B. Jost solutions $f^{\pm}(k,r)$

These solutions are defined by boundary conditions imposed at infinity. They are also called irregular solutions since they are not regular at r = 0. $f^+(k,r)$ and $f^-(k,r)$ are linearly independent except for k = 0. The boundary conditions are3

$$\lim_{r \to \infty} e^{\pm ikr} f^{\pm}(k,r) = 1 \tag{12a}$$

and

$$\lim_{r \to \infty} e^{\pm ikr} f^{\pm \prime}(k,r) = \pm ik. \tag{12b}$$

The condition (12b) is not usually seen, but is to be understood when only (12a) is written. Choosing any two linearly independent solutions to Eq. (8) leads (as it should) to the same single-point Green's function as before, Eq. (10). Imposing the boundary condition (12) we find after interchange of the limits.

$$f^{\pm}(k,r) = e^{\pm ikr} - k^{-1} \int_{r}^{\infty} \sin k(r - r')v(r')f^{\pm}(k,r')dr'.$$
 (13)

C. Physical solutions $\psi^{\pm}(k,r)$

The physical solutions are defined to be zero at the origin and to have a specific asymptotic form at infinity. There are many equivalent asymptotic forms that are encountered when studying the physical solution. The three standard forms are [to avoid confusion we deal with $\psi^+(k,r)$ only

$$\lim_{r \to \infty} \psi^{+}(k,r) \to (i/2)[e^{-ikr} - S(k)e^{ikr}] \quad (14a)$$

$$\rightarrow \sin kr + T(k)e^{ikr}$$
 (14b)

$$\rightarrow e^{i\delta}\sin(kr+\delta), \tag{14c}$$

where the functions S(k), T(k), and $\delta(k)$ are referred to as the S matrix, T matrix, and phase shift, respectively. However, to illustrate the boundary conditions (6) it is more convenient to use the following form:

$$\lim_{r \to \infty} e^{ikr} [\psi^{+}(k,r) + ik^{-1}\psi^{+\prime}(k,r)] = i.$$
 (15)

By substitution it is easily seen that each form of Eq. (14) satisfies Eq. (15). The boundary condition at the origin u(0)= 0 can be expressed in the notation of Eq. (6) by choosing $C_1 = 1$, $D_1 = 0$, and $U_a = 0$. One of the appropriate homogeneous solutions is then obtained according to Eq. (7) with the above values of C_1 and D_1 by the condition

$$u_1(0) = 0, (16a)$$

which is satisfied by choosing $u_1(r) = \sin kr$. The other suitable solution $u_2(r)$ must satisfy Eq. (7) in the form $C_2 u_2(\infty) + D_2 u_2'(\infty) = 0$. The ratio of D_2/C_2 is determined from a comparison of Eqs. (6) and (15) to have the value i/k. Thus u_2 must satisfy the equation

$$u_2(\infty) + ik^{-1}u_2'(\infty) = 0,$$
 (16b)

which is satisfied by choosing $u_2(r) = e^{ikr}$. Substituting $u_1(r)$ and $u_2(r)$ into Eq. (5) for the Green's function gives

$$G_T(r,r') = \begin{cases} -k^{-1} \sin kr' e^{ikr}, & 0 \le r' \le r \\ -k^{-1} e^{ikr'} \sin kr, & r \le r' \le \infty \end{cases}$$
(17)

The constants A and B in the general solution Eq. (4) are easily evaluated. The boundary condition at the origin requires B = 0 and the condition at infinity, Eq. (4) requires A = 1. The complete solution is then

$$\psi^{+}(k,r) = \sin kr$$

$$-k^{-1}e^{ikr} \int_{0}^{r} \sin kr'v(r')\psi^{+}(k,r')dr'$$

$$-k^{-1}\sin kr \int_{0}^{\infty} e^{ikr'}v(r')\psi^{+}(k,r')dr'. \quad (18)$$

Similarly for $\psi^-(k,r)$ with Eq. (15) replaced by $\lim_{r\to\infty} e^{-ikr} [\psi^-(r) - ik^{-1}\psi^-(r)'] = -i$ we find

$$\psi^{-}(k,r) = \sin kr - k^{-1}e^{-ikr} \int_{0}^{r} \sin kr'v(r')\psi^{-}(k,r')dr' - k^{-1}\sin kr \int_{0}^{\infty} e^{-ikr'}v(r')\psi^{-}(k,r')dr'.$$
 (19)

III. SOLUTIONS FOR A SQUARE-WELL POTENTIAL

In this section we solve the Eqs. (11), (13), and (18) for a square-well potential defined by

$$v(r) = -v_{0}, \quad r \le a$$

= 0, $r > a$. (20)

Any solution for the square-well potential can now be written

$$u(r) = u_1(r)\theta(a-r) + u_2(r)\theta(r-a),$$
 (21)

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where θ is a step function defined by

$$\theta(r - r') = 1 \quad r > r'$$

$$= \frac{1}{2} \quad r = r'$$

$$= 0, \quad r < r'.$$
(22)

Using for u(r) in Eq. (21) the desired functions φ , f^{\pm} , and ψ^{\pm} we can write down the integral equations for each of the solutions.

A. Regular solution $\varphi(k,r)$

Writing

$$\varphi(k,r) = \varphi_1(k,r)\theta(a-r) + \varphi_2(k,r)\theta(r-a), \quad (23)$$

and using Eq. (20) in (11) we get two equations,

$$\varphi_1(k,r) = k^{-1} \sin kr$$

$$-\frac{v_0}{k} \int_0^r \sin k(r-r') \varphi_1(k,r') dr', \quad (24a)$$

and

 $\varphi_2(k,r) = k^{-1} \sin kr$

$$-\frac{v_0}{k} \int_0^a \sin k(r-r')\varphi_1(k,r')dr'. \quad (24b)$$

Since Eq. (24a) is a Voltérra equation, the solution is difficult to obtain. However, from the differential equation for region one we can immediately infer that in order to satisfy the initial conditions, Eq. (9), the solution must be of the form

$$\varphi_1(k,r) = k_0^{-1} \sin k_0 r. \tag{25}$$

Substituting Eq. (25) in (24a), we see that for Eq. (25) to be a solution

$$k_0^2 = k^2 + v_0. (26)$$

Next we substitute Eq. (25) in (24b) and get

$$\varphi_2(k,r) = A_2 \sin kr + B_2 \cos kr, \tag{27}$$

where

$$A_2 = \frac{1}{kk_0} (k \sin ka \sin k_0 a + k_0 \cos ka \cos k_0 a), \quad (28a)$$

and

$$B_2 = \frac{1}{kk_0} (k \sin k_0 a \cos k a - k_0 \sin k a \cos k_0 a).$$
 (28b)

It is interesting to note that solutions φ_1 and φ_2 automatically satisfy the usual matching conditions at r = a, $\varphi_1(k,a) = \varphi_2(k,a)$, and $\varphi_1(k,a) = \varphi_2(k,a)$.

B. Jost solutions $f^{\pm}(k,r)$

Writing

$$f^{+}(k,r) = f_{1}^{+}(k,r)\theta(a-r) + f_{2}^{+}(k,r)\theta(r-a), \quad (29)$$

Eq. (13) can be reduced to

$$f_1^+(k,r) = e^{ikr} + \frac{v_o}{k} \int_r^a \sin k(r - r') f_1^+(k,r') dr'$$
 (30a)

and

$$f_2^+(k,r) = e^{ikr}$$
. (30b)

To solve Eq. (30a) we assume

$$f_1^+(k,r) = A_1 e^{ik_0 r} + B_1 e^{-ik_0 r}. (31)$$

Since the boundary conditions, Eq. (12), are imposed not at the origin but at infinity, where they are satisfied by f_2^+ , Eq. (30b), we must use two unknown constants A and B for f_1^+ . Substituting Eq. (31) in (30a) and setting to zero the coefficient of $e^{\pm ik_0 r}$, we get

$$k_0^2 = k^2 + v_0 \tag{32}$$

as expected. Setting to zero the coefficient of $e^{\pm ikr}$, we get

$$A_1 = [(k_0 + k)/2k_0] e^{-i(k_0 - k)a}$$
(33)

and

$$B_1 = [(k_0 - k)/2k_0]e^{i(k_0 + k)a}.$$
 (34)

A similar procedure for $f^-(k,r)$ leads to the result

$$f^{-}(k,r) = f^{+}(k,r)^{*},$$
 (35)

where the asterisk denotes complex conjugation.

C. Physical solution $\psi^{\pm}(k,r)$

If ψ^+ is written

$$\psi^{+}(k,r) = \psi_{1}^{+}(k,r)\theta(a-r) + \psi_{2}^{+}(k,r)\theta(r-a), \quad (36)$$

Eq. (18) becomes

$$\psi_1^+(k,r) = \sin kr$$

$$+\frac{v_0}{k}e^{ikr}\int_0^r \sin kr' \psi_1^+(k,r')dr'$$
$$+\frac{v_0}{k}\sin kr\int_r^a e^{ikr'} \psi_1^+(k,r')dr' \qquad (37a)$$

and

$$\psi_2^+(k,r) = \sin kr$$

$$+\frac{v_0}{k}e^{ikr}\int_0^a \sin kr'\psi_1^+(k,r')dr'. \quad (37b)$$

To solve Eq. (37a) we note from Eq. (16a) the condition $\psi_1^+(k,0) = 0$ and therefore try

$$\psi_1^+ = C \sin k_0 r. \tag{38}$$

Again setting to zero the coefficients of $e^{\pm ik_0r}$ we get $k_0^2 = k^2 + v_0$, and doing the same for the coefficients of $e^{\pm ikr}$ we get

$$C = 2k[(k_0 - k)e^{i(k_0 + k)a} + (k_0 + k)e^{-i(k_0 - k)a}]^{-1}.$$
 (39)

Substituting Eq. (38) into (37b) we find

 $\psi_2^+(k,r) = \sin kr$

$$-\frac{2(k_0 \sin ka \cos k_0 a - k \cos ka \sin k_0 a)}{(k_0 - k)e^{i(k_0 + k)a} + (k_0 + k)e^{-i(k_0 - k)a}} \times e^{ikr}.$$
(40)

Similar for ψ^- using Eq. (19) we find

$$\psi^{-}(k,r) = \psi^{+}(k,r)^{*}, \tag{41}$$

which completes our list of solutions.

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IV. ASYMPTOTIC FORMS OF SOLUTIONS AND PHASE SHIFT

In this section we discuss the asymptotic behavior of $\varphi(k,r)$ and $\psi^+(k,r)$ at infinity and of $f^+(k,r)$ at the origin, and extract an expression for phase shift. We show that the expression for the phase shift is the same for the three cases. We also derive expressions for the S matrix and T matrix in terms of the phase shift.

Using Eq. (27) we can write for r > a,

$$\varphi(k,r) = \varphi_2(k,r) = R\sin(kr + \delta), \tag{42}$$

where

$$\tan\delta = \frac{k \tan k_0 a - k_0 \tan k a}{k_0 + k \tan k a \tan k_0 a} \tag{43}$$

and

$$R = \frac{1}{kk_0} (k_0^2 \cos^2 k_0 a + k^2 \sin^2 k_0 a)^{1/2}.$$
 (44)

With some manipulation and using

$$\tan(\alpha + \beta) = \frac{\tan\alpha + \tan\beta}{1 - \tan\alpha \tan\beta},$$

we obtain the familiar result,8

$$\delta = -ka + \tan^{-1}[(k/k_0)\tan k_0 a]. \tag{45}$$

The phase shift can also be determined from the Jost solutions. However, for the Jost solutions the incoming plane wave is at $r = \infty$ and therefore the phase shift can be found from the (asymptotic) behavior at r = 0. From Eq. (31), (33), and (34) we have for r = 0,

$$f^{+}(k,0) = f_{1}^{+}(k,0)$$

$$= \frac{1}{2k_{0}} [(k_{0} + k)e^{-i(k_{0} - k)a} + (k_{0} - k)e^{i(k_{0} + k)a}]$$

$$= \frac{1}{k_{0}} [(k_{0}\cos ka\cos k_{0}a + k\sin ka\sin k_{0}a) + i(k_{0}\sin ka\cos k_{0}a - k\cos ka\sin k_{0}a)]. \tag{46}$$

This function, the Jost solution evaluated at r = 0, is called the Jost function.³

Equation (46) is standardly written in polar form³ to exhibit the phase shift δ ,

$$f^{+}(k,0) = |f^{+}(k,0)|e^{-i\delta}. \tag{47}$$

where clearly

$$\tan \delta = -\operatorname{Im} f^{+}(k,0)/\operatorname{Re} f^{+}(k,0),$$
 (48)

where Re and Im refer to the real and imaginary parts, respectively. With the aid of Eq. (46), Eq. (48) can be shown to be identical to Eq. (43) confirming that the solutions $\varphi(k,r)$ and $f^+(k,r)$ lead to the same phase shift. Alternatively we could have used $f^-(k,0)$ to write

$$f^{-}(k,0) = |f^{-}(k,0)|e^{i\delta}$$
 (49)

and, from Eq. (35), $|f^-(k,0)| = |f^+(k,0)|$. The sign of the phase in Eq. (47) is the result of the use of Newton's boundary conditions which are now standard but are dif-

ferent from the boundary conditions originally introduced by Jost, as mentioned in Ref. 3.

With the aid of Eq. (46) we can see from Eq. (44) that $R = k^{-1}|f^+(k,0)|$, and thus Eq. (42) becomes, for r > a.

$$\varphi(k,r) = k^{-1} |f^{+}(k,0)| \sin(kr + \delta). \tag{50}$$

To get an expression for the phase shift from the asymptotic behavior of the physical solution $\psi^+(k,r)$ it is convenient to first express $\psi^+(k,r)$ in terms of $\varphi(k,r)$. Using Eqs. (25), (27), (38), (39), (40), and (46) and after some manipulation we find

$$\psi^{+}(k,r) = k\varphi(k,r)/f^{+}(k,0). \tag{51}$$

This is the standard relation between $\psi^+(k,r)$ and $\varphi(k,r)$. Using Eqs. (47) and (50) we easily deduce the form of $\psi^+(k,r)$ at r > a,

$$\psi^{+}(k,r) = \frac{kk^{-1}|f^{+}(k,0)|\sin(kr+\delta)}{|f^{+}(k,0)|e^{-i\delta}}
= e^{i\delta}\sin(kr+\delta),$$
(52)

which is in agreement with the boundary condition, Eq. (14c).

It is customary to express the boundary condition for $\psi^+(k,r)$ at infinity in terms of the T matrix [see Eq. (14b)] or the S matrix [see Eq. (14a)]. Thus we can also obtain solutions for these functions. From Eqs. (14b), (40), and (46) we find that

$$T(k) = -\frac{k_0 \sin ka \cos k_0 a - k \cos ka \sin k_0 a}{k_0 f^+(k, 0)}$$
$$= -\frac{\text{Im} f^+(k, 0)}{f^+(k, 0)},$$

Since $\sin \delta = -\text{Im} f^+(k,0)/|f^+(k,0)|$ the expression for T(k) can be rewritten in the more familiar form,⁹

$$T(k) = e^{i\delta} \sin\delta. \tag{53}$$

Similarly putting Eq. (40) in the form of Eq. (14a) we arrive at the standard result⁹ for the S matrix

$$S(k) = e^{2i\delta}. (54)$$

Finally, by comparing Eqs. (53) and (54) we obtain the usual relation between S and T as

$$S = 1 + 2iT. \tag{55}$$

V. CONCLUSIONS

In this paper we have introduced the Green's function appropriate to different solutions and have shown how the phase shift, T matrix, and S matrix can be derived from these solutions. In order to illustrate the ideas most simply we limited ourselves to the s-wave analysis of an attractive square-well potential, its solutions being very well known. Obtaining the solutions to the above-mentioned integral equations involves some integration and is therefore (for the square well) more difficult than the familiar algebraic method of solution, which involves matching by invoking the continuity of the solution and its derivative at r = a. Nevertheless we feel that an introduction to the Green's function integral equation approach is important for several reasons: (i) matching may not be an available alternative, (ii) advanced treatments^{3,10} of scattering theory emphasize

the Green's function approach, (iii) the integral equation formulation is a very convenient starting point for the introduction of approximations, ¹¹ e.g., the familiar Born approximation where the wave function to be integrated is replaced by its plane wave counterpart, and (iv) in the study of nonlocal potentials ¹² the radial Schrödinger equation is an integrodifferential equation and the integral equation approach is more natural.

Solutions for l > 0 can be obtained in exactly the same manner as for l = 0 except that the presence of $l(l+1)/r^2$ term in Eq. (9) introduces spherical Bessel and Neumann functions in place of the sine and cosine functions encountered for l = 0. Although we have assumed E > 0 in this work the negative energy or bound state problem can be equally easily handled by this approach (this will be reported in a forthcoming communication).

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