Recursive analytical formula for the Green's function of a Hamiltonian having a sum of one-dimensional arbitrary delta-function potentials

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The Green's functions of one-dimensional Hamiltonians containing, respectively, one and two delta-function potentials are derived by analytically summing over the corresponding Lippmann-Schwinger series. A generalization of this procedure leads to an explicit recursive formula for the Green's function $G^{(n+1)}$ corresponding to a Hamiltonian containing a sum of $n+1$ delta-function potentials of arbitrary positions and strengths in terms of $G^{(n)}$ and the additional $n+1$ delta-function potential parameters.

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I. INTRODUCTION

Delta-function potentials serve both as feasible representations of physical potentials in various contexts and as useful paradigms for the solution of quantum-mechanical problems. Given the solvability feature of these potentials in many cases, relevant information can be obtained[1] about other potentials that are approximated by these but otherwise unsolvable. Delta-function potentials are also helpful in areas as varied as condensed-matter physics to simulate, for example, scatterers in electronic transport, to describe periodic potentials as in the Kronig-Penney model,[2] and in nuclear physics, for example, to model short-range potentials[3] or optical potentials.[4] Many of these problems can be usefully reduced to one-dimensional problems. In particular, the delta-function potential

$$U(x)=\sum_i V_i=\sum_i U_i\delta(x-a_i), \tag{1}$$

formed of a series of V_i representing delta-potentials of strength U_i and located at a_i, has the advantage that it can be solved analytically, albeit with rather complicated expressions.[5,6] Thus, one possible application of the potential $U(x)$ lies in modeling other potentials. Indeed, a local potential can be expressed as a sum of delta-function contributions

$$V(x)=\int dx'\,\delta(x-x')V(x'). \tag{2}$$

By making an adequate approximation

$$V(x)\approx\sum_i U_i\delta(x-a_i), \tag{3}$$

we find that this could serve as an approximative method for the calculation of the wave function or the Green's function for any potential, using the solvability property of the potential in Eq. (1), and provided the method is relatively simple.

In this report we find a recursive formula for the Green's function G of the Hamiltonian

$$H'=\frac{p^2}{2m}+U, \tag{4}$$

with U given Eq. (1), which can serve the purpose of simplifying the calculation of G. We shall arrive at it in the next section by first analyzing the Green's function for U terms with one- and two-delta potentials, and for which we obtain explicit expressions. In the last section we shall discuss some implications of this formula, with regard to physical problems.

II. GREEN'S FUNCTION FOR ONE-, TWO- AND MANY-DELTA POTENTIALS

The Green's function $G(E)$ for a given Hamiltonian H, with argument E satisfies

$$(E-H)G=1 \quad \text{and} \quad G(E-H)=1, \tag{5}$$

and it contains information on the solutions of the Schrödinger equation. In particular, by choosing G with the adequate boundary conditions, one can obtain from it the scattering wave function, and the on-shell and off-shell scattering matrix; the T matrix, proportional to the latter, can be obtained from

$$T=V+VGV. \tag{6}$$

In the task of calculating G we start by considering the Green's function for a free particle with Hamiltonian $H_0=p^2/2m$

$$G_{0\pm}(E)=\frac{1}{E-H_0\pm i\epsilon}, \tag{7}$$

where the energy argument is $E=k^2/2m$ and the $+$ or $-$ indexes refer, respectively, to advanced or retarded Green's functions. $G_{0\pm}$ is diagonal in momentum space and is interpreted as a free particle propagator. From here on we shall concentrate on the advanced Green's functions $G_0\equiv G_{0+}$, while similar manipulations can be carried out for the other type of resolvent.

The representation of the matrix elements of the Green's function for H' in Eq. (4) in configuration space shall prove useful. The corresponding expression for $G_0(E)$ is given by

$$\langle x'|G_0|x\rangle=\frac{-im}{k}e^{ik|x'-x|}, \tag{8}$$

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where we use plane wave functions with normalization taken to be

$$\psi = e^{ikx}. \tag{9}$$

The presence of an interaction modifies the function in Eq. (8) and the Green's function with an interacting Hamiltonian $H = H_0 + V$

$$G(E) = \frac{1}{E - H + i\epsilon}, \tag{10}$$

now satisfies the Lippmann-Schwinger equation

$$G = G_0 + G_0 V G. \tag{11}$$

Eq. (11) is an integral equation for which a perturbative series expression can be arrived at by substituting the intial approximation $G \approx G_0$ on the right-hand side term of G, and successively repeating this process for the obtained G on the left-hand side. This gives rise to the series

$$G = G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \ldots. \tag{12}$$

A. One-delta potential

The analysis of the first terms of the series in Eq. (12) can lead to interesting information on its general form as in other applications.[7] In the case of the Hamiltonian $H_1 = p^2/2m + V_1$ with $V_1 = U_1 \delta(x - a_1)$ the series for the corresponding Green's function

$$G^{(1)} = G_0 + G_0 V_1 G_0 + G_0 V_1 G_0 V_1 G_0 + , \ldots, \tag{13}$$

gives rise to a geometric series that can be summed into an exact expression. The origin of this simplification is in the fact that the delta potentials separate the internal terms in Eq. (13) and convert them into numbers. For example, by carrying out the integration over the internal coordinates, the first-order term in V_1 becomes

$$\begin{aligned} \langle x'|G_0 V_1 G_0|x\rangle &= U_1 \left(\frac{-im}{k}\right)^2 \int dx'' e^{ik|x' - x''|} \\ &\quad \times \delta(x'' - a_1) e^{ik|x'' - x|}, \\ &= U_1 \left(\frac{-im}{k}\right)^2 e^{ik|x' - a_1|} e^{ik|a_1 - x|}, \end{aligned} \tag{14}$$

while the second-order term in V_1 can be similarly obtained and is

$$\langle x'|G_0 V_1 G_0 V_1 G_0|x\rangle = U_1^2 \left(\frac{-im}{k}\right)^3 e^{ik|x' - a_1|} e^{ik|a_1 - x|}. \tag{15}$$

In general, by performing the integral over the internal coordinates of terms in the series (13) of the form $\ldots V_1 G_0 V_1 \ldots$, they lose their coordinate dependence and become constants. The series obtained for $\langle x'|G^{(1)}|x\rangle$ transforms into a geometric series $1/(1-c) = 1 + c + c^2 + c^3 + \ldots$, whose sum gives

$$\begin{aligned} \langle x'|G^{(1)}|x\rangle &= \left(\frac{-im}{k}\right) e^{ik|x' - x|} \\ &\quad + \frac{\left(\frac{-im}{k}\right)^2 U_1 e^{ik|x' - a_1|} e^{ik|a_1 - x|}}{1 + \frac{im}{k} U_1}. \end{aligned} \tag{16}$$

Similar sums can be obtained for the scattering matrix,[8] using Eq. (6).

B. Two-delta potential

Modified Lippmann-Schwinger series can be constructed by separating the Hamiltonian in various ways.[9] For the case of the Green's function $G^{(2)}$ corresponding to two delta-function potentials $V_1 + V_2$, one may use $G^{(1)}$ and expand in V_2. One gets

$$G^{(2)} = G^{(1)} + G^{(1)} V_2 G^{(2)}, \tag{17}$$

with the corresponding expansion

$$G^{(2)} = G^{(1)} + G^{(1)} V_2 G^{(1)} + G^{(1)} V_2 G^{(1)} V_2 G^{(1)} + \ldots. \tag{18}$$

Then

$$\langle x'|G^{(1)} V_2 G^{(1)}|x\rangle = U_2 \langle x'|G^{(1)}|a_2\rangle \langle a_2|G^{(1)}|x\rangle. \tag{19}$$

The second-order term in V_2 can be obtained similarly to Eq. (15), and is given by

$$\begin{aligned} &\langle x'|G^{(1)} V_2 G^{(1)} V_2 G^{(1)}|x\rangle \\ &\quad = U_2^2 \langle x'|G^{(1)}|a_2\rangle \langle a_2|G^{(1)}|x\rangle \\ &\qquad \times \left(\frac{-im}{k} + \frac{\left(\frac{-im}{k}\right)^2 e^{i2k|a_1 - a_2|} U_1}{1 + \frac{im}{k} U_1} \right), \\ &\quad = U_2^2 \langle x'|G^{(1)}|a_2\rangle \langle a_2|G^{(1)}|x\rangle \langle a_2|G^{(1)}|a_2\rangle. \end{aligned} \tag{20}$$

By repeating this procedure for higher-order terms, we obtain again a geometrical series whose sum can be expressed as

$$\langle x'|G^{(2)}|x\rangle = \langle x'|G^{(1)}|x\rangle + \frac{U_2 \langle x'|G^{(1)}|a_2\rangle \langle a_2|G^{(1)}|x\rangle}{1 - U_2 \langle a_2|G^{(1)}|a_2\rangle}. \tag{21}$$

Explicitly,

$$\langle x'|G^{(2)}|x\rangle = a/b \tag{22}$$

where

$$a=-i\frac{k}{m}e^{ik|x-x'|}+e^{ik|x-x'|}(U_1+U_2)$$
$$-e^{ik(|x-a_1|+|a_1-x'|)}U_1-e^{ik(|x-a_2|+|a_2-x'|)}U_2$$
$$+\frac{-im}{k}[e^{ik(|x-x'|+2|a_1-a_2|)}-e^{ik|x-x'|}$$
$$+e^{ik(|x-a_1|+|a_1-x'|)}+e^{ik(|x-a_2|+|a_2-x'|)}$$
$$-e^{ik(|x-a_2|+|a_1-a_2|+|a_1-x'|)}$$
$$-e^{ik(|x-a_1|+|a_1-a_2|+|a_2-x'|)}]U_1U_2, \quad (23)$$

and

$$b=\left(\frac{k}{m}\right)^2+i\frac{k}{m}(U_1+U_2)+(e^{2ik|a_1-a_2|}-1)U_1U_2. \quad (24)$$

C. General recursive formula

The procedure we have followed to deduce the matrix element of $G^{(2)}$ in Eq. (21) in terms of the matrix element of $G^{(1)}$ and U_2 depends on the fact that under integration with the delta potential, the internal elements of the Lippmann-Schwinger series become a geometrical series of powers of separate numbers that can be summed into a single analytical formula. By repeating this procedure, in the case of an arbitrary $U(x)$, we obtain a recursive formula for $G^{(n+1)}$ in terms of $G^{(n)}$, U_{n+1}, a_{n+1}, given by

$$\langle x'|G^{(n+1)}|x\rangle=\langle x'|G^{(n)}|x\rangle + \frac{U_{n+1}\langle x'|G^{(n)}|a_{n+1}\rangle\langle a_{n+1}|G^{(n)}|x\rangle}{1-U_{n+1}\langle a_{n+1}|G^{(n)}|a_{n+1}\rangle}. \quad (25)$$

III. OUTLOOK

It is interesting to note that the Green's function in Eq. (25) need not be assumed to come from a Hamiltonian with a kinetic and a delta-function potential part; in fact, the derivations we have made do not depend on the type of nonperturbed Hamiltonian H_0, and therefore, can serve also for any Hamiltonian to which an arbitrary delta-function potential is added, and it is enough to have an initial numerical value for its Green's function to carry out the calculation.

While the analytical expressions that can be obtained for the Green's function with a series of delta potentials are rather elaborate, the derived recursive formula in Eq. (25) could be useful computationally or numerically as the number of calculations necessary to obtain a matrix element grows like the number of potential terms, that is, if N is the number of potential elements, the number of necessary calculations is proportional to N, unlike the exact formulas whose determinants may require an order of the number calculations as large as $N!$. Also, this method can be useful for calculations with large memory demands as it is necessary to keep only one complex number for each Green's function matrix element when carrying out this calculation.

The formula obtained in Eq. (25) leads to a known recursive procedure for the consideration of one-dimensional scatterings in terms of the transfer matrix. Given that no restrictions are put on the arguments of Eq. (25), it is clear this formula extends this method by allowing also for consideration of off-the-energy-shell states (after transforming to momentum space).

In addition, the recursive formula could provide new information in areas where it has been useful, namely, in applications in the description of both periodic and nonperiodic, discrete and continuous potentials in nuclear and condensed-matter physics, in the investigation of coherent and incoherent effects, in mesoscopic systems, etc. It could also serve in theoretical studies requiring descriptions of the Green's function for nonanalytically solvable potentials; as mentioned, this formula is also utile to obtain analytical information on the solutions of a problem with a potential expressed as a discrete series of delta-function potentials that is approached when adding ever more terms.

In order to know more about how to adequately calculate with this method properties of any potential approximated by series of delta functions, and in particular, the convergence quality of successively approximated values of the wave function, the energy eigenvalues, and the scattering amplitude, further study is required.

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