Exact Green's Functions for Delta-Function Potentials and Renormalization in Quantum Mechanics

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Recebido em 14 de junho, 1998

We present a simple recipe to construct the Green's function associated with a Hamiltonian of the form $H = H_0 + \lambda \delta(x)$, where H_0 is a Hamiltonian for which the associated Green's function is known. We apply this result to the case in which H_0 is the Hamiltonian of a free particle in D dimensions. Field theoretic concepts such as regularization, renormalization, dimensional transmutation and triviality are introduced naturally in order to deal with an infinity which shows up in the formal expression of the Green's function for D > 2.

I Introduction

Quantum electrodynamics (QED), like most quantum field theories, is plagued with infinities. It was a major accomplishment when Schwinger, Feynman, Tomonaga and Dyson [1] showed how to extract meaningful information from QED, in spite of such infinities. In a renormalizable theory, like QED, such infinities can be dealt with in a two-step process: (i) its short distance (or high energy) behavior is modified with the introduction of a cut-off, which gives rise to finite answers, and (ii) the parameters of the theory are redefined in order to absorb the divergences which appear when the cut-off is removed. These steps are the regularization and renormalization of the theory, respectively.

Infinities of this sort also occur in non-relativistic quantum mechanics if the potential is singular enough, for instance the Dirac delta-function potential in two or more dimensions [2-9] and the Aharonov-Bohm potential [7,9]. This provides a unique framework in which the important concepts of regularization and renormalization can be explained free from the technical complications usually found in quantum field theory.

In this paper we study the Dirac delta-function potential. This problem has been previously studied in the literature using a variety of techniques: exact solutions of the Schrödinger equation [4,5] (or its integral version, the Lippman-Schwinger equation [6-8]), the self-adjoint extension method [2,3], and Green's function techniques [9,10]. Here we use the latter, which have a closer resemblance with the techniques usually

employed in quantum field theory. Besides that, it is very easy to find the Green's function associated with a Hamiltonian of the form $H=H_0+\lambda\delta(\mathbf{x})$ when the Green's function associated with H_0 is known; this is the content of Sec. II. In Sec. III, we apply this result to the case in which H_0 is the Hamiltonian of a free particle in D dimensions. For $D\geq 2$ an infinity shows up in the formal expression of the Green's function. In the two- and three-dimensional cases, this infinity can be removed in a consistent way, in what amounts to be a simple exercise in regularization and renormalization. Finally, in the Appendix we show how the technique, presented in Sec. II, can be adapted to the calculation of the scattering amplitude.

II Green's functions for deltafunction potentials

The Green's function $G(E; \mathbf{x}, \mathbf{y})$ associated with the Hamiltonian H is the solution of the differential equation

$$(E - H)G(E; \mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y}) \tag{1}$$

satisfying the boundary condition

$$\lim_{|\mathbf{x} - \mathbf{y}| \to \infty} G(E; \mathbf{x}, \mathbf{y}) = 0.$$
 (2)

Here \mathbf{x} and \mathbf{y} are points in D-dimensional Euclidean space and, correspondingly, $\delta(\mathbf{x} - \mathbf{y})$ is a D-dimensional Dirac delta-function.

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One can use the completeness of the eigenfunctions of H to write the solution of (1) as

$$G(E; \mathbf{x}, \mathbf{y}) = \sum_{n} \frac{\psi_n(\mathbf{x})\psi_n^*(\mathbf{y})}{E - E_n},$$
 (3)

where E_n and ψ_n are the eigenvalues and eigenfunctions of H, respectively. Now, let suppose that the Hamiltonian can be written as the sum of two terms,

$$H = H_0 + \lambda \delta(\mathbf{x}),\tag{4}$$

and that the Green's function $G_0(E; \mathbf{x}, \mathbf{y})$ associated with H_0 is known. Then, as we shall show below, there is a very simple recipe to write G in terms of G_0 .

Let us rewrite Eq.(1) in integral form [11] (for simplicity we omit the dependence on E):

$$G(\mathbf{x}, \mathbf{y}) = G_0(\mathbf{x}, \mathbf{y}) + \int d^D z G_0(\mathbf{x}, \mathbf{z}) \lambda \delta(\mathbf{z}) G(\mathbf{z}, \mathbf{y})$$
$$= G_0(\mathbf{x}, \mathbf{y}) + \lambda G_0(\mathbf{x}, \mathbf{0}) G(\mathbf{0}, \mathbf{y}).$$
(5)

Now we put $\mathbf{x} = \mathbf{0}$ in the expression above and solve it for $G(\mathbf{0}, \mathbf{y})$; then, inserting the result in (5), we obtain an explicit expression for the Green's function associated with H:

$$G(\mathbf{x}, \mathbf{y}) = G_0(\mathbf{x}, \mathbf{y}) + \frac{G_0(\mathbf{x}, \mathbf{0})G_0(\mathbf{0}, \mathbf{y})}{\frac{1}{\lambda} - G_0(\mathbf{0}, \mathbf{0})}.$$
 (6)

It is worth to note that successive applications of this procedure allows one to find the Green's function for a potential with an arbitrary number of delta-functions.

III Bound states and renormalization

In this section, we shall investigate the bound states of the Hamiltonian (4), with H_0 the Hamiltonian of a free particle in D dimensions (we use units such that $\hbar = 2m = 1$):

$$H_0 = -\nabla^2 \equiv -\sum_{i=1}^D \frac{\partial^2}{\partial x_i^2}.$$
 (7)

It follows from (3) that the energy levels of bound states are given by the real poles of the Green's function. Since there are no bound states in the free particle problem, such poles can only appear as zeros of the denominator of the second term on the r.h.s. of Eq.(6). In order to obtain $G_0(E; \mathbf{x}, \mathbf{y})$, we Fourier transform Eq. (1) (with H replaced with H_0), thus finding

$$G_0(E; \mathbf{x}, \mathbf{y}) = \int \frac{d^D k}{(2\pi)^D} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{E - k^2}.$$
 (8)

Therefore, in order to find the energy of the bound states we must solve the equation $(K^2 \equiv -E)$

$$\frac{1}{\lambda} + \int \frac{d^D k}{(2\pi)^D} \frac{1}{k^2 + K^2} = 0. \tag{9}$$

In what follows we shall examine Eq. (9) for different values of D.

$$\mathbf{A} \cdot D = 1$$

Performing the integral in Eq. (9), we find

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{1}{k^2 + K^2} = \frac{1}{2K}.$$
 (10)

Then, solving Eq.(9) for K, we obtain

$$K = -\frac{\lambda}{2} \quad \text{and} \quad E_B = -\frac{\lambda^2}{4} \ . \tag{11}$$

Note that λ must be negative, for K was implicitly taken positive in Eq. (10). Physically, this means that the potential must be attractive in order to create a bound state.

For the sake of comparison, we present an alternative more elementary derivation of this result. The time-independent Schrödinger equation for a particle in the potential $V(x) = \lambda \delta(x)$ is

$$-\frac{d^2}{dx^2}\psi(x) + \lambda\delta(x)\psi(x) = E\psi(x). \tag{12}$$

For $x \neq 0$ this equation is that of a free particle; solving it for $E = -K^2 < 0$ and imposing continuity at the origin, we find

$$\psi(x) = Ae^{-K|x|} . (13)$$

A restriction on the possible values of K is obtained by integrating Eq. (12) from $-\epsilon$ to $+\epsilon$ and letting $\epsilon \to 0^+$:

$$-\psi'(0^+) + \psi'(0^-) + \lambda\psi(0) = 0, \tag{14}$$

from which follows that $K = -\lambda/2$. Therefore, both methods give the same results.

$$\mathbf{B} \cdot D = 2$$

In this case, a problem occurs that is absent in $D = 1 : G_0(E; \mathbf{0}, \mathbf{0})$ is (logarithmically) divergent. To deal with this problem, we must introduce a cut-off in the integral which appears in Eq. (9) and absorb the dependence on the cutoff in a redefinition of the parameters of the theory (in this case, the "coupling constant" λ). In quantum field theory this procedure is known as

regularization and renormalization. Let us demonstrate it explicitly. The first step is to regularize the integral:

$$\int \frac{d^2k}{(2\pi)^2} \frac{1}{k^2 + K^2} = \frac{1}{2\pi} \int_0^{\Lambda} \frac{kdk}{k^2 + K^2}$$
$$= \frac{1}{4\pi} \ln\left(\frac{\Lambda^2 + K^2}{K^2}\right). \quad (15)$$

The next step is to absorb the divergent part of the above result in a redefinition of the coupling constant:

$$\frac{1}{\lambda_R} \equiv \frac{1}{\lambda} + \frac{1}{4\pi} \ln \left(\frac{\Lambda^2}{\mu^2} \right) \tag{16}$$

(The parameter μ is arbitrary, and is introduced in order to keep the argument of the logarithm dimensionless.) We now take the limit $\Lambda \to \infty$, varying the bare coupling constant λ in such a way that the renormalized coupling constant λ_R remains finite; Eq. (9) then becomes

$$\frac{1}{\lambda_R} - \frac{1}{4\pi} \ln \left(\frac{K^2}{\mu^2} \right). \tag{17}$$

Solving this equation for K^2 we find the energy of the bound state:

$$E_B = -K^2 = -\mu^2 \exp\left(\frac{4\pi}{\lambda_R}\right). \tag{18}$$

A curious thing happens here: although the Hamiltonian contains only one parameter (λ) , we have obtained an energy (E_B) depending on two parameters $(\lambda_R \text{ and } \mu)$. However, this doubling of parameters is illusory. In fact, it is possible to show that the Green's function depends on a sole parameter (besides E, \mathbf{x} and \mathbf{y} , of course). To see this, let us write the denominator of the second term on the r.h.s. of Eq. (6) in regularized form:

$$\frac{1}{\lambda} - G_0(E; \mathbf{0}, \mathbf{0}) = \frac{1}{\lambda} + \frac{1}{2\pi} \int_0^{\Lambda} \frac{k dk}{k^2 + E}$$

$$= \frac{1}{\lambda} + \frac{1}{4\pi} \ln \left(\frac{\Lambda^2 + E}{-E} \right). (19)$$

On the other hand, according to Eqs. (16)-(18), $\lambda^{-1} = -(1/4\pi) \ln(-\Lambda^2/E_B)$; substituting this in the expression above and taking the limit $\Lambda \to \infty$, we obtain

$$\frac{1}{\lambda} - G_0(E; \mathbf{0}, \mathbf{0}) = -\frac{1}{4\pi} \ln \left(\frac{E}{E_B} \right). \tag{20}$$

This is an instance of the so-called dimensional transmutation [12]. Having started with a Hamiltonian containing only dimensionless parameters (in this case, the coupling constant λ), we ended up with a theory

containing a dimensional parameter (E_B) . This happens because during the renormalization process we had to introduce the dimensionful parameter μ , thus breaking the scale invariance of the theory.

$$\mathbf{C} \cdot D = 3$$

As in the case D = 2, $G_0(E; \mathbf{0}, \mathbf{0})$ is divergent, and so the bare Green's function, given by Eq. (6), is ill-defined. To deal with this problem, we proceed as in the previous subsection: we regularize the integral which appears in Eq. (9),

$$\int \frac{d^3k}{(2\pi)^3} \frac{1}{k^2 + K^2} = \frac{1}{2\pi^2} \int_0^{\Lambda} \frac{k^2 dk}{k^2 + K^2}$$
$$= \frac{1}{2\pi^2} \left[\Lambda - K \arctan\left(\frac{\Lambda}{K}\right) \right], \tag{21}$$

and absorb the divergent part of this result in a redefinition of the coupling constant,

$$\frac{1}{\lambda_R} \equiv \frac{1}{\lambda} + \frac{\Lambda}{2\pi^2}.\tag{22}$$

Taking the limit $\Lambda \to \infty$ in Eq. (9) while keeping λ_R fixed, we obtain

$$\frac{1}{\lambda_B} - \frac{K}{4\pi} = 0,\tag{23}$$

from which it follows that

$$K = \frac{4\pi}{\lambda_R}$$
 and $E_B = -\left(\frac{4\pi}{\lambda_R}\right)^2$. (24)

Here too we can eliminate all reference to λ_R in favor of E_B , the energy of the bound state. In fact, as a simple calculation shows, the denominator of the second term on the r.h.s. of Eq. (6) can be rewritten as

$$\frac{1}{\lambda} - G_0(E; \mathbf{0}, \mathbf{0}) = \frac{\sqrt{-E_B} - \sqrt{-E}}{4\pi}.$$
 (25)

$$\mathbf{D} \cdot D > 4$$

Let us now consider D = 4. In this case, the regularized form of the integral in Eq.(9) is

$$\frac{1}{8\pi^2} \int_0^{\Lambda} \frac{k^3 dk}{k^2 + K^2} = \frac{1}{16\pi^2} \left[\Lambda^2 - K^2 \ln\left(\frac{\Lambda^2 + K^2}{K^2}\right) \right]. \tag{26}$$

The quadratically divergent term $\Lambda^2/16\pi^2$ may be absorbed in a redefinition of the coupling constant, similar to (16) and (22). However, the second term on

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the r.h.s., which is also divergent, cannot be eliminated this way, as it is intrinsically dependent on K. The same problem occurs for D > 4. This is part of Friedman's theorem [13]: it is not possible to define a contact (i.e., zero-range) potential in more than three dimensions possessing bound states with finite energy. To present the other piece of that theorem, let us note that in order that λ_R be finite (in D=2 and 3), λ must tend to 0⁻ when the cut-off is removed [see Eqs. (16) and (22). On the other hand, if one insists to keep λ finite, then one of these two alternatives will follow: (i) if $\lambda < 0$, the Hamiltonian is unbounded from below (the energy of the bound state depends on the cut-off Λ , and tends to $-\infty$ when $\Lambda \to \infty$), or (ii) if $\lambda > 0$, there is no way to avoid the denominator of the second term on the r.h.s. of Eq. (6) of diverging, and so the Green's function is the same as that in the absence of the potential. This is precisely the other piece of Friedman's theorem: a repulsive delta-function potential in more than one dimension does not scatter, and so it is said to be trivial.

Acknowledgments

I thank Carlos Alberto Aragão de Carvalho for a critical reading of this paper. This work had financial support from the Conselho Nacional de Desenvolvimento Científico e Tecnológico, and was supported in part by the National Science Foundation under Grant No. PHY94-07194.

Appendix A

Here we show how to obtain scattering amplitudes for a Dirac delta-function potential. First let us recall that for positive energies $E=k^2$ the Schrödinger equation is equivalent to the Lippman-Schwinger equation

$$\psi(\mathbf{x}) = \psi_0(\mathbf{x}) + \int d^D x' G_0^R(\mathbf{x}, \mathbf{x}') V(\mathbf{x}') \psi(\mathbf{x}'), \quad (A1)$$

where ψ_0 is a solution of the free Schrödinger equation and $G_0^R(\mathbf{x}, \mathbf{x}') \equiv G_0(E + i\epsilon; \mathbf{x}, \mathbf{x}')$ is the free retarded Green's function. For $V(\mathbf{x}') = \lambda \delta(\mathbf{x}')$, Eq. (A1) gives

$$\psi(\mathbf{x}) = \psi_0(\mathbf{x}) + \lambda G_0^R(\mathbf{x}, \mathbf{0}) \psi(\mathbf{0}). \tag{A2}$$

Now we put $\mathbf{x} = \mathbf{0}$ in this expression and solve it for $\psi(\mathbf{0})$; inserting the result in (A2), we obtain

$$\psi(\mathbf{x}) = \psi_0(\mathbf{x}) + \frac{G_0^R(\mathbf{x}, \mathbf{0})\psi_0(\mathbf{0})}{\frac{1}{\lambda} - G_0^R(\mathbf{0}, \mathbf{0})}.$$
 (A3)

Note that for two and three dimensions the denominator of this term is divergent, but it becomes finite after renormalization.

From the asymptotic behavior of this expression as $r \equiv |\mathbf{x}| \to \infty$ one can extract the scattering amplitude. As an example, let us consider the three-dimensional scattering problem. In this case, the free Green's function is given by

$$G_0(E + i\epsilon; \mathbf{x}, \mathbf{x}') = -\frac{e^{i\sqrt{E}|\mathbf{x} - \mathbf{x}'|}}{4\pi|\mathbf{x} - \mathbf{x}'|}.$$
 (A4)

Substituting this expression and Eq. (25) in Eq. (A3), taking $\psi_0(\mathbf{x}) = \exp(ikz)$ (which represents a particle moving along the positive z direction), and comparing the result with the asymptotic expression of the wave function,

$$\psi(\mathbf{x}) \approx e^{ikz} + f(k, \theta, \phi) \frac{e^{ikr}}{r} \qquad (r \to \infty), \qquad (A5)$$

we find the following expression for the scattering amplitude:

$$f(k,\theta,\phi) = -\frac{1}{\sqrt{-E_B - ik}}. (A6)$$

As expected, the scattering is isotropic, since only the s-waves "see" the zero-range potential located at the origin.

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¹ By treating the delta-function as the limit of a sequence of spherical cores, one can verify [14] that in two or more dimensions the s-waves are the same as those of a free particle, except at the origin, where they drop to zero discontinuously (the other partial waves are not affected by the potential, since they vanish at the origin). Therefore, the assertion made in Ref. [4], that a repulsive delta-function potential in two or more dimensions expels the s-waves from the Hilbert space, is wrong.

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