On the Green function of linear evolution equations for a region with a boundary

George Krylov†‡ and Marko Robnik†

†Center for Applied Mathematics and Theoretical Physics, University of Maribor, Krekova 2, SI–2000 Maribor, Slovenia
‡Department of Physics, Belarusian State University, Fr. Skariny av. 4, 220050 Minsk, Belarus

Abstract. We derive a closed form expression for the Green function of linear evolution equation with the Dirichlet boundary condition for an arbitrary region, based on singular perturbation approach to boundary problems.

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1 Introduction

The boundary value problem for linear operators in non-trivial regions leads to complications and quite often it is necessary to resort to the numerical analysis even for the simplest operators which possess a known kernel in the whole space, such as e.g. Laplace operator in the $\mathbb{R}^n$ [1].

The possibility of a new approach to these problems appeared along with developing the theory of point interactions in quantum mechanics, firstly stimulated by the famous Kronig-Penney model [2], and systematically investigated in [3] where self-adjoint extensions for Hamiltonian with point-like interactions have been constructed so that the explicit form for resolvent has been obtained for some physically significant systems. It is in reference [3] that it has been already pointed out that the limiting case of infinitely strong point interaction allows effectively to split the space in two separated regions that lead to two boundary problems on half line.

This important trick has been successfully developed in [4, 5, 6] and it allows one to write down the explicit expressions for the Green function of Schrödinger equation for the particle in one dimensional and radial boxes with Dirichlet and Neumann boundary conditions provided the appropriate problem in the whole space has been solved. The technique that has been successfully used for such a derivation is a direct summation of perturbation series (Dyson series [7]), effectively leading to geometrical progression due to the specific form of the perturbation. We would like to stress here, that numerous analytical results obtained up to now are related to quantum one-dimensional problems (as e.g., Krein’s formula [3]), effective one-dimensional problems after variables’ separation (‘radial problem’), and point-like interactions (see [3, 8] and recent book [9] for detailed references which include both solvable $\delta$-perturbation cases and boundary value problems).

The question naturally arising here is whether it is possible to generalize these constructions to higher dimensional boundary problems. As we will see, and this will be the main aim of this work, it can be done at least for Dirichlet boundary conditions for arbitrary linear evolution operators in topologically trivial region (homeomorphic to a ball in $\mathbb{R}^d$), when assuming some natural conditions for the propagator of “free particle” to be fulfilled. It is worthwhile to mention here that we intend neither to construct the self-adjoint extension of appropriate singular perturbed operators [3], nor to perform a detailed investigation of convergence properties of appropriate perturbation series (as is well known the answer may be negative even for regular perturbations, see e.g. [1]). To the contrary, we intend to propose explicit construction of Green function for non-separable case and demonstrate its validity by known examples. Generally speaking the problem we will solve can be formulated on an abstract level of the theory of linear operators by
introducing some generalization of projector operators, but we expect that it could only shadow simple foundation of the approach we use. Moreover, although, admittedly, the manipulations with perturbation series and the subsequent limit of infinitely large coupling constant are rather formal, we do not know another way to obtain the Green function representation for general boundary problem that we will construct in this paper.

2 Series summation for singular perturbed system

Let us have a linear evolution equation in $\mathbb{R}^d$ of the form

$$\left( \frac{\partial}{\partial t} - \hat{\mathcal{L}} \right) \Psi(x) = 0,$$

with explicitly time independent operator $\hat{\mathcal{L}}$ acting on the function defined over $\mathbb{R}^d$ and obeying Dirichlet boundary condition $\Psi|_\Gamma = 0$, where $\Gamma = \{ x : P(x) = 0 \}$ is the boundary (hyper-surface) of the region $\mathcal{B}$ under consideration, in which we seek the solutions of equation (1).

We start from a consideration of the “free particle”, omitting the boundary condition, and assuming that propagator for that case, given by

$$K^0(x', x''; t) = |x''\rangle \langle x'| e^{\hat{\mathcal{L}}t} |x'\rangle > \theta(t),$$

is already known. Here $\theta$ is the Heaviside unit-step function, incorporated into (2) to ensure causality property $K(x', x''; t) = 0$, when $t < 0$. The propagator $K$ possesses the composition property

$$K(x', x''; t) = \int_{\mathbb{R}^d} dx_1 K(x', x_1; t_1) K(x_1, x''; t - t_1).$$

which follows from the semi-group property with respect to the time evolution, which in turn is automatically fulfilled for an explicitly time-independent operator $\hat{\mathcal{L}}$ and the decomposition of unity in an appropriate functional space, namely

$$\text{Id} = \sum_x |x\rangle \langle x|,$$

where summation (integration) is performed over discrete (continuous) index enumerating states (see e.g. [7]). These properties are natural for most of physically significant models so that our consideration is not very restrictive.

Now we will emulate the boundary condition by introducing into (1) the additional singular potential term of the form $V^\delta = -\gamma \delta_P(x)$. The generalized $\delta$-function used here is a distribution concentrated on the hyper-surface
In the limiting case of $\gamma \to \infty$ the corresponding one dimensional problem turns out to be a Dirichlet boundary problem on the half line $\mathbb{R}$ (see the discussion in introduction). We will demonstrate explicitly that the same situation is met in higher dimensions.

We will use the method expounded in \cite{3, 4, 5, 6, 11}, performing a perturbation expansion, starting from the formula for the propagator of the singular perturbed problem

$$K(x', x''; t) = \left. x'' \right| e^{(\hat{L} + V\delta)t} \left| x' > \theta(t) \right. .$$

The formal perturbation series over powers of $V\delta$ can be constructed as in the quantum mechanics \cite{12} and reads

$$K^\delta(x', x''; t) = K^0(x', x''; t) + \sum_{n=1}^{\infty} \gamma^n \int_0^t dt_1 \int_{\mathbb{R}^d} dx_1 K^0(x', x_1; t_1 - 0) \delta_P(x_1) \times$$

$$\prod_{j=2}^{n} \left[ \int_0^t dt_j \int_{\mathbb{R}^d} dx_j K^0(x_{j-1}, x_j; t_j - t_{j-1}) \delta_P(x_j) \right] K^0(x_n, x''; t - t_n).$$

The convergence questions appearing at this moment should be treated for every problem considered separately, e.g. for Schrödinger equation the existence of well defined Green function has been proven rigorously in some cases \cite{3}. For arbitrary linear evolution equation we must stay on the formal level only to go further.

After performing the Laplace transformation for the Green function, defined by

$$G(x', x''; E) = \int_0^\infty e^{-Et} K(x', x''; t) dt,$$

the following series representation can be written

$$G^\delta(x', x''; E) = G^0(x', x''; E) + \sum_{n=1}^{\infty} \gamma^n \int_{\mathbb{R}^d} dx_1 G^0(x', x_1; E) \delta_P(x_1) \times$$

$$\prod_{j=2}^{n} \left[ \int_{\mathbb{R}^d} dx_j G^0(x_{j-1}, x_j; E) \delta_P(x_j) \right] G^0(x_n, x''; E).$$

The behaviour of $G^0(x', x''; E)$ at coincident space arguments in spaces with $d > 2$ may lead to divergence of integrals in (8), but we will not discuss this in details, since the appropriate procedures of regularizations are well known (for point-like perturbations in quantum mechanics see e.g., \cite{3, 11}). We only point out that for most interesting cases of two and three-dimensional quantum problems there are no singularities within our approach, opposite
to the models described in [11]. Indeed, the short distance behaviour of the Green function in d-dimensional spaces is [9], f.6.2.1.2

\[ G(x', x'', k) \propto |x' - x''|^{1-d/2} Y_{1-d/2}(k|x' - x''|), \]  

(9)

where \( Y_n(x) \) is Bessel function [13], so that the relevant underlying singularities are integrable for d=2,3. For higher dimension (or) and other operator \( \mathcal{L} \), some sort of regularization should be used as e.g. in [11].

Returning to our problem, now we can introduce new coordinates by the map \( F : x = \{x_1,..,x_d\} \mapsto y = \{y_1,..,y_d\} \) with Jacobian \( J = \frac{\partial x}{\partial y} \) so that the equation of hyper-surface \( P \) will be given by \( y_d = \eta \) (see e.g., [10]). We designate all coordinates except the last one namely \( \{y_i : i = 1,..,d - 1\} \), by \( \Omega \), so that \( y = \{\Omega, y_d\} \). Then, the integrations over \( \delta \)-functions are simply projections on the submanifold, defined by \( y_d = \eta \) and we get

\[ G(\delta(x', x''; E) = G^0(x', x''; E) + \sum_{n=1}^{\infty} \gamma^n \int_P \sqrt{g_1} d\Omega_1 G^0(\Omega', (y_d)', \Omega_1, \eta; E) \times \prod_{\beta=2}^{n} \left[ \int_P \sqrt{g_{\beta\beta}} d\Omega_{\beta} G^0(\Omega_{\beta-1}, \eta, \Omega_{\beta}, \eta; E) \right] G^0(\Omega_n, \eta, \Omega', (y_d)''); E), \]  

(10)

where the integration is performed over the hyper-surface \( P \), \( g = \det(g^{\mu\nu}) \), \( g^{\mu\nu} = \frac{\partial x^\mu}{\partial y^\nu} \) is an induced metric tensor on \( P \) and we introduce coordinates \( \Omega, y_d \) corresponding to the initial and final points \( x', x'' \). Now we want to expand the Green function \( G^0(\Omega_{j-1}, \eta, \Omega_j, \eta; E) \) in a series of functions defined on \( P \). Let us choose an appropriate full (complete) orthonormal system of functions \( \{f_\kappa(\Omega)\} \) on the boundary \( \Gamma \) of the region \( \mathcal{B} \), where \( \kappa \) is some multi-index enumerating the system \( f \), with a standard \( L_2(\Omega) \) scalar product

\[ < f_\kappa, f_{\kappa'} > = \int_\Omega \sqrt{g(\Omega)} f_\kappa(\Omega) f_{\kappa'}(\Omega) d\Omega = \delta_{\kappa,\kappa'}. \]  

(11)

For example, the case of axially symmetric closed surfaces has been recently treated by Prodan [14], where the projection of the resolvent operator on such surfaces has been investigated.

We represent \( G^0 \) in the form

\[ G^0(\Omega', \xi, \Omega'', \eta; E) = \sum_{\kappa',\kappa''} G_{\kappa',\kappa''}(\xi, \eta; E) f_{\kappa'}(\Omega') \bar{f}_{\kappa''}(\Omega'') \]  

(12)

so that the coefficient \( G_{\kappa',\kappa''}(\xi, \eta; E) \) is expressed as

\[ G_{\kappa',\kappa''}(\xi, \eta; E) = \int \sqrt{g(\Omega') g(\Omega'')} G^0(\Omega', \xi, \Omega'', \eta; E) f_{\kappa'}(\Omega') \bar{f}_{\kappa''}(\Omega'') d\Omega' d\Omega'' \]  

(13)
Then, substituting (12) into (10) we get

\[ G^\delta(x', x''; E) = G^0(x', x''; E) + \sum_{n=1}^{\infty} \gamma^n \int_{\lambda} \sqrt{g_1} d\Omega_1 \sum_{\kappa', \kappa_1} \mathcal{G}_{\kappa', \kappa_1}((y_d)', \eta; E) \times \]

\[ f_{\kappa'}(\Omega') \bar{f}_{\kappa_1}(\Omega_1) \prod_{j=2}^{n} \left[ \int_{\lambda} \sqrt{g_j} d\Omega_j \sum_{\kappa_j-1, \kappa_j} \mathcal{G}_{\kappa_{j-1}, \kappa_j}(\eta, \eta; E)f_{\kappa_{j-1}}(\Omega_{j-1}) \bar{f}_{\kappa_j}(\Omega) \right] \times \]

\[ \sum_{\kappa_n, \kappa''} \mathcal{G}_{\kappa_n, \kappa''}((y_d)'', \eta; E)f_{\kappa_n}(\Omega_n) \bar{f}_{\kappa''}(\Omega'') = \]

\[ G^0(x', x''; E) + \gamma \sum_{\kappa', \kappa_1, \kappa_n, \kappa''} \mathcal{G}_{\kappa', \kappa_1}((y_d)', \eta; E)\mathcal{G}_{\kappa_n, \kappa''}((y_d)'', \eta; E)f_{\kappa'}(\Omega') \bar{f}_{\kappa''}(\Omega'') \times \]

\[ \left[ \delta_{\kappa_1, \kappa_n} + \gamma \mathcal{G}_{\kappa_1, \kappa_n}(\eta, \eta; E) + \gamma^2 \sum_{\kappa_2} \mathcal{G}_{\kappa_1, \kappa_2}(\eta, \eta; E)\mathcal{G}_{\kappa_2, \kappa_n}(\eta, \eta; E) + \ldots \right] (14) \]

where we used the orthonormality of the functions (11). After summing up the geometrical progression we obtain

\[ G^\delta(x', x''; E) = G^0(x', x''; E) + \]

\[ \sum_{\kappa', \kappa''} \left[ \mathcal{G}((y_d)', \eta; E)(\gamma^{-1} - \mathcal{G}(\eta, \eta; E))^{-1} \mathcal{G}(\eta, (y_d)'', E) \right]_{\kappa', \kappa''} f_{\kappa'}(\Omega') \bar{f}_{\kappa''}(\Omega''). (15) \]

For the brevity of notation we used matrix form within the square brackets, and \((\gamma \mathcal{G})^n\) is an ordinary matrix power. Taking the limit \(\gamma \to \infty\) we get finally

\[ G^\delta(x', x''; E) = G^0(x', x''; E) - \]

\[ \sum_{\kappa', \kappa''} \left[ \mathcal{G}((y_d)', \eta; E)\mathcal{G}(\eta, \eta; E)^{-1} \mathcal{G}(\eta, (y_d)'', E) \right]_{\kappa', \kappa''} f_{\kappa'}(\Omega') \bar{f}_{\kappa''}(\Omega''), \]

(16)

which is the main result of our paper.

3 Discussion

As it is easily seen, the last formula solves an appropriate Dirichlet boundary problem. Indeed, the statement that the object constructed above satisfies the differential equation (11) is evident from the construction and, if \((y_d)' = \eta\) or \((y_d)''' = \eta\), that is if the initial or the final points are on a boundary, the term in the square brackets simply gives the free Green function expansion coefficient and the whole sum becomes the free Green function cancelling the first term in (13), which means that the Dirichlet boundary condition is obeyed.

It is worthwhile to point out here that the spectrum of the system under consideration is given by such values of \(E\) that \(\mathcal{G}(\eta, \eta; E)\) is non-invertible.
In two dimensional case the multi-index \( \kappa \) becomes an ordinary one and we obtain the condition of vanishing determinant
\[
\text{Det } G(\eta, \eta; E) = 0. \tag{17}
\]

From the last equation it is easily seen that our approach looks like some alternative and generalization of the boundary integral method \([13, 16]\), where the spectrum of 2-D billiard can be obtained based on an integral of Green function’s normal derivative over the boundary.

It is also easy to demonstrate that formula \((16)\) leads to a known one for the case of the separability of variables. Let us do it explicitly for the 2-D case of quantum particle in a circular region \((\Gamma = \{ x : |x| = R \})\). An appropriate formula for the Green function in polar coordinates \((r, \phi)\) reads \([4]\) (see also \([17]\) for alternative derivation)
\[
G(r, r'; E) = \sum_{m=-\infty}^{\infty} G^0_l(r, r'; E) e^{im(\phi' - \phi)}, \tag{18}
\]

Where
\[
G^0_l(r, r'; E) = G^0_l(r', R; E)G^0_l(R, r'; E) \frac{1}{G^0_l(R, R; E)}. \tag{19}
\]

A natural choice of the functions’ family is of course \(f_m(\phi) = \exp{im\phi}\). Expanding the free particle Green function in the same manner as in \((13)\) and calculating the coefficient of equation \((12)\) one can see that
\[
G_{mm'}(r, r'; E) = G^0_m(r, r'; E)\delta_{mm'}, \tag{20}
\]

so that the matrix inversion becomes trivial and after the substitution of \((20)\) into \((16)\), formula \((19)\) follows immediately. Similar arguments may be used for other separable quantum problems.

Thus, we see, that indeed we have successfully constructed the explicit representation for the Green function of linear evolutional equation with Dirichlet boundary condition, based on Green function in the whole space, thereby generalizing results already known in separable cases in quantum mechanics.

The formula \((16)\) can be rewritten in a more formal way, introducing the series expansion of \(G^\delta(x', x''; E)\) in a manner like \((12)\) for \(G^0\). Then,
\[
G^\delta_{\kappa',\kappa''}((y_d)', (y_d)''; E) = G^0_{\kappa',\kappa''}((y_d)', (y_d)''; E) - \left[ G((y_d)', \eta; E)G(\eta, \eta; E)^{-1}G(\eta, (y_d)''; E) \right]_{\kappa',\kappa''}, \tag{21}
\]

or in operator notation
\[
\hat{G}^\delta((y_d)', (y_d)''; E) = \hat{G}((y_d)', (y_d)''; E) - \hat{G}((y_d)', \eta; E)\hat{G}(\eta, \eta; E)^{-1}\hat{G}(\eta, (y_d)''; E). \tag{22}
\]
The last expression is suitable for further formal manipulations in the case of double δ-perturbation $V = \gamma(\delta(y_d - a) + \delta(y_d - b))$, where the system is being ”squeezed” into a narrow shell $a \leq \eta \leq b$, simulating the quantization on a hyper-surface in the limit $a \to b$ in a manner similar to [4] (see the equation 2.15 in [4]), but the detailed analysis will be published elsewhere.

It should be mentioned also, that our approach can be modified also to be used for more general perturbation of the form $\tilde{V} = -\gamma h(x)\delta P(x)$ with arbitrary function $h$. Then similar arguments show that the only difference from the case considered above is that one should change $\sqrt{g}$ to $\sqrt{gh(\Omega, \eta)}$. Then, we should use another function family for the expansion or, it may be more convenient to expand into the series not the Green function but the product

$$\sqrt{h(\Omega; \xi)h(\Omega', \eta)G^0(\Omega', \xi, \Omega'', \eta; E)} = \sum_{\kappa', \kappa''} \tilde{G}_{\kappa', \kappa''}(\xi, \eta; E) f_{\kappa'}(\Omega') \tilde{f}_{\kappa''}(\Omega''),$$

and the final formula becomes

$$\tilde{G}^\delta(\mathbf{x}', \mathbf{x}''; E) = G^0(\mathbf{x}', \mathbf{x}''; E) - \sum_{\kappa', \kappa''} \frac{f_{\kappa'}(\Omega') \tilde{f}_{\kappa''}(\Omega'')}{\sqrt{h(\Omega'', (y_d)')}h(\Omega'', (y_d)'')}} \times$$

$$\left[ \tilde{G}((y_d)', \eta; E)\tilde{G}(\eta, \eta; E)^{-1} \tilde{G}(\eta, (y_d)''; E) \right]_{\kappa', \kappa''}. \quad (24)$$

Such a generalization may be useful for the systems with the boundary whose initial shape is not very convenient for the construction of the function family set $f_{\kappa}$ and when it is easy to perform some transformations before using the proposed approach. In this case, after a transformation to the new coordinates (and, e.g., accompanied by the “local time rescaling” [18]), the initially pure δ-function perturbation really transforms to a non-uniform one like discussed above.

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