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1999 J. Phys. A: Math. Gen. 32 1261

(http://iopscience.iop.org/0305-4470/32/7/015)

J. Phys. A: Math. Gen. **32** (1999) 1261–1267. Printed in the UK PII: S0305-4470(99)97748-X

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

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Received 22 September 1998, in final form 5 November 1998

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

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 numerical analysis even for the simplest operators which possess a known kernel in the whole space, such as the Laplace operator in $\mathbb{R}^n$ [1], for example.

The possibility of a new approach to these problems appeared along with the development of the theory of point interactions in quantum mechanics, first stimulated by the famous Kronig–Penney model [2], and systematically investigated in [3] where self-adjoint extensions for a Hamiltonian with point-like interactions were constructed so that the explicit form of the resolvent was obtained for some physically significant systems. It had already been pointed out in [3] that the limiting case of an infinitely strong point interaction allows one effectively to split the space into two separate regions which leads to two boundary problems on the half-line.

This important trick was successfully developed in [4–6] and it allows one to write down the explicit expressions for the Green function of the Schrödinger equation for a 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 (the 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 (such as Krein's formula [3], for example), effective one-dimensional problems after separation of variables (the 'radial problem'), and point-like interactions (see [3, 8] and the recent book [9] for detailed references which include both solvable δ-perturbation cases and boundary value problems).

The question that naturally arises here is whether it is possible to generalize these constructions to higher-dimensional boundary problems. As we shall see, and this will be the

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0305-4470/99/071261+07$19.50

main aim of this paper, it can be done at least for Dirichlet boundary conditions for arbitrary linear evolution operators in a topologically trivial region (homeomorphic to a ball in R^d), with the assumption that some natural conditions for the propagator of the 'free particle' are fulfilled. It is worthwhile mentioning here that we intend neither to construct the self-adjoint extension of the appropriate singular perturbed operators [3], nor to perform a detailed investigation of the convergence properties of the appropriate perturbation series (as is well known the answer may be negative even for regular perturbations, see [7], for example). In contrast, we propose to construct the Green function for the non-separable case explicitly, and to 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 the projector operators, but we expect that this would only shadow the simple foundation of the approach we use. Moreover, although the manipulations with perturbation series and the subsequent limit of infinitely large coupling constant are admittedly rather formal, we do not know of another way of obtaining the Green-function representation for the general boundary problem which we will construct in this paper.

2. Series summation for a singular perturbed system

Let us have a linear evolution equation in R^d of the form

$$\left(\frac{\partial}{\partial t} - \hat{\mathcal{L}}\right) \Psi(\mathbf{x}) = 0 \tag{1}$$

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

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

$$K^0(\boldsymbol{x}', \boldsymbol{x}''; t) = \langle \boldsymbol{x}'' | \mathrm{e}^{\hat{\mathcal{L}}t} | \boldsymbol{x}' \rangle \theta(t) \tag{2}$$

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

$$K(\boldsymbol{x}', \boldsymbol{x}''; t) = \int_{\mathrm{R}^d} \mathrm{d}\boldsymbol{x}_1 \, K(\boldsymbol{x}', \boldsymbol{x}_1; t_1) K(\boldsymbol{x}_1, \boldsymbol{x}''; t - t_1) \tag{3}$$

which follows from the semi-group property with respect to 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

$$\mathrm{Id} = \sum_x |x\rangle\langle x| \tag{4}$$

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

Now we will emulate the boundary condition by introducing in (1) the additional singular potential term of the form $V^\delta = -\gamma \delta_P(\boldsymbol{x})$. The generalized δ-function used here is a distribution concentrated on the hypersurface P [10]. 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 [3] (see the discussion in introduction). We will demonstrate explicitly that the same situation occurs for higher dimensions.

We will use the method expounded in [3–6, 11], performing a perturbation expansion, starting from the formula for the propagator of the singular perturbed problem

$$K(\boldsymbol{x}', \boldsymbol{x}''; t) = \langle \boldsymbol{x}''|\mathrm{e}^{(\hat{\mathcal{L}}+V^{\delta})t}|\boldsymbol{x}'\rangle\theta(t). \tag{5}$$

The formal perturbation series over powers of V^{δ} can be constructed as in quantum mechanics [12], and reads

$$K^{\delta}(\boldsymbol{x}', \boldsymbol{x}''; t) = K^0(\boldsymbol{x}', \boldsymbol{x}''; t) + \sum_{n=1}^{\infty} \gamma^n \int_0^t \mathrm{d}t_1 \int_{\mathrm{R}^d} \mathrm{d}\mathbf{x}_1\, K^0(\boldsymbol{x}', \boldsymbol{x}_1; t_1 - 0)\delta_P(\boldsymbol{x}_1)$$
$$\times \prod_{j=2}^{n} \left[\int_0^t \mathrm{d}t_j \int_{\mathrm{R}^d} \mathrm{d}\mathbf{x}_j\, K^0(\boldsymbol{x}_{j-1}, \boldsymbol{x}_j; t_j - t_{j-1})\delta_P(\boldsymbol{x}_j) \right] K^0(\boldsymbol{x}_n, \boldsymbol{x}''; t - t_n). \tag{6}$$

The convergence questions appearing at this moment should be treated separately for every problem considered, e.g., for the Schrödinger equation the existence of a well-defined Green function has been proved rigorously in some cases [3]. For an arbitrary linear evolution equation we must remain only at the formal level to go further.

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

$$G(\boldsymbol{x}', \boldsymbol{x}''; E) = \int_0^{\infty} \mathrm{e}^{-Et} K(\boldsymbol{x}', \boldsymbol{x}''; t)\, \mathrm{d}t \tag{7}$$

the following series representation can be written:

$$G^{\delta}(\boldsymbol{x}', \boldsymbol{x}''; E) = G^0(\boldsymbol{x}', \boldsymbol{x}''; E) + \sum_{n=1}^{\infty} \gamma^n \int_{\mathrm{R}^d} \mathrm{d}\mathbf{x}_1\, G^0(\boldsymbol{x}', \boldsymbol{x}_1; E)\delta_P(\boldsymbol{x}_1)$$
$$\times \prod_{j=2}^{n} \left[\int_{\mathrm{R}^d} \mathrm{d}\mathbf{x}_j\, G^0(\boldsymbol{x}_{j-1}, \boldsymbol{x}_j; E)\delta_P(\boldsymbol{x}_j) \right] G^0(\boldsymbol{x}_n, \boldsymbol{x}''; E). \tag{8}$$

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

$$G(\mathbf{x}', \mathbf{x}'', k) \propto |\mathbf{x}' - \mathbf{x}''|^{1-d/2} Y_{1-d/2}(k|\mathbf{x}' - \mathbf{x}''|) \tag{9}$$

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

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

$$G^{\delta}(\boldsymbol{x}', \boldsymbol{x}''; E) = G^0(\boldsymbol{x}', \boldsymbol{x}''; E) + \sum_{n=1}^{\infty} \gamma^n \int_P \sqrt{g}_1 \mathrm{d}\Omega_1\, G^0(\Omega', (y_d)', \Omega_1, \eta; E)$$

$$\times \prod_{j=2}^{n} \left[\int_P \sqrt{g}_j \mathrm{d}\Omega_j\, G^0(\Omega_{j-1}, \eta, \Omega_j, \eta; E) \right] G^0(\Omega_n, \eta, \Omega'', (y_d)''; E) \qquad (10)$$

where the integration is performed over the hypersurface P, $g = \det(g^{\mu\nu})$, $g^{\mu\nu} = \frac{\partial x^\mu}{\partial y^\nu}\Big|_P$ is an induced metric tensor on P and we introduce coordinates Ω, y_d corresponding to the initial and final points $\boldsymbol{x}', \boldsymbol{x}''$. 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 Γ of the region $\mathcal{B}$, where κ is some multi-index enumerating the system f, with a standard $L_2(\Omega)$ scalar product

$$\langle f_\kappa, f_{\kappa'} \rangle = \int_\Omega \sqrt{g(\Omega)}\, \bar{f}_\kappa(\Omega) f_{\kappa'}(\Omega)\, \mathrm{d}\Omega = \delta_{\kappa,\kappa'}. \qquad (11)$$

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

We represent G^0 in the form

$$G^0(\Omega', \xi, \Omega'', \eta; E) = \sum_{\kappa', \kappa''} \mathcal{G}_{\kappa', \kappa''}(\xi, \eta; E) f_{\kappa'}(\Omega') \bar{f}_{\kappa''}(\Omega'') \qquad (12)$$

so that the coefficient $\mathcal{G}_{\kappa',\kappa''}(\xi, \eta; E)$ is expressed as

$$\mathcal{G}_{\kappa',\kappa''}(\xi, \eta; E) = \int \sqrt{g(\Omega')g(\Omega'')}\, G^0(\Omega', \xi, \Omega'', \eta; E) f_{\kappa'}(\Omega') \bar{f}_{\kappa''}(\Omega'')\, \mathrm{d}\Omega'\, \mathrm{d}\Omega''. \qquad (13)$$

Then, substituting (12) in (10) we get

$$G^{\delta}(\boldsymbol{x}', \boldsymbol{x}''; E) = G^0(\boldsymbol{x}', \boldsymbol{x}''; E) + \sum_{n=1}^{\infty} \gamma^n \int_P \sqrt{g}_1 \mathrm{d}\Omega_1 \sum_{\kappa', \kappa_1} \mathcal{G}_{\kappa', \kappa_1}((y_d)', \eta; E)$$

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

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

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

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

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

$$G^{\delta}(\boldsymbol{x}', \boldsymbol{x}''; E) = G^0(\boldsymbol{x}', \boldsymbol{x}''; E) + \Bigg(\sum_{\kappa', \kappa''} \Big[\mathcal{G}((y_d)', \eta; E)(\gamma^{-1} - \mathcal{G}(\eta, \eta; E))^{-1}$$

$$\times \mathcal{G}(\eta, (y_d)''; E) \Big]_{\kappa', \kappa''} f_{\kappa'}(\Omega') \bar{f}_{\kappa''}(\Omega'') \Bigg). \qquad (15)$$

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

$$G^\delta(\boldsymbol{x}', \boldsymbol{x}''; E) = G^0(\boldsymbol{x}', \boldsymbol{x}''; E) - \left(\sum_{\kappa',\kappa''}\Big[\mathcal{G}((y_d)', \eta; E)\mathcal{G}(\eta, \eta; E)^{-1}\mathcal{G}(\eta, (y_d)''; E)\Big]_{\kappa',\kappa''} \times f_{\kappa'}(\Omega')\bar{f}_{\kappa''}(\Omega'')\right) \tag{16}$$

which is the main result of our paper.

3. Discussion

As can easily be seen, the propagator (16) solves an appropriate Dirichlet boundary problem. Indeed, the statement that the object constructed above satisfies the differential equation (1) is evident from the construction and, if $(y_d)' = \eta$ or $(y_d)'' = \eta$, i.e. if the initial or 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 (16), which means that the Dirichlet boundary condition is obeyed.

It is worthwhile pointing 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 the two-dimensional case the multi-index κ becomes an ordinary one and we obtain the condition of vanishing determinant

$$\operatorname{Det}\mathcal{G}(\eta, \eta; E) = 0. \tag{17}$$

From the last equation it can easily be seen that our approach looks like an alternative to and generalization of the boundary integral method [15, 16], where the spectrum of a 2D billiard can be obtained based on an integral of the normal derivative of the Green function over the boundary.

It is also easy to demonstrate that equation (16) leads to a known formula for the case of separability of variables. Let us perform this explicitly for the 2D case of a quantum particle in a circular region ($\Gamma = \{\boldsymbol{x} : |\boldsymbol{x}| = R\}$). An appropriate formula for the Green function in polar coordinates (r, ϕ) [4] (see also [17] for an alternative derivation) reads

$$G(\boldsymbol{x}, \boldsymbol{x}'; E) = \sum_{m=-\infty}^{\infty} G_l(r, r', E)\mathrm{e}^{\mathrm{i}m(\phi'-\phi)} \tag{18}$$

$$G_l(r, r'; E) = G_l^0(r, r'; E) - \frac{G_l^0(r', R; E)G_l^0(R, r'; E)}{G_l^0(R, R; E)}. \tag{19}$$

A natural choice of family for the functions is of course $f_m(\phi) = \exp\{\mathrm{i}m\phi\}$. Expanding the free particle Green function in the same manner as in (18) and calculating the coefficient of equation (12) one can see that

$$\mathcal{G}_{mm'}(r, r'; E) = G_m^0(r, r'; E)\delta_{mm'} \tag{20}$$

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

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

Equation (16) can be rewritten in a more formal way, introducing the series expansion of $G^\delta(\boldsymbol{x}', \boldsymbol{x}''; E)$ in a manner like (12) for G^0. Then

$$\begin{aligned}\mathcal{G}^\delta_{\kappa'\kappa''}((y_d)', (y_d)''; E) \\ = \mathcal{G}_{\kappa'\kappa''}((y_d)', (y_d)''; E) - \left[\mathcal{G}((y_d)', \eta; E)\mathcal{G}(\eta, \eta; E)^{-1}\mathcal{G}(\eta, (y_d)''; E)\right]_{\kappa',\kappa''} \quad (21)\end{aligned}$$

or in operator notation

$$\hat{\mathcal{G}}^\delta((y_d)', (y_d)''; E) = \hat{\mathcal{G}}((y_d)', (y_d)''; E) - \hat{\mathcal{G}}((y_d)', \eta; E)\hat{\mathcal{G}}(\eta, \eta; E)^{-1}\hat{\mathcal{G}}(\eta, (y_d)''; E). \quad (22)$$

The last expression is suitable for further formal manipulation in the case of the double δ-perturbation $V = \gamma(\delta(y_d - a) + \delta(y_d - b))$, where the system is being 'squeezed' into a narrow shell $a \leqslant \eta \leqslant b$, simulating the quantization on a hypersurface in the limit $a \to b$ in a manner similar to [4] (see [4, equation 2.15]), but the detailed analysis will be published elsewhere.

It should be mentioned that our approach can also be modified to be used for more general perturbation of the form $\tilde{V}^\delta = -\gamma h(\boldsymbol{x})\delta_P(\boldsymbol{x})$ 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 $\sqrt{g}\ h(\Omega, \eta)$. Then, we should use another family of functions for the expansion, or, rather than expand the Green function, it may be more convenient to perform a series expansion of the product

$$\sqrt{h(\Omega; \xi)h(\Omega'', \eta)}G^0(\Omega', \xi, \Omega'', \eta; E) = \sum_{\kappa',\kappa''} \tilde{\mathcal{G}}_{\kappa',\kappa''}(\xi, \eta; E) f_{\kappa'}(\Omega')\bar{f}_{\kappa''}(\Omega'') \quad (23)$$

where the final formula becomes

$$\begin{aligned}\tilde{G}^\delta(\boldsymbol{x}', \boldsymbol{x}''; E) = G^0(\boldsymbol{x}', \boldsymbol{x}''; E) - \sum_{\kappa',\kappa''} \frac{f_{\kappa'}(\Omega')\bar{f}_{\kappa''}(\Omega'')}{\sqrt{h(\Omega'', (y_d)')h(\Omega'', (y_d)'')}} \\ \times \left[\tilde{\mathcal{G}}((y_d)', \eta; E)\tilde{\mathcal{G}}(\eta, \eta; E)^{-1}\tilde{\mathcal{G}}(\eta, (y_d)''; E)\right]_{\kappa',\kappa''}. \quad (24)\end{aligned}$$

Such a generalization may be useful for systems with a boundary whose initial shape is not very convenient for the construction of the function family set f_κ and where 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 'local-time rescaling' [18]), the initially pure δ-function perturbation really transforms to a non-uniform one as discussed above.

Acknowledgments

Financial support from the Ministry of Science and Technology of the Republic of Slovenia is acknowledged with thanks. This work was also supported by the Rector's Fund of the University of Maribor. GK acknowledges financial support under postdoctoral Grant No SZF-CAMTP01-MZS/1997 of the Slovenian Science Foundation.

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