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A trace formula for Dirac Green's functions related by Darboux transformations

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Abstract
We construct Green's functions and a trace formula for pairs of stationary Dirac equations under Sturm–Liouville boundary conditions, where the equations are related to each other by a Darboux transformation. Our findings generalize former results (Pozdeeva E 2008 *J. Phys. A: Math. Theor* at press).

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1. Introduction

The Darboux transformation is one of the major tools for constructing integrable cases of quantum-mechanical equations. While originally it had been developed for equations of stationary Schrödinger type [5], the Darboux transformation has been proved generalizable to a variety of linear and nonlinear equations. Examples of linear equations include generalizations of the stationary Schrödinger equation, such as the time-dependent case [3, 6], the effective mass Schrödinger equation [13, 14] and the Schrödinger equation with weighted energy [16, 17]. Besides, the Darboux transformation has been found to be applicable to the stationary Dirac equation [8, 11], which we focus on in the present paper. In particular, we consider a Dirac equation with Sturm–Liouville boundary conditions on a real interval and study the behavior of the associated Green's function and its trace under Darboux transformations. The interest in the trace of the Green's function that belongs to a stationary Dirac equation lies in the fact that its imaginary part gives the spectral density (density of energy levels). For Schrödinger equations and effective mass Schrödinger equations it has been shown [9, 15] that traces of Green's functions that are related by Darboux transformations, fulfil a surprisingly simple relation (trace formula). In the present paper we show that the same trace formula is valid for Green's functions of Dirac equations with Sturm–Liouville boundary conditions

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that are related to each other by a Darboux transformation. In particular, we state the Green's function of the boundary value problem and its trace in closed form, then we show how the Sturm–Liouville boundary conditions change under the Darboux transformation, and finally we derive the trace formula. Note that the results in this paper generalize former findings [10], as in the present case we generalize the potential used in the Dirac equation and the boundary conditions. Our generalized boundary conditions involve linear combinations of the solution's values at the interval border points; such boundary conditions are frequently used in applications, e.g. in modeling fermions on a terminated honeycomb lattice [1], inverse spectral problems [2] and the study of relativistic supersymmetric systems with singularities [18]. An overview on Dirac equations with generalized boundary conditions can be found in [4]. For the sake of completeness, in section 2 we review basic facts about the Darboux transformation for the Dirac equation. Section 3 contains a summary of our results, which we prove in section 4. Finally, section 5 is devoted to an example.

2. Preliminaries: the Darboux transformation

Let σ_j, $j = 1, 2, 3$, denote the Pauli matrices, let I be the identity matrix and let $\gamma = \mathrm{i}\sigma_2$. The stationary Dirac equation in one dimension can be written in the form

$$\gamma\Psi'(x) + V_0(x)\Psi(x) = EI\Psi(x), \tag{1}$$

where Ψ is a two-component spinor, the constant E denotes the energy and the (2×2)-matrix potential V_0 reads as

$$V_0(x) = r(x)I + p(x)\sigma_1 + q(x)\sigma_3 = \begin{pmatrix} r(x)+q(x) & p(x) \\ p(x) & r(x)-q(x) \end{pmatrix}. \tag{2}$$

Here r, p and q are real-valued functions. Now, let the two spinors u_1 and u_2 be linearly independent solutions of the Dirac equation (1) at energies $\lambda_1 \neq E$ and $\lambda_2 \neq E$, respectively, with $\lambda_1 \neq \lambda_2$, such that the matrix $u(x) = (u_1(x), u_2(x))$ is invertible. Define the Darboux transformation $\tilde{\Psi}$ of Ψ as

$$\tilde{\Psi}(x) = \Psi'(x) - u'(x)u^{-1}(x)\Psi(x). \tag{3}$$

Then this function $\tilde{\Psi}$ solves the Dirac equation

$$\gamma\tilde{\Psi}'(x) + V_1(x)\tilde{\Psi}(x) = EI\tilde{\Psi}(x), \tag{4}$$

where the transformed potential V_1 is given by

$$V_1(x) = V_0(x) + [\gamma, u'(x)u^{-1}(x)].$$

For more details on the Darboux transformation for the Dirac equation see e.g. [11] and references therein.

3. Summary of results

For two arbitrary real numbers α and β we consider the following Dirac equation with homogeneous boundary value conditions on the interval $[a, b] \subset \mathbb{R}$:

$$\gamma\Psi'(x) + (V_0(x) - EI)\Psi(x) = 0 \tag{5}$$

$$(\cos(\alpha), \sin(\alpha))\Psi(a) = 0 \tag{6}$$

$$(\cos(\beta), \sin(\beta))\Psi(b) = 0. \tag{7}$$

The Hamiltonian associated with the Dirac equation (6) has discrete spectrum, if the boundary conditions (6) and (7) are present (this prevents Green's function trace from divergence) [7]. Let Ψ_1 be a solution of the Dirac equation (5) that fulfils the boundary condition (6) and let Ψ_2 be a solution of the Dirac equation (5) that fulfils the boundary condition (7).

3.1. Green's function

Green's function G of the Dirac equation (5) with boundary conditions (6), (7) is given by

$$G(x, y) = \frac{1}{C}\big(\Psi_2(x)\Psi_1^T(y)\theta(x-y) + \Psi_1(x)\Psi_2^T(y)\theta(y-x)\big), \tag{8}$$

where θ stands for the Heaviside distribution and C is a constant that is determined by the choice of Ψ_1 and Ψ_2.

3.2. The boundary conditions

Let $\tilde{\Psi}_1$ and $\tilde{\Psi}_2$ be the Darboux transformed solutions Ψ_1 and Ψ_2, respectively, as defined in (3). Recall that Ψ_1 satisfies the first boundary condition (6) and that Ψ_2 satisfies the second boundary condition (7). If the corresponding auxiliary functions u_1, u_2 solve the boundary value problem (5) at energy λ_1 and λ_2, respectively, and fulfil both boundary conditions (6) and (7), then the functions $\tilde{\Psi}_1$ and $\tilde{\Psi}_2$ satisfy

$$\tilde{\Psi}_1(a) = \tilde{\Psi}_2(b) = 0, \tag{9}$$

generally in the sense of a limit. Furthermore, Green's function $\tilde{G}$ of the Darboux transformed Dirac equation (4) with boundary condition (9) is given by

$$\tilde{G}(x, y) = \frac{1}{\tilde{C}}(\tilde{\Psi}_2(x)\tilde{\Psi}_1^T(y)\theta(x-y) + \tilde{\Psi}_1(x)\tilde{\Psi}_2^T(y)\theta(y-x)), \tag{10}$$

where $\tilde{C}$ is a constant that is determined by the explicit form of $\tilde{\Psi}_1$ and $\tilde{\Psi}_2$.

3.3. The trace formula

The following relation (trace formula) holds between Green's functions G and $\tilde{G}$:

$$\int_a^b \mathrm{tr}(\tilde{G}(x, x) - G(x, x))\, \mathrm{d}x = \frac{1}{E-\lambda_1} + \frac{1}{E-\lambda_2}, \tag{11}$$

where tr denotes the matrix trace.

4. Proof of results

In the following we show that the three statements given in the previous section hold.

4.1. Green's function

We must show that the function G in (8) is symmetric in its variables, that it fulfils the boundary conditions (6), (7) and that application of the left-hand side of the Dirac equation (5) to G gives a delta $\delta(x-y)I$. First, it is apparent that function (8) is invariant under the exchange of x and y. In order to show that it satisfies the boundary conditions (6) and (7), let us assume that $x \geqslant y$ in (8), which implies $\theta(x-y)=1, \theta(y-x)=0$. Writing $\Psi_j=(\Psi_{j,1},\Psi_{j,2})^T$ for $j=1,2$, we find

$$
\begin{aligned}
(\cos(\alpha),\sin(\alpha))G(a,y) &= (\cos(\alpha),\sin(\alpha))\frac{1}{C}\Psi_2(a)\Psi_1^T(y)\\
&= \frac{1}{C}\begin{pmatrix}\cos(\alpha)\Psi_{2,1}(a)\Psi_{1,1}(y)+\sin(\alpha)\Psi_{2,2}(a)\Psi_{1,1}(y)\\ \cos(\alpha)\Psi_{2,1}(a)\Psi_{1,2}(y)+\sin(\alpha)\Psi_{2,2}(a)\Psi_{1,2}(y)\end{pmatrix}^T\\
&= 0,
\end{aligned}
$$

because of the second boundary condition (6). In the same way one shows that the second boundary condition (7), when applied to G, is satisfied. If $x < y$, then G also fulfils the boundary conditions due to its symmetry in x and y. It remains to show that substitution of G in the Dirac equation gives a delta. Making use of the differentiation rules $\theta_x(\pm x \mp y) = \pm\delta(x-y)$ and the Dirac equation (5), we get

$$
\begin{aligned}
&\gamma\frac{\partial}{\partial x}G(x,y)+(V_0(x)-EI)G(x,y)\\
&\quad= \gamma\frac{1}{C}\big(\Psi_2'(x)\Psi_1^T(y)\theta(x-y)+\Psi_1'(x)\Psi_2^T(y)\theta(y-x)\big)\\
&\qquad+\gamma\frac{1}{C}\big(\Psi_2(x)\Psi_1^T(y)-\Psi_1(x)\Psi_2^T(y)\big)\delta(x-y)\\
&\qquad+(V_0(x)-EI)\frac{1}{C}\big(\Psi_2(x)\Psi_1^T(y)\theta(x-y)+\Psi_1(x)\Psi_2^T(y)\theta(y-x)\big)\\
&\quad= \frac{1}{C}\big((EI-V_0(x))\Psi_2(x)\Psi_1^T(y)\theta(x-y)+(EI-V_0(x))\Psi_1(x)\Psi_2^T(y)\theta(y-x)\\
&\qquad+\gamma\frac{1}{C}\big(\Psi_2(x)\Psi_1^T(y)-\Psi_1(x)\Psi_2^T(y)\big)\delta(x-y)\\
&\qquad+(V_0(x)-EI)\frac{1}{C}\big(\Psi_2(x)\Psi_1^T(y)\theta(x-y)+\Psi_1(x)\Psi_2^T(y)\theta(y-x)\big)\\
&\quad= \gamma\frac{1}{C}\big(\Psi_2(x)\Psi_1^T(y)-\Psi_1(x)\Psi_2^T(y)\big)\delta(x-y).
\end{aligned}
\tag{12}
$$

We cannot continue until we evaluate explicitly the components of the latter expression. We find

$$
\begin{aligned}
&\gamma\big(\Psi_2(x)\Psi_1^T(y)-\Psi_1(x)\Psi_2^T(y)\big)\\
&\quad= \begin{pmatrix}\Psi_{2,2}(x)\Psi_{1,1}(y)-\Psi_{1,2}(x)\Psi_{2,1}(y) & \Psi_{2,2}(x)\Psi_{1,2}(y)-\Psi_{1,2}(x)\Psi_{2,2}(y)\\ \Psi_{1,1}(x)\Psi_{2,1}(y)-\Psi_{2,1}(x)\Psi_{1,1}(y) & \Psi_{1,1}(x)\Psi_{2,2}(y)-\Psi_{2,1}(x)\Psi_{1,2}(y)\end{pmatrix}.
\end{aligned}
\tag{13}
$$

Restriction to $y=x$ gives

$$
\begin{aligned}
&\gamma\big(\Psi_2(x)\Psi_1^T(x)-\Psi_1(x)\Psi_2^T(x)\big)\\
&\quad= \begin{pmatrix}\Psi_{2,2}(x)\Psi_{1,1}(x)-\Psi_{1,2}(x)\Psi_{2,1}(x) & 0\\ 0 & \Psi_{1,1}(x)\Psi_{2,2}(x)-\Psi_{2,1}(x)\Psi_{1,2}(x)\end{pmatrix},
\end{aligned}
\tag{14}
$$

that is, the matrix takes diagonal form, where the diagonal elements are the same. We will now show that these elements are constants with respect to x by proving that their derivative vanishes. To this end, we write them in matrix form:

$$\Psi_{1,1}(x)\Psi_{2,2}(x)-\Psi_{1,2}(x)\Psi_{2,1}(x)=\Psi_1^T(x)\gamma\Psi_2(x).$$

We compute the derivative of the latter expression, using the fact that $\gamma^T = -\gamma$:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\Psi_1^T(x)\gamma\Psi_2(x)\right) = \left(\Psi_1^T\right)'(x)\gamma\Psi_2(x) + \Psi_1^T(x)\gamma\Psi_2'(x)$$
$$= -(\gamma\Psi_1'(x))^T\Psi_2(x) + \Psi_1^T(x)\gamma\Psi_2'(x). \quad (15)$$

Now we make use of the Dirac equation (5), that is, for $j = 1, 2$ we have

$$\gamma\Psi_j'(x) = (EI - V_0(x))\Psi_j(x),$$

which we insert into expression (15) and arrive at

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\Psi_1^T(x)\gamma\Psi_2(x)\right) = ((V_0(x) - EI)\Psi_1(x))^T\Psi_2(x) + \Psi_1^T(x)(EI - V_0(x))\Psi_2(x)$$
$$= \Psi_1^T(x)((V_0(x) - EI)^T + EI - V_0(x))\Psi_2(x).$$

From the explicit form (2) of the potential V_0 we infer $V_0^T = V_0$. Since furthermore EI is diagonal, we have that

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\Psi_1^T(x)\gamma\Psi_2(x)\right) = \Psi_1^T(x)(V_0(x) - EI + EI - V_0(x))\Psi_2(x)$$
$$= 0.$$

Thus, $-\Psi_1^T(x)\gamma\Psi_2(x)$ is a constant and we define the constant C via

$$C = \Psi_1^T(x)\gamma\Psi_2(x). \quad (16)$$

Insertion of this C into (12) finally gives by means of (13) and (14) that

$$\left[\frac{1}{C}\gamma\left(\Psi_2(x)\Psi_1^T(y) - \Psi_1(x)\Psi_2^T(y)\right)\right]_{|y=x}\delta(x-y)$$
$$= \left[\frac{1}{\Psi_1^T(x)\gamma\Psi_2(x)}\gamma\left(\Psi_2(x)\Psi_1^T(y) - \Psi_1(x)\Psi_2^T(y)\right)\right]_{|y=x}\delta(x-y)$$
$$= \delta(x-y)I.$$

This, together with (12), gives the final result

$$\gamma\frac{\partial}{\partial x}G(x,y) + (V_0(x) - EI)G(x,y) = \delta(x-y)I.$$

This proves the first statement in the previous section.

4.2. The boundary conditions

For $j = 1, 2$ let $u_j = (u_{j,1}, u_{j,2})^T$ be the auxiliary solutions of the Dirac equation (5) at energies $\lambda_1 \neq E, \lambda_2 \neq E$ with $\lambda_1 \neq \lambda_2$, that fulfil the boundary conditions (6) and (7). Furthermore, let $u = (u_{jk})$ be the (2×2)-matrix that contains the auxiliary solutions in its columns and let λ be the diagonal matrix that has λ_1 and λ_2 as its diagonal elements. The matrix u satisfies the Dirac equation (5) in the following sense:

$$\gamma u'(x) = u(x)\lambda - V_0(x)u(x). \quad (17)$$

We need to show that the Darboux transformed solution $\tilde{\Psi}_1$, as given in (3), fulfils the boundary conditions (9), if Ψ_1 fulfills the first boundary condition (6). Afterward, we show that $\tilde{\Psi}_2$ fulfils (9), if Ψ_2 fulfils the second boundary condition (7). As for the first case, consider the Darboux transformation (3):

$$\tilde{\Psi}_1(x) = \Psi_1'(x) - u'(x)u^{-1}(x)\Psi_1(x). \quad (18)$$

We cannot evaluate this expression at $x = a$ (as the matrix u^{-1} is singular there), but we can take the limit $x \to a$ in (18). To this end, we need the explicit form of u^{-1}, given by

$$u^{-1}(x) = \frac{1}{\det(u(x))} \begin{pmatrix} u_{22}(x) & -u_{12}(x) \\ -u_{21}(x) & u_{11}(x) \end{pmatrix}.$$

This we can use to write the last two factors on the right-hand side of (18) in components. Using $\Psi_1 = (\Psi_{11}, \Psi_{12})^T$, we get

$$u^{-1}(x)\Psi_1(x) = \frac{1}{\det(u(x))} \begin{pmatrix} u_{22}(x)\Psi_{11}(x) - u_{12}(x)\Psi_{12}(x) \\ -u_{21}(x)\Psi_{11}(x) + u_{11}(x)\Psi_{12}(x) \end{pmatrix}. \tag{19}$$

We now compute the limit $x \to a$ of the latter expression, employing the rule of de l'Hopital. To this end, we differentiate numerator and denominator of each component in (19). We find

$$\left[\frac{\mathrm{d}}{\mathrm{d}x}(u_{22}(x)\Psi_{11}(x) - u_{12}(x)\Psi_{12}(x))\right]\left(\frac{\mathrm{d}}{\mathrm{d}x}\det(u(x))\right)^{-1}$$
$$= \frac{u'_{22}(x)\Psi_{11}(x) + u_{22}(x)\Psi'_{11}(x) - u'_{12}(x)\Psi_{12}(x) - u_{12}(x)\Psi'_{12}(x)}{u'_{11}(x)u_{22}(x) + u_{11}(x)u'_{22}(x) - u'_{21}(x)u_{12}(x) - u_{21}(x)u'_{12}(x)}$$
$$\left[\frac{\mathrm{d}}{\mathrm{d}x}(-u_{21}(x)\Psi_{11}(x) + u_{11}(x)\Psi_{12}(x))\right]\left(\frac{\mathrm{d}}{\mathrm{d}x}\det(u(x))\right)^{-1}$$
$$= \frac{-u'_{21}(x)\Psi_{11}(x) - u_{21}(x)\Psi'_{11}(x) + u'_{11}(x)\Psi_{12}(x) + u_{11}(x)\Psi'_{12}(x)}{u'_{11}(x)u_{22}(x) + u_{11}(x)u'_{22}(x) - u'_{21}(x)u_{12}(x) - u_{21}(x)u'_{12}(x)}.$$

This we evaluate at $x = a$ and obtain together with (19) that

$$u^{-1}(a)\Psi_1(a) = \begin{pmatrix} \dfrac{u'_{22}(a)\Psi_{11}(a) + u_{22}(a)\Psi'_{11}(a) - u'_{12}(a)\Psi_{12}(a) - u_{12}(a)\Psi'_{12}(a)}{u'_{11}(a)u_{22}(a) + u_{11}(a)u'_{22}(a) - u'_{21}(a)u_{12}(a) - u_{21}(a)u'_{12}(a)} \\ \dfrac{-u'_{21}(a)\Psi_{11}(a) - u_{21}(a)\Psi'_{11}(a) + u'_{11}(a)\Psi_{12}(a) + u_{11}(a)\Psi'_{12}(a)}{u'_{11}(a)u_{22}(a) + u_{11}(a)u'_{22}(a) - u'_{21}(a)u_{12}(a) - u_{21}(a)u'_{12}(a)} \end{pmatrix}. \tag{20}$$

We substitute the latter expression into the Darboux transformation (18) and evaluated at $x = a$:

$$\tilde{\Psi}_1(a) = \left(\frac{\mathrm{d}}{\mathrm{d}x}\det(u(x))_{|x=a}\right)^{-1}(A\Psi_1(a) + B\Psi'_1(a)), \tag{21}$$

where the constant A and the matrix B are given by

$$A = u'_{12}(a)u'_{21}(a) - u'_{11}(a)u'_{22}(a)$$
$$B = \begin{pmatrix} u_{11}(a)u'_{22}(a) - u_{12}(a)u'_{21}(a) & u'_{11}(a)u_{12}(a) - u'_{12}(a)u_{11}(a) \\ u'_{22}(a)u_{21}(a) - u'_{21}(a)u_{22}(a) & u_{22}(a)u'_{11}(a) - u'_{12}(a)u_{21}(a) \end{pmatrix}. \tag{22}$$

Since the auxiliary functions satisfy the boundary conditions (6) and (7), we obtain from (22) that

$$(\cos(\alpha), \sin(\alpha))B = 0. \tag{23}$$

Now we can show that the Darboux transformed solution $\tilde{\Psi}_1 = (\tilde{\Psi}_{11}, \tilde{\Psi}_{22})^T$ satisfies the boundary condition (6). Application of $(\cos(\alpha), \sin(\alpha))$ to (21) gives

$$(\cos(\alpha), \sin(\alpha))\tilde{\Psi}_1(a) = \left(\frac{\mathrm{d}}{\mathrm{d}x}\det(u(x))_{|x=a}\right)^{-1}$$
$$\times [A(\cos(\alpha), \sin(\alpha))\Psi_1(a) + (\cos(\alpha), \sin(\alpha))B\Psi'_1(a)].$$

The latter expression vanishes, since Ψ_1 satisfies the boundary condition (6) and because of (23):

$$(\cos(\alpha), \sin(\alpha))\tilde{\Psi}_1(a) = 0. \tag{24}$$

Before we continue here, we need a reformulation of the Darboux transformation (18), where we substitute the derivatives of Ψ and u by means of (5) and (17):

$$\begin{aligned}\tilde{\Psi}_1(x) &= \Psi_1'(x) - u'(x)u^{-1}(x)\Psi_1(x)\\ &= \gamma^{-1}(EI - V_0(x))\Psi_1(x) - (\gamma^{-1}u(x)\lambda - \gamma^{-1}V_0(x)u(x))u^{-1}(x)\Psi_1(x)\\ &= \gamma^{-1}(EI - u(x)\lambda u^{-1}(x))\Psi_1(x).\end{aligned} \tag{25}$$

We evaluate the latter Darboux transformation at $x = a$ (the term $u^{-1}(a)\Psi_1(a)$ being given by (20)), and apply $(\sin(\alpha), -\cos(\alpha))$ from the left. This renders (25) in the following form:

$$\begin{aligned}(\sin(\alpha), -\cos(\alpha))\tilde{\Psi}_1(a) &= (\sin(\alpha), -\cos(\alpha))\gamma^{-1}EI\Psi_1(a)\\ &\quad - (\sin(\alpha), -\cos(\alpha))\gamma^{-1}u(a)\lambda u^{-1}(a)\Psi_1(a)\\ &= (\cos(\alpha), \sin(\alpha))EI\Psi_1(a) - (\cos(\alpha), \sin(\alpha))u(a)\lambda u^{-1}(a)\Psi_1(a)\\ &= 0,\end{aligned} \tag{26}$$

because $(\sin(\alpha), -\cos(\alpha))$ commutes with the diagonal matrix EI, and because Ψ_1 and the columns of u fulfil the boundary condition (6). If we combine (24) and (26), then we obtain that each component of $\tilde{\Psi}_1$ must vanish, that is,

$$\tilde{\Psi}_1(a) = 0,$$

which is the desired result. In a completely analogous way one obtains $\tilde{\Psi}_2(b) = 0$.

4.3. The trace formula

Before we can derive the trace formula (11), we need to establish a relation between the constant C as defined in (16) and its counterpart $\tilde{C}$, given by

$$\begin{aligned}C &= \Psi_1^T(x)\gamma\Psi_2(x) = (\Psi_{1,1}(x)\Psi_{2,2}(x) - \Psi_{1,2}(x)\Psi_{2,1}(x))\\ \tilde{C} &= \tilde{\Psi}_1^T(x)\gamma\tilde{\Psi}_2(x) = (\tilde{\Psi}_{1,1}(x)\tilde{\Psi}_{2,2}(x) - \tilde{\Psi}_{1,2}(x)\tilde{\Psi}_{2,1}(x)).\end{aligned}$$

These expressions are in fact constants, as we have seen in (16). In order to relate the constants to each other, let us consider $\tilde{C}$, taking into account that $\gamma^T\gamma = I$ and that the matrix product inside a trace is commutative:

$$\begin{aligned}\tilde{C} &= \mathrm{tr}\left(\gamma\tilde{\Psi}_2(x)\tilde{\Psi}_1^T(x)\right)\\ &= \mathrm{tr}\left(\gamma\tilde{\Psi}_2(x)\tilde{\Psi}_1^T(x)\gamma^T\gamma\right)\\ &= \mathrm{tr}\left(\gamma\tilde{\Psi}_2(x)(\gamma\tilde{\Psi}_1(x))^T\gamma\right).\end{aligned} \tag{27}$$

Next, we replace the function $\tilde{\Psi}_j$, $j = 1, 2$ by the form given in (25), that is,

$$\tilde{\Psi}_j(x) = \gamma^{-1}(EI - u(x)\lambda u^{-1}(x))\Psi_j(x).$$

Substitution of these expressions into (27) gives

$$\begin{aligned}\tilde{C} &= \mathrm{tr}\left(\gamma(EI - u(x)\lambda u^{-1}(x))\Psi_2(x)\Psi_1^T(x)(EI - u(x)\lambda u^{-1}(x))^T\right)\\ &= \mathrm{tr}\big[E^2\gamma\Psi_2(x)\Psi_1^T(x) - E\left(\gamma u(x)\lambda u^{-1}(x) + (u(x)\lambda u^{-1}(x))^T\gamma\right)\Psi_2(x)\Psi_1^T(x)\\ &\quad + [u(x)\lambda u^{-1}(x)]^T\gamma u(x)\lambda u^{-1}(x)\Psi_2(x)\Psi_1^T(x)\big].\end{aligned} \tag{28}$$

The coefficients of $\Psi_2\Psi_1^T$ in the trace take a very simple explicit form:

$$\begin{aligned}&\gamma u(x)\lambda u^{-1}(x) + (u(x)\lambda u^{-1}(x))^T\gamma = \gamma(\lambda_1 + \lambda_2)\\ &(u(x)\lambda u^{-1}(x))^T\gamma u(x)\lambda u^{-1}(x) = \gamma\lambda_1\lambda_2.\end{aligned} \tag{29}$$

If we insert these relations into trace (28), we get

$$\begin{aligned}\tilde{C} &= \mathrm{tr}\big[E^2\gamma\Psi_2(x)\Psi_1^T(x) - E\,(\gamma(\lambda_1+\lambda_2))\,\Psi_2(x)\Psi_1^T(x) + \gamma\lambda_1\lambda_2\Psi_2(x)\Psi_1^T(x)\big] \\ &= \big(E^2 - E(\lambda_1+\lambda_2) + \lambda_1\lambda_2\big)\,\mathrm{tr}\big[\gamma\Psi_2(x)\Psi_1^T(x)\big] \\ &= (E-\lambda_1)(E-\lambda_2)C. \end{aligned} \tag{30}$$

This is the relation between $\tilde{C}$ and C that we wanted to derive. Now we are ready to derive the trace formula (11). To this end, consider Green's function G as given in (8). Its trace reads for $y = x$

$$\begin{aligned}\mathrm{tr}(G(x,x)) &= \frac{1}{C}\mathrm{tr}\big(\Psi_1(x)\Psi_2^T(x)\big) \\ &= \frac{1}{C}\mathrm{tr}\left(\Psi_2(x)\Psi_1^T(x)\right). \end{aligned} \tag{31}$$

Since the expressions in the latter two lines are the same, we can choose either of them as a representation of Green's function's trace. Let us take the first one (31) and consider Green's function $\tilde{G}$, as given in (10):

$$\begin{aligned}\mathrm{tr}(\tilde{G}(x,x)) &= \frac{1}{\tilde{C}}\mathrm{tr}\left(\tilde{\Psi}_1(x)\tilde{\Psi}_2^T(x)\right) \\ &= \frac{1}{\tilde{C}}\tilde{\Psi}_1^T(x)\tilde{\Psi}_2(x). \end{aligned} \tag{32}$$

We will now insert the Darboux transformation (3) for $\tilde{\Psi}_1$, which can be rewritten by means of the identity $-u'u^{-1} = u(u^{-1})'$:

$$\tilde{\Psi}_1(x) = u(x)\frac{\mathrm{d}}{\mathrm{d}x}(u^{-1}(x)\Psi_1(x)). \tag{33}$$

This we substitute in (32) and arrive at

$$\begin{aligned}\mathrm{tr}(\tilde{G}(x,x)) &= \frac{1}{\tilde{C}}\frac{\mathrm{d}}{\mathrm{d}x}(u^{-1}(x)\Psi_1(x))^T u^T(x)\tilde{\Psi}_2(x) \\ &= \frac{1}{\tilde{C}}\left[\frac{\mathrm{d}}{\mathrm{d}x}\big(\Psi_1^T(x)\tilde{\Psi}_2(x)\big) - \Psi_1^T(x)(u^{-1}(x))^T\frac{\mathrm{d}}{\mathrm{d}x}(u^T(x)\tilde{\Psi}_2(x))\right]. \end{aligned} \tag{34}$$

Let us now have a look at the second term on the right-hand side of the latter equality:

$$\begin{aligned}\Psi_1^T(x)(u^{-1}(x))^T\frac{\mathrm{d}}{\mathrm{d}x}(u^T(x)\tilde{\Psi}_2(x)) &= \Psi_1^T(x)(u^{-1}(x))^T((u'(x))^T\tilde{\Psi}_2(x) + u^T(x)\tilde{\Psi}_2'(x)) \\ &= \Psi_1^T(x)(\tilde{\Psi}_2'(x) + (u'(x)u^{-1}(x))^T\tilde{\Psi}_2(x)). \end{aligned}$$

If we now insert the explicit form of the Darboux transformation (3) for $\tilde{\Psi}_2$, then we get

$$\Psi_1^T(x)(u^{-1}(x))^T\frac{\mathrm{d}}{\mathrm{d}x}(u^T(x)\tilde{\Psi}_2(x)) = \left(\frac{\mathrm{d}}{\mathrm{d}x} + (u'(x)u^{-1}(x))^T\right)\left(\frac{\mathrm{d}}{\mathrm{d}x} - u'(x)u^{-1}(x)\right)\Psi_2(x). \tag{35}$$

Since the coefficients in the Dirac equation (5) are real-valued, the matrix u can be chosen to have real-valued entries. In this case, the two differential operators on the right-hand side of (35) correspond to the Darboux operator and its adjoint [11]. Application of these two operators gives

$$\Psi_1^T(x)(u^{-1}(x))^T\frac{\mathrm{d}}{\mathrm{d}x}(u^T(x)\tilde{\Psi}_2(x)) = -(E-\lambda_1)(E-\lambda_2)\Psi_1^T(x)\Psi_2(x).$$

This we insert into Green's functions trace (34) and obtain by means of relation (30)

$$\begin{aligned}\operatorname{tr}(\tilde{G}(x,x)) &= \frac{1}{\tilde{C}}\left[\frac{\mathrm{d}}{\mathrm{d}x}\left(\Psi_1^T(x)\tilde{\Psi}_2(x)\right) + (E-\lambda_1)(E-\lambda_2)\Psi_1^T(x)\Psi_2(x)\right] \\ &= \frac{1}{(E-\lambda_1)(E-\lambda_2)C}\frac{\mathrm{d}}{\mathrm{d}x}\left(\Psi_1^T(x)\tilde{\Psi}_2(x)\right) + \operatorname{tr}(G(x,x)).\end{aligned}$$

Thus, we find for the trace of Green's functions difference

$$\operatorname{tr}(\tilde{G}(x,x) - G(x,x)) = \frac{1}{(E-\lambda_1)(E-\lambda_2)C}\frac{\mathrm{d}}{\mathrm{d}x}\left(\Psi_1^T(x)\tilde{\Psi}_2(x)\right). \tag{36}$$

Recall that we used the explicit form of the Darboux transformation for the function $\tilde{\Psi}_1$ in (33). If we instead had substituted the Darboux transformation for $\tilde{\Psi}_2$, we would have arrived at the following Green functions difference:

$$\operatorname{tr}(\tilde{G}(x,x) - G(x,x)) = \frac{1}{(E-\lambda_1)(E-\lambda_2)C}\frac{\mathrm{d}}{\mathrm{d}x}\left(\tilde{\Psi}_1^T(x)\Psi_2(x)\right). \tag{37}$$

Before we proceed with the integration of the trace, let us derive a relation between the right-hand sides of (36) and (37). Their difference is zero and thus,

$$\tilde{\Psi}_1^T(x)\Psi_2(x) - \Psi_1^T(x)\tilde{\Psi}_2(x) = K,$$

for a constant K, the explicit form of which we will derive now. To this end, recall that Ψ_1, Ψ_2 solve the Dirac equation (5), that the matrix u fulfils (17) and that $\gamma^{-1} = \gamma^T = -\gamma$:

$$\begin{aligned}&\tilde{\Psi}_1^T(x)\Psi_2(x) - \Psi_1^T(x)\tilde{\Psi}_2(x) \\ &\quad = \Psi_1^T(x)(((u(x)\lambda u^{-1}(x))^T - E)\gamma^T - \gamma(u(x)\lambda u^{-1}(x) - E))\Psi_2(x) \\ &\quad = 2E\Psi_1^T(x)\gamma\Psi_2(x) - \Psi_1^T(x)((u(x)\lambda u^{-1}(x))^T\gamma + \gamma u(x)\lambda u^{-1}(x))\Psi_2(x).\end{aligned}$$

We make use of our result (29) and arrive at

$$\tilde{\Psi}_1^T(x)\Psi_2(x) - \Psi_1^T(x)\tilde{\Psi}_2(x) = (2E - \lambda_1 - \lambda_2)C. \tag{38}$$

We now integrate (36), using the latter relation (38) and the boundary conditions (9) for the transformed functions $\tilde{\Psi}_1$ and $\tilde{\Psi}_2$:

$$\begin{aligned}\int_a^b \operatorname{tr}(\tilde{G}(x,x) - G(x,x)) &= \frac{1}{(E-\lambda_1)(E-\lambda_2)C}\left(\Psi_1^T(x)\tilde{\Psi}_2(x)\right)\Big|_a^b \\ &= -\frac{1}{(E-\lambda_1)(E-\lambda_2)C}\left(\Psi_1^T(a)\tilde{\Psi}_2(a)\right) \\ &= -\frac{1}{(E-\lambda_1)(E-\lambda_2)C}\left(\tilde{\Psi}_1^T(a)\Psi_2(a) - (2E-\lambda_1-\lambda_2)C\right) \\ &= \frac{(2E-\lambda_1-\lambda_2)C}{(E-\lambda_1)(E-\lambda_2)C} \\ &= \frac{1}{E-\lambda_1} + \frac{1}{E-\lambda_2}.\end{aligned}$$

This is the trace formula (11) that was to be proved.

5. Application

In the following we present a simple example that illustrates our results.

5.1. The boundary value problem

We consider (5)–(7) for the settings $V_0 = q\sigma_3$ for a constant q, $\alpha = \beta = 0$ and $a = 0$, $b = 1$, that is,

$$\gamma\Psi'(x) + (q\sigma_3 - EI)\Psi(x) = 0 \tag{39}$$

$$(1,0)\Psi(0) = 0 \tag{40}$$

$$(1,0)\Psi(1) = 0. \tag{41}$$

The Hamiltonian associated with equation (39) has discrete spectrum, which consists of positive and negative energies λ_n^+ and λ_n^-, respectively:

$$\lambda_n^{\pm} = \pm\sqrt{(n\pi)^2 + q^2}, \tag{42}$$

where n is a natural number or zero. Let c be an arbitrary real constant, then the solutions Ψ_n^+ and Ψ_n^- corresponding to λ_n^+ and λ_n^-, respectively, have the form

$$\begin{aligned} \Psi_0^{\pm}(x) &= \begin{pmatrix} 0 \\ c \end{pmatrix} \\ \Psi_n^{\pm}(x) &= \begin{pmatrix} \sin(n\pi x) \\ -\frac{n\pi}{\pm\sqrt{(n\pi)^2+q^2}+q}\cos(n\pi x) \end{pmatrix}, \qquad n \in \mathbb{N}. \end{aligned} \tag{43}$$

The functions $\Psi_n^{\pm}$ fulfil the boundary conditions (6) and (7), as can be verified by straightforward substitution.

5.2. Green's functions trace

We are now ready to construct the Green's function of the boundary value problem (39)–(7) according to (8). To this end, let E be a real number such that $E \neq \lambda_n^{\pm}$ for all $n \in \mathbb{N}_0$. Furthermore, let Ψ_1 and Ψ_2 be defined as

$$\Psi_1(x) = \begin{pmatrix} \sin(\sqrt{E^2-q^2}x) \\ -\frac{\sqrt{E^2-q^2}}{E+q}\cos(\sqrt{E^2-q^2}x) \end{pmatrix} \tag{44}$$

$$\Psi_2(x) = \begin{pmatrix} \sin(\sqrt{E^2-q^2}(x-1)) \\ -\frac{\sqrt{E^2-q^2}}{E+q}\cos(\sqrt{E^2-q^2}(x-1)) \end{pmatrix}. \tag{45}$$

Note that these functions Ψ_1 and Ψ_2 also satisfy the boundary conditions (40) and (41). Now we can set up Green's functions trace according to (32):

$$\begin{aligned} \mathrm{tr}(G(x,x)) &= \frac{1}{C}\Psi_1^T(x)\Psi_2(x) \\ &= \frac{1}{C}\left[\frac{E}{E+q}\cos(\sqrt{E^2-q^2}) - \frac{q}{E+q}\cos(\sqrt{E^2-q^2}(2x-1))\right]. \end{aligned} \tag{46}$$

Note that the explicit form of the constant C as given in (16) is not needed now and will be inserted later.

5.3. The Darboux transformation

We want to apply the Darboux transformation (3) to the solutions Ψ_1 and Ψ_2 of (39), that are given in (44) and (45), respectively. To this end, we need the matrix u that contains two auxiliary solutions u_1 and u_2, which we take from the set (43):

$$u_1(x) = \Psi_0^-(x)$$
$$u_2(x) = \Psi_1^-(x).$$

These auxiliary solutions belong to the following energies (42):

$$\lambda_0^- = -q \tag{47}$$

$$\lambda_1^- = -\sqrt{\pi^2 + q^2}. \tag{48}$$

The matrix u of auxiliary solutions then reads $u = (u_1, u_2)$, that is,

$$u(x) = \begin{pmatrix} 0 & \sin(\pi x) \\ c & \dfrac{\pi}{\sqrt{\pi^2 + q^2} - q}\cos(\pi x) \end{pmatrix}.$$

This gives for the term $u'u^{-1}$ that occurs in the Darboux transformation (3):

$$u'(x)u^{-1}(x) = \begin{pmatrix} \pi \operatorname{cotan}(\pi x) & 0 \\ -\sqrt{\pi^2 + q^2} - q & 0 \end{pmatrix}.$$

On employing this result, we can write down the Darboux transformation (3), applied to the function Ψ_1 as given in (44):

$$\begin{aligned}\tilde{\Psi}_1(x) &= \Psi_1'(x) - u'(x)u^{-1}(x)\Psi_1(x) \\ &= \begin{pmatrix} \sqrt{E^2 - q^2}\cos(\sqrt{E^2 - q^2}x) - \pi \operatorname{cotan}(\pi x)\sin(\sqrt{E^2 - q^2}x) \\ (E + \sqrt{\pi^2 + q^2})\sin(\sqrt{E^2 - q^2}x) \end{pmatrix}. \end{aligned} \tag{49}$$

In the same way we obtain the Darboux transformed solution $\tilde{\Psi}_2$, if we apply the Darboux transformation (3) to the solution Ψ_2 as given in (45), this time using the auxiliary functions $u_1 = \Psi_0^+$ and $u_2 = \Psi_1^-$. This process yields

$$\begin{aligned}\tilde{\Psi}_2(x) &= \Psi_2'(x) - u'(x)u^{-1}(x)\Psi_2(x) \\ &= \begin{pmatrix} \sqrt{E^2 - q^2}\cos(\sqrt{E^2 - q^2}(x-1)) - \pi \operatorname{cotan}(\pi x)\sin(\sqrt{E^2 - q^2}(x-1)) \\ (E + \sqrt{\pi^2 + q^2})\sin(\sqrt{E^2 - q^2}(x-1)) \end{pmatrix}. \end{aligned} \tag{50}$$

We observe that the functions $\tilde{\Psi}_1$ and $\tilde{\Psi}_2$ fulfil the boundary conditions (9) that read in the present case $a = 0$ and $b = 1$:

$$\tilde{\Psi}_1(0) = \tilde{\Psi}_2(1) = 0,$$

where evaluation of the functions $\tilde{\Psi}_1$ and $\tilde{\Psi}_2$ is understood in the sense of a limit.

5.4. The transformed trace and the trace formula

We can now construct the trace of Green's function $\tilde{G}$ that corresponds to the functions $\tilde{\Psi}_1$ and $\tilde{\Psi}_2$. To this end, we employ (32), inserting (49) and (50):

$$\begin{aligned}\operatorname{tr}(\tilde{G}(x,x)) &= \frac{1}{\tilde{C}}\tilde{\Psi}_1^T(x)\tilde{\Psi}_2(x) \\ &= \frac{1}{\tilde{C}}[(E + \sqrt{\pi^2 + q^2})^2 \sin(\sqrt{E^2 - q^2}x)\sin(\sqrt{E^2 - q^2}(x-1)) \\ &\quad + (\sqrt{E^2 - q^2}\cos(\sqrt{E^2 - q^2}x) - \pi \operatorname{cotan}(\pi x)\sin(\sqrt{E^2 - q^2}x)) \\ &\quad \times (\sqrt{E^2 - q^2}\cos(\sqrt{E^2 - q^2}(x-1)) - \pi \operatorname{cotan}(\pi x)\sin(\sqrt{E^2 - q^2}(x-1)))]. \end{aligned} \tag{51}$$

We are now ready to verify the trace formula (11) for the present example. Integration of trace (46) gives

$$\int_0^1 \operatorname{tr}(G(x,x))\,\mathrm{d}x = \frac{1}{C}\left[\frac{E}{E+q}\cos(\sqrt{E^2-q^2}) - \frac{q}{\sqrt{E-q}(E+q)^{\frac{3}{2}}}\sin(\sqrt{E^2-q^2})\right]. \quad (52)$$

Next, integration of trace (51) yields the result

$$\int_0^1 \operatorname{tr}(\tilde{G}(x,x)) = \frac{1}{\tilde{C}}\Bigg[E(E+\sqrt{\pi^2+q^2})\cos(\sqrt{E^2-q^2}) + \frac{q^2-2E^2-E\sqrt{\pi^2+q^2}}{\sqrt{E^2-q^2}}\sin(\sqrt{E^2-q^2})\Bigg]. \quad (53)$$

In the final step we need the explicit form of the constant C that appears in (52). From (16) and (44), (45) we infer that

$$C = \Psi_1^T(x)\gamma\Psi_2(x) = -\sqrt{\frac{E-q}{E+q}}\sin(\sqrt{E^2-q^2}). \quad (54)$$

We now replace $\tilde{C}$ in (53) via relation (30), insert the explicit form of C as given in (54), and compute the difference of (53) and (52). This gives after simplification

$$\int_0^1 \operatorname{tr}(\tilde{G}(x,x) - G(x,x))\,\mathrm{d}x = \frac{1}{E+q} + \frac{1}{E+\sqrt{\pi^2+q^2}}.$$

This is precisely the trace formula (11), where λ_1 and λ_2 are given by (47) and (48), respectively.

6. Concluding remarks

In this paper we have established a simple trace formula for Dirac equations with Sturm–Liouville boundary conditions that are related to each other by a Darboux transformation. The presence of Sturm–Liouville boundary conditions guarantees the existence of a discrete spectrum, which in turn prevents the trace of Green's functions from divergence. This fact has also been an issue in the context of Schrödinger equations [12] and effective mass Schrödinger equations [9], where in the first case it has been resolved. Existence and form of trace formulae for the case of Dirac equations with more general boundary conditions will be subject to further study.

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