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Discontinuities in Dirac eigenfunction expansions

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An expansion, over a finite interval, of a two-component function in a basis of eigenfunctions of a one-dimensional regular Dirac differential operator with separated homogeneous boundary conditions imposed at ends of the interval is considered. It is shown that at the ends of the domain the expansion does not converge to the expanded function unless the latter obeys at these points the same homogeneous boundary conditions as the basis eigenfunctions. General results obtained in the work are illustrated by an analytically solvable example. The problem is related to the R-matrix theory for Dirac particles. [DOI: 10.1063/1.1389471]

I. INTRODUCTION

In theoretical physics one frequently encounters the situation that a given function, defined over some domain, is expanded in a functional basis. Among a variety of bases used in such expansions, those generated by differential eigenvalue problems are of major importance. Properties of expansions in series of eigenfunctions of differential operators were extensively investigated by generations of mathematicians and mathematical physicists and their results are contained in a vast literature of the subject (cf. Refs. 1–6 and references therein).

Expansions, over a finite interval, of a given two-component function in a basis of eigenfunctions of a one-dimensional regular Dirac differential operator with separated homogeneous boundary conditions were studied, for instance, in Refs. 5 and 6. However, in these monographs only a particular case, when at ends of an interval an expanded function obeys the same boundary conditions as basis eigenfunctions, was considered. One may imagine expansion problems in which at end points a two-component function to be expanded is admitted to satisfy boundary conditions that differ from those obeyed by basis eigenfunctions. Problems of that kind are not of purely academic interest and are met in applications of relativistic quantum mechanics (e.g., in the R-matrix theory for Dirac particles[7–9]). It is also very likely that they may be encountered in a mathematical modeling of one-dimensional magnetohydrodynamical phenomena where differential operators of the Dirac type occur.[10,11] We have not found any mathematical study of such problems in available literature and it is a purpose of this work to fill in this gap to some extent. We concentrate on the interesting and important question concerning convergence of an eigenfunction expansion at ends of a domain. We prove that at these points the expansion does not converge to the expanded function unless the latter obeys there the same homogeneous boundary conditions as the basis functions. (That result is by no means obvious since in an analogous problem concerning expansions of one-component functions in bases generated by second-order Sturm–Liouville eigensystems the expansions do converge at the end points except the very special case when basis eigenfunctions are forced to vanish at these points!) Still we show that magnitudes of jumps in both components of the expansion may be precisely determined and we provide relevant expressions. These general results are illustrated by an analytically solvable example.

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II. THE PROBLEM

Consider the eigenproblem consisting of the Dirac differential system

$$\begin{pmatrix} p(x)-\lambda_n\rho(x) & -d/dx+t(x) \\ d/dx+t(x) & q(x)-\lambda_n\rho(x) \end{pmatrix}\begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix}=0 \quad (x_1\leqslant x\leqslant x_2) \tag{2.1}$$

augmented by the separated boundary conditions

$$f_n(x_i)\cos\alpha_i+g_n(x_i)\sin\alpha_i=0 \quad (i=1,2). \tag{2.2}$$

It is assumed that the interval $[x_1,x_2]\subset\mathbb{R}$ is finite, that $p(x)$, $q(x)$, $t(x)$, and $\rho(x)$ are real, bounded and continuous functions of the variable $x\in[x_1,x_2]$, with the additional constraint $\rho(x)>0$, and that α_1 and α_2 are real parameters. Under these assumptions the eigensystem (2.1) and (2.2) has an infinite number of discrete nondegenerate real eigenvalues λ_n.[5,6] The associated eigenfunctions are orthogonal in the sense of

$$\int_{x_1}^{x_2}dx\,\rho(x)[f_n(x)f_{n'}(x)+g_n(x)g_{n'}(x)]=0 \quad (\lambda_n\neq\lambda_{n'}). \tag{2.3}$$

If they are chosen to be real and normalized so that

$$\int_{x_1}^{x_2}dx\,\rho(x)[f_n(x)f_{n'}(x)+g_n(x)g_{n'}(x)]=\delta_{nn'}, \tag{2.4}$$

they obey the closure relation

$$\sum_{n=-\infty}^{\infty}\begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix}(f_n(x') \quad g_n(x'))=\frac{\delta(x-x')}{\sqrt{\rho(x)\rho(x')}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (x_1<x,x'<x_2), \tag{2.5}$$

where $\delta(x-x')$ is the Dirac delta function defined so that[12–14]

$$\int_a^b dx'\,\delta(x-x')\,\phi(x')=\begin{cases} 0 & \text{for } x<a<b \text{ or } a<b<x, \\ \phi(x) & \text{for } a<x<b, \\ \frac{1}{2}\phi(x) & \text{for } a=x<b \text{ or } a<x=b \end{cases} \tag{2.6}$$

for any interval $[a,b]\subset\mathbb{R}$ and any sufficiently regular function $\phi(x)$ defined on $[a,b]$.

Let $(F(x)\;G(x))^{\mathrm{T}}$ be an arbitrary two-component function with continuous components of bounded variation in $[x_1,x_2]$. Its expansion in the set of eigenfunctions of the problem (2.1) and (2.2) is defined as

$$\begin{pmatrix} \overline{F}(x) \\ \overline{G}(x) \end{pmatrix}=\sum_{n=-\infty}^{\infty}C_n\begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix} \quad (x_1\leqslant x\leqslant x_2) \tag{2.7}$$

with the coefficients

$$C_n=\int_{x_1}^{x_2}dx\,\rho(x)[f_n(x)F(x)+g_n(x)G(x)]. \tag{2.8}$$

The closure relation (2.5) implies that

$$\begin{pmatrix} F(x) \\ G(x) \end{pmatrix} = \begin{pmatrix} \overline{F}(x) \\ \overline{G}(x) \end{pmatrix} \quad (x_1 < x < x_2). \tag{2.9}$$

The validity of Eqs. (2.5) and (2.9) is restricted to the *open* interval (x_1, x_2). Since both functions $(F(x) \quad G(x))^{\mathrm{T}}$ and $(\overline{F}(x) \quad \overline{G}(x))^{\mathrm{T}}$ are defined in the *closed* interval $[x_1, x_2]$, we ask the question: how are these functions related at the end points x_1 and x_2?

III. THE SOLUTION

To answer the question posed above, we have to consider an extension of the closure relation (2.5) to the case when one of the variables is fixed at x_i. In analogy with (2.5), we postulate

$$\sum_{n=-\infty}^{\infty} \begin{pmatrix} f_n(x_i) \\ g_n(x_i) \end{pmatrix} (f_n(x) \quad g_n(x)) = \frac{\delta(x-x_i)}{\rho(x_i)} \begin{pmatrix} I_i & J_i \\ K_i & L_i \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2), \tag{3.1}$$

where I_i, J_i, K_i, and L_i are yet unknown constants. Notice that, because of the boundary conditions (2.2), these constants are not independent but are related through

$$J_i = K_i = -I_i \cot \alpha_i, \quad L_i = I_i \cot^2 \alpha_i. \tag{3.2}$$

Hence, it follows that Eq. (3.1) may be rewritten in the form

$$\sum_{n=-\infty}^{\infty} \begin{pmatrix} f_n(x_i) \\ g_n(x_i) \end{pmatrix} (f_n(x) \quad g_n(x)) = \frac{I_i \delta(x-x_i)}{\rho(x_i)} \begin{pmatrix} 1 & -\cot \alpha_i \\ -\cot \alpha_i & \cot^2 \alpha_i \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2). \tag{3.3}$$

From Eqs. (2.7) and (2.8) we have

$$\begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \int_{x_1}^{x_2} dx \rho(x) \sum_{n=-\infty}^{\infty} \begin{pmatrix} f_n(x_i) \\ g_n(x_i) \end{pmatrix} (f_n(x) \quad g_n(x)) \begin{pmatrix} F(x) \\ G(x) \end{pmatrix}, \tag{3.4}$$

and, on substituting here Eq. (3.3) and performing integration, we obtain

$$\begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \begin{pmatrix} \frac{1}{2} I_i F(x_i) - \frac{1}{2} I_i G(x_i) \cot \alpha_i \\ \frac{1}{2} I_i G(x_i) \cot^2 \alpha_i - \frac{1}{2} I_i F(x_i) \cot \alpha_i \end{pmatrix}. \tag{3.5}$$

Equation (3.5) implies

$$\overline{F}(x_i) \cos \alpha_i + \overline{G}(x_i) \sin \alpha_i = 0, \tag{3.6}$$

which might be also inferred from Eqs. (2.7) and (2.2).

To answer completely the question raised at the end of Sec. II, we have to determine the constants I_1 and I_2. To this end, let us choose

$$\begin{pmatrix} F(x) \\ G(x) \end{pmatrix} = \begin{pmatrix} f_k(x) \\ g_k(x) \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2), \tag{3.7}$$

where the function on the right is an eigenfunction of the system (2.1) and (2.2). Because of the orthonormality relation (2.4), in this particular case from Eq. (2.8) we infer

$$C_n = \delta_{nk} \tag{3.8}$$

and thus

$$\begin{pmatrix} \overline{F}(x) \\ \overline{G}(x) \end{pmatrix} = \begin{pmatrix} f_k(x) \\ g_k(x) \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2). \tag{3.9}$$

Utilizing Eqs. (3.7) and (3.9) in Eq. (3.5), we arrive at the homogeneous algebraic system

$$\begin{pmatrix} \frac{1}{2} I_i - 1 & -\frac{1}{2} I_i \cot \alpha_i \\ -\frac{1}{2} I_i \cot \alpha_i & \frac{1}{2} I_i \cot^2 \alpha_i - 1 \end{pmatrix} \begin{pmatrix} f_k(x_i) \\ g_k(x_i) \end{pmatrix} = 0. \tag{3.10}$$

Since $f_k(x_i)$ and $g_k(x_i)$ do not vanish simultaneously, one has

$$\det \begin{pmatrix} \frac{1}{2} I_i - 1 & -\frac{1}{2} I_i \cot \alpha_i \\ -\frac{1}{2} I_i \cot \alpha_i & \frac{1}{2} I_i \cot^2 \alpha_i - 1 \end{pmatrix} = 0, \tag{3.11}$$

hence, it follows that

$$I_i = 2 \sin^2 \alpha_i . \tag{3.12}$$

In Appendix A we present an alternative derivation of that result.

Having determined the constants I_i, from Eqs. (3.3), (3.5), and (3.12) we deduce

$$\sum_{n=-\infty}^{\infty} \begin{pmatrix} f_n(x_i) \\ g_n(x_i) \end{pmatrix} (f_n(x) \quad g_n(x)) = \frac{\delta(x - x_i)}{\rho(x_i)} \begin{pmatrix} 2 \sin^2 \alpha_i & -\sin 2\alpha_i \\ -\sin 2\alpha_i & 2 \cos^2 \alpha_i \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2) \tag{3.13}$$

and

$$\begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \begin{pmatrix} F(x_i) \sin^2 \alpha_i - \frac{1}{2} G(x_i) \sin 2\alpha_i \\ G(x_i) \cos^2 \alpha_i - \frac{1}{2} F(x_i) \sin 2\alpha_i \end{pmatrix}. \tag{3.14}$$

These two equations constitute the main result of this article.

If Eq. (3.14) is rewritten in the form

$$\begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \begin{pmatrix} F(x_i) - [F(x_i) \cos \alpha_i + G(x_i) \sin \alpha_i] \cos \alpha_i \\ G(x_i) - [F(x_i) \cos \alpha_i + G(x_i) \sin \alpha_i] \sin \alpha_i \end{pmatrix}, \tag{3.15}$$

it is immediately seen that, since the sine and the cosine never vanish simultaneously, at the end point $x = x_i$ one has

$$\begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \begin{pmatrix} F(x_i) \\ G(x_i) \end{pmatrix} \tag{3.16}$$

if and only if

$$F(x_i) \cos \alpha_i + G(x_i) \sin \alpha_i = 0, \tag{3.17}$$

i.e., if and only if the function to be expanded obeys at $x = x_i$ the same homogeneous boundary condition as the basis eigenfunctions. If the boundary condition (3.17) is not satisfied, Eqs. (2.9) and (3.15) imply that at $x = x_i$ the eigenfunction expansion (2.7) has a discontinuity

$$\lim_{x \to x_i} \begin{pmatrix} \overline{F}(x) \\ \overline{G}(x) \end{pmatrix} - \begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \begin{pmatrix} F(x_i) \cos^2 \alpha_i + \frac{1}{2} G(x_i) \sin 2\alpha_i \\ \frac{1}{2} F(x_i) \sin 2\alpha_i + G(x_i) \sin^2 \alpha_i \end{pmatrix}. \tag{3.18}$$

This fact was not realized in early formulations of the R-matrix theory for Dirac particles[7,8] which resulted in errors corrected by Szmytkowski and Hinze.[15,16]

It should be emphasized that the previous results are specific for bases generated by Dirac differential eigenproblems; the reader is asked to consult Appendix B on the analogous problem for second-order Sturm–Liouville eigensystems.

It is interesting to consider Eqs. (3.13) and (3.14) in two particular cases. The first case is

$$\cos \alpha_i = 0 \Rightarrow \sin \alpha_i = \pm 1. \tag{3.19}$$

Then Eqs. (3.13) and (3.14) become, respectively,

$$\sum_{n=-\infty}^{\infty} \begin{pmatrix} f_n(x_i) \\ g_n(x_i) \end{pmatrix} (f_n(x) \quad g_n(x)) = \frac{\delta(x-x_i)}{\rho(x_i)} \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2), \tag{3.20}$$

$$\begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \begin{pmatrix} F(x_i) \\ 0 \end{pmatrix}. \tag{3.21}$$

It is seen that in this case the expansion converges at $x = x_i$ in the upper component but fails to converge in the lower one unless $G(x_i) = 0$. The second case to be considered is

$$\sin \alpha_i = 0 \Rightarrow \cos \alpha_i = \pm 1. \tag{3.22}$$

Then

$$\sum_{n=-\infty}^{\infty} \begin{pmatrix} f_n(x_i) \\ g_n(x_i) \end{pmatrix} (f_n(x) \quad g_n(x)) = \frac{\delta(x-x_i)}{\rho(x_i)} \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2) \tag{3.23}$$

and

$$\begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \begin{pmatrix} 0 \\ G(x_i) \end{pmatrix}, \tag{3.24}$$

i.e., at $x = x_i$ the expansion converges in the lower component but fails to converge in the upper one unless $F(x_i) = 0$.

IV. AN ILLUSTRATIVE EXAMPLE

As an example illustrating the general results obtained earlier, in this section we discuss the particular case when the Dirac eigenvalue problem (2.1) and (2.2) is

$$\begin{pmatrix} -\lambda_n & -d/dx \\ d/dx & -\lambda_n \end{pmatrix} \begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix} = 0 \quad (0 \leqslant x \leqslant b), \tag{4.1}$$

$$f_n(0) = 0, \quad f_n(b)\cos\beta + g_n(b)\sin\beta = 0. \tag{4.2}$$

Comparing Eqs. (4.1) and (4.2) with (2.1) and (2.2), one identifies

$$\rho(x) \equiv 1, \quad x_1 = 0, \quad x_2 = b, \quad \alpha_1 = 0, \quad \alpha_2 = \beta. \tag{4.3}$$

Solving the system (4.1) and (4.2), one finds that its eigenvalues are

$$\lambda_n = \frac{\pi n - \beta}{b}, \quad n = 0, \pm 1, \pm 2, \ldots, \tag{4.4}$$

while corresponding eigenfunctions, normalized according to

$$\int_0^b dx[f_n(x)f_{n'}(x)+g_n(x)g_{n'}(x)]=\delta_{nn'}, \tag{4.5}$$

are

$$\begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix}=\frac{1}{\sqrt{b}}\begin{pmatrix} \sin\lambda_n x \\ \cos\lambda_n x \end{pmatrix} \quad (0\leqslant x\leqslant b). \tag{4.6}$$

A. The closure relation and its extension

To verify that eigensolutions to the system (4.1) and (4.2) do obey Eqs. (2.5) and (3.13), we should investigate the series

$$\sum_{n=-\infty}^{\infty}\begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix}(f_n(x') \quad g_n(x'))=\begin{pmatrix} I(x,x') & J(x,x') \\ K(x,x') & L(x,x') \end{pmatrix} \tag{4.7}$$

in the domain $0\leqslant x,x'\leqslant b$. We begin with considering the series

$$I(x,x')=\sum_{n=-\infty}^{\infty} f_n(x)f_n(x') \tag{4.8}$$

in the extended domain $-\infty<x,x'<\infty$. To sum it, we construct a sequence of finite sums

$$I_N(x,x')=\sum_{n=-N}^{N} f_n(x)f_n(x')=\frac{1}{b}\sum_{n=-N}^{N}\sin[(\pi n-\beta)x/b]\sin[(\pi n-\beta)x'/b]. \tag{4.9}$$

Obviously, one has

$$I(x,x')=\lim_{N\to\infty} I_N(x,x'). \tag{4.10}$$

The sum in Eq. (4.9) is easily found to be

$$I_N(x,x')=\frac{\sin[\pi(2N+1)(x-x')/2b]}{2b\sin[\pi(x-x')/2b]}\cos[\beta(x-x')/b] - \frac{\sin[\pi(2N+1)(x+x')/2b]}{2b\sin[\pi(x+x')/2b]}\cos[\beta(x+x')/b]. \tag{4.11}$$

With the aid of the formula

$$\lim_{N\to\infty}\frac{\sin(2N+1)\pi x}{\sin\pi x}=\sum_{n=-\infty}^{\infty}\delta(x-n) \quad (N\in\mathbb{N}), \tag{4.12}$$

which is well known in the theory of Fourier series,[17] from Eqs. (4.10) and (4.11) we infer

$$I(x,x')=\sum_{n=-\infty}^{\infty}[\delta(x-x'-2nb)-\delta(x+x'-2nb)]\cos 2n\beta. \tag{4.13}$$

Let us now restrict to the case when $0<x,x'<b$. Then

$$-b<x-x'<b, \quad 0<x+x'<2b. \tag{4.14}$$

It is evident that under the constraints (4.14) the argument of the first delta in the summand in Eq. (4.13) may vanish if and only if $n=0$, while the argument of the second delta never vanishes. Consequently, in this case all but one term on the right side of Eq. (4.13) are effectively zero and the latter equation reduces to

$$I(x,x')=\delta(x-x') \quad (0<x,x'<b), \tag{4.15}$$

in agreement with the result that may be inferred from Eqs. (2.5) and (4.3).

Next we concentrate on the case $0\leqslant x\leqslant b$ and $x'=0$. This case is the simplest one since then Eq. (4.13) becomes

$$I(x,0)=\sum_{n=-\infty}^{\infty}[\delta(x-2nb)-\delta(x-2nb)]\cos 2n\beta=0 \quad (0\leqslant x\leqslant b), \tag{4.16}$$

which agrees with the result that may be obtained from Eqs. (4.3) and (3.13).

Finally, we consider the most interesting case $x'=b$. Then

$$\begin{aligned} I(x,b)&=\sum_{n=-\infty}^{\infty}[\delta(x-(2n+1)b)-\delta(x-(2n-1)b)]\cos 2n\beta \\ &=2\sin\beta\sum_{n=-\infty}^{\infty}\delta(x-(2n+1)b)\sin[(2n+1)\beta] \quad (-\infty<x<\infty). \end{aligned} \tag{4.17}$$

If $0\leqslant x\leqslant b$, the argument of the delta may vanish if and only if $n=0$; the remaining terms in the series are effectively zero and Eq. (4.17) reduces to

$$I(x,b)=2\sin^2\beta\,\delta(x-b) \quad (0\leqslant x\leqslant b), \tag{4.18}$$

which again agrees with the result that may be deduced from Eqs. (4.3) and (3.13).

The reader will find no difficulty in verifying that in the domain $0\leqslant x,x'\leqslant b$ the remaining three matrix elements on the right side of Eq. (4.7) are identical with those deduced from Eqs. (2.5), (4.3), and (3.13).

B. The expansion problem

Consider now the expansion of the two-component function

$$\begin{pmatrix} F(x) \\ G(x) \end{pmatrix}=\frac{1}{\sqrt{b}}\begin{pmatrix} \sin\lambda x \\ \cos\lambda x \end{pmatrix} \quad (0\leqslant x\leqslant b), \tag{4.19}$$

where λ is a real parameter, in the basis (4.6). The expansion is

$$\begin{pmatrix} \overline{F}(x) \\ \overline{G}(x) \end{pmatrix}=\sum_{n=-\infty}^{\infty}\frac{C_n}{\sqrt{b}}\begin{pmatrix} \sin\lambda_n x \\ \cos\lambda_n x \end{pmatrix} \quad (0\leqslant x\leqslant b) \tag{4.20}$$

with the expansion coefficients given by

$$C_n=\frac{1}{b}\int_0^b dx[\sin\lambda_n x\sin\lambda x+\cos\lambda_n x\cos\lambda x]=\frac{\sin(\lambda_n-\lambda)b}{(\lambda_n-\lambda)b}. \tag{4.21}$$

On utilizing the relationship

$$\sin(\lambda_n-\lambda)b=\frac{\sin(\lambda b+\beta)\sin\lambda_n b}{\sin\beta}, \tag{4.22}$$

which stems from elementary trigonometry and from the boundary condition (4.2), the expansion (4.20) becomes

$$\begin{pmatrix} \overline{F}(x) \\ \overline{G}(x) \end{pmatrix} = \frac{\sin(\lambda b+\beta)}{\sqrt{b}\sin\beta} \sum_{n=-\infty}^{\infty} \frac{\sin\lambda_n b}{(\lambda_n-\lambda)b} \begin{pmatrix} \sin\lambda_n x \\ \cos\lambda_n x \end{pmatrix} \quad (0\leqslant x\leqslant b). \tag{4.23}$$

Below we shall attempt to sum the series on the right side of Eq. (4.23) at the end points $x=0$ and $x=b$.

Let us begin with the end point $x=0$. Then the expansion (4.23) becomes

$$\begin{pmatrix} \overline{F}(0) \\ \overline{G}(0) \end{pmatrix} = \frac{\sin(\lambda b+\beta)}{\sqrt{b}\sin\beta} \sum_{n=-\infty}^{\infty} \frac{\sin\lambda_n b}{(\lambda_n-\lambda)b} \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{4.24}$$

It is obvious that $\overline{F}(0)=0$ while evaluation of $\overline{G}(0)$ requires summation of the series

$$S_1 = \sum_{n=-\infty}^{\infty} \frac{\sin\lambda_n b}{(\lambda_n-\lambda)b}. \tag{4.25}$$

To perform the summation, we rewrite S_1 as follows:

$$S_1 = \sum_{n=-\infty}^{\infty} \frac{(-)^{n+1}\sin\beta}{\pi n-(\lambda b+\beta)} = \sin\beta\left[\frac{1}{\lambda b+\beta} + \sum_{n=1}^{\infty} (-)^n \frac{2(\lambda b+\beta)}{(\lambda b+\beta)^2-(\pi n)^2}\right]. \tag{4.26}$$

On making use of the known[18] partial fraction expansion of $1/\sin z$,

$$\frac{1}{\sin z} = \frac{1}{z} + \sum_{n=1}^{\infty} (-)^n \frac{2z}{z^2-(\pi n)^2}, \tag{4.27}$$

we obtain

$$S_1 = \frac{\sin\beta}{\sin(\lambda b+\beta)}, \tag{4.28}$$

hence, it follows that

$$\begin{pmatrix} \overline{F}(0) \\ \overline{G}(0) \end{pmatrix} = \frac{1}{\sqrt{b}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{4.29}$$

The same result may be inferred from Eqs. (3.14), (4.3), and (4.19).

Next we turn to the case of the end point $x=b$. Then the object of our interest is the series

$$\begin{pmatrix} \overline{F}(b) \\ \overline{G}(b) \end{pmatrix} = \frac{\sin(\lambda b+\beta)}{\sqrt{b}\sin\beta} \sum_{n=-\infty}^{\infty} \frac{\sin\lambda_n b}{(\lambda_n-\lambda)b} \begin{pmatrix} \sin\lambda_n b \\ \cos\lambda_n b \end{pmatrix}. \tag{4.30}$$

To sum it, we have to consider the series

$$S_2 = \sum_{n=-\infty}^{\infty} \frac{\sin^2\lambda_n b}{(\lambda_n-\lambda)b}, \tag{4.31}$$

$$S_3 = \sum_{n=-\infty}^{\infty} \frac{\sin\lambda_n b\cos\lambda_n b}{(\lambda_n-\lambda)b}. \tag{4.32}$$

Of these, only S_2 has to be investigated since, because of Eqs. (4.2) and (4.6), we have

$$S_3 = -S_2 \cot\beta. \tag{4.33}$$

To deal with the series S_2, we rewrite it in the following way:

$$S_2 = \sum_{n=-\infty}^{\infty} \frac{\sin^2\beta}{\pi n-(\lambda b+\beta)} = -\sin^2\beta\left[\frac{1}{\lambda b+\beta}+\sum_{n=1}^{\infty}\frac{2(\lambda b+\beta)}{(\lambda b+\beta)^2-(\pi n)^2}\right]. \tag{4.34}$$

Hence, because of the known[18] partial fraction expansion of $\cot z$,

$$\cot z = \frac{1}{z}+\sum_{n=1}^{\infty}\frac{2z}{z^2-(\pi n)^2}, \tag{4.35}$$

we find

$$S_2 = -\sin^2\beta\cot(\lambda b+\beta). \tag{4.36}$$

Consequently, Eq. (4.30) becomes

$$\begin{pmatrix} \bar{F}(b) \\ \bar{G}(b) \end{pmatrix} = \frac{1}{\sqrt{b}}\begin{pmatrix} -\sin\beta\cos(\lambda b+\beta) \\ \cos\beta\cos(\lambda b+\beta) \end{pmatrix}. \tag{4.37}$$

The same result may be inferred from Eqs. (3.14), (4.3), and (4.19).

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APPENDIX A: AN ALTERNATIVE DERIVATION OF EQ. (3.12)

Consider an auxiliary inhomogeneous boundary value problem

$$\begin{pmatrix} p(x)-\lambda\rho(x) & -d/dx+t(x) \\ d/dx+t(x) & q(x)-\lambda\rho(x) \end{pmatrix}\begin{pmatrix} f(x) \\ g(x) \end{pmatrix} = 0 \quad (x_1 \leqslant x \leqslant x_2), \tag{A1}$$

$$f(x_i)\cos\alpha_i + g(x_i)\sin\alpha_i = A_i \quad (i=1,2), \tag{A2}$$

where the functions $p(x)$, $q(x)$, $t(x)$ and $\rho(x)$ are the same that appear in Eq. (2.1), $\lambda\in\mathbb{R}$, $\lambda \neq \lambda_n$, $A_i\in\mathbb{R}$, and $A_1^2+A_2^2\neq 0$. We construct the series

$$\begin{pmatrix} \bar{f}(x) \\ \bar{g}(x) \end{pmatrix} = \sum_{n=-\infty}^{\infty} c_n \begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2) \tag{A3}$$

with the coefficients defined by

$$c_n = \int_{x_1}^{x_2} dx\,\rho(x)[f_n(x)f(x)+g_n(x)g(x)]. \tag{A4}$$

It is obvious that, because of regularity of $(f(x) \quad g(x))^{\mathrm{T}}$ [implied by Eq. (A1)], one has

$$\begin{pmatrix} \overline{f}(x) \\ \overline{g}(x) \end{pmatrix} = \begin{pmatrix} f(x) \\ g(x) \end{pmatrix} \quad (x_1 < x < x_2) \tag{A5}$$

[cf. Eq. (2.9)] but, because of Eq. (2.2) and the definition (A3),

$$\overline{f}(x_i)\cos\alpha_i + \overline{g}(x_i)\sin\alpha_i = 0. \tag{A6}$$

To find a convenient expression for the coefficients (A4), we premultiply Eq. (2.1) by $(f(x) \quad g(x))^{\mathrm{T}}$, Eq. (A1) by $(f_n(x) \quad g_n(x))^{\mathrm{T}}$, subtract and integrate the result over the interval $[x_1, x_2]$. This yields

$$(\lambda_n - \lambda)\int_{x_1}^{x_2} dx\,\rho(x)[f_n(x)f(x) + g_n(x)g(x)] = [f_n(x)g(x) - f(x)g_n(x)]\big|_{x_1}^{x_2}, \tag{A7}$$

hence, on making use of the boundary conditions (2.2) and (A2) and the definition (A4), it follows

$$c_n = \frac{A_2 f_n(x_2)}{(\lambda_n - \lambda)\sin\alpha_2} - \frac{A_1 f_n(x_1)}{(\lambda_n - \lambda)\sin\alpha_1}. \tag{A8}$$

Next, let us operate from the left on both sides of Eq. (A9) with the differential operator appearing in Eq. (A1). Because of Eq. (2.1), this gives

$$\begin{pmatrix} p(x) - \lambda\rho(x) & -d/dx + t(x) \\ d/dx + t(x) & q(x) - \lambda\rho(x) \end{pmatrix} \begin{pmatrix} \overline{f}(x) \\ \overline{g}(x) \end{pmatrix} = \rho(x)\sum_{n=-\infty}^{\infty} c_n(\lambda_n - \lambda)\begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2) \tag{A9}$$

or, after utilizing the result (A8),

$$\left[\frac{d}{dx} + t(x)\right]\overline{f}(x) + [q(x) - \lambda\rho(x)]\overline{g}(x) = \frac{A_2}{\sin\alpha_2}\rho(x)\sum_{n=-\infty}^{\infty} f_n(x_2)g_n(x) - \frac{A_1}{\sin\alpha_1}\rho(x)\sum_{n=-\infty}^{\infty} f_n(x_1)g_n(x) \quad (x_1 \leqslant x \leqslant x_2) \tag{A10}$$

and

$$\left[-\frac{d}{dx} + t(x)\right]\overline{g}(x) + [p(x) - \lambda\rho(x)]\overline{f}(x) = \frac{A_2}{\sin\alpha_2}\rho(x)\sum_{n=-\infty}^{\infty} f_n(x_2)f_n(x) - \frac{A_1}{\sin\alpha_1}\rho(x)\sum_{n=-\infty}^{\infty} f_n(x_1)f_n(x) \quad (x_1 \leqslant x \leqslant x_2). \tag{A11}$$

Right sides of Eqs. (A10) and (A11) may be transformed if one makes use of Eq. (3.3). This results in

$$\left[\frac{d}{dx} + t(x)\right]\overline{f}(x) + [q(x) - \lambda\rho(x)]\overline{g}(x) = -\frac{A_2 I_2 \cot\alpha_2}{\sin\alpha_2}\,\delta(x - x_2) + \frac{A_1 I_1 \cot\alpha_1}{\sin\alpha_1}\,\delta(x - x_1) \quad (x_1 \leqslant x \leqslant x_2), \tag{A12}$$

$$\left[-\frac{d}{dx}+t(x)\right]\overline{g}(x)+[p(x)-\lambda\rho(x)]\overline{f}(x)=\frac{A_2I_2}{\sin\alpha_2}\delta(x-x_2)-\frac{A_1I_1}{\sin\alpha_1}\delta(x-x_1)$$
$$(x_1\leqslant x\leqslant x_2). \tag{A13}$$

In the following step, we integrate Eqs. (A12) and (A13) either from x_1 to $x<x_2$, passing then to the limit $x\downarrow x_1$, or from $x>x_1$ to x_2, passing then to the limit $x\uparrow x_2$. The results may be compactly written as

$$f(x_i)-\overline{f}(x_i)=\frac{A_iI_i\cot\alpha_i}{2\sin\alpha_i}, \tag{A14}$$

$$g(x_i)-\overline{g}(x_i)=\frac{A_iI_i}{2\sin\alpha_i}. \tag{A15}$$

After supplementing Eqs. (A14) and (A15) by the boundary condition (A6), we obtain a set of three linear algebraic equations for three unknowns I_i, $\overline{f}(x_i)$ and $\overline{g}(x_i)$. Solving this set for I_i, one obtains

$$I_i=2\sin^2\alpha_i, \tag{A16}$$

which coincides with Eq. (3.12).

APPENDIX B: EXPANSIONS IN EIGENFUNCTIONS OF SECOND-ORDER STURM–LIOUVILLE SYSTEMS

Consider the second-order Sturm–Liouville eigensystem

$$\frac{d}{dx}\left(p(x)\frac{df_n(x)}{dx}\right)+q(x)f_n(x)-\lambda_n\rho(x)f_n(x)=0\quad(x_1\leqslant x\leqslant x_2), \tag{B1}$$

$$f_n(x_i)\cos\alpha_i+p(x_i)f_n'(x_i)\sin\alpha_i=0\quad(i=1,2) \tag{B2}$$

on the finite interval $[x_1,x_2]\subset\mathbb{R}$. Here $p(x)$, $q(x)$, and $\rho(x)$ are real, bounded and continuous functions of the variable $x\in[x_1,x_2]$, with the additional constraints $\rho(x)>0$, $p(x)\in C^1([x_1,x_2])$, and $p(x)\neq 0$, while α_1 and α_2 are real constants. Provided the eigenfunctions to the system (B1) and (B2) have been normalized according to

$$\int_{x_1}^{x_2}dx\,\rho(x)f_n(x)f_{n'}(x)=\delta_{nn'}, \tag{B3}$$

it holds

$$\sum_{n=0}^{\infty}f_n(x)f_n(x')=\frac{\delta(x-x')}{\sqrt{\rho(x)\rho(x')}}\quad(x_1<x,x'<x_2) \tag{B4}$$

and

$$\sum_{n=0}^{\infty}f_n(x_i)f_n(x)=\frac{I_i\delta(x-x_i)}{\rho(x_i)}\quad(x_1\leqslant x\leqslant x_2), \tag{B5}$$

where

$$I_i=\begin{cases}2 & \text{for } \sin\alpha_i\neq 0\\ 0 & \text{for } \sin\alpha_i=0.\end{cases} \tag{B6}$$

Equations (B5) and (B6) may be obtained in a way similar to that in which Eq. (3.13) has been derived.

Let $F(x)$ be any continuous function of bounded variation in $[x_1,x_2]$. Then, it follows from Eqs. (B4)–(B6) that its eigenfunction expansion, defined as

$$\overline{F}(x)=\sum_{n=0}^{\infty} f_n(x)\int_{x_1}^{x_2}dx'\,\rho(x')f_n(x')F(x') \quad (x_1\leqslant x\leqslant x_2), \tag{B7}$$

has the following properties:

$$\overline{F}(x)=F(x) \quad (x_1<x<x_2), \tag{B8}$$

$$\overline{F}(x_i)=\begin{cases}F(x_i) & \text{for } \sin\alpha_i\neq 0,\\ 0 & \text{for } \sin\alpha_i=0.\end{cases} \tag{B9}$$

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[12] In some cases it is convenient to define the Dirac delta function in the following way (Ref. 13):

$$\int_a^b dx'\,\delta(x-x')\phi(x')=\begin{cases}0 & \text{for } x<a<b \text{ or } a<b<x\\ \phi(x) & \text{for } a\leqslant x\leqslant b\end{cases},$$

for any interval $[a,b]\subset\mathbb{R}$ and any function $\phi(x)$ that is sufficiently regular in $[a,b]$. This definition, which differs from the one used in the present work, is usually adopted in the R-matrix theory when a Bloch operator is employed (Ref. 14). Either definition of the delta is correct as long as it is used consistently.
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