Physics Open 15 (2023) 100151

Contents lists available at ScienceDirect

Physics Open

journal homepage: www.elsevier.com/locate/physo

General pseudo self-adjoint boundary conditions for a 1D KFG particle in a box

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ARTICLE INFO

Handling Editor: Matteo Paris

Keywords:
1D Klein–Fock–Gordon wave equation
1D Feshbach–Villars wave equation
Pseudo-Hermitian operator
Pseudo self-adjoint operator
Boundary conditions

ABSTRACT

We consider a 1D Klein–Fock–Gordon particle in a finite interval, or box. We construct for the first time the most general set of pseudo self-adjoint boundary conditions for the Hamiltonian operator that is present in the first order in time 1D Klein–Fock–Gordon wave equation, or the 1D Feshbach–Villars wave equation. We show that this set depends on four real parameters and can be written in terms of the one-component wavefunction for the second order in time 1D Klein–Fock–Gordon wave equation and its spatial derivative, both evaluated at the endpoints of the box. Certainly, we write the general set of pseudo self-adjoint boundary conditions also in terms of the two-component wavefunction for the 1D Feshbach–Villars wave equation and its spatial derivative, evaluated at the ends of the box; however, the set actually depends on these two column vectors each multiplied by the singular matrix that is present in the kinetic energy term of the Hamiltonian. As a consequence, we found that the two-component wavefunction for the 1D Feshbach–Villars equation and its spatial derivative do not necessarily satisfy the same boundary condition that these quantities satisfy when multiplied by the singular matrix. In any case, given a particular boundary condition for the one-component wavefunction of the standard 1D Klein–Fock–Gordon equation and using the pair of relations that arise from the very definition of the two-component wavefunction for the 1D Feshbach–Villars equation, the respective boundary condition for the latter wavefunction and its derivative can be obtained. Our results can be extended to the problem of a 1D Klein–Fock–Gordon particle moving on a real line with a point interaction (or a hole) at one point.

1. Introduction

As is well known, the three-dimensional (3D) Klein–Fock–Gordon (KFG) wave equation in its standard form plays an important role in relativistic quantum mechanics [1–5]. As an example, when potentials fail to create particle–antiparticle pairs, the 3D KFG wave equation can be used to describe spin-zero particles, for example, the pion, a composite particle, and the Higgs boson, an apparently elementary particle. Clearly, this equation is one of the most widely used in relativistic quantum mechanics. Naturally, the search for exact solutions to this equation in specific and representative potentials has always been of interest, mainly because these solutions can be useful for modeling real physical processes. In the study of exactly solvable problems, various methods have been introduced and developed. Examples include supersymmetric quantum mechanics (SUSY QM) and/or the factorization method [6–10] and the Nikiforov–Uvarov (UV) method [8,9,11], among others [12–15]. It is worth mentioning that in recent years, new computational schemes or methods have been applied to obtain solutions of nonlinear partial differential equations that are related in some way to the KFG equation. See, for example, Refs. [16–18] and references therein.

In reviewing the literature on KFG theory, it is immediately apparent that the 3D KFG wave equation in Hamiltonian form, i.e., the so-called 3D Feshbach–Villars (FV) wave equation [19], has not received the same attention as the standard 3D KFG equation. Certainly, both equations are equivalent, and connecting their corresponding solutions seems to be straightforward. However, the 3D FV partial differential equation is first order in time and second order in space, that is, it includes a second-order Hamiltonian operator in the spatial derivative (for a nice discussion of the procedure used by Feshbach and Villars to obtain a linear equation in the time derivative, see Ref. [20]. For a brief and concise historical discussion of similar work, but prior to that of Feshbach and Villars, see again Ref. [20], specifically, the commentary written in its reference number 3, page 191).

Similarly, the one-dimensional (1D) FV wave equation has also not received sufficient attention when considering problems within the KFG theory in (1+1) dimensions. Certainly, the 1D KFG equation in its standard form is much more popular. In this regard, there is an issue within the 1D KFG theory that has received practically no attention and that we can raise with the following questions: What are the boundary

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https://doi.org/10.1016/j.physo.2023.100151
Received 7 January 2023; Received in revised form 23 February 2023; Accepted 7 March 2023
Available online 9 March 2023
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conditions that the 1D FV equation can support? Can general families of boundary conditions be written for this equation? Specifically, what are the appropriate boundary conditions for this equation in the problem of a 1D KFG particle inside an interval? For example, some unexpected boundary conditions for the solutions of the 1D FV wave equation in simple physical situations were presented in Refs. [21–23]. In general, the boundary conditions for the solutions of the second-order KFG equation in 3D and 1D appear to be similar to those supported by the corresponding Schrödinger wavefunction (see, for example, Refs. [21, 23–25]), but we do not have at our disposal a wave equation that could have boundary conditions similar to those of the 1D FV equation (the presence of a singular matrix in the kinetic energy term of the Hamiltonian has much to do with this). In general, the physically acceptable boundary conditions for a wave equation that is written in Hamiltonian form must ensure that the respective Hamiltonian operator retains its essential attribute, namely, that of being self-adjoint (if that is the case). In the case of the 1D FV equation, it is known that its Hamiltonian is a formally pseudo-Hermitian operator (or a formally pseudo self-adjoint operator) [2,4], and, in principle, we could find families of general boundary conditions that agree with the property of being a pseudo self-adjoint operator, i.e., not just formally. In fact, here, we show that indeed a general four-parameter family of boundary conditions can be found for the solutions of the 1D FV equation and that it is consistent with the latter property. Incidentally, to do this is essentially to specify the domain of the Hamiltonian and that of its generalized adjoint (as is done in the case of Hamiltonians that are self-adjoint in the standard way), but, in addition, these two domains must be equal, i.e., they must always contain the same boundary condition (once the four parameters are fixed).

The article is organized as follows. In Section 2, we begin by introducing the KFG equations in their standard and Hamiltonian versions and the relations linking their solutions. In addition, we introduce the pseudo inner product for the two-component solutions of the 1D FV equation and briefly discuss its relation to other distinctive inner products of quantum mechanics. In particular, we note that this pseudo inner product can also be considered the scalar product for the one-component solutions of the KFG equation in its standard form. Moreover, as might be expected, this pseudo inner product does not possess the property of positive definiteness but can be independent of time. Thus, the corresponding pseudo norm can be a constant, and because this implies that the probability current density takes the same value at each end of the box, the Hamiltonian for this problem can be a pseudo-Hermitian operator. In fact, the Hamiltonian is formally pseudo-Hermitian, and we find in this section a general four-parameter set of boundary conditions that ensures that it is indeed a pseudo-Hermitian operator. We write this set in terms of the one-component wavefunction for the 1D KFG wave equation and its spatial derivative, both evaluated at the ends of the interval. Here, we also consider the nonrelativistic approximation of the general set of boundary conditions, and the results support the idea that this set is indeed the most general. In Section 3, we finally write the general set of boundary conditions in terms of the two-component column vector for the 1D FV wave equation and its spatial derivative, evaluated at the ends of the interval. To be precise, the set must be written in terms of the latter two column vectors each multiplied by the singular matrix that is present in the kinetic energy term of the Hamiltonian (remember that a singular matrix does not have an inverse). In Appendix A, we check that the time derivative of the pseudo inner product of two solutions of the 1D FV equation in a nonzero electric potential, but expressed in terms of the respective solutions of the standard KFG equation in the same potential, is proportional to a term evaluated at the ends of the box that also does not depend on the potential, i.e., it is a boundary term. In Appendix B, we show that the Hamiltonian operator for a 1D KFG particle in a box is in fact a pseudo self-adjoint operator; that is, the general matrix boundary condition, i.e., the general set of boundary conditions, ensures that the domains of the Hamiltonian and its generalized adjoint are equal. From the results shown in this section, it follows that the boundary term that arose in Appendix A always vanishes (certainly, for any boundary condition included in the general family of boundary conditions); consequently, the value of the pseudo inner product in this problem is conserved. Finally, concluding remarks are presented in Section 4.

2. Boundary conditions for the 1D KFG particle in a box I

Let us begin by writing the 1D KFG wave equation in Hamiltonian form,

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi=\hat{\mathrm{h}}\Psi, \tag{1}$$

where

$$\hat{\mathrm{h}}=-\frac{\hbar^2}{2\mathrm{m}}\left(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2\right)\frac{\partial^2}{\partial x^2}+\mathrm{m}c^2\hat{\tau}_3+V(x)\hat{\mathrm{I}}_2, \tag{2}$$

is, let us say, the KFG Hamiltonian differential operator. Here, $\hat{\tau}_3=\hat{\sigma}_z$ and $\hat{\tau}_2=\hat{\sigma}_y$ are Pauli matrices and $V(x)\in\mathbb{R}$ is the external electric potential ($\hat{\mathrm{I}}_2$ is the 2×2 identity matrix). The (matrix) operator $\hat{\mathrm{h}}$ acts on (complex) two-component column state vectors of the form $\Psi=\Psi(x,t)=\left[\psi_1(x,t)\ \psi_2(x,t)\right]^{\mathrm{T}}$ (the symbol $^{\mathrm{T}}$ represents the transpose of a matrix). Eq. (1) with $\hat{\mathrm{h}}$ given in Eq. (2) is the 1D FV wave equation [2–4,19].

The 1D KFG wave equation in its standard form, or the second order in time KFG equation in one spatial dimension [1,5] is given by

$$\left[\mathrm{i}\hbar\frac{\partial}{\partial t}-V(x)\right]^2\psi=\left[-\hbar^2c^2\frac{\partial^2}{\partial x^2}+(\mathrm{m}c^2)^2\right]\psi, \tag{3}$$

where $\psi=\psi(x,t)$ is a (complex) one-component state vector or one-component wavefunction.

The relation between ψ and Ψ can be defined as follows:

$$\Psi=\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}=\frac{1}{2}\begin{bmatrix}\psi+\mathrm{i}\tau\left(\frac{\partial}{\partial t}-\frac{V}{\mathrm{i}\hbar}\right)\psi\\ \psi-\mathrm{i}\tau\left(\frac{\partial}{\partial t}-\frac{V}{\mathrm{i}\hbar}\right)\psi\end{bmatrix}, \tag{4}$$

where $\tau\equiv\hbar/\mathrm{m}c^2$. The Compton wavelength is precisely $\lambda_{\mathrm{C}}\equiv c\tau$; thus, τ is the time taken for a ray of light to travel the distance λ_{C}. The expression given in Eq. (3) is fully equivalent to Eq. (1) (with $\hat{\mathrm{h}}$ given in Eq. (2)) [2,3]. Note that, from Eq. (4), the solution ψ of Eq. (3) depends only on the components of the column vector Ψ, namely,

$$\psi=\psi_1+\psi_2. \tag{5}$$

Additionally,

$$\left(\mathrm{i}\hbar\frac{\partial}{\partial t}\psi-V\psi\right)\frac{1}{\mathrm{m}c^2}=\psi_1-\psi_2. \tag{6}$$

Certainly, all the results we have presented so far are well known.

Let us now consider a 1D KFG particle moving in the interval $x\in\Omega=[a,b]$, i.e., in a box. The corresponding Hamiltonian operator given in Eq. (2) acts on two-component column state vectors of the form $\Psi=\left[\psi_1\ \psi_2\right]^{\mathrm{T}}$ and $\Phi=\left[\phi_1\ \phi_2\right]^{\mathrm{T}}$, and the scalar product for these two state vectors must be defined as

$$\langle\langle\Psi,\Phi\rangle\rangle\equiv\int_\Omega \mathrm{d}x\,\Psi^\dagger\hat{\tau}_3\Phi \tag{7}$$

(the symbol † denotes the usual Hermitian conjugate, or the usual formal adjoint, of a matrix and an operator) [2–4,19]. Additionally, the square of the corresponding norm (or rather, pseudo norm) is $|||\Psi|||^2\equiv\langle\langle\Psi,\Psi\rangle\rangle=\int_\Omega \mathrm{d}x\,\varrho$, where $\varrho=\varrho(x,t)=\Psi^\dagger\hat{\tau}_3\Psi=|\psi_1|^2-|\psi_2|^2$ is the 1D KFG probability density. Certainly, ϱ is not positive definite and calling it probability density is not absolutely correct (although it can be interpreted as a charge density) [2–4,19]. Note that the integral in (7) can also be identified with the usual scalar product in Dirac's theory in (1+1) dimensions, namely, $\langle\Psi,\Phi\rangle_{\mathrm{D}}\equiv\int_\Omega \mathrm{d}x\,\Psi^\dagger\Phi$, which is an inner product on the Hilbert space of two-component square-integrable wavefunctions, $\mathcal{L}^2(\Omega)\oplus\mathcal{L}^2(\Omega)$; therefore,

$$\langle\langle\Psi,\Phi\rangle\rangle\equiv\langle\Psi,\hat{\tau}_3\Phi\rangle_{\mathrm{D}}, \tag{8}$$

and $\langle\Psi,\Phi\rangle_{\rm D} = \langle\langle\Psi,\hat{\tau}_3\Phi\rangle\rangle$. Because $\langle\langle\Psi,\Psi\rangle\rangle$ can be a negative quantity, the scalar product in Eq. (7) is an indefinite (or improper) inner product, or a pseudo inner product, on an infinite-dimensional complex vector space. In general, such a vector space itself is not necessarily a Hilbert space.

Similarly, writing Ψ and Φ in the integrand in (7) in terms of their respective components, that is, using the relations that arise from Eq. (4) and other analogous relations for Φ (which are obtained from Eq. (4) by making the replacements $\Psi \to \Phi$, $\psi_1 \to \phi_1$, $\psi_2 \to \phi_2$ and $\psi \to \phi$), we obtain

$$\langle\langle\Psi,\Phi\rangle\rangle = \frac{\mathrm{i}\hbar}{2\mathrm{m}c^2}\int_\Omega \mathrm{d}x\,\left(\psi^*\phi_t - \psi_t^*\phi - \frac{2V}{\mathrm{i}\hbar}\psi^*\phi\right) \tag{9}$$

(where the asterisk * denotes the complex conjugate, and $\psi_t \equiv \partial\psi/\partial t$, etc.), or also,

$$\langle\langle\Psi,\Phi\rangle\rangle = \frac{\mathrm{i}\hbar}{2\mathrm{m}c^2}\left(\langle\psi,\phi_t\rangle_{\rm S} - \langle\psi_t,\phi\rangle_{\rm S} - \frac{2}{\mathrm{i}\hbar}\langle\psi,V\phi\rangle_{\rm S}\right) \equiv \langle\psi,\phi\rangle_{\rm KFG}, \tag{10}$$

where $\langle\psi,\phi\rangle_{\rm KFG}$ can be considered the scalar product for the one-component solutions of the 1D KFG equation in Eq. (3) (see Appendix A). Note that $\langle\ ,\ \rangle_{\rm S}$ denotes the usual scalar product in the Schrödinger theory in one spatial dimension, namely, $\langle\psi,\phi\rangle_{\rm S} \equiv \int_\Omega \mathrm{d}x\,\psi^*\phi$, which is an inner product on the Hilbert space of one-component square-integrable wavefunctions, $\mathcal{L}^2(\Omega)$. Certainly, ψ and ψ_t, and ϕ, $V\phi$, and ϕ_t, must belong to $\mathcal{L}^2(\Omega)$ to ensure that $\langle\psi,\phi\rangle_{\rm KFG}$ exists [26].

It can be noted that there is an isomorphism between the vectorial space of the solutions ψ of the standard 1D KFG equation for the corresponding 1D particle, namely,

$$\left[\left(\partial_t - \frac{V}{\mathrm{i}\hbar}\right)^2 + \hat{\mathrm{d}}\right]\psi = 0 \tag{11}$$

(Eq. (3)), where $\hat{\mathrm{d}} \equiv -c^2\partial_{xx} + \tau^{-2}$ ($\partial_t \equiv \partial/\partial t$ and $\partial_{xx} \equiv \partial^2/\partial x^2$, etc.) and the vectorial space of the initial state vectors of the 1D KFG equation in Hamiltonian form for this 1D particle, namely, Eq. (1) with $\hat{\mathrm{h}}$ given in Eq. (2) [27]. In effect, a possible initial state vector, for example, at $t = 0$, would have the form

$$\Psi(0) = \begin{bmatrix}\psi_1(0)\\ \psi_2(0)\end{bmatrix} = \frac{1}{2}\begin{bmatrix}\psi(0) + \mathrm{i}\tau\left(\psi_t(0) - \frac{V}{\mathrm{i}\hbar}\psi(0)\right)\\ \psi(0) - \mathrm{i}\tau\left(\psi_t(0) - \frac{V}{\mathrm{i}\hbar}\psi(0)\right)\end{bmatrix}, \tag{12}$$

that arises immediately from the relation given in Eq. (4). Thus, giving an initial state vector as $\Psi(0)$ is equivalent to providing the initial data for the solution vector ψ, namely, $\psi(0)$ and $\psi_t(0)$. Incidentally, operators $\hat{\mathrm{d}}$, which can act on the one-component state vectors ψ, and $\hat{\mathrm{h}}$, which can act on the two-component state vectors Ψ, are related as follows:

$$\hat{\mathrm{h}} = +\frac{\hbar}{2}\tau\left(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2\right)\hat{\mathrm{d}} + \frac{\hbar}{2}\tau^{-1}\left(\hat{\tau}_3 - \mathrm{i}\hat{\tau}_2\right) + V(x)\hat{\mathrm{I}}_2. \tag{13}$$

Although the scalar product in Eqs. (7) and (10) does not possess the property of positive definiteness (i.e., $\langle\langle\Psi,\Psi\rangle\rangle < 0$), it is a time-independent scalar product. Indeed, using Eq. (3) for ψ and ψ^*, and for ϕ and ϕ^*, it can be demonstrated that the following relation is verified:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle\Psi,\Phi\rangle\rangle = -\frac{\mathrm{i}\hbar}{2\mathrm{m}}\left[\psi_x^*\phi - \psi^*\phi_x\right]\Big|_a^b = \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi,\phi\rangle_{\rm KFG}, \tag{14}$$

where $[\,g\,]_a^b \equiv g(b,t) - g(a,t)$, and $\psi_x \equiv \partial\psi/\partial x$, etc. This result is also valid when the external potential V is different from zero inside the box (see Appendix A). The term evaluated at the endpoints of the interval Ω must vanish due to the boundary condition satisfied by ψ and ϕ, or Ψ and Φ (see Appendix B). Additionally, if we make $\psi = \phi$, or $\Psi = \Phi$, in Eq. (14), we obtain the result

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle\Psi,\Psi\rangle\rangle = -\,[\,j\,]_a^b = \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi,\psi\rangle_{\rm KFG}, \tag{15}$$

where $j = j(x,t) = (\mathrm{i}\hbar/2\mathrm{m})(\psi_x^*\psi - \psi^*\psi_x)$ would be the probability current density, although we know that this quantity, as well as ϱ, cannot be interpreted as probability quantities [2,3]. The disappearance of the boundary term in Eq. (15) implies that the pseudo norm remains constant, and because $j(a,t) = j(b,t)$, we have that $\hat{\mathrm{h}}$ must be a pseudo-Hermitian operator. In the case that $\Omega = \mathbb{R}$, the scalar product $\langle\langle\Psi,\Phi\rangle\rangle$ is a time-independent constant whenever Ψ and Φ are two normalizable solutions, i.e., solutions that have their pseudo norm finite. The square of the pseudo norm of these functions could be negative, but their magnitude cannot be infinite if the boundary term in Eq. (14) is expected to be zero.

Next, we use the pseudo inner product given in Eq. (7), which is defined over an indefinite inner product space [20]. For a collection of basic properties of this scalar product (but also of general results on Hamiltonians of the type given in Eq. (2)), see Ref. [27]. Using integration by parts twice, it can be demonstrated that the Hamiltonian differential operator $\hat{\mathrm{h}}$ in Eq. (2) satisfies the following relation:

$$\langle\langle\Psi,\hat{\mathrm{h}}\Phi\rangle\rangle = \langle\langle\hat{\mathrm{h}}_{\rm adj}\Psi,\Phi\rangle\rangle + f[\Psi,\Phi], \tag{16}$$

where the boundary term $f[\Psi,\Phi]$ is given by

$$f[\Psi,\Phi] \equiv \frac{\hbar^2}{2\mathrm{m}}\left[\Psi_x^\dagger\,\hat{\tau}_3\,(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)\Phi - \Psi^\dagger\,\hat{\tau}_3\,(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)\Phi_x\right]\Big|_a^b. \tag{17}$$

This quantity can also be written in a way that will be especially important, namely,

$$f[\Psi,\Phi] \equiv \frac{\hbar^2}{2\mathrm{m}}\,\frac{1}{2}\left[\left((\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)\Psi_x\right)^\dagger(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)\Phi - \left((\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)\Psi\right)^\dagger(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)\Phi_x\right]\Big|_a^b. \tag{18}$$

The latter somewhat unexpected expression is true because the singular matrix $\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2$ obeys the following relation: $(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)^\dagger(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2) = 2\hat{\tau}_3\,(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)$; however, $(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)^2 = \hat{0}$. The differential operator $\hat{\mathrm{h}}_{\rm adj}$ in Eq. (16) is the generalized Hermitian conjugate, or the formal generalized adjoint of $\hat{\mathrm{h}}$, namely,

$$\hat{\mathrm{h}}_{\rm adj} = \hat{\eta}^{-1}\,\hat{\mathrm{h}}^\dagger\,\hat{\eta} = \hat{\tau}_3\,\hat{\mathrm{h}}^\dagger\,\hat{\tau}_3 \tag{19}$$

($\hat{\eta} = \hat{\tau}_3 = \hat{\eta}^{-1}$ is sometimes called the metric operator; in this case, $\hat{\eta}$ is a bounded operator and satisfies $\hat{\eta}^3 = \hat{\eta}$) and therefore (just formally, i.e., by using only the scalar product definition given in Eq. (7)),

$$\langle\langle\Psi,\hat{\mathrm{h}}\Phi\rangle\rangle = \langle\langle\hat{\mathrm{h}}_{\rm adj}\Psi,\Phi\rangle\rangle. \tag{20}$$

The latter is essentially the relation that defines the generalized adjoint differential operator $\hat{\mathrm{h}}_{\rm adj}$ on an indefinite inner product space. Clearly, the latter definition requires that $f[\Psi,\Phi]$ in Eq. (16) vanishes.

The Hamiltonian operator in Eq. (2) also formally satisfies the following relation:

$$\hat{\mathrm{h}} = \hat{\mathrm{h}}_{\rm adj}, \tag{21}$$

that is, $\hat{\mathrm{h}}$ is formally pseudo-Hermitian (or formally generalized Hermitian), or formally pseudo self-adjoint (or formally generalized self-adjoint). However, if the boundary conditions imposed on Ψ and Φ at the endpoints of the interval Ω lead to the cancellation of the boundary term in Eq. (16), then the differential operator $\hat{\mathrm{h}}$ is indeed pseudo-Hermitian (or generalized Hermitian), and as shown in Appendix B, it is also pseudo self-adjoint (or generalized self-adjoint), i.e.,

$$\langle\langle\Psi,\hat{\mathrm{h}}\Phi\rangle\rangle = \langle\langle\hat{\mathrm{h}}\Psi,\Phi\rangle\rangle. \tag{22}$$

Precisely, we want to obtain a general set of boundary conditions for the pseudo-Hermitian Hamiltonian differential operator. Thus, if we impose $\Psi = \Phi$ in the latter relation and in Eq. (16) (with the result in Eq. (21)), we obtain the following condition:

$$f[\Psi,\Psi] = \frac{\hbar}{\mathrm{i}}\,[\,j\,]_a^b = 0 \quad (\Rightarrow\ j(b,t) = j(a,t)), \tag{23}$$

where $j = j(x,t)$ is given by

$$j = \frac{\mathrm{i}\hbar}{2\mathrm{m}}\,\frac{1}{2}\left[\left((\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)\Psi_x\right)^\dagger(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)\Psi - \left((\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)\Psi\right)^\dagger(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)\Psi_x\right] \tag{24}$$

(see Eq. (18)). But also because $\hat{\tau}_3\,(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)=\hat{1}_2+\hat{\sigma}_x$ (the latter if we use the expression given by Eq. (17)), and the result in Eq. (5), we obtain

$$j=\frac{\mathrm{i}\hbar}{2\mathrm{m}}\left(\psi_x^*\psi-\psi^*\psi_x\right), \tag{25}$$

as expected (see the comment made just after Eq. (15)). Certainly, all the generalized Hermitian boundary conditions must lead to the equality of j at the endpoints of the interval Ω. Furthermore, we also obtain the result $\langle\langle\Psi,\hat{\mathrm{h}}\Psi\rangle\rangle=\langle\langle\hat{\mathrm{h}}\Psi,\Psi\rangle\rangle=\langle\langle\Psi,\hat{\mathrm{h}}\Psi\rangle\rangle^*$ (the superscript * denotes the complex conjugate); therefore, $\langle\langle\Psi,\hat{\mathrm{h}}\Psi\rangle\rangle\equiv\langle\langle\hat{\mathrm{h}}\rangle\rangle_\Psi\in\mathbb{R}$, i.e., the generalized mean value of the Hamiltonian operator is real valued. Other typical properties of operators that are Hermitian in the usual sense hold here as well; for example, the eigenvalues are real (see, for example, Refs. [2,4]).

Substituting j from Eq. (25) into Eq. (23), we obtain the result (we omit the variable t in the expressions that follow)

$$\begin{aligned}\lambda\frac{2\mathrm{m}}{\hbar^2}f[\Psi,\Psi]&=\left[\psi\,\lambda\psi_x^*-\psi^*\lambda\psi_x\right]\Big|_a^b\\&=\left[\psi(b)\,\lambda\psi_x^*(b)-\psi^*(b)\,\lambda\psi_x(b)\right]-\left[\psi(a)\,\lambda\psi_x^*(a)-\psi^*(a)\,\lambda\psi_x(a)\right]=0,\end{aligned} \tag{26}$$

where $\lambda\in\mathbb{R}$ is a parameter required for dimensional reasons. It is very convenient to rewrite the latter two terms using the following identity:

$$\begin{aligned}z_1z_2^*-z_1^*z_2&=\frac{\mathrm{i}}{2}\left[(z_1+\mathrm{i}z_2)(z_1+\mathrm{i}z_2)^*-(z_1-\mathrm{i}z_2)(z_1-\mathrm{i}z_2)^*\right]\\&=\frac{\mathrm{i}}{2}\left(\left|z_1+\mathrm{i}z_2\right|^2-\left|z_1-\mathrm{i}z_2\right|^2\right),\end{aligned} \tag{27}$$

where z_1 and z_2 are complex numbers. Then, the following result is obtained:

$$\begin{aligned}\lambda\frac{2\mathrm{m}}{\hbar^2}f[\Psi,\Psi]&=\frac{\mathrm{i}}{2}\left(\left|\psi(b)+\mathrm{i}\lambda\psi_x(b)\right|^2-\left|\psi(b)-\mathrm{i}\lambda\psi_x(b)\right|^2\right)\\&\quad-\frac{\mathrm{i}}{2}\left(\left|\psi(a)+\mathrm{i}\lambda\psi_x(a)\right|^2-\left|\psi(a)-\mathrm{i}\lambda\psi_x(a)\right|^2\right)\\&=\frac{\mathrm{i}}{2}\left(\left|\psi(b)+\mathrm{i}\lambda\psi_x(b)\right|^2+\left|\psi(a)-\mathrm{i}\lambda\psi_x(a)\right|^2\right)\\&\quad-\frac{\mathrm{i}}{2}\left(\left|\psi(b)-\mathrm{i}\lambda\psi_x(b)\right|^2+\left|\psi(a)+\mathrm{i}\lambda\psi_x(a)\right|^2\right)=0,\end{aligned} \tag{28}$$

that is,

$$\begin{aligned}\lambda\frac{2\mathrm{m}}{\hbar^2}f[\Psi,\Psi]&=\frac{\mathrm{i}}{2}\begin{bmatrix}\psi(b)+\mathrm{i}\lambda\psi_x(b)\\\psi(a)-\mathrm{i}\lambda\psi_x(a)\end{bmatrix}^\dagger\begin{bmatrix}\psi(b)+\mathrm{i}\lambda\psi_x(b)\\\psi(a)-\mathrm{i}\lambda\psi_x(a)\end{bmatrix}\\&\quad-\frac{\mathrm{i}}{2}\begin{bmatrix}\psi(b)-\mathrm{i}\lambda\psi_x(b)\\\psi(a)+\mathrm{i}\lambda\psi_x(a)\end{bmatrix}^\dagger\begin{bmatrix}\psi(b)-\mathrm{i}\lambda\psi_x(b)\\\psi(a)+\mathrm{i}\lambda\psi_x(a)\end{bmatrix}=0.\end{aligned} \tag{29}$$

Let us now consider the following general matrix boundary condition:

$$\begin{bmatrix}\psi(b)+\mathrm{i}\lambda\psi_x(b)\\\psi(a)-\mathrm{i}\lambda\psi_x(a)\end{bmatrix}=\hat{\mathrm{M}}\begin{bmatrix}\psi(b)-\mathrm{i}\lambda\psi_x(b)\\\psi(a)+\mathrm{i}\lambda\psi_x(a)\end{bmatrix}, \tag{30}$$

where $\hat{\mathrm{M}}$ is an arbitrary complex matrix. By substituting Eq. (30) into Eq. (29), we obtain

$$\frac{\mathrm{i}}{2}\begin{bmatrix}\psi(b)-\mathrm{i}\lambda\psi_x(b)\\\psi(a)+\mathrm{i}\lambda\psi_x(a)\end{bmatrix}^\dagger\left(\hat{\mathrm{M}}^\dagger\hat{\mathrm{M}}-\hat{1}_2\right)\begin{bmatrix}\psi(b)-\mathrm{i}\lambda\psi_x(b)\\\psi(a)+\mathrm{i}\lambda\psi_x(a)\end{bmatrix}=0;$$

therefore, $\hat{\mathrm{M}}$ is a unitary matrix (the justification for this result is given in the comment that follows Eq. (A.14)). Thus, a general set of generalized Hermitian boundary conditions for the 1D KFG particle in a box can be written as follows:

$$\begin{bmatrix}\psi(b)-\mathrm{i}\lambda\psi_x(b)\\\psi(a)+\mathrm{i}\lambda\psi_x(a)\end{bmatrix}=\hat{\mathrm{U}}_{(2\times2)}\begin{bmatrix}\psi(b)+\mathrm{i}\lambda\psi_x(b)\\\psi(a)-\mathrm{i}\lambda\psi_x(a)\end{bmatrix}, \tag{31}$$

where $\hat{\mathrm{U}}_{(2\times2)}=\hat{\mathrm{M}}^{-1}$ is also unitary. This family of boundary conditions is similar to the one corresponding to the problem of the 1D Schrödinger particle enclosed in a box; for example, see Eq. (28) in Ref. [28]. In relation to this, we can also take the nonrelativistic approximation of the general boundary condition given in Eq. (31). For that purpose, it is convenient to first write the KFG wavefunction $\psi=\psi(x,t)$ as follows: $\psi=\psi_{\mathrm{S}}\exp(-\mathrm{i}\,\mathrm{m}c^2t/\hbar)$, where $\psi_{\mathrm{S}}=\psi_{\mathrm{S}}(x,t)$ is the Schrödinger wavefunction. Because in this approximation we have that $\left|\mathrm{i}\hbar(\psi_{\mathrm{S}})_t\right|\ll\mathrm{m}c^2\left|\psi_{\mathrm{S}}\right|$, we can write $\psi_t=(-\mathrm{i}\,\mathrm{m}c^2t/\hbar)\psi$, and therefore $\psi_1=\left(1-\frac{V}{2\mathrm{m}c^2}\right)\psi$ and $\psi_2=\frac{V}{2\mathrm{m}c^2}\psi$ (see Eq. (4)). Thus, for weak external potentials and to the lowest order in v/c (and for positive energy solutions), $\psi_1\approx\psi$ satisfies the Schrödinger equation in the potential $V+\mathrm{m}c^2$ (the latter $\mathrm{m}c^2$ can be eliminated by using the expression $\psi_1\approx\psi=\psi_{\mathrm{S}}\exp(-\mathrm{i}\,\mathrm{m}c^2t/\hbar)$) but also $(\psi_1)_x\approx\psi_x$ (see, for example, Refs. [2,19,23]). It is then clear that, in the problem of the particle in a box, the one-component KFG wavefunction satisfies the same boundary conditions as the one-component Schrödinger wavefunction. Incidentally, a similar result to Eq. (31) had already been obtained by taking the nonrelativistic limit of the most general family of boundary conditions for the 1D Dirac particle enclosed in a box [29]. Additionally, in the analogous problem of a 1D Schrödinger particle in the presence of a point interaction at the point $x=0$ (or a hole at the origin), the most general family of boundary conditions is similar to that given in Eq. (31) [30]. Indeed, all these results substantiate that the set of boundary conditions dependent on the four real parameters given in Eq. (31) is also the most general for a 1D KFG particle in the interval $[a,b]$. Moreover, by making the replacements $a\to0+$ and $b\to0-$ in Eq. (31), we obtain the respective most general set of boundary conditions for the case in which the 1D KFG particle moves along the real line with a hole at the origin. Some examples of boundary conditions for this system can be seen in Refs. [21,23] and will be briefly discussed in Section 3.

For all the boundary conditions that are part of the general set of boundary conditions in Eq. (31), $\hat{\mathrm{h}}$ is a pseudo-Hermitian operator, but it is also a pseudo self-adjoint operator (see Appendix B). Certainly, the result in Eq. (31) is given in terms of the wavefunction ψ, but if the relation in Eq. (5) is used, it can also be written in terms of the components of $\Psi=\begin{bmatrix}\psi_1&\psi_2\end{bmatrix}^{\mathrm{T}}$, i.e., in terms of $\psi_1+\psi_2$, and its spatial derivative $(\psi_1)_x+(\psi_2)_x$, evaluated at the edges $x=a$ and $x=b$. Actually, the general family of boundary conditions given in Eq. (31) must be written in terms of $(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\Psi$ and $(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\Psi_x$ evaluated at the ends of the box. We work on this in the next section. We give below some examples of boundary conditions that are contained in Eq. (31): $\psi(a)=\psi(b)=0$ ($\hat{\mathrm{U}}_{(2\times2)}=-\hat{1}_2$), i.e., ψ can satisfy the Dirichlet boundary condition; $\psi_x(a)=\psi_x(b)=0$ ($\hat{\mathrm{U}}_{(2\times2)}=+\hat{1}_2$), i.e., ψ can satisfy the Neumann boundary condition; $\psi(a)=\psi(b)$ and $\psi_x(a)=\psi_x(b)$ ($\hat{\mathrm{U}}_{(2\times2)}=+\hat{\sigma}_x$), ψ can satisfy the periodic boundary condition; $\psi(a)=-\psi(b)$ and $\psi_x(a)=-\psi_x(b)$ ($\hat{\mathrm{U}}_{(2\times2)}=-\hat{\sigma}_x$), ψ can satisfy the antiperiodic boundary condition; $\psi(a)=\psi_x(b)=0$ ($\hat{\mathrm{U}}_{(2\times2)}=\hat{\sigma}_z$), i.e., ψ can satisfy a mixed boundary condition; $\psi_x(a)=\psi(b)=0$ ($\hat{\mathrm{U}}_{(2\times2)}=-\hat{\sigma}_z$), i.e., ψ can satisfy another mixed boundary condition; $\psi(a)-\lambda\psi_x(a)=0$ and $\psi(b)+\lambda\psi_x(b)=0$ ($\hat{\mathrm{U}}_{(2\times2)}=\mathrm{i}\hat{1}_2$), ψ can satisfy a kind of Robin boundary condition. In fact, the latter boundary condition would be the KFG version of the boundary condition commonly used in the so-called (one-dimensional) MIT bag model for hadronic structures (see, for example, Ref. [29]). All these boundary conditions are typical of wave equations that are of the second order in the spatial derivative.

Of all the boundary conditions included in the four-parameter family of boundary conditions, only those arising from a diagonal unitary matrix describe a particle in an impenetrable box. This is because, for these boundary conditions, the probability current density satisfies the relation $j(b)=j(a)=0$ for all t. Thus, the most general family of confining boundary conditions for a 1D KFG particle in a box only has two (real) parameters. The latter result is due to the similarity between the general set of boundary conditions given in Eq. (31) and the general sets of boundary conditions for the 1D Dirac and Schrödinger particles, and because we already know that the confining boundary conditions come from a matrix $\hat{\mathrm{U}}_{(2\times2)}$ that is diagonal [29].

3. Boundary conditions for the 1D KFG particle in a box II

Here, we obtain the most general set of pseudo self-adjoint boundary conditions for the Hamiltonian operator in the 1D FV equation, that is, we write the latter set in terms of Ψ and Ψ_x evaluated at the endpoints of the box. More specifically, in terms of $(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)\Psi$ and $(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_2)\Psi_x$. Indeed, following a procedure similar to that used above to obtain Eq. (26), namely, substituting j from Eq. (24) into Eq. (23), we obtain

$$\begin{aligned}\lambda\frac{2\mathrm{m}}{\hbar^2}f[\Psi,\Psi] &= \frac{1}{2}\Big[\left((\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\lambda\Psi_x\right)^\dagger(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\Psi \\ &\quad -\left((\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\Psi\right)^\dagger(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\lambda\Psi_x\Big]\Big|_a^b \\ &= \frac{1}{2}\Big[\left((\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\lambda\Psi_x(b)\right)^\dagger(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\Psi(b) \\ &\quad -\left((\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\Psi(b)\right)^\dagger(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\lambda\Psi_x(b)\Big] \\ &\quad -\frac{1}{2}\Big[\left((\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\lambda\Psi_x(a)\right)^\dagger(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\Psi(a) \\ &\quad -\left((\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\Psi(a)\right)^\dagger(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\lambda\Psi_x(a)\Big] = 0, \end{aligned} \tag{32}$$

where again, we insert the real parameter λ for dimensional reasons. Now, we use the following matrix identity twice:

$$\hat{Z}_2^\dagger\hat{Z}_1 - \hat{Z}_1^\dagger\hat{Z}_2 = \frac{\mathrm{i}}{2}\left[(\hat{Z}_1+\mathrm{i}\hat{Z}_2)^\dagger(\hat{Z}_1+\mathrm{i}\hat{Z}_2) - (\hat{Z}_1-\mathrm{i}\hat{Z}_2)^\dagger(\hat{Z}_1-\mathrm{i}\hat{Z}_2)\right]. \tag{33}$$

Then, we obtain the following result:

$$\begin{aligned}\lambda\frac{2\mathrm{m}}{\hbar^2}f[\Psi,\Psi] &= \frac{1}{2}\frac{\mathrm{i}}{2}\Big[\left((\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(b)\right)^\dagger(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(b) \\ &\quad -\left((\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(b)\right)^\dagger(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(b)\Big] \\ &\quad -\frac{1}{2}\frac{\mathrm{i}}{2}\Big[\left((\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(a)\right)^\dagger(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(a) \\ &\quad -\left((\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(a)\right)^\dagger(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(a)\Big] = 0, \end{aligned} \tag{34}$$

that is,

$$\begin{aligned}&\lambda\frac{2\mathrm{m}}{\hbar^2}f[\Psi,\Psi] \\ &\quad = \frac{1}{2}\frac{\mathrm{i}}{2}\begin{bmatrix}(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(b)\\(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(a)\end{bmatrix}^\dagger\begin{bmatrix}(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(b)\\(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(a)\end{bmatrix} \\ &\quad -\frac{1}{2}\frac{\mathrm{i}}{2}\begin{bmatrix}(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(b)\\(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(a)\end{bmatrix}^\dagger\begin{bmatrix}(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(b)\\(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(a)\end{bmatrix} = 0. \end{aligned} \tag{35}$$

Now, we propose writing a general matrix boundary condition as follows:

$$\begin{bmatrix}(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(b)\\(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(a)\end{bmatrix} = \hat{\mathrm{A}}\begin{bmatrix}(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(b)\\(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(a)\end{bmatrix}, \tag{36}$$

where $\hat{\mathrm{A}}$ is an arbitrary 4×4 complex matrix. By substituting Eq. (36) into Eq. (35), we obtain

$$\frac{1}{2}\frac{\mathrm{i}}{2}\begin{bmatrix}(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(b)\\(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(a)\end{bmatrix}^\dagger\left(\hat{\mathrm{A}}^\dagger\hat{\mathrm{A}}-\hat{\mathrm{I}}_4\right)\begin{bmatrix}(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(b)\\(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(a)\end{bmatrix} = 0,$$

then $\hat{\mathrm{A}}$ is a unitary matrix ($\hat{\mathrm{I}}_4$ is the 4×4 identity matrix). Note that the components of the column vectors in Eq. (36) are themselves 2×1 column matrices and are given by

$$(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi\pm\mathrm{i}\lambda\Psi_x)(x) = \begin{bmatrix}(\psi\pm\mathrm{i}\lambda\psi_x)(x)\\-(\psi\pm\mathrm{i}\lambda\psi_x)(x)\end{bmatrix}, \quad x=a,b. \tag{37}$$

Thus, the general boundary condition in Eq. (36) can be written as follows:

$$\begin{bmatrix}(\psi+\mathrm{i}\lambda\psi_x)(b)\\-(\psi+\mathrm{i}\lambda\psi_x)(b)\\(\psi-\mathrm{i}\lambda\psi_x)(a)\\-(\psi-\mathrm{i}\lambda\psi_x)(a)\end{bmatrix} = \hat{\mathrm{A}}\begin{bmatrix}(\psi-\mathrm{i}\lambda\psi_x)(b)\\-(\psi-\mathrm{i}\lambda\psi_x)(b)\\(\psi+\mathrm{i}\lambda\psi_x)(a)\\-(\psi+\mathrm{i}\lambda\psi_x)(a)\end{bmatrix}. \tag{38}$$

On the other hand, this relation can also be written as follows:

$$\begin{bmatrix}(\psi+\mathrm{i}\lambda\psi_x)(b)\\(\psi-\mathrm{i}\lambda\psi_x)(a)\\(\psi+\mathrm{i}\lambda\psi_x)(b)\\(\psi-\mathrm{i}\lambda\psi_x)(a)\end{bmatrix} = \hat{\mathrm{S}}\hat{\mathrm{A}}\hat{\mathrm{S}}^\dagger\begin{bmatrix}(\psi-\mathrm{i}\lambda\psi_x)(b)\\(\psi+\mathrm{i}\lambda\psi_x)(a)\\(\psi-\mathrm{i}\lambda\psi_x)(b)\\(\psi+\mathrm{i}\lambda\psi_x)(a)\end{bmatrix}, \tag{39}$$

where $\hat{\mathrm{S}}$ is given by

$$\hat{\mathrm{S}} = \begin{bmatrix}1&0&0&0\\0&0&1&0\\0&-1&0&0\\0&0&0&-1\end{bmatrix}$$

$$= \frac{1}{2}\left(\hat{\sigma}_z\otimes\hat{\mathrm{I}}_2 + \mathrm{i}\hat{\sigma}_y\otimes\hat{\sigma}_x + \mathrm{i}\hat{\sigma}_x\otimes\hat{\sigma}_y + \hat{\mathrm{I}}_2\otimes\hat{\sigma}_z\right), \tag{40}$$

where $\otimes$ denotes the Zehfuss–Kronecker product of matrices, or the matrix direct product

$$\hat{\mathrm{F}}\otimes\hat{\mathrm{G}} \equiv \begin{bmatrix}\mathrm{F}_{11}\hat{\mathrm{G}} & \cdots & \mathrm{F}_{1n}\hat{\mathrm{G}}\\ \vdots & \ddots & \vdots\\ \mathrm{F}_{m1}\hat{\mathrm{G}} & \cdots & \mathrm{F}_{mn}\hat{\mathrm{G}}\end{bmatrix}, \tag{41}$$

which is bilinear and associative and satisfies, among other properties, the mixed-product property: $(\hat{\mathrm{F}}\otimes\hat{\mathrm{G}})(\hat{\mathrm{J}}\otimes\hat{\mathrm{K}}) = (\hat{\mathrm{F}}\hat{\mathrm{J}}\otimes\hat{\mathrm{G}}\hat{\mathrm{K}})$ (see, for example, Ref. [31]). The matrix $\hat{\mathrm{S}}$ is unitary, and therefore, $\hat{\mathrm{S}}\hat{\mathrm{A}}\hat{\mathrm{S}}^\dagger$ is also a unitary matrix. Now, notice that the left-hand side of the relation in Eq. (39) is given by (see Eq. (30))

$$\begin{aligned}\begin{bmatrix}\begin{bmatrix}(\psi+\mathrm{i}\lambda\psi_x)(b)\\(\psi-\mathrm{i}\lambda\psi_x)(a)\end{bmatrix}\\ \begin{bmatrix}(\psi+\mathrm{i}\lambda\psi_x)(b)\\(\psi-\mathrm{i}\lambda\psi_x)(a)\end{bmatrix}\end{bmatrix} &= \begin{bmatrix}\hat{\mathrm{M}}\begin{bmatrix}(\psi-\mathrm{i}\lambda\psi_x)(b)\\(\psi+\mathrm{i}\lambda\psi_x)(a)\end{bmatrix}\\ \hat{\mathrm{M}}\begin{bmatrix}(\psi-\mathrm{i}\lambda\psi_x)(b)\\(\psi+\mathrm{i}\lambda\psi_x)(a)\end{bmatrix}\end{bmatrix} \\ &= \begin{bmatrix}\hat{\mathrm{M}}&\hat{0}\\\hat{0}&\hat{\mathrm{M}}\end{bmatrix}\begin{bmatrix}(\psi-\mathrm{i}\lambda\psi_x)(b)\\(\psi+\mathrm{i}\lambda\psi_x)(a)\\(\psi-\mathrm{i}\lambda\psi_x)(b)\\(\psi+\mathrm{i}\lambda\psi_x)(a)\end{bmatrix}, \end{aligned} \tag{42}$$

and substituting the latter relation into Eq. (39), we obtain

$$\hat{\mathrm{S}}\hat{\mathrm{A}}\hat{\mathrm{S}}^\dagger = \begin{bmatrix}\hat{\mathrm{M}}&\hat{0}\\\hat{0}&\hat{\mathrm{M}}\end{bmatrix} = \hat{\mathrm{I}}_2\otimes\hat{\mathrm{M}} \tag{43}$$

(because $\hat{\mathrm{M}}$ is a unitary matrix, the block diagonal matrix in Eq. (43) is also unitary). Then, from Eq. (43), we can write the matrix $\hat{\mathrm{A}}$ as follows:

$$\hat{\mathrm{A}} = \hat{\mathrm{S}}^\dagger\begin{bmatrix}\hat{\mathrm{M}}&\hat{0}\\\hat{0}&\hat{\mathrm{M}}\end{bmatrix}\hat{\mathrm{S}} = \hat{\mathrm{S}}^\dagger(\hat{\mathrm{I}}_2\otimes\hat{\mathrm{M}})\hat{\mathrm{S}}. \tag{44}$$

Thus, the most general family of pseudo self-adjoint boundary conditions for the 1D KFG particle in a box, that is, for the Hamiltonian operator in the 1D FV wave equation, can be written as follows (see Eq. (36)):

$$\begin{bmatrix}(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(b)\\(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(a)\end{bmatrix} = \hat{\mathrm{U}}_{(4\times4)}\begin{bmatrix}(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi+\mathrm{i}\lambda\Psi_x)(b)\\(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)(\Psi-\mathrm{i}\lambda\Psi_x)(a)\end{bmatrix}, \tag{45}$$

where

$$\begin{aligned}\hat{\mathrm{U}}_{(4\times4)} = \hat{\mathrm{A}}^{-1} = \hat{\mathrm{A}}^\dagger &= \hat{\mathrm{S}}^\dagger\begin{bmatrix}\hat{\mathrm{M}}^\dagger&\hat{0}\\\hat{0}&\hat{\mathrm{M}}^\dagger\end{bmatrix}\hat{\mathrm{S}} = \hat{\mathrm{S}}^\dagger\begin{bmatrix}\hat{\mathrm{M}}^{-1}&\hat{0}\\\hat{0}&\hat{\mathrm{M}}^{-1}\end{bmatrix}\hat{\mathrm{S}} \\ &= \hat{\mathrm{S}}^\dagger\begin{bmatrix}\hat{\mathrm{U}}_{(2\times2)}&\hat{0}\\\hat{0}&\hat{\mathrm{U}}_{(2\times2)}\end{bmatrix}\hat{\mathrm{S}} = \hat{\mathrm{S}}^\dagger(\hat{\mathrm{I}}_2\otimes\hat{\mathrm{U}}_{(2\times2)})\hat{\mathrm{S}} \end{aligned} \tag{46}$$

(to reach this result, we use Eq. (44) and the fact that $\hat{\mathrm{U}}_{(2\times2)} = \hat{\mathrm{M}}^{-1}$, the latter two results and only some properties of the matrix direct product could also be used). Note that the general matrix boundary condition in Eq. (45) could also be written as follows:

$$(\hat{\mathrm{I}}_2\otimes(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2))\begin{bmatrix}(\Psi-\mathrm{i}\lambda\Psi_x)(b)\\(\Psi+\mathrm{i}\lambda\Psi_x)(a)\end{bmatrix}$$

$$= \hat{U}_{(4\times4)}(\hat{I}_2 \otimes (\hat{\tau}_3 + i\hat{\tau}_2)) \begin{bmatrix} (\Psi + i\lambda\Psi_x)(b) \\ (\Psi - i\lambda\Psi_x)(a) \end{bmatrix}; \quad (47)$$

however, the matrix $\hat{I}_2 \otimes (\hat{\tau}_3 + i\hat{\tau}_2)$ does not have an inverse and the column vector on the left side of this relation cannot be cleared. Thus, the expression given in Eq. (47) is an elegant way to write the general boundary condition, but it is not functional and could lead to errors.

The boundary conditions that were presented just before the last paragraph of Section 2 can be extracted from Eq. (45) if the matrix $\hat{U}_{(2\times2)}$ is known. In effect, the Dirichlet boundary condition is $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi(a) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi(b) = 0$ ($\hat{U}_{(4\times4)} = -\hat{I}_4 = -\hat{I}_2 \otimes \hat{I}_2$); the Neumann boundary condition is $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(a) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(b) = 0$ ($\hat{U}_{(4\times4)} = +\hat{I}_4 = +\hat{I}_2 \otimes \hat{I}_2$); the periodic boundary condition is $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi(a) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi(b)$ and $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(a) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(b)$ ($\hat{U}_{(4\times4)} = \hat{\sigma}_x \otimes \hat{I}_2$); the antiperiodic boundary condition is $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi(a) = -(\hat{\tau}_3 + i\hat{\tau}_2)\Psi(b)$ and $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(a) = -(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(b)$ ($\hat{U}_{(4\times4)} = -\hat{\sigma}_x \otimes \hat{I}_2$); a mixed boundary condition is $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi(a) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(b) = 0$ ($\hat{U}_{(4\times4)} = \hat{\sigma}_z \otimes \hat{I}_2$); another mixed boundary condition is $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(a) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi(b) = 0$ ($\hat{U}_{(4\times4)} = -\hat{\sigma}_z \otimes \hat{I}_2$); a kind of Robin boundary condition (and a kind of MIT bag boundary condition for a 1D KFG particle) is $(\hat{\tau}_3 + i\hat{\tau}_2)(\Psi(a) - \lambda\Psi_x(a)) = 0$ and $(\hat{\tau}_3 + i\hat{\tau}_2)(\Psi(b) + \lambda\Psi_x(b)) = 0$ ($\hat{U}_{(4\times4)} = i\hat{I}_4 = i\hat{I}_2 \otimes \hat{I}_2$). Then, to write all these boundary conditions in terms of $\psi(a)$ and $\psi(b)$, and $\psi_x(a)$ and $\psi_x(b)$, we must use the fact that $\Psi = \begin{bmatrix} \psi_1 & \psi_2 \end{bmatrix}^T$ and $\psi = \psi_1 + \psi_2$ (Eq. (5)). If we wish to obtain explicit relations between the components of Ψ and Ψ_x at $x = a$ and Ψ and Ψ_x at $x = b$, we must use the relations given in Eqs. (5) and (6). Additionally, it can be shown that when the matrix $\hat{U}_{(2\times2)}$ is diagonal, then the matrix $\hat{U}_{(4\times4)}$ is also diagonal; consequently, diagonal matrices $\hat{U}_{(4\times4)}$ in Eq. (45) lead to confining boundary conditions (see the last paragraph of Section 2).

In general, the boundary conditions imposed on $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi$ and $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x$ at the endpoints of the box do not imply that Ψ and Ψ_x must also satisfy them. For example, let us consider the problem of the 1D KFG particle in the step potential ($V(x) = V_0\,\Theta(x)$, where $\Theta(x)$ is the Heaviside step function). This problem was also considered in Refs. [21,23]. The step potential is a (soft) point interaction in the neighborhood of the origin, that is, between the points $x = a \to 0+$ and $x = b \to 0-$, and the boundary condition is the periodic boundary condition, which in this case becomes the continuity condition of $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi$ and $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x$ at $x = 0$, i.e., $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi(0-) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi(0+)$ and $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(0-) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(0+)$. As we know, from this condition, it is obtained that $\psi(0-) = \psi(0+)$ and $\psi_x(0-) = \psi_x(0+)$. If the relations $\psi_1 + \psi_2 = \psi$ (Eq. (5)) and $\psi_1 - \psi_2 = (E - V)\psi/mc^2$ (Eq. (6)) are used (in the latter, we also assumed that ψ is an energy eigenstate), one can find relations between $\{\Psi(0+), \Psi_x(0+)\}$ and $\{\Psi(0-), \Psi_x(0-)\}$. We find that the relation given in Eq. (30) in Ref. [21] is none other than the boundary condition $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi(0-) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi(0+)$, with Eqs. (5) and (6) evaluated at $x = 0\pm$. Likewise, the relation given in Eq. (31) of the same reference is none other than $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(0-) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(0+)$, with the spatial derivatives of Eqs. (5) and (6) also evaluated at $x = 0\pm$. Finally, adding the latter two boundary conditions, we obtain Eq. (32) of Ref. [21]. Clearly, if the height of the step potential is not zero, then $\Psi(0+)$ is different from $\Psi(0-)$, and $\Psi_x(0+)$ is different from $\Psi_x(0-)$. Similarly, in Ref. [23], it was explicitly proven that $\Psi(0+) \neq \Psi(0-)$ and $\Psi_x(0+) \neq \Psi_x(0-)$ (see Eqs. (19) and (20) in that reference), but it was also shown that the boundary condition should be written in the form $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi(0-) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi(0+)$ and $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(0-) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x(0+)$. Incidentally, in the same reference, it was shown that the latter boundary condition can be obtained by integrating the 1D FV equation from $x = 0-$ to $x = 0+$.

On the other hand, in the problem of the 1D KFG particle inside the box $\Omega = [a, b]$, and subjected to the potential V, with the Dirichlet boundary condition, $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi(a) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi(b) = 0$, we know that ψ also satisfies this condition, namely, $\psi(a) = \psi(b) = 0$. The latter boundary condition together with Eqs. (5) and (6) lead us to the boundary condition $\Psi(a) = \Psi(b) = 0$. Indeed, in addition to $\psi_1(a) + \psi_2(a) = \psi_1(b) + \psi_2(b) = 0$, $\psi_1(a) - \psi_2(a) = \psi_1(b) - \psi_2(b) = 0$ (because $\psi_t(a, t) = \psi_t(b, t) = 0$ also holds). Finally, Ψ also satisfies the Dirichlet boundary condition at the edges of the box (the latter boundary condition was precisely the one used in Ref. [22]).

In short, let us suppose that the one-component wavefunction ψ can vanish at a point on the real line, for example, at $x = 0$ (also $V(0+)$ and $V(0-)$ must be finite numbers there). The latter is the Dirichlet boundary condition, namely, $\psi(0-) = \psi(0+) = 0 \equiv \psi(0)$. Certainly, this result is obtained from the disappearance of $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi$ at that same point, i.e., from the fact that the Hamiltonian operator with the latter boundary condition is a pseudo self-adjoint operator; then, the latter condition implies that the entire two-component wavefunction Ψ has to disappear at that point (use Eqs. (5) and (6)). In other words, the 1D FV wave equation is a second-order equation in the spatial derivative that accepts the vanishing of the entire two-component wavefunction at a point. On the other hand, let us now suppose that ψ_x can vanish at a point on the real line, for example, at $x = 0$, but ψ is nonzero there (also $V_x(0+)$ and $V_x(0-)$ must be finite numbers there). The latter is the Neumann boundary condition, namely, $\psi_x(0-) = \psi_x(0+) = 0 \equiv \psi_x(0)$. Indeed, we also have that $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x$ vanishes at that same point. Then, it can be shown that $(\psi_1)_x$ and $(\psi_2)_x$ do not have to vanish at the point in question, and therefore, Ψ_x is not zero there either (use Eqs. (5) and (6)).

4. Concluding remarks

The KFG Hamiltonian operator, or the Hamiltonian that is present in the first order in time 1D KFG wave equation, i.e., the 1D FV wave equation, is formally pseudo-Hermitian. This is a well-known fact, and its verification does not require knowledge of the domain of the Hamiltonian or its adjoint. We have shown that this operator is also a pseudo-Hermitian operator, but in addition, it is a pseudo self-adjoint operator when it describes a 1D KFG particle in a finite interval. Consequently, we constructed the most general set of boundary conditions for this operator, which is characterized by four real parameters and is consistent with the last two properties. All these results can be extended to the problem of a 1D KFG particle moving on a real line with a penetrable or an impenetrable obstacle at one point, i.e., with a point interaction (or a hole) there. For instance, assuming the point is $x = 0$, it suffices to make the replacements $x = a \to 0+$ and $x = b \to 0-$ in the general set of boundary conditions for the particle in the interval $[a, b]$.

As we have shown, the general set of boundary conditions can be written in terms of the one-component wavefunction for the second order in time 1D KFG wave equation, that is, ψ, and its derivative ψ_x, both evaluated at the ends of the box. Certainly, we showed that the general set can also be written in terms of the two-component column vectors for the 1D FV wave equation, that is, $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi$ and $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x$, evaluated at the ends of the box. We only used algebraic arguments and simple concepts that are within the general theory of linear operators on a space with indefinite inner product to build these sets of boundary conditions.

From the results presented in Section 3, we also found that Ψ and Ψ_x do not necessarily satisfy the same boundary condition that $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi$ and $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x$ satisfy. In any case, given a particular boundary condition that ψ and ψ_x satisfy at the ends of the box and using the relations that arise between the components of the column vector Ψ, that is, ψ_1 and ψ_2, and quantities ψ, ψ_t, and the potential V (see Eqs. (5) and (6)), the respective boundary condition on Ψ and Ψ_x can be obtained.

We think that our article will be of interest to those interested in the fundamental and technical aspects of relativistic wave equations. Furthermore, to the best of our knowledge, the main results of our article, i.e., those related to general pseudo self-adjoint sets of boundary conditions in the 1D KFG theory, do not appear to have been considered before.

Declaration of competing interest

The author declares that he has no known competing financial interest or personal relationship that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

Acknowledgment

The author wishes to thank the referees for their comments and suggestions.

Appendix A

The 1D KFG wave equation given in Eq. (3) can also be written as follows:

$$\left[-\hbar^2\frac{\partial^2}{\partial t^2}-\mathrm{i}2\hbar\, V(x)\frac{\partial}{\partial t}+(V(x))^2\right]\psi=\left[-\hbar^2c^2\frac{\partial^2}{\partial x^2}+(\mathrm{m}c^2)^2\right]\psi, \tag{A.1}$$

and therefore,

$$\psi_{tt}=c^2\psi_{xx}-\left(\frac{\mathrm{m}c^2}{\hbar}\right)^2\psi+\frac{2V}{\mathrm{i}\hbar}\psi_t+\frac{V^2}{\hbar^2}\psi. \tag{A.2}$$

The scalar product for the two-component column state vectors $\boldsymbol{\Psi}=\left[\psi_1\ \psi_2\right]^{\mathrm{T}}$ and $\boldsymbol{\Phi}=\left[\phi_1\ \phi_2\right]^{\mathrm{T}}$, where $\psi_1+\psi_2=\psi$ and $\phi_1+\phi_2=\phi$, is given by

$$\begin{aligned}\langle\langle\boldsymbol{\Psi},\boldsymbol{\Phi}\rangle\rangle&\equiv\int_\Omega \mathrm{d}x\,\boldsymbol{\Psi}^\dagger\hat{\tau}_3\boldsymbol{\Phi}\\&=\frac{\mathrm{i}\hbar}{2\mathrm{m}c^2}\int_\Omega \mathrm{d}x\left[\psi^*\left(\frac{\partial}{\partial t}-\frac{V}{\mathrm{i}\hbar}\right)\phi-\left(\left(\frac{\partial}{\partial t}-\frac{V}{\mathrm{i}\hbar}\right)\psi\right)^*\phi\right]\\&=\frac{\mathrm{i}\hbar}{2\mathrm{m}c^2}\int_\Omega \mathrm{d}x\left(\psi^*\phi_t-\psi_t^*\phi-\frac{2V}{\mathrm{i}\hbar}\psi^*\phi\right)\equiv\langle\psi,\phi\rangle_{\mathrm{KFG}}.\end{aligned} \tag{A.3}$$

The latter quantity is preserved in time; in fact, taking its time derivative and using the result in Eq. (A.2), and a similar relation for ϕ (ψ and ϕ are solutions of the 1D KFG wave equation in its standard form), one obtains the same relation given in Eq. (14), namely,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle\boldsymbol{\Psi},\boldsymbol{\Phi}\rangle\rangle=\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi,\phi\rangle_{\mathrm{KFG}}=-\frac{\mathrm{i}\hbar}{2\mathrm{m}}\left[\psi_x^*\phi-\psi^*\phi_x\right]\Big|_a^b. \tag{A.4}$$

As follows from the results obtained in Appendix B, if ψ and ϕ both satisfy any boundary condition included in the most general set of boundary conditions, the boundary term in Eq. (A.4) always vanishes.

Appendix B

The goal of this section is to show that if the functions belonging to the domain of $\hat{\mathrm{h}}$ (considered a densely defined operator) obey any of the boundary conditions included in Eq. (31), then the functions of the domain of $\hat{\mathrm{h}}_{\mathrm{adj}}$ must obey the same boundary condition. This means that for the general family of boundary conditions given in Eq. (31), the operator $\hat{\mathrm{h}}=\hat{\mathrm{h}}_{\mathrm{adj}}$ is pseudo self-adjoint. Our results are obtained using simple arguments that are part of the general theory of linear operators in an indefinite inner product space (see, for example, Refs. [32,33]).

Let us return to the result given in Eq. (16), namely,

$$\langle\langle\Xi,\hat{\mathrm{h}}\boldsymbol{\Phi}\rangle\rangle=\langle\langle\hat{\mathrm{h}}_{\mathrm{adj}}\Xi,\boldsymbol{\Phi}\rangle\rangle+f[\Xi,\boldsymbol{\Phi}], \tag{A.5}$$

where $f[\Xi,\boldsymbol{\Phi}]$ is given by (see Eq. (18))

$$f[\Xi,\boldsymbol{\Phi}]\equiv\frac{\hbar^2}{2\mathrm{m}}\frac{1}{2}\left[\left((\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\Xi_x\right)^\dagger(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\boldsymbol{\Phi}-\left((\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\Xi\right)^\dagger(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\boldsymbol{\Phi}_x\right]\Big|_a^b. \tag{A.6}$$

Here, $\hat{\mathrm{h}}$ can act on column vectors $\boldsymbol{\Phi}=\left[\phi_1\ \phi_2\right]^{\mathrm{T}}\in\mathcal{D}(\hat{\mathrm{h}})$, where $\mathcal{D}(\hat{\mathrm{h}})$ is the domain of $\hat{\mathrm{h}}$, a set of column vectors on which we allow the differential operator $\hat{\mathrm{h}}$ to act ($\mathcal{D}(\hat{\mathrm{h}})$ is a linear subset of the indefinite inner product space), which fundamentally includes boundary conditions, and $\hat{\mathrm{h}}_{\mathrm{adj}}$ can act on column vectors $\Xi=\left[\xi_1\ \xi_2\right]^{\mathrm{T}}\in\mathcal{D}(\hat{\mathrm{h}}_{\mathrm{adj}})$ (in general, $\mathcal{D}(\hat{\mathrm{h}}_{\mathrm{adj}})$ may not coincide with $\mathcal{D}(\hat{\mathrm{h}})$). By virtue of the result given in Eq. (5), the respective solutions of Eq. (3) are the following:

$$\phi_1+\phi_2=\phi\quad\text{and}\quad\xi_1+\xi_2=\xi. \tag{A.7}$$

The boundary term in Eq. (A.6) can be written in terms of ϕ and ξ, namely,

$$f[\Xi,\boldsymbol{\Phi}]=\frac{\hbar^2}{2\mathrm{m}}\left[\xi_x^*\phi-\xi^*\phi_x\right]\Big|_a^b. \tag{A.8}$$

First, let us suppose that every column vector $\boldsymbol{\Phi}\in\mathcal{D}(\hat{\mathrm{h}})$ satisfies the boundary conditions $(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\boldsymbol{\Phi}(a)=(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\boldsymbol{\Phi}(b)=0$ and $(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\boldsymbol{\Phi}_x(a)=(\hat{\tau}_3+\mathrm{i}\hat{\tau}_2)\boldsymbol{\Phi}_x(b)=0$, or, equivalently, $\phi(a)=\phi(b)=0$ and $\phi_x(a)=\phi_x(b)=0$ (remember the first relation in Eq. (A.7)). In this case, the boundary term in Eq. (A.5) vanishes, and we have the result

$$\langle\langle\Xi,\hat{\mathrm{h}}\boldsymbol{\Phi}\rangle\rangle=\langle\langle\hat{\mathrm{h}}_{\mathrm{adj}}\Xi,\boldsymbol{\Phi}\rangle\rangle. \tag{A.9}$$

The latter relation is precisely the one that defines the generalized adjoint differential operator. It is clear that its verification did not require the imposition of any boundary condition on the vectors $\Xi\in\mathcal{D}(\hat{\mathrm{h}}_{\mathrm{adj}})$. Thus, until now, we have that $\mathcal{D}(\hat{\mathrm{h}})\neq\mathcal{D}(\hat{\mathrm{h}}_{\mathrm{adj}})$ (in fact, we have that $\mathcal{D}(\hat{\mathrm{h}})\subset\mathcal{D}(\hat{\mathrm{h}}_{\mathrm{adj}})$, i.e., $\mathcal{D}(\hat{\mathrm{h}})$ is a restriction of $\mathcal{D}(\hat{\mathrm{h}}_{\mathrm{adj}})$).

If the operator $\hat{\mathrm{h}}$ is to be a pseudo self-adjoint differential operator, the relation given in Eq. (21), namely, $\hat{\mathrm{h}}=\hat{\mathrm{h}}_{\mathrm{adj}}$, must be verified, and therefore, $\mathcal{D}(\hat{\mathrm{h}})=\mathcal{D}(\hat{\mathrm{h}}_{\mathrm{adj}})$. To achieve this, we must allow every vector $\boldsymbol{\Phi}\in\mathcal{D}(\hat{\mathrm{h}})$ to satisfy more general boundary conditions, that is, we must relax the domain of $\hat{\mathrm{h}}$. Let us suppose that we have a set of boundary conditions to be imposed on a vector $\boldsymbol{\Phi}\in\mathcal{D}(\hat{\mathrm{h}})$; if the cancellation of the boundary term $f[\Xi,\boldsymbol{\Phi}]$ by these boundary conditions only depends on imposing the same boundary conditions on the vector $\Xi\in\mathcal{D}(\hat{\mathrm{h}}_{\mathrm{adj}})$, then $\hat{\mathrm{h}}$ will be a pseudo self-adjoint differential operator.

First, from Eq. (A.8), we write the boundary term in Eq. (A.5) as follows:

$$\begin{aligned}\lambda\frac{2\mathrm{m}}{\hbar^2}f[\Xi,\boldsymbol{\Phi}]&=\left[\phi\,\lambda\xi_x^*-\xi^*\lambda\phi_x\right]\Big|_a^b\\&=\left[\phi(b)\,\lambda\xi_x^*(b)-\xi^*(b)\,\lambda\phi_x(b)\right]-\left[\phi(a)\,\lambda\xi_x^*(a)-\xi^*(a)\,\lambda\phi_x(a)\right]=0.\end{aligned} \tag{A.10}$$

It is fairly convenient to rewrite the latter two terms using the following identity:

$$z_1z_2^*-z_3^*z_4=\frac{\mathrm{i}}{2}\left[(z_1+\mathrm{i}z_4)(z_3+\mathrm{i}z_2)^*-(z_1-\mathrm{i}z_4)(z_3-\mathrm{i}z_2)^*\right], \tag{A.11}$$

where z_1, z_2, z_3 and z_4 are complex numbers. The latter relation is the generalization of that given in Eq. (27). In fact, making the replacements $z_3\to z_1$ and $z_4\to z_2$ in Eq. (A.11), the relation given in Eq. (27) is obtained. Then, the following result is derived:

$$\begin{aligned}\lambda\frac{2\mathrm{m}}{\hbar^2}f[\Xi,\boldsymbol{\Phi}]&=\frac{\mathrm{i}}{2}\left[\left(\phi(b)+\mathrm{i}\lambda\phi_x(b)\right)\left(\xi(b)+\mathrm{i}\lambda\xi_x(b)\right)^*\right.\\&\quad\left.-\left(\phi(b)-\mathrm{i}\lambda\phi_x(b)\right)\left(\xi(b)-\mathrm{i}\lambda\xi_x(b)\right)^*\right]\\&\quad-\frac{\mathrm{i}}{2}\left[\left(\phi(a)+\mathrm{i}\lambda\phi_x(a)\right)\left(\xi(a)+\mathrm{i}\lambda\xi_x(a)\right)^*\right.\\&\quad\left.-\left(\phi(a)-\mathrm{i}\lambda\phi_x(a)\right)\left(\xi(a)-\mathrm{i}\lambda\xi_x(a)\right)^*\right]\\&=\frac{\mathrm{i}}{2}\left[\left(\phi(b)+\mathrm{i}\lambda\phi_x(b)\right)\left(\xi(b)+\mathrm{i}\lambda\xi_x(b)\right)^*\right.\\&\quad\left.+\left(\phi(a)-\mathrm{i}\lambda\phi_x(a)\right)\left(\xi(a)-\mathrm{i}\lambda\xi_x(a)\right)^*\right]\\&\quad-\frac{\mathrm{i}}{2}\left[\left(\phi(b)-\mathrm{i}\lambda\phi_x(b)\right)\left(\xi(b)-\mathrm{i}\lambda\xi_x(b)\right)^*\right.\\&\quad\left.+\left(\phi(a)+\mathrm{i}\lambda\phi_x(a)\right)\left(\xi(a)+\mathrm{i}\lambda\xi_x(a)\right)^*\right]=0,\end{aligned}$$

this means that

$$\lambda\frac{2\mathrm{m}}{\hbar^2}f[\Xi,\boldsymbol{\Phi}]=\frac{\mathrm{i}}{2}\begin{bmatrix}\xi(b)+\mathrm{i}\lambda\xi_x(b)\\ \xi(a)-\mathrm{i}\lambda\xi_x(a)\end{bmatrix}^{\dagger}\begin{bmatrix}\phi(b)+\mathrm{i}\lambda\phi_x(b)\\ \phi(a)-\mathrm{i}\lambda\phi_x(a)\end{bmatrix}$$
$$-\frac{\mathrm{i}}{2}\begin{bmatrix}\xi(b)-\mathrm{i}\lambda\xi_x(b)\\ \xi(a)+\mathrm{i}\lambda\xi_x(a)\end{bmatrix}^{\dagger}\begin{bmatrix}\phi(b)-\mathrm{i}\lambda\phi_x(b)\\ \phi(a)+\mathrm{i}\lambda\phi_x(a)\end{bmatrix}=0. \tag{A.12}$$

Let us now consider a more general set of boundary conditions to be imposed on a vector $\boldsymbol{\Phi}\in D(\hat{\mathrm{h}})$ (i.e., more general than the boundary conditions that we presented after Eq. (A.8)), namely,

$$\begin{bmatrix}\phi(b)+\mathrm{i}\lambda\phi_x(b)\\ \phi(a)-\mathrm{i}\lambda\phi_x(a)\end{bmatrix}=\hat{\mathrm{N}}\begin{bmatrix}\phi(b)-\mathrm{i}\lambda\phi_x(b)\\ \phi(a)+\mathrm{i}\lambda\phi_x(a)\end{bmatrix}, \tag{A.13}$$

where $\hat{\mathrm{N}}$ in an arbitrary complex matrix. By substituting the latter relation in Eq. (A.12), we obtain the following result:

$$\lambda\frac{2\mathrm{m}}{\hbar^2}f[\Xi,\boldsymbol{\Phi}]$$
$$=\frac{\mathrm{i}}{2}\left\{\left(\begin{bmatrix}\xi(b)+\mathrm{i}\lambda\xi_x(b)\\ \xi(a)-\mathrm{i}\lambda\xi_x(a)\end{bmatrix}^{\dagger}\hat{\mathrm{N}}\right.\right.$$
$$\left.\left.-\begin{bmatrix}\xi(b)-\mathrm{i}\lambda\xi_x(b)\\ \xi(a)+\mathrm{i}\lambda\xi_x(a)\end{bmatrix}^{\dagger}\right)\begin{bmatrix}\phi(b)-\mathrm{i}\lambda\phi_x(b)\\ \phi(a)+\mathrm{i}\lambda\phi_x(a)\end{bmatrix}\right\}=0,$$

and therefore,

$$\begin{bmatrix}\xi(b)+\mathrm{i}\lambda\xi_x(b)\\ \xi(a)-\mathrm{i}\lambda\xi_x(a)\end{bmatrix}^{\dagger}\hat{\mathrm{N}}=\begin{bmatrix}\xi(b)-\mathrm{i}\lambda\xi_x(b)\\ \xi(a)+\mathrm{i}\lambda\xi_x(a)\end{bmatrix}^{\dagger} \tag{A.14}$$

(This result is because, at this point, we cannot impose any boundary conditions that would completely annul the column vectors in Eq. (A.13), for example). Every vector $\Xi\in D(\hat{\mathrm{h}}_{\mathrm{adj}})$ should satisfy the same boundary conditions that $\boldsymbol{\Phi}\in D(\hat{\mathrm{h}})$ satisfies, i.e., the boundary conditions in Eq. (A.13), namely,

$$\begin{bmatrix}\xi(b)+\mathrm{i}\lambda\xi_x(b)\\ \xi(a)-\mathrm{i}\lambda\xi_x(a)\end{bmatrix}=\hat{\mathrm{N}}\begin{bmatrix}\xi(b)-\mathrm{i}\lambda\xi_x(b)\\ \xi(a)+\mathrm{i}\lambda\xi_x(a)\end{bmatrix}. \tag{A.15}$$

Taking the Hermitian conjugate of the matrix relation in Eq. (A.14) and substituting this result into Eq. (A.15), we obtain

$$\begin{bmatrix}\xi(b)+\mathrm{i}\lambda\xi_x(b)\\ \xi(a)-\mathrm{i}\lambda\xi_x(a)\end{bmatrix}=\hat{\mathrm{N}}\hat{\mathrm{N}}^{\dagger}\begin{bmatrix}\xi(b)+\mathrm{i}\lambda\xi_x(b)\\ \xi(a)-\mathrm{i}\lambda\xi_x(a)\end{bmatrix};$$

therefore, $\hat{\mathrm{N}}$ is a unitary matrix. Thus, the most general family of pseudo self-adjoint, or generalized self-adjoint boundary conditions, for the 1D KFG particle in a box can be written in the form given by Eq. (31), namely,

$$\begin{bmatrix}\xi(b)-\mathrm{i}\lambda\xi_x(b)\\ \xi(a)+\mathrm{i}\lambda\xi_x(a)\end{bmatrix}=\hat{\mathrm{U}}\begin{bmatrix}\xi(b)+\mathrm{i}\lambda\xi_x(b)\\ \xi(a)-\mathrm{i}\lambda\xi_x(a)\end{bmatrix}, \tag{A.16}$$

where $\hat{\mathrm{U}}=\hat{\mathrm{N}}^{-1}$. The fact that the boundary condition for $\boldsymbol{\Phi}\in D(\hat{\mathrm{h}})$ (for example, given in terms of ϕ) is the same boundary condition for $\Xi\in D(\hat{\mathrm{h}}_{\mathrm{adj}})$ (given in terms of ξ) ensures that $D(\hat{\mathrm{h}})=D(\hat{\mathrm{h}}_{\mathrm{adj}})$; therefore, $\hat{\mathrm{h}}$, which was already a pseudo-Hermitian operator, is also a pseudo self-adjoint operator. Additionally, the boundary term given in Eq. (14), or in Eq. (A.4), vanishes, and therefore, the pseudo inner product is conserved.

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