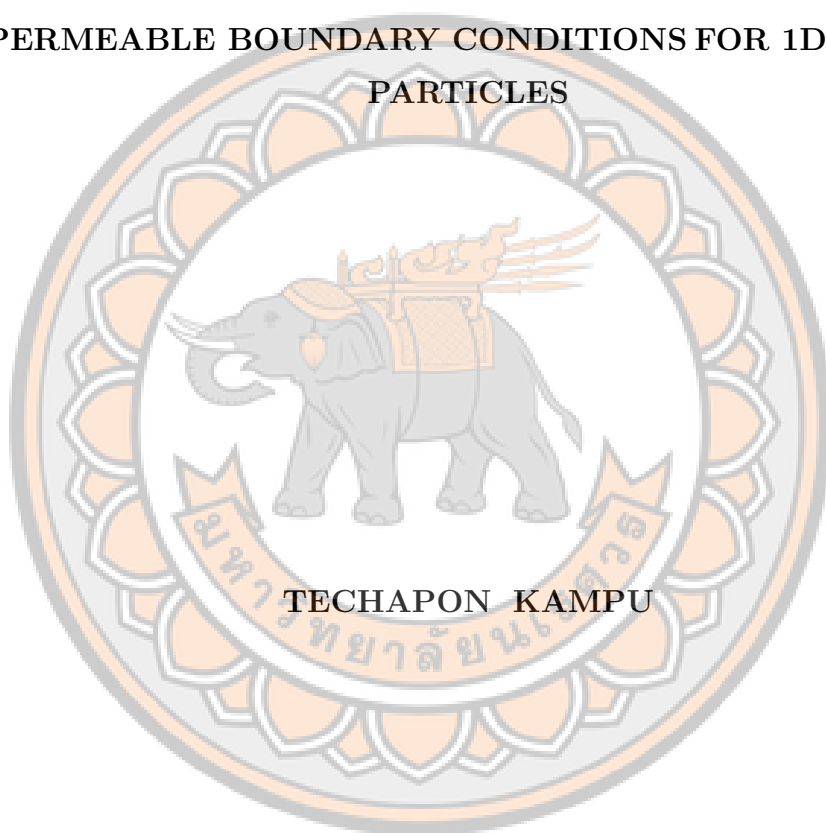




NONTRIVIAL LOCAL OBSERVABLES AND IMPERMEABLE AND
PERMEABLE BOUNDARY CONDITIONS FOR 1D KFGM
PARTICLES



TECHAPON KAMPU

A Thesis Submitted to Graduate School of Naresuan University
in Partial Fulfillment of the Requirements
for the Master of Science Program in Theoretical Physics

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Thesis entitled “Nontrivial local observables and impermeable and permeable
boundary conditions for 1D KFGM particles”

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the requirement for the Master of Science Program in Theoretical Physics of
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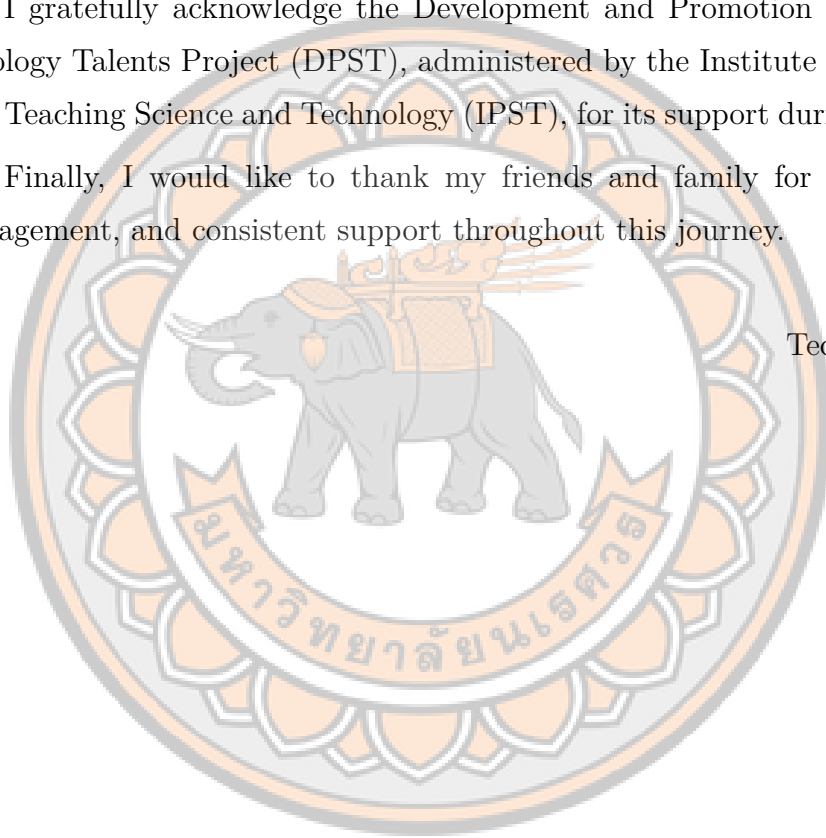
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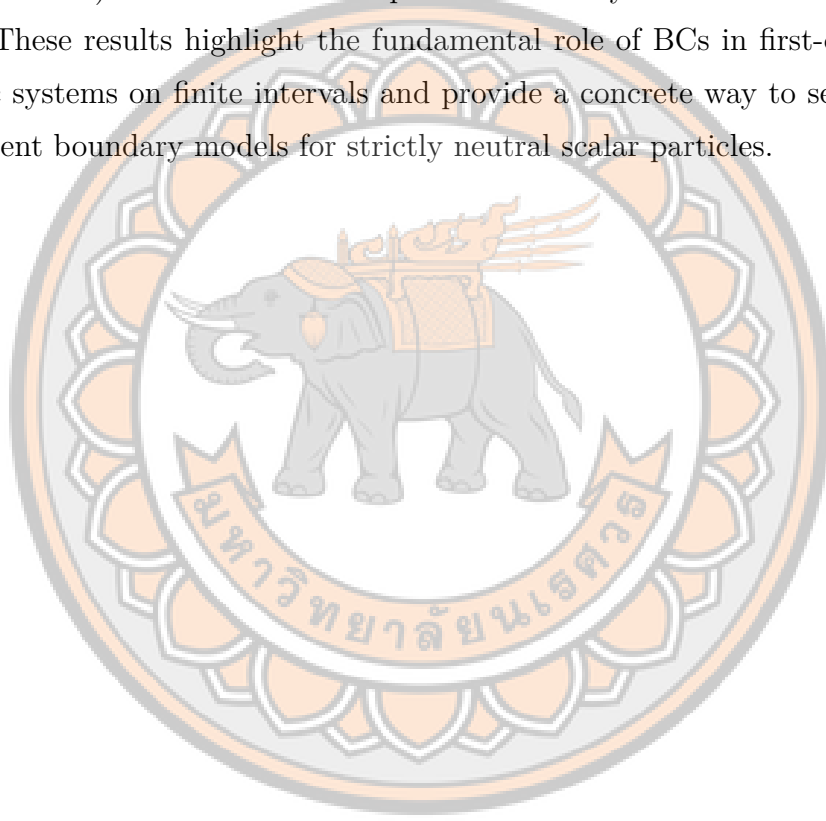


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ABSTRACT

Real solutions of the one-dimensional Klein-Fock-Gordon (KFG) equation make the usual two-vector current density vanish identically; as a result, the associated continuity equation becomes trivial, no nontrivial globally conserved quantity is obtained, and the usual current cannot distinguish between impermeable and permeable boundary conditions (BCs). This becomes an issue especially when the equation is used to describe a strictly neutral particle, namely a one-dimensional Klein-Fock-Gordon-Majorana (KFGM) particle. In this thesis, we address this limitation by introducing the simplest nontrivial local observables for the 1D KFGM system—an energy density and an energy current density. Working within the Feshbach-Villars (FV) framework on a finite interval, we derive these observables and establish their reality and conservation properties under the Majorana constraint. The acceptable BCs are obtained from the pseudo self-adjointness of the FV Hamiltonian together with two Majorana conditions. We show that the proposed energy density and energy current density, which form components of

an unusual energy-momentum tensor, satisfy a continuity equation and yield a conserved quantity for all acceptable BCs, whether the corresponding walls are impermeable or permeable. Additionally, the energy current density alone provides a complete local characterization of these BCs. By contrast, the standard energy current constructed from the usual energy-momentum tensor does not characterize all BCs correctly, and its associated energy density does not in general lead to a conserved global quantity. We further determine the conditions under which both sets of observables become equally satisfactory. This occurs only for four confining (impermeable) BCs and for a one-parameter family of nonconfining (permeable) BCs. These results highlight the fundamental role of BCs in first-quantized relativistic systems on finite intervals and provide a concrete way to select physically consistent boundary models for strictly neutral scalar particles.



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CHAPTER I

INTRODUCTION

In relativistic wave mechanics, a strictly neutral particle is one that is identical with its antiparticle. The term “Majorana” is historically associated with real wave equations for strictly neutral fermions [1], and related ideas also appear in discussions of neutrinos, dark-matter candidates, and condensed-matter Majorana modes. In the present thesis, however, these examples serve only as physical motivation. The technical subject is narrower: a massive, first-quantized, strictly neutral scalar particle on a finite interval. In this scalar setting, a one-dimensional Klein-Fock-Gordon-Majorana (1D KFGM) particle is represented by a real or purely imaginary solution of the KFG equation, together with the corresponding Majorana condition.

Recently, strictly neutral scalar particles have been studied in a system with one spatial and one temporal dimension. In particular, De Vincenzo analyzed one-dimensional (1D) Klein-Fock-Gordon (KFG) particles defined on a finite spatial interval and treated them as strictly neutral particles in $(1 + 1)$ -dimensional spacetime [5]. We refer to these systems as 1D KFGM particles. At the level of first quantization, their dynamics can be described either by the standard 1D KFG equation or by the 1D Feshbach-Villars (FV) equation, each with a real Lorentz scalar potential and a Majorana condition; see Refs. [6–9]. The standard FV decomposition used in this thesis contains factors proportional to $(mc^2)^{-1}$ and is therefore restricted to $m \neq 0$. The massless case requires a generalized FV/CFFV construction and is mentioned here only as a limitation and future direction. As emphasized in Ref. [5], first-order equations in the time derivative that do not have Hamiltonian form can also describe these particles; such equations are called first-order 1D Majorana equations.

Consider, for instance, the standard 1D KFG equation, namely,

$$\hat{O}_{\text{KFG}}\psi \equiv [\hat{E}^2 - (c\hat{p})^2 - (mc^2)^2 - 2mc^2S]\psi = 0, \quad (1.1)$$

where $\psi = \psi(x, t)$ is a one-component wavefunction, $\hat{E} = i\hbar \partial/\partial t$ is the energy operator, $\hat{p} = -i\hbar \partial/\partial x$ is the momentum operator, and here S is taken to be a real Lorentz scalar interaction. The strictly neutral (Majorana-type) restriction is implemented by imposing a real-field condition on ψ . One convenient way to express this is to impose the reality condition $\psi = \psi^*$, where the superscript $*$ denotes complex conjugation. An equivalent possibility is to impose $\psi = -\psi^*$, which makes ψ purely imaginary; in this case a simple redefinition, $(\psi - \psi^*)/2i = \psi/i$, makes the field real [5]. In either formulation, the essential point is that the physical state can be represented by a real wavefunction.

In Eq. (1.1), the scalar interaction $S(x, t)$ is real and Lorentz scalar: it modifies the mass-like part of the relativistic wave equation through the term $2mc^2S$, rather than entering as the time component of a vector potential. Thus S is not introduced in the same way as the additive potential energy $V(x)$ in the nonrelativistic Schrödinger equation. Nevertheless, for a weak, time-independent scalar interaction and a positive-energy solution written as $E = mc^2 + E_{\text{NR}}$ with $|E_{\text{NR}}| \ll mc^2$, Eq. (1.1) gives, to leading order, $E_{\text{NR}} \simeq p^2/(2m) + S$. In this limited nonrelativistic sense, S contributes like a potential-energy term, while its relativistic origin remains scalar and mass-like.

The usual local observables associated with Eq. (1.1) are the density ϱ and current j , which for a general complex solution are defined by

$$\varrho(x, t) = \frac{1}{2mc^2} [\psi^*(\hat{E}\psi) - (\hat{E}\psi^*)\psi] = \frac{1}{mc^2} \text{Re}[\psi^*(\hat{E}\psi)], \quad (1.2)$$

and

$$j(x, t) = \frac{1}{2m} [\psi^*(\hat{p}\psi) - (\hat{p}\psi^*)\psi] = \frac{1}{m} \text{Re}[\psi^*(\hat{p}\psi)], \quad (1.3)$$

and they satisfy a continuity equation of the form $\hat{E}\varrho - \hat{p}j = 0$. Accordingly, on an interval $\Omega = [a, b]$ we obtain the conservation law $\int_{\Omega} dx \varrho = \text{const.}$

If, however, a Majorana condition is imposed with ψ real ($\psi = \psi^*$) or purely imaginary ($\psi = -\psi^*$, which can again be made real by a trivial redefinition), then $\hat{E}\psi^* = \hat{E}\psi$ and $\hat{p}\psi^* = \hat{p}\psi$. Substituting these identities into Eqs. (1.2)–(1.3) gives $\psi^*(\hat{E}\psi) - (\hat{E}\psi^*)\psi = \psi[(\hat{E}\psi) - (\hat{E}\psi)] = 0$ and $\psi^*(\hat{p}\psi) - (\hat{p}\psi^*)\psi = 0$; consequently, the quantities in Eqs. (1.2)–(1.3) vanish. In other words, when ψ satisfies a Majorana condition, the usual density and current reduce to

$$\varrho(x, t) = 0 \quad \text{and} \quad j(x, t) = 0, \quad (1.4)$$

and the continuity equation is satisfied in a trivial way (because ϱ and j are quantities ultimately associated with the electric charge of the particle). Consequently, if the particle is strictly neutral, ϱ and j are expected to vanish.

Hence, when the solutions ψ of the standard KFG equation are real, the vanishing of j implies that the current at the boundaries of the finite interval $\Omega = [a, b]$ satisfies $j(b, t) = j(a, t) = 0$. For the equation in (1.1), we may always choose a real solution, but we are not required to impose this restriction: complex solutions also exist (we do not refer here to purely imaginary ones). This freedom is related to the fact that the operator $\hat{O}_{\text{KFG}}$ in Eq. (1.1) obeys $(\hat{O}_{\text{KFG}}\psi)^* = \hat{O}_{\text{KFG}}\psi^*$; hence $\hat{O}_{\text{KFG}}$ is a real operator. When $\psi \in \mathbb{C}$, the current j is generally nonzero, and we can use it to distinguish between confining (or impermeable, or impenetrable) boundary conditions (BCs) and nonconfining (or permeable, or penetrable) BCs [11]. In this context, confining BCs correspond to the condition $j(b, t) = j(a, t) = 0$, while nonconfining BCs are characterized by $j(b, t) = j(a, t)$, with the common value not necessarily vanishing. For such nonconfining BCs, the solutions ψ must be genuinely complex.

Thus, when the solutions of Eq. (1.1) are real-valued, i.e., when the equation is used to describe a 1D KFGM particle, the vanishing of j in Eq. (1.4) means

that we can no longer distinguish confining from nonconfining BCs by examining the current density j alone. The usual pair of local observables $\{\varrho, j\}$ therefore becomes unsuitable for characterizing the behavior at the boundaries in the strictly neutral case. This suggests that a different local current density is needed in order to characterize the boundary behavior of a 1D KFGM particle at the walls of the interval. The main objective of the study is to introduce a nontrivial local observable—a current density—which remains well-defined for 1D KFGM particles confined to a finite interval or enclosed within a box with transparent walls. A second objective is to exhibit explicit BCs corresponding to these two physical situations and to investigate whether this current can be embedded into a continuity equation together with a suitable local density. It is worth recalling that the need to employ local observables other than j and ϱ when the standard 1D KFG equation describes a strictly neutral particle was briefly mentioned by Feshbach and Villars in their seminal 1958 work [9]. More specifically, this thesis addresses the characterization of impermeable and permeable BCs for first-quantized 1D KFGM particles using local observables that remain real-valued and nontrivial under the Majorana condition.

The finite interval setting is not merely a technical convenience. Boundary-sensitive scalar models occur in idealized boxes, point-interaction limits, and Casimir-type configurations. These connections motivate the present analysis, but the thesis does not attempt a full condensed-matter model, second-quantized vacuum calculation, or higher-dimensional boundary field theory.

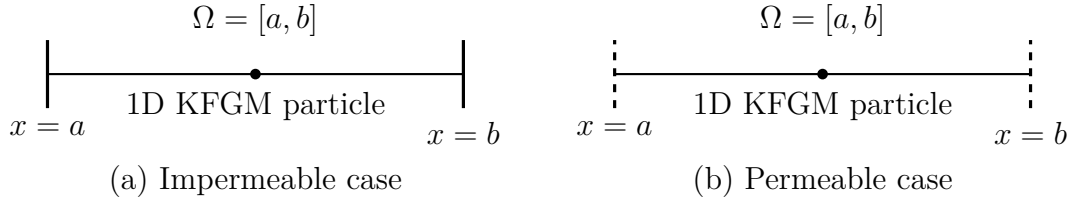


Figure 1 Schematic of the finite interval $\Omega = [a, b]$ under impermeable and permeable BCs. In panel (a), the relevant nontrivial current density vanishes at both ends of the interval; in panel (b), it has equal values at the two ends but need not vanish.

This thesis is organized as follows. Chapter II presents the pseudo self-adjoint Hamiltonian arising in the one-dimensional Feshbach-Villars formulation and summarizes the operator-theoretic tools needed for its physical interpretation. In this chapter, general notions from operator theory that apply to this Hamiltonian are recalled and used to analyze the meaning and consequences of its pseudo self-adjointness in the 1D FV setting. This analysis leads to the determination of the most general set of quantum BCs on a finite interval for which the FV Hamiltonian remains pseudo self-adjoint; if the solutions of the 1D KFG equation are complex, this set depends on four real parameters.

In Chapter III, three energy densities and two energy current densities are introduced and related to the usual density ϱ and current density j . We show that, for a given BC, only one of the two energy current densities always takes the same value at the two ends of the interval, a property enforced by pseudo self-adjointness of the FV Hamiltonian. This “acceptable” energy current density and its associated energy density are shown to satisfy a continuity equation whenever the Lorentz scalar potential does not explicitly depend on time, i.e., $\partial_t S = 0$ (a situation that is valid on-shell). Although these two local observables are generally complex for complex-valued ψ , imposing a Majorana condition makes them real and, crucially, nontrivial. Moreover, the energy expectation value $\int_a^b dx \varrho_E = \langle\langle \Psi, \hat{E} \Psi \rangle\rangle$ need not

be negative: for suitable BCs and for a nonnegative Lorentz scalar potential that does not explicitly depend on time on Ω , it can be positive. On the other hand, the other energy current density—namely the component cT^1_0 of the standard energy-momentum tensor for this $(1+1)$ -dimensional system—and the remaining two energy densities, one of which coincides with the component T^0_0 of T^μ_ν , are always real quantities. However, for a fixed BC, cT^1_0 does not necessarily take the same value at $x = a$ and $x = b$, and this behavior at $x = a$ and $x = b$ is itself sensitive to the chosen BCs.

In Chapter IV, the local observables obtained in Chapter III are used to characterize the BCs for the 1D KFGM particle. The pair of observables that remain real and nontrivial under a Majorana condition is shown to be appropriate for characterizing a 1D KFGM particle on an interval, whereas the standard pair $\{T^0_0, cT^1_0\}$ turns out to be incomplete for this purpose. Throughout the chapter, explicit examples of BCs are analyzed to support this conclusion. When a Majorana condition is imposed on the four-parameter family of BCs found in Chapter II, we obtain a three-parameter family suitable for strictly neutral particles. Within this family, a condition defining confining BCs for 1D KFGM particles is derived, and the most general two-parameter subset of confining BCs is identified. In addition, the mathematical conditions under which the incomplete energy current density cT^1_0 attains the same value at $x = a$ and $x = b$ are determined; these conditions also guarantee that the mean value of the energy operator is positive and that this mean value coincides with the spatial integrals of both the acceptable energy density and T^0_0 . In such cases, these two densities become equally acceptable, even though they differ by the gradient of a function. Only four typical impenetrable BCs (Dirichlet, Neumann, and two mixed BCs) satisfy these conditions, together with a one-parameter family of nonconfining BCs. In all these situations, the two energy current densities behave in an analogous way at the walls: the same condition holds at the boundaries while the currents still differ by a total derivative.

For all other BCs that do not meet these conditions, only the acceptable energy current density correctly captures whether the interval is confining or not. We also determine when the spatial integrals of the two energy current densities coincide; within the confining class, this occurs only for Dirichlet BCs, while a one-parameter nonconfining family shares the same property. Chapter V concludes the thesis, clarifies its scope and limitations, and presents physical examples. The results that complement the main text are collected in Appendices A–G: Appendix A verifies that $\hat{h}_{\text{adj}}$ has the same action as $\hat{h}$; Appendix B proves $\langle\langle \hat{h}_{\text{adj}} \Psi, \Phi \rangle\rangle = \langle\langle \Psi, \hat{h} \Phi \rangle\rangle$; Appendix C summarizes pseudo-Hermiticity consequences (real mean value/eigenvalues and pseudo-orthogonality); Appendix D gives an example with unequal domains $\mathcal{D}(\hat{h}) \subsetneq \mathcal{D}(\hat{h}_{\text{adj}})$; Appendix E shows that a unitary matrix equalizes the domains and ensures pseudo self-adjointness; Appendix F constructs the $(1 + 1)$ energy-momentum/energy current density tensors and Appendix G provides the tabulated catalog of BCs.

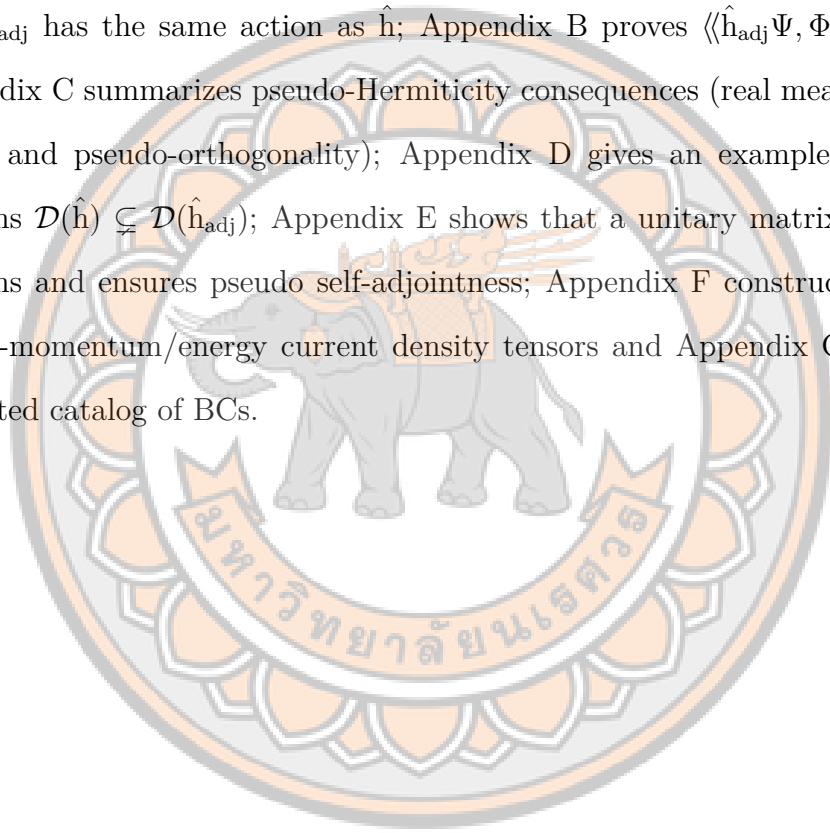


Table 1 Summary of key literature relevant to this thesis.

Reference	Main role	Relation to this thesis
Feshbach and Villars (1958)	FV first-order formulation and energy current density motivation	Supplies the two-component framework used here.
De Vincenzo (2023)	General pseudo self-adjoint BCs for 1D KFG particles	Provides the four-parameter BC family before the Majorana reduction.
De Vincenzo (2024)	Characterization of 1D KFGM particles	Identifies the KFGM setup and BC problem, but not the full energy current density characterization.
Mostafazadeh and Zamani (2006)	KFG Hilbert space localization and related structures	Useful comparison point, but not the finite interval BC characterization developed here.
Albeverio et al. (2009)	Indefinite metric and extension theory background	Supports the pseudo self-adjoint/Krein space language.
Asorey and Muñoz-Castañeda (2013)	Boundary effects and Casimir-type applications	Future work motivation only, not part of the derivation.

Table 2 Notation conventions used in the thesis.

Symbol	Meaning
$\hat{E}$	Energy operator, $i\hbar \partial_t$.
$\hat{p}$	Momentum operator, $-i\hbar \partial_x$.
$\hat{h}$	FV Hamiltonian operator.
$\hat{h}_{\text{adj}}$	Generalized adjoint of $\hat{h}$ with respect to the indefinite product.
$\mathcal{D}(\hat{h})$	Domain of $\hat{h}$, including the imposed BCs.
$\hat{U}$ and $\hat{M}$	Boundary unitary matrix and boundary transfer matrix, respectively.
ϱ, j	Usual KFG density and current density.
ϱ_E, j_E	Energy density and energy current density used for the KFGM BC characterization.
T^0_0, cT^1_0	Standard energy density and energy current density components from the energy-momentum tensor, used for comparison.

CHAPTER II

THEORETICAL FRAMEWORK

In this chapter we introduce and analyze the pseudo self-adjoint Hamiltonian operator obtained from the 1D FV equation, which is a first-order reformulation of the 1D KFG equation. We recall the basic notions from operator theory that are required to study this Hamiltonian, paying particular attention to the mathematical structure and physical interpretation of pseudo self-adjointness in an indefinite inner product (Krein) space. We also present the most general family of BCs on a finite interval that guarantees the pseudo self-adjointness of the Hamiltonian. For complex solutions of the 1D KFG equation, this family of BCs involves four real parameters, reflecting the large variety of possible BCs.

2.1 Definition of the FV Hamiltonian and wave equation

For spin-0 particles, the FV formalism rewrites the KFG equation, which is second order in time, into a Schrödinger-like first-order equation, $i\hbar \frac{\partial}{\partial t} \Psi = \hat{h} \Psi$, by introducing a two-component wavefunction. The Hamiltonian operator $\hat{h}$ governs the time evolution of the system, and its eigenvalues represent the energy spectrum. In one spatial dimension, we consider the Hamiltonian operator of the FV wave equation

$$\hat{h} = \frac{\hat{p}^2}{2m}(\hat{\tau}_3 + i\hat{\tau}_2) + mc^2\hat{\tau}_3 + S(\hat{\tau}_3 + i\hat{\tau}_2), \quad (2.1)$$

where $\hat{\tau}_3 = \hat{\sigma}_z$ and $\hat{\tau}_2 = \hat{\sigma}_y$ denote Pauli matrices. The corresponding FV equation takes the form

$$\hat{O}_{\text{FV}} \Psi \equiv (\hat{E}\hat{1}_2 - \hat{h})\Psi = 0 \quad (2.2)$$

(with $\hat{1}_2$ the 2×2 identity matrix), and it can describe a 1D KFGM particle if a Majorana condition is imposed. The operator $\hat{h}$ acts on two-component wavefunctions of the form $\Psi = \Psi(x, t) = [\psi_1 \ \psi_2]^T = [\psi_1(x, t) \ \psi_2(x, t)]^T$, where ^{T} indicates

matrix transposition.

The FV equation should also be distinguished from the Dirac equation. Both use two-component wavefunctions in $(1 + 1)$ dimensions, but their Hamiltonians have different orders in the spatial derivative. The FV Hamiltonian $\hat{h}$ contains the squared momentum operator $\hat{p}^2 = -\hbar^2 \partial_x^2$ and is therefore second order in the spatial derivative, whereas the Dirac Hamiltonian $\hat{h}_D$ contains the momentum operator $\hat{p} = -i\hbar \partial_x$ and is first order in the spatial derivative. Consequently, the acceptable BCs belong to different Hamiltonian domains. In particular, the FV form of the Dirichlet BC, $(\hat{\tau}_3 + i\hat{\tau}_2)\Psi(a, t) = (\hat{\tau}_3 + i\hat{\tau}_2)\Psi(b, t) = 0$, is an acceptable BC in the pseudo self-adjoint domain of the FV Hamiltonian and is equivalent to the KFG form of the Dirichlet BC $\psi(a, t) = \psi(b, t) = 0$. In contrast, the Dirac form of the Dirichlet BC, $\Psi_D(a, t) = \Psi_D(b, t) = 0$, is not included in the self-adjoint domain of the Dirac Hamiltonian.

A Pauli-Lubanski spin classification is not available in the present $(1 + 1)$ -dimensional setting. In spacetime dimension D , the generalized Pauli-Lubanski object has rank $D - 3$; for $D = 2$, this would formally give rank -1 ; therefore, no Pauli-Lubanski object is defined. The spin-zero character of the FV formulation is therefore inferred from its equivalence to the scalar KFG equation in the nonzero-mass case.

In Eq. (2.1), the parameter m is assumed to be nonzero. This is not an accidental detail: the standard Feshbach-Villars (FV) variables used here contain $(mc^2)^{-1}$ and therefore become singular at $m = 0$. The massless case can instead be treated by generalized Feshbach-Villars (FV) or generalized Case-Foldy-Feshbach-Villars (CFFV) constructions, where the mass appearing in the two-component reduction is replaced by an auxiliary nonzero parameter. These generalized constructions are useful for comparison, but they are not used in the present thesis; throughout this work we use the standard massive FV Hamiltonian in Eq. (2.1) and restrict

attention to the massive first-quantized 1D KFGM problem.

2.2 Pseudo-adjoint and indefinite inner product

To analyze $\hat{h}$ in an indefinite inner product space, we introduce its generalized Hermitian conjugate (or generalized adjoint), denoted $\hat{h}_{\text{adj}}$. It is defined by

$$\hat{h}_{\text{adj}} \equiv \hat{\tau}_3 \hat{h}^\dagger \hat{\tau}_3 = \frac{\hat{p}^2}{2m}(\hat{\tau}_3 + i\hat{\tau}_2) + mc^2 \hat{\tau}_3 + S(\hat{\tau}_3 + i\hat{\tau}_2) \quad (2.3)$$

(the symbol † stands for the conventional Hermitian conjugation of matrices and operators). Thus, when acting on wavefunctions, $\hat{h}_{\text{adj}}$ has exactly the same differential form as $\hat{h}$. An equivalent way of stating this definition is through the relation

$$\langle\langle \hat{h}_{\text{adj}} \Psi, \Phi \rangle\rangle = \langle\langle \Psi, \hat{h} \Phi \rangle\rangle, \quad (2.4)$$

where we have used $\hat{\tau}_3 = \hat{\tau}_3^\dagger = \hat{\tau}_3^{-1}$ and introduced the scalar product

$$\langle\langle \Psi, \Phi \rangle\rangle \equiv \int_{\Omega} dx \Psi^\dagger \hat{\tau}_3 \Phi = \langle\langle \Phi, \Psi \rangle\rangle^*, \quad (2.5)$$

with $\Psi = [\psi_1 \ \psi_2]^T$ and $\Phi = [\phi_1 \ \phi_2]^T$, and $*$ denoting complex conjugation. Equation (2.4) is precisely the defining property of the generalized adjoint with respect to the indefinite inner product determined by $\hat{\tau}_3$ (the $\hat{\tau}_3$ -space) [12].

The Hamiltonian $\hat{h}$ is understood as a formal differential operator together with a domain. For a given imposed BC, the domain of $\hat{h}$ is specified as the following subset of $\mathcal{V}$:

$$\mathcal{D}(\hat{h}) = \{\Phi \in \mathcal{V} : \hat{h}\Phi \in \mathcal{V} \text{ and } \Phi \text{ satisfies the imposed BC}\}.$$

Here $\mathcal{V}$ denotes the underlying $\hat{\tau}_3$ -space. The formal generalized adjoint $\hat{h}_{\text{adj}} = \hat{\tau}_3 \hat{h}^\dagger \hat{\tau}_3$ has the same differential action as $\hat{h}$, but its domain is determined separately.

The corresponding generalized-adjoint domain is formally specified by

$$\mathcal{D}(\hat{h}_{\text{adj}}) = \{\Psi \in \mathcal{V} : \hat{h}_{\text{adj}}\Psi \in \mathcal{V} \text{ and the boundary condition below holds}\}.$$

The boundary condition is that $[(\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x]^\dagger(\hat{\tau}_3 + i\hat{\tau}_2)\Phi - ((\hat{\tau}_3 + i\hat{\tau}_2)\Psi)^\dagger(\hat{\tau}_3 + i\hat{\tau}_2)\Phi_x]_a^b = 0$ for every $\Phi \in \mathcal{D}(\hat{h})$. Equivalently, the BCs defining $\mathcal{D}(\hat{h}_{\text{adj}})$ are those

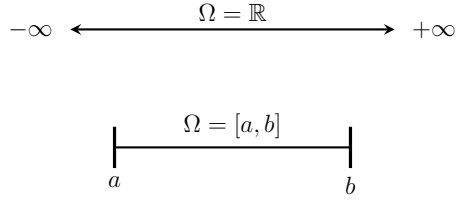
restrictions on Ψ that cancel this boundary term against all functions Φ satisfying the imposed BCs in $\mathcal{D}(\hat{h})$.

Thus, the functions on which $\hat{h}$ and $\hat{h}_{\text{adj}}$ act are not arbitrary; they must belong to the corresponding domains, and the BCs are part of these domains. In general, $\mathcal{D}(\hat{h})$ and $\mathcal{D}(\hat{h}_{\text{adj}})$ need not be equal; Appendix D gives an explicit example of this situation. When the imposed BCs belong to the pseudo self-adjoint family, the boundary term vanishes with the same BCs imposed on both Ψ and Φ . In that case, $\hat{h}$ and $\hat{h}_{\text{adj}}$ have the same differential action and the same domain; hence $\mathcal{D}(\hat{h}_{\text{adj}}) = \mathcal{D}(\hat{h})$ and $\hat{h}_{\text{adj}} = \hat{h}$, as illustrated in Appendix E. For any $\Psi \in \mathcal{V}$, the quantity $\langle\langle \Psi, \Psi \rangle\rangle$ is real but may be positive, negative, or zero, reflecting the indefinite character of the inner product.

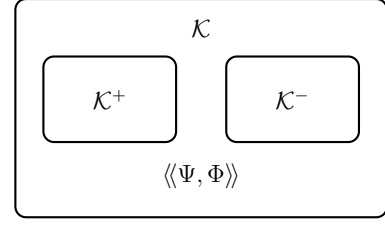
2.3 Integration by parts and boundary terms

In first-quantized KFG theory, the possibility that $\langle\langle \Psi, \Psi \rangle\rangle$ can take either sign is physically acceptable: it reproduces the integral of the usual density ϱ , which plays the role of a charge density and is therefore not constrained to be nonnegative.

More generally, an indefinite inner product space, namely an infinite-dimensional complex vector space endowed with an indefinite form, is usually accompanied by an associated positive-definite scalar product. In the present case, this positive-definite structure is the standard Dirac scalar product in one spatial dimension, $\langle \Psi, \Phi \rangle_{\text{D}} \equiv \langle\langle \Psi, \hat{\tau}_3 \Phi \rangle\rangle$. Using $\hat{\tau}_3^2 = \hat{1}_2$, one also has $\langle\langle \Psi, \Phi \rangle\rangle = \langle \Psi, \hat{\tau}_3 \Phi \rangle_{\text{D}}$ (see Eq. (2.5)). The product $\langle \Psi, \Phi \rangle_{\text{D}}$ is positive definite because $\langle \Psi, \Psi \rangle_{\text{D}} = \int_{\Omega} dx \Psi^{\dagger} \Psi$ and $\Psi^{\dagger} \Psi = |\psi_1|^2 + |\psi_2|^2 \geq 0$. Thus, the pair consisting of the indefinite scalar product $\langle\langle \cdot, \cdot \rangle\rangle$ and the positive-definite Dirac product defines a Krein space structure [12, 13].



(a) Spatial settings.



(b) Krein space structure.

Figure 2 Spatial setting and Krein space structure. Panel (a) contrasts $\Omega = \mathbb{R}$ with the finite interval $\Omega = [a, b]$ used for the BC analysis. Panel (b) illustrates the decomposition $\mathcal{K} = \mathcal{K}^+ \oplus \mathcal{K}^-$ into mutually orthogonal positive and negative subspaces with respect to the indefinite inner product $\langle\langle \Psi, \Phi \rangle\rangle$.

Table 3 Self-adjointness and pseudo self-adjointness.

Feature	Self-adjointness	Pseudo self-adjointness
Inner product	Positive-definite $\langle \cdot, \cdot \rangle$	Indefinite $\langle\langle \cdot, \cdot \rangle\rangle$.
Adjoint relation	$\hat{H} = \hat{H}^\dagger$ on $\mathcal{D}(\hat{H})$	$\hat{h} = \hat{h}_{\text{adj}}$ on $\mathcal{D}(\hat{h})$.
BC	Cancels the boundary term associated with the Hilbert space inner product	Cancels the boundary term associated with the Krein space inner product.
Domain role	BCs give $\mathcal{D}(\hat{H}) = \mathcal{D}(\hat{H}^\dagger)$	BCs give $\mathcal{D}(\hat{h}) = \mathcal{D}(\hat{h}_{\text{adj}})$.
Physical consequence	(i) $\langle \hat{H} \rangle_\Phi \in \mathbb{R}$ and $\hat{H}\Phi = E\Phi \Rightarrow E \in \mathbb{R}$. (ii) $i\hbar \partial_t \Phi = \hat{H}\Phi \Rightarrow \frac{d}{dt} \langle \Phi, \Phi \rangle = 0$ (on-shell). (iii) $[j]_a^b = 0$, hence $j(b, t) = j(a, t)$.	(i) $\langle\langle \hat{h} \rangle\rangle_\Psi \in \mathbb{R}$ and $\hat{h}\Psi = E\Psi \Rightarrow E \in \mathbb{R}$. (ii) $i\hbar \partial_t \Psi = \hat{h}\Psi \Rightarrow \frac{d}{dt} \langle\langle \Psi, \Psi \rangle\rangle = 0$ (on-shell). (iii) $[j]_a^b = 0$, hence $j(b, t) = j(a, t)$.

As will be shown later, if Ψ and Φ are solutions of the 1D FV equation, the scalar product $\langle\langle\Psi, \Phi\rangle\rangle$ is conserved in time. Because $\hat{h}$ and $\hat{h}_{\text{adj}}$ coincide as differential operators, the Hamiltonian in Eq. (2.1) is pseudo-Hermitian in the *formal* sense (equivalently, formally generalized Hermitian). The qualifier “formally” indicates that we are, at this stage, ignoring domain issues. For unbounded operators, however, the choice of BCs is essential, as BCs effectively specify the domains on which the operators act.

By integrating by parts twice, we can show that $\hat{h}$ and $\hat{h}_{\text{adj}}$, which has the same differential action as $\hat{h}$, obey the relation [11]

$$\langle\langle\hat{h}_{\text{adj}}\Psi, \Phi\rangle\rangle = \langle\langle\Psi, \hat{h}\Phi\rangle\rangle - \frac{\hbar^2}{4m} \left[((\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi - ((\hat{\tau}_3 + i\hat{\tau}_2)\Psi)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi_x \right] \Big|_a^b. \quad (2.6)$$

Here $\Psi \in \mathcal{D}(\hat{h}_{\text{adj}})$ and $\Phi \in \mathcal{D}(\hat{h})$, $[f]_a^b \equiv f(b, t) - f(a, t)$, and $\Psi_x \equiv \partial\Psi/\partial x$, etc. Equation (2.6) makes explicit how the difference between the two generalized expectation values is encoded in a boundary contribution evaluated at $x = a$ and $x = b$. Whenever the BCs are chosen to make the bracketed term vanish, $\hat{h}$ becomes pseudo-Hermitian (or generalized Hermitian) in the genuine, domain-dependent sense.

The BCs that accomplish this cancellation need not be identical for the two domains $\mathcal{D}(\hat{h})$ and $\mathcal{D}(\hat{h}_{\text{adj}})$; in principle, we may have $\mathcal{D}(\hat{h}) \neq \mathcal{D}(\hat{h}_{\text{adj}})$. It can even happen that no BCs are imposed on Ψ while Φ is constrained at the boundaries. For instance, within $\mathcal{D}(\hat{h})$ we may require $(\hat{\tau}_3 + i\hat{\tau}_2)\Phi(a, t) = (\hat{\tau}_3 + i\hat{\tau}_2)\Phi(b, t) = 0$ and $(\hat{\tau}_3 + i\hat{\tau}_2)\Phi_x(a, t) = (\hat{\tau}_3 + i\hat{\tau}_2)\Phi_x(b, t) = 0$. Under these conditions, the boundary term in Eq. (2.6) vanishes for all $\Psi \in \mathcal{D}(\hat{h}_{\text{adj}})$, even if no explicit BCs are enforced in $\mathcal{D}(\hat{h}_{\text{adj}})$, and we then have $\mathcal{D}(\hat{h}) \subset \mathcal{D}(\hat{h}_{\text{adj}})$ (see Appendix D for further details).

In Ref. [11], the most general family of BCs that ensures the cancellation of the boundary term in Eq. (2.6) is obtained. For any choice of BCs in this family, the operator $\hat{h}$ is simultaneously pseudo-Hermitian and pseudo self-adjoint, meaning

that it satisfies

$$\langle\langle \hat{h}\Psi, \Phi \rangle\rangle = \langle\langle \Psi, \hat{h}\Phi \rangle\rangle. \quad (2.7)$$

In particular, we then have $\mathcal{D}(\hat{h}_{\text{adj}}) = \mathcal{D}(\hat{h})$; hence $\hat{h} = \hat{h}_{\text{adj}}$ can be regarded as an operator identity on that common domain (see Appendix E for further details). Thus, the general BCs are implemented consistently in both domains. Even at the purely formal level, Eq. (2.7) encodes several properties that resemble those of ordinary Hermitian operators. For example, the generalized expectation value of the Hamiltonian is real: $\langle\langle \hat{h} \rangle\rangle_{\Psi} \equiv \langle\langle \Psi, \hat{h}\Psi \rangle\rangle = \langle\langle \hat{h}\Psi, \Psi \rangle\rangle = \langle\langle \Psi, \hat{h}\Psi \rangle\rangle^* [10, 14, 15]$.

2.4 Time evolution and conservation law

We can also verify the following relation:

$$\frac{d}{dt} \langle\langle \Psi, \Phi \rangle\rangle = \frac{1}{i\hbar} \frac{\hbar^2}{4m} [((\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi - ((\hat{\tau}_3 + i\hat{\tau}_2)\Psi)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi_x] \Big|_a^b. \quad (2.8)$$

Here, Ψ and Φ are required to satisfy the 1D FV equation. Comparing Eq. (2.6) with Eq. (2.8), we see that if $\hat{h}$ is pseudo self-adjoint (i.e., $\hat{h} = \hat{h}_{\text{adj}}$ and Eq. (2.7) holds), then the inner product $\langle\langle \Psi, \Phi \rangle\rangle$ defined in Eq. (2.5) is conserved in time. Indeed, when $\hat{h} = \hat{h}_{\text{adj}}$, the boundary term in Eq. (2.6) vanishes, and the boundary term in Eq. (2.8) must also be zero. In fact, the boundary term in Eq. (2.6) is equal to $-i\hbar$ times the boundary term in Eq. (2.8). Thus, any BCs that eliminate the boundary contribution in Eq. (2.6) also remove the boundary term in Eq. (2.8), guaranteeing the conservation of $\langle\langle \Psi, \Phi \rangle\rangle$.

2.5 Relations between one-component and two-component wavefunctions

The relation between the two-component wavefunctions Ψ and Φ (solutions of the 1D FV equation) and the corresponding one-component wavefunctions ψ and ϕ

(solutions of the standard 1D KFG equation) is

$$\Psi = \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} \psi + \frac{1}{mc^2} \hat{E}\psi \\ \psi - \frac{1}{mc^2} \hat{E}\psi \end{bmatrix} \quad \text{and} \quad \Phi = \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} \phi + \frac{1}{mc^2} \hat{E}\phi \\ \phi - \frac{1}{mc^2} \hat{E}\phi \end{bmatrix}, \quad (2.9)$$

which immediately implies $\psi_1 + \psi_2 = \psi$, $\phi_1 + \phi_2 = \phi$, $\psi_1 - \psi_2 = (\hat{E}\psi/mc^2)$, and $\phi_1 - \phi_2 = (\hat{E}\phi/mc^2)$. Conversely, Eq. (2.9) also makes explicit why the standard KFG equation and the FV equation are equivalent for $m \neq 0$. Starting from a one-component solution ψ of $\hat{O}_{\text{KFG}}\psi \equiv [\hat{E}^2 - (c\hat{p})^2 - (mc^2)^2 - 2mc^2S]\psi = 0$, one defines $\psi_1 = \frac{1}{2}[\psi + (mc^2)^{-1}\hat{E}\psi]$ and $\psi_2 = \frac{1}{2}[\psi - (mc^2)^{-1}\hat{E}\psi]$. Substitution gives the two FV component equations $\hat{E}\psi_1 = [\hat{p}^2/(2m) + S](\psi_1 + \psi_2) + mc^2\psi_1$ and $\hat{E}\psi_2 = -[\hat{p}^2/(2m) + S](\psi_1 + \psi_2) - mc^2\psi_2$, or equivalently $(\hat{E}\hat{1}_2 - \hat{h})\Psi = 0$. Conversely, if $\Psi = [\psi_1 \ \psi_2]^T$ satisfies the FV equation, then adding its two component equations gives $\hat{E}\psi = mc^2(\psi_1 - \psi_2)$, where $\psi = \psi_1 + \psi_2$, while subtracting them gives $\hat{E}(\psi_1 - \psi_2) = [\hat{p}^2/m + 2S + mc^2]\psi$. Combining these two identities yields $[\hat{E}^2 - (c\hat{p})^2 - (mc^2)^2 - 2mc^2S]\psi = 0$. Thus, Eq. (2.9) reconstructs the FV wavefunction from the KFG wavefunction, while the FV equation recovers the original KFG equation.

Nonrelativistic limit. The notation $\hat{E} = i\hbar \partial_t$ denotes the energy operator, not a numerical energy by itself. The replacement $\hat{E}\psi \mapsto E\psi$ is therefore justified only after restricting to a KFG solution with a definite-energy sign. For the free KFG equation, the energy branches are $E = \pm E_p$, where $E_p = (c^2p^2 + m^2c^4)^{1/2}$ [14, 16]. On the positive-energy branch one writes $E = mc^2 + E_{\text{NR}}$, with $|E_{\text{NR}}| \ll mc^2$. The identity $E^2 - (mc^2)^2 = (E - mc^2)(E + mc^2) \simeq 2mc^2E_{\text{NR}}$ gives $E_{\text{NR}} \simeq p^2/(2m)$ from the free KFG relation. Equivalently, $E/(mc^2) = +E_p/(mc^2) \rightarrow +1$ in the positive-energy nonrelativistic regime, whereas $E/(mc^2) = -E_p/(mc^2) \rightarrow -1$ on the negative-energy branch.

Substituting these limiting behaviors into Eq. (2.9) gives $\Psi^{(+)} \xrightarrow{\text{NR}} \begin{bmatrix} \psi^{(+)} \\ 0 \end{bmatrix}$ and $\Psi^{(-)} \xrightarrow{\text{NR}} \begin{bmatrix} 0 \\ \psi^{(-)} \end{bmatrix}$. The nonrelativistic limit therefore associates the upper FV

component with the positive-energy branch and the lower FV component with the negative-energy branch. For the plane-wave solutions $\psi_p^{(\pm)} \propto \exp[i(px \mp E_p t)/\hbar]$, one obtains $\hat{E}\psi_p^{(\pm)} = \pm E_p \psi_p^{(\pm)}$.

In the KFG operator in Eq. (1.1), $S = S(x, t)$ appears as a real-valued Lorentz scalar interaction; it is not required to be independent of time. For stationary states, one takes $S = S(x)$ and writes $\psi(x, t) = \psi_E(x) \exp(-iEt/\hbar)$, with $\hat{E}\psi = E\psi$. Under this assumption, the KFG equation can be written as $[E^2 - (mc^2)^2]\psi_E/(2mc^2) = [\hat{p}^2/(2m) + S]\psi_E$, which gives $E_{\text{NR}}\psi_E \simeq [\hat{p}^2/(2m) + S]\psi_E$ on the positive-energy branch. In this limited Schrödinger limit, S appears as the potential energy in the corresponding Schrödinger equation. This does not make S an electric potential: an electric potential enters through $\hat{E} - V$ and changes sign under charge conjugation, whereas a real Lorentz scalar interaction is the same for particles and antiparticles. The equivalence between the standard 1D KFG and 1D FV wave equations used above assumes that $m \neq 0$. The nonrelativistic limit of the real scalar field may also be obtained from the recently introduced first-order 1D Majorana equations, although the procedure is more subtle and is discussed separately in Ref. [5].

2.6 Inner product in terms of one-component fields

The scalar product defined in Eq. (2.5) can be rewritten in terms of the one-component fields as

$$\langle\langle \Psi, \Phi \rangle\rangle = \frac{1}{2mc^2} \int_{\Omega} dx [\psi^*(\hat{E}\phi) - (\hat{E}\psi^*)\phi]. \quad (2.10)$$

This expression follows directly by substituting Eq. (2.9) into Eq. (2.5) and simplifying. Using Eq. (2.10), we can rederive Eq. (2.8) in an equivalent form, now expressed in terms of ψ and ϕ :

$$\frac{d}{dt} \langle\langle \Psi, \Phi \rangle\rangle = -\frac{1}{2m} [\psi^*(\hat{p}\phi) - (\hat{p}\psi^*)\phi] \Big|_a^b. \quad (2.11)$$

2.7 Consequences and implications

It should be emphasized that Eqs. (2.8) and (2.11) hold on-shell for Ψ , Φ , ψ , and ϕ satisfying their respective equations of motion. Setting $\Psi = \Phi$ and $\psi = \phi$ in Eq. (2.11) yields $d\langle\langle\Psi, \Psi\rangle\rangle/dt = -[j]_a^b$ (see Eq. (1.3)). Moreover, by explicit integration by parts in the defining relation of pseudo self-adjointness (cf. Eqs. (2.6) and (2.7)), we find that for $\hat{h} = \hat{h}_{\text{adj}}$ the only possible obstruction comes from a boundary term, namely $\langle\langle\hat{h}\Psi, \Psi\rangle\rangle = \langle\langle\Psi, \hat{h}\Psi\rangle\rangle - \frac{\hbar}{i}[j]_a^b$. Therefore, pseudo self-adjointness forces $[j]_a^b = 0$, i.e., $j(b, t) = j(a, t)$. In the one-component representation this implies

$$j(b, t) = j(a, t) \implies \text{Re}[\psi^*(\hat{p}\psi)]|_a^b = 0 \quad (2.12)$$

(see Eq. (1.3)). The condition $j(b, t) = j(a, t)$ is a straightforward consequence of the pseudo self-adjointness of $\hat{h}$.

2.8 General set of BCs

The four-parameter family of BCs for solutions ψ of the standard 1D KFG equation, under which the operator $\hat{h}$ in the 1D FV equation is pseudo self-adjoint, can be written as

$$\begin{bmatrix} \psi(b, t) - i\lambda\psi_x(b, t) \\ \psi(a, t) + i\lambda\psi_x(a, t) \end{bmatrix} = \hat{U}_{(2 \times 2)} \begin{bmatrix} \psi(b, t) + i\lambda\psi_x(b, t) \\ \psi(a, t) - i\lambda\psi_x(a, t) \end{bmatrix} \quad (2.13)$$

where $\lambda \in \mathbb{R}$ is a parameter introduced for dimensional consistency, and the 2×2 unitary matrix $\hat{U}_{(2 \times 2)}$ is given by

$$\hat{U}_{(2 \times 2)} = e^{i\mu} \begin{bmatrix} m_0 - im_3 & -m_2 - im_1 \\ m_2 - im_1 & m_0 + im_3 \end{bmatrix}, \quad (2.14)$$

with $\mu \in [0, \pi)$ and real parameters m_0, m_1, m_2 , and m_3 satisfying $(m_0)^2 + (m_1)^2 + (m_2)^2 + (m_3)^2 = 1$ (see Ref. [11]).

The parameter λ has the dimension of length and is introduced to ensure that $\lambda\psi_x$ has the same dimension as ψ in the boundary vector. A natural choice is the Compton wavelength $\hbar/(mc)$, but the BC characterization does not depend on this particular choice of length.

2.9 An expression for $j(x, t)$ at the boundaries

An explicit formula for the current density at $x = a$ in Eq. (1.3) is

$$j(a, t) = -\frac{\hbar}{m} \frac{1}{\lambda} \operatorname{Im}\left[\left(\frac{m_1 + im_2}{m_0 + \cos(\mu)}\right)\psi^*(a, t)\psi(b, t)\right] = j(b, t), \quad (2.15)$$

By pseudo self-adjointness, the same value is obtained at $x = b$. From Eq. (2.15), it is evident that setting $m_1 = m_2 = 0$ yields $j(a, t) = j(b, t) = 0$. This case defines confining BCs when ψ is complex. On the other hand, if ψ is real or purely imaginary, then the condition $m_2 = 0$ follows from the general BCs in Eq. (2.13) (because both ψ and ψ^* must satisfy Eq. (2.13)). Because the imaginary part of a real number vanishes, Eq. (2.15) again gives $j(a, t) = j(b, t) = 0$, which is consistent with the fact that $j(x, t) = 0$ whenever $\psi \in \mathbb{R}$ (see Eq. (1.1)).

This formula is obtained as follows. Starting from the boundary relation in Eq. (2.13), one solves the two equations at $x = a$ and $x = b$ for $\lambda\psi_x(a, t)$ and $\lambda\psi_x(b, t)$ in terms of $\psi(a, t)$ and $\psi(b, t)$, for the case $m_0 + \cos \mu \neq 0$. Substitution of these derivatives at $x = a$ and $x = b$ into $j = (1/m) \operatorname{Re}[\psi^* \hat{p}\psi]$ then gives Eq. (2.15) at both ends of the interval. Therefore, the equality $j(a, t) = j(b, t)$ is not an additional assumption, but follows from the pseudo self-adjoint BCs.

2.10 Representative spectral examples

Although a comprehensive spectral analysis is beyond the scope of this thesis, two representative cases are considered: Dirichlet and periodic BCs. Taking the left end as the origin, the interval is written as $\Omega = [0, L]$, where $L = b - a$.

First, consider Dirichlet BCs, given by $\psi_N(0, t) = \psi_N(L, t) = 0$. For $S = 0$, the spatial dependence is proportional to $\sin(kx)$. The condition at $x = L$ gives $\sin(kL) = 0$, hence $kL = N\pi$. Thus the allowed labels are $N = 1, 2, \dots$: the value $N = 0$ gives the trivial zero function, and negative values only reproduce the same mode up to an overall sign because $\sin(-N\pi x/L) = -\sin(N\pi x/L)$. This is the standard one-dimensional KFG/FV box result: the spatial dependence is proportional to $\sin(px/\hbar)$, and the condition at $x = L$ gives $pL = N\pi\hbar$ [36]. Therefore the momentum magnitude is $P_N = N\pi\hbar/L$, and the two KFG energy branches can be expressed as $E_N = \pm\sqrt{c^2 P_N^2 + m^2 c^4}$, equivalently $E_N^2 = m^2 c^4 + c^2 \hbar^2 (N\pi/L)^2$.

Second, consider periodic BCs. The imposed BCs are $\psi_N(L, t) = \psi_N(0, t)$ and $\psi_{N,x}(L, t) = \psi_{N,x}(0, t)$. The spatial dependence of $\psi_N(x, t)$ may be written as $\psi_N(x, t) \propto \exp(ikx)$. The condition $\psi_N(L, t) = \psi_N(0, t)$ gives $\exp(ikL) = 1$. By Euler's identity, this requires $\cos(kL) = 1$ and $\sin(kL) = 0$, and hence $kL = 2\pi N$ with $N \in \mathbb{Z}$. Thus the allowed labels are $N = 0, \pm 1, \pm 2, \dots$, and the spatial dependence may be written as $\psi_N(x, t) \propto \exp(i2\pi Nx/L)$. Here $N = 0$ is allowed because the spatial dependence is constant and nonzero, whereas the labels N and $-N$ with $N \neq 0$ describe opposite momentum directions. The associated signed momentum values are $P_N = 2\pi\hbar N/L$, and the KFG energy branches are $E_N = \pm\sqrt{c^2 P_N^2 + m^2 c^4}$, or equivalently $E_N^2 = m^2 c^4 + c^2 \hbar^2 (2\pi N/L)^2$. Because the energy depends on N^2 , the periodic spectrum is degenerate for every nonzero N : within the positive-energy branch one has $E_{+N}^{(+)} = E_{-N}^{(+)}$, and within the negative-energy branch one has $E_{+N}^{(-)} = E_{-N}^{(-)}$, for $N = 1, 2, \dots$. Here the superscripts $(+)$ and $(-)$ denote the positive- and negative-energy branches, respectively. The $N = 0$ state is not degenerate in this sense because the two momentum labels coincide.

These two cases are included only as representative spectral examples. The boundary characterization in this thesis is based on current relations at the ends of the interval and the BC parameters, rather than on solving every spectral problem.

CHAPTER III

NONTRIVIAL LOCAL OBSERVABLES

This chapter introduces a set of local observables—specifically, three energy densities and two energy current densities—and examines how they relate to the usual density ϱ and the usual current density j . For acceptable BCs, only one of the two energy currents, namely j_E , is guaranteed to take equal values at the ends of the interval; this equality at the ends of the interval follows from the pseudo self-adjointness of the FV Hamiltonian and, when $\dot{S} = 0$, from the associated continuity statement (see Appendix F for further details). Moreover, the pair $\{\varrho_E, j_E\}$ satisfies a continuity equation when the Lorentz scalar potential does not explicitly depend on time (i.e., $\dot{S} = 0$, on-shell). These two local observables are generally complex when $\psi \in \mathbb{C}$, but they become real for real (Majorana-type) fields; importantly, they are not forced to vanish under the Majorana constraint. In this regime, the spatial integral $\int_{\Omega} \varrho_E dx$ is constant in time, although it is not guaranteed to be positive. In particular, the expectation value of the energy operator is not necessarily positive definite: it depends on the imposed BCs and on the positivity of a scalar potential that is time independent on the interval. By contrast, the remaining energy current density, $\tilde{j}_E \equiv cT^1_0$, and the two real energy densities ($\tilde{\varrho}_E$ and T^0_0) are real for all wavefunctions; however, $\tilde{j}_E$ requires an additional boundary cancellation to match at the ends of the interval and may otherwise take different values at $x = a$ and $x = b$. In this setting, $\langle\langle \Psi, \hat{E}\Psi \rangle\rangle$ is real on-shell, because $\hat{E}\Psi = \hat{h}\Psi$ for solutions. However, its positivity is not automatic; under certain realizable conditions, depending on the imposed BCs, and provided that $S \geq 0$ on Ω , this expectation value can be a positive quantity. Finally, $\{\varrho_E, j_E\}$ can be embedded into an unusual second-rank Lorentz tensor $K^\mu{}_\nu$, giving a Lorentz-covariant continuity relation (see Appendix F for further details).

The guiding principle is to select the simplest nontrivial local observables involving $\hat{E}$ that remain useful after the usual charge-like observables ϱ and j vanish under the Majorana condition. In this thesis, an observable pair is called acceptable if it is nontrivial under the Majorana condition, real for KFGM fields, compatible with the equality of the current values at $x = a$ and $x = b$ for all acceptable BCs, and able to satisfy the corresponding continuity equation when $\dot{S} = 0$. An observable pair is called incomplete if it is meaningful in special cases but fails either this equality condition or the full characterization of impermeable and permeable BCs.

3.1 Further results involving the generalized adjoint of $\hat{h}$

An additional relation, analogous to Eq. (2.6), holds for the Hamiltonian operator $\hat{h}$ and its generalized adjoint $\hat{h}_{\text{adj}}$:

$$\langle\langle \hat{h}_{\text{adj}}\Psi, \hat{E}\Phi \rangle\rangle = \langle\langle \Psi, \hat{h}\hat{E}\Phi \rangle\rangle - \frac{i\hbar^3}{4m} \left[((\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\dot{\Phi} - ((\hat{\tau}_3 + i\hat{\tau}_2)\Psi)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\dot{\Phi}_x \right] \Big|_a^b \quad (3.1)$$

Here $\dot{\Phi}$ denotes the time derivative, i.e., $\dot{\Phi} = \partial\Phi/\partial t$. If $\Phi \in \mathcal{D}(\hat{h})$, then $\hat{E}\Phi = i\hbar\dot{\Phi} \in \mathcal{D}(\hat{h})$. Indeed, if Φ satisfies a BC, then $\dot{\Phi}$ satisfies that same BC. Consequently, any BC included in the most general set of BCs that cancels the boundary term in Eq. (2.6) also cancels the boundary term in Eq. (3.1). We recall that, for any BC within this general family, $\hat{h}$ is pseudo self-adjoint, i.e., $\hat{h} = \hat{h}_{\text{adj}}$, meaning that $\hat{h}$ and $\hat{h}_{\text{adj}}$ act in the same way and $\mathcal{D}(\hat{h}) = \mathcal{D}(\hat{h}_{\text{adj}})$ [11].

The following relation can also be written:

$$\begin{aligned} \frac{d}{dt} \langle\langle \Psi, \hat{E}\Phi \rangle\rangle &= \frac{\hbar^2}{2m} \frac{1}{2} [((\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\dot{\Phi} - ((\hat{\tau}_3 + i\hat{\tau}_2)\Psi)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\dot{\Phi}_x] \Big|_a^b \\ &\quad + \frac{1}{2} \int_{\Omega} dx \dot{S} ((\hat{\tau}_3 + i\hat{\tau}_2)\Psi)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi, \end{aligned} \quad (3.2)$$

where $\dot{S} = \partial S/\partial t$. Here, Ψ and Φ must satisfy the 1D FV wave equation. If S does not explicitly depend on time, then the pseudo self-adjointness of $\hat{h}$ implies

that $\langle\langle\Psi, \hat{E}\Phi\rangle\rangle$ remains constant in time, because the boundary term in Eq. (3.1) vanishes under $\hat{h} = \hat{h}_{\text{adj}}$, which also ensures that the boundary term in Eq. (3.2) vanishes (the boundary term in Eq. (3.1) is $-i\hbar$ times that of Eq. (3.2)).

Using the relations in Eq. (2.9), the scalar product $\langle\langle\Psi, \hat{E}\Phi\rangle\rangle$ may also be expressed as

$$\langle\langle\Psi, \hat{E}\Phi\rangle\rangle = \frac{1}{2mc^2} \int_{\Omega} dx [\psi^*(\hat{E}^2\phi) - (\hat{E}\psi^*)(\hat{E}\phi)]. \quad (3.3)$$

Taking the time derivative of this expression yields another form of Eq. (3.2):

$$\frac{d}{dt} \langle\langle\Psi, \hat{E}\Phi\rangle\rangle = -\frac{1}{2mc} [\psi^*(c\hat{p}\hat{E}\phi) - (c\hat{p}\psi^*)(\hat{E}\phi)]_a^b + \int_{\Omega} dx \dot{S} \psi^* \phi. \quad (3.4)$$

3.2 Proper energy density and energy current density

Setting $\Psi = \Phi$ and $\psi = \phi$ in Eq. (3.4) gives

$$\frac{d}{dt} \langle\langle\Psi, \hat{E}\Psi\rangle\rangle = \frac{d}{dt} \left(\int_{\Omega} dx \varrho_E \right) = -[j_E]_a^b + \int_{\Omega} dx \dot{S} |\psi|^2, \quad (3.5)$$

where

$$\varrho_E(x, t) = \frac{1}{2mc^2} [\psi^*(\hat{E}^2\psi) - (\hat{E}\psi^*)(\hat{E}\psi)] \quad (3.6)$$

defines a type of complex energy density, and

$$j_E(x, t) = \frac{1}{2mc} [\psi^*(c\hat{p}\hat{E}\psi) - (c\hat{p}\psi^*)(\hat{E}\psi)] \quad (3.7)$$

defines a type of complex energy current density. It is convenient to collect these quantities into the two-component object $j_E^\mu = (c\varrho_E, j_E)$. When $\dot{S} = 0$, this pair satisfies the continuity equation $\partial_\mu j_E^\mu = 0$. More generally, it can be expressed as $\partial_\mu j_E^\mu = \dot{S}|\psi|^2$. More precisely, ϱ_E and j_E are the components K^0_0 and cK^1_0 of the second-rank Lorentz tensor K^μ_ν constructed in Appendix F. For $\nu = 0$, the identity $\partial_\mu K^\mu_0 = (\partial_0 S)|\psi|^2$ reproduces the local form of the FV/Krein energy balance in Eq. (3.5), namely $d(\int_{\Omega} \varrho_E dx)/dt = -[j_E]_a^b + \int_{\Omega} \dot{S} |\psi|^2 dx$. Thus j_E is the current selected by the pseudo self-adjoint boundary form. By contrast, the usual energy-momentum tensor gives $\tilde{j}_E \equiv cT^1_0$, and Eq. (3.13) gives

$j_E = \frac{i}{2mc} \hat{E} [\text{Im}(\psi^*(c\hat{p}\psi))] + \frac{1}{2} \hat{E} j + \tilde{j}_E$, hence, using $j(b, t) = j(a, t)$, the equality $\tilde{j}_E(b, t) = \tilde{j}_E(a, t)$ still requires the extra cancellation $\frac{i}{2mc} \hat{E} [\text{Im}(\psi^*(c\hat{p}\psi))]_a^b = 0$. Therefore $T^\mu{}_\nu$ is not discarded. Rather, the equality $\tilde{j}_E(b, t) = \tilde{j}_E(a, t)$, where $\tilde{j}_E \equiv cT^1{}_0$, depends on the imposed BCs, whereas j_E satisfies $j_E(b, t) = j_E(a, t)$ directly from the pseudo self-adjoint boundary form. The quantities ϱ_E and j_E are generally complex when ψ is complex-valued. Under $\psi = \pm\psi^*$, the quantities ϱ_E and j_E become real and remain nontrivial. Similarly, taking $\Psi = \Phi$ and hence $\psi = \phi$ in Eq. (3.1) yields

$$j_E(b, t) = j_E(a, t). \quad (3.8)$$

The equality $j_E(b, t) = j_E(a, t)$ is enforced by pseudo self-adjointness of $\hat{h}$.

The quantities ϱ_E and j_E admit reformulations that make their connections to the usual densities, to additional real densities, and to the relevant derivative terms explicit. In particular,

$$\varrho_E = -\frac{i}{2mc^2} \hat{E} [\text{Im}(\psi^*(\hat{E}\psi))] + \frac{1}{2} \hat{E} \varrho + \tilde{\varrho}_E, \quad (3.9)$$

where

$$\tilde{\varrho}_E = \frac{1}{2mc^2} [\psi^*(\hat{E}^2\psi) + (\hat{E}^2\psi)^*\psi] = \frac{1}{mc^2} \text{Re}[\psi^*(\hat{E}^2\psi)], \quad (3.10)$$

is a real energy density. Alternatively, using the standard 1D KFG equation (Eq. (1.1)) together with the continuity equation $\hat{E}\varrho - \hat{p}j = 0$, Eq. (3.9) may be written as

$$\varrho_E = \frac{i}{2mc^2} c\hat{p} [\text{Im}(\psi^*(c\hat{p}\psi))] + \frac{1}{2} \hat{E}\varrho + T^0{}_0, \quad (3.11)$$

where

$$T^0{}_0 = \frac{1}{2mc^2} [-(\hat{E}\psi^*)(\hat{E}\psi) - (c\hat{p}\psi^*)(c\hat{p}\psi) + (mc^2)^2\psi^*\psi + 2mc^2 S\psi^*\psi], \quad (3.12)$$

is another real energy density; in particular, it is positive when $S \geq 0$ in Ω . It constitutes a component of the standard energy-momentum tensor associated with

KFG theory in $(1+1)$ dimensions (see Ref. [16]). Equations (3.9) and (3.11) show that when ψ is complex, ϱ_E is also complex because $\hat{E}\varrho$ is complex (indeed, purely imaginary). However, if ψ is real, then $\hat{E}\varrho = 0$ and ϱ_E becomes real, as expected. Similarly,

$$j_E = \frac{i}{2mc} \hat{E} [\text{Im}(\psi^*(c\hat{p}\psi))] + \frac{1}{2} \hat{E}j + \tilde{j}_E, \quad (3.13)$$

where

$$\tilde{j}_E \equiv cT^1_0 = -\frac{1}{2mc} [(\hat{E}\psi^*)(c\hat{p}\psi) + (c\hat{p}\psi^*)(\hat{E}\psi)] = -\frac{1}{mc} \text{Re}[(\hat{E}\psi^*)(c\hat{p}\psi)], \quad (3.14)$$

is a real energy current density, directly proportional to the component T^1_0 of the standard energy-momentum tensor in 1D KFG theory (see Ref. [16]). Moreover, when ψ is complex, j_E in Eq. (3.13) is generally complex because $\hat{E}j$ is complex (in fact purely imaginary). However, if ψ is real, then $\hat{E}j = 0$ and j_E reduces to a real quantity. For a general complex KFG solution, j remains the correct boundary quantity that characterizes the BCs. Using pseudo self-adjointness of $\hat{h}$ (see the discussion preceding Eq. (2.12) and also Eq. (3.8)), Eq. (3.13) implies

$$0 = \frac{i}{2mc} \hat{E} [\text{Im}(\psi^*(c\hat{p}\psi))] \Big|_a^b + [\tilde{j}_E] \Big|_a^b. \quad (3.15)$$

For BCs that do not cancel the first boundary term in Eq. (3.15), only the “acceptable” current j_E can be used to characterize impermeability/permeability; the “incomplete” current cT^1_0 fails to take the same value at the two ends. When both currents are acceptable, they differ by the gradient of a function; hence they satisfy the same wall condition while remaining distinct as local observables. Thus, if the first term evaluated at the boundaries in Eq. (3.15) vanishes (depending on the BCs), it follows that

$$\tilde{j}_E(b, t) = \tilde{j}_E(a, t). \quad (3.16)$$

However, not all physically acceptable BCs for this problem lead to the vanishing of the boundary term $\frac{i}{2mc} \hat{E} [\text{Im}(\psi^*(c\hat{p}\psi))] \Big|_a^b$ in Eq. (3.15), and therefore

not all acceptable BCs ensure the validity of Eq. (3.16). This issue will be examined in more detail in the next chapter, where a specific case involving a 1D KFGM particle is discussed. In Ref. [9], the energy current density $\tilde{j}_E$ was introduced directly, without a discussion of its origin, and only a single BC was considered—namely, that the wavefunction ψ tends to zero as $x \rightarrow \pm\infty$ for a strictly neutral particle on the real line. This point will also be revisited in the next chapter.

Thus, ϱ_E and j_E satisfy $\hat{E}\varrho_E - \hat{p}j_E = (\hat{E}S)\psi^*\psi$, which holds on-shell. This becomes a continuity equation only when S is not explicitly dependent on time (equivalently, $\partial_t S = 0$), or in the trivial case $S \equiv 0$. In such cases, integrating over $\Omega = [a, b]$ and using Eq. (3.8) yields $\int_{\Omega} dx \varrho_E = \text{const.}$ Equivalently, if the scalar potential does not explicitly depend on time, pseudo self-adjointness of $\hat{h}$ guarantees that $\langle\langle \Psi, \hat{E}\Psi \rangle\rangle = \text{const.}$ for any solution of the equations of motion (see Eq. (3.5)). Moreover, ϱ_E and j_E can be identified with K^0_0 and cK^1_0 of an unusual energy-momentum tensor K^μ_ν , and we have $\hat{E}\varrho_E - \hat{p}j_E = \hat{E}T^0_0 - \hat{p}\tilde{j}_E = i\hbar c \partial_\mu T^\mu_0$. Because $i\hbar c \partial_\mu T^\mu_0$ is a Lorentz scalar, $\hat{E}\varrho_E - \hat{p}j_E$ is also a Lorentz scalar; in this sense, the continuity equation built from $\{\varrho_E, j_E\}$ can be written in Lorentz-covariant form (see Appendix F for further details). Similarly, if S does not depend explicitly on position, we obtain an additional conservation law associated with $\partial_\mu K^\mu_1 = 0$ (not pursued here).

Likewise, T^0_0 and $cT^1_0 \equiv \tilde{j}_E$ satisfy $\hat{E}T^0_0 - c\hat{p}T^1_0 = (\hat{E}S)\psi^*\psi$, or equivalently, $\partial_\mu T^\mu_0 = (\partial_0 S)\psi^*\psi$, which again holds on-shell. From this, if $\dot{S} = 0$, then $\int_{\Omega} dx T^0_0 = \text{const.}$ is obtained only if Eq. (3.16) holds—i.e., only if the BCs eliminate the first boundary term in Eq. (3.15). It is precisely in this sense, depending on the imposed BCs, that T^0_0 and cT^1_0 are often regarded as the standard local energy observables. However, the conclusion depends on the imposed BCs: the pair $\{T^0_0, cT^1_0\}$ does not necessarily yield a conserved quantity in general.

Furthermore, $\partial_\mu T^\mu_\nu = (\partial_\nu S)\psi^*\psi$. Here T^0_1 and T^1_1 are the remaining

components of $T^\mu{}_\nu$ (with $T^{01} = T^{10}$ for a scalar field) [9]. By contrast, $\{\varrho_E, \tilde{j}_E\}$ (i.e., $\{\varrho_E, cT^1{}_0\}$) does not lead to a continuity equation when $\dot{S} = 0$. Thus, when S does not explicitly depend on time, $\int_\Omega T^0{}_0 dx$ is conserved if and only if $[cT^1{}_0]_a^b = 0$; conservation depends on the imposed BCs.

In summary, if $\hat{h} = \hat{h}_{\text{adj}}$ and Ψ and Φ satisfy the 1D FV equation, then $\langle\langle \Psi, \Phi \rangle\rangle = \text{const}$, and consequently, $\langle\langle \Psi, \Psi \rangle\rangle = \int_\Omega dx \varrho$ is also constant. This latter quantity is real, but it is not necessarily positive. On the other hand, if $\hat{h} = \hat{h}_{\text{adj}}$ with $\dot{S} = 0$ and Ψ and Φ again satisfy the 1D FV equation, then $\langle\langle \Psi, \hat{E}\Phi \rangle\rangle = \text{const}$, and therefore, $\langle\langle \Psi, \hat{E}\Psi \rangle\rangle = \int_\Omega dx \varrho_E$ is also constant. This quantity, which represents a type of expectation value of the energy operator in the state Ψ , is also real. Moreover, because the system is on-shell, it coincides with the mean value of the Hamiltonian in the same state, i.e., $\langle\langle \Psi, \hat{h}\Psi \rangle\rangle$. Under certain realizable conditions, $\langle\langle \Psi, \hat{E}\Psi \rangle\rangle$ can be positive.

It is useful to distinguish this quantity from the ordinary Dirac product expression $\langle \Psi, \hat{E}\Psi \rangle_D := \int_\Omega dx \Psi^\dagger \hat{E}\Psi$. The FV/Krein product is related to the Dirac product by insertion of the metric operator: $\langle\langle \Psi, \Phi \rangle\rangle = \langle \Psi, \hat{\tau}_3 \Phi \rangle_D$. Applying this identity to the case $\Phi = \hat{E}\Psi$ gives $\langle\langle \Psi, \hat{E}\Psi \rangle\rangle = \langle \Psi, \hat{\tau}_3 \hat{E}\Psi \rangle_D$. It follows from these identities that the two expressions are related by the metric operator $\hat{\tau}_3$, but they are not generally equal. In the present FV formulation, the conserved and pseudo self-adjoint structure is the indefinite product; the ordinary Dirac product is positive definite as a norm, but it is not the product with respect to which the FV Hamiltonian in Eq. (2.1) is pseudo self-adjoint or with respect to which the energy balance above is obtained.

3.3 Local observables, continuity, and boundary term

Using the Hamiltonian operator given in Eq. (2.1), we may write

$$\langle\langle \Psi, \hat{E}\Psi \rangle\rangle = \langle\langle \Psi, \hat{h}\Psi \rangle\rangle = \langle\langle \Psi, \hat{T}\Psi \rangle\rangle + \langle\langle \Psi, mc^2 \hat{\tau}_3 \Psi \rangle\rangle + \langle\langle \Psi, S(\hat{\tau}_3 + i\hat{\tau}_2)\Psi \rangle\rangle, \quad (3.17)$$

where $\hat{T}$ denotes a kinetic-energy operator of the form

$$\hat{T} = \frac{\hat{\mathbf{p}}^2}{2m}(\hat{\tau}_3 + i\hat{\tau}_2). \quad (3.18)$$

From this, we obtain

$$\begin{aligned} \langle\langle \Psi, \hat{E}\Psi \rangle\rangle &= \frac{\hbar}{2mc} \operatorname{Im} [\psi^*(c\hat{\mathbf{p}}\psi)] \Big|_a^b + \frac{1}{mc^2} \int_{\Omega} dx |c\hat{\mathbf{p}}\psi|^2 + \frac{1}{2}mc^2 \int_{\Omega} dx |\psi|^2 \\ &+ \frac{1}{2mc^2} \int_{\Omega} dx |\hat{E}\psi|^2 + \int_{\Omega} dx S |\psi|^2. \end{aligned} \quad (3.19)$$

To obtain Eq. (3.19) from Eq. (3.17), the term $\langle\langle \Psi, \hat{T}\Psi \rangle\rangle$ is integrated by parts once. The resulting boundary contribution is then rewritten by separating $\psi^*\hat{\mathbf{p}}\psi$ into its real and imaginary parts, together with Eq. (2.12). The term $\langle\langle \Psi, mc^2\hat{\tau}_3\Psi \rangle\rangle$ is similarly reduced to an expression involving ψ , using the definition of Ψ in Eq. (2.9).

Thus, $\langle\langle \Psi, \hat{E}\Psi \rangle\rangle$ in Eq. (3.19) is real. This quantity is the spatial integral of ϱ_E and, on-shell, coincides with the mean value of the FV Hamiltonian. Its positivity is not automatic; it depends on the imposed BCs and on the scalar potential. In particular, if the boundary contribution in Eq. (3.19) vanishes and $S(x) \geq 0$ on Ω , then the remaining terms in Eq. (3.19) are nonnegative; hence $\langle\langle \Psi, \hat{E}\Psi \rangle\rangle$ can be a positive quantity. It is also useful to note that if the boundary term in Eq. (3.19) vanishes, then the corresponding boundary term in Eq. (3.15) vanishes as well. The expression in Eq. (3.19) may also be obtained by integrating the energy density ϱ_E over Ω .

Furthermore, because $\int_{\Omega} dx \varrho = \text{const}$, the spatial integral of the imaginary part of ϱ_E vanishes. Hence, while ϱ_E is a complex local observable (for $\psi \in \mathbb{C}$), its integral over Ω is always real, ensuring its physical relevance (see Eqs. (3.9) and (3.11)). The result in Eq. (3.19) can also be written in terms of T^0_0 and the boundary contribution appearing in that expression:

$$\langle\langle \Psi, \hat{E}\Psi \rangle\rangle = \int_{\Omega} dx \varrho_E = \frac{\hbar}{2mc} \operatorname{Im} [\psi^*(c\hat{\mathbf{p}}\psi)] \Big|_a^b + \int_{\Omega} dx T^0_0. \quad (3.20)$$

Essentially, although the “surface term” and the spatial integral of T^0_0 in Eq. (3.20) may each be time dependent, their sum, $\langle\langle\Psi, \hat{E}\Psi\rangle\rangle$, remains constant in time provided that $\dot{S} = 0$. This follows by taking the total time derivative of Eq. (3.20) and using $\hat{E}T^0_0 - c\hat{p}T^1_0 = (\hat{E}S)\psi^*\psi = 0$, together with Eq. (3.8) and its complex conjugate. In scalar-field applications it is common to neglect the boundary contribution in Eq. (3.20) by imposing Dirichlet BCs at $x = a$ and $x = b$ (or at infinity when Ω is the whole real line). Finally, Eq. (3.19) is consistent with Eq. (3.9), as expected.

All the results above apply to the 1D KFG particle. The next chapter imposes the additional KFGM constraints and derives the conditions under which the boundary terms in Eqs. (3.19)–(3.20) and Eq. (3.15) vanish. Examples of BCs satisfying or failing these conditions will also be given. In particular, the vanishing of the boundary term in Eq. (3.20) also ensures the vanishing of the boundary term in Eq. (3.15).

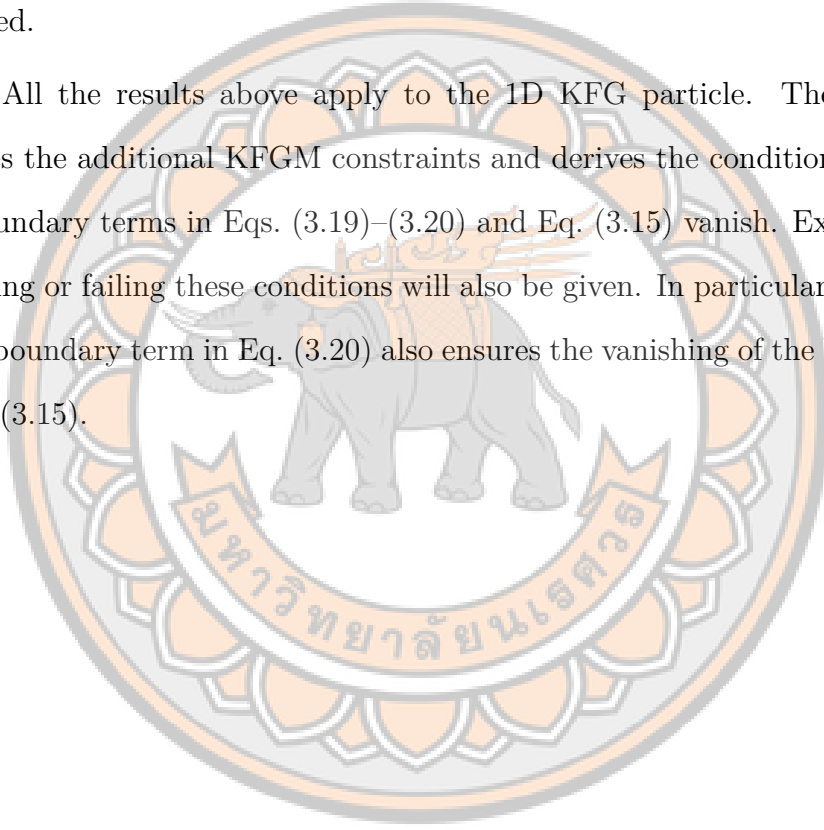


Table 4 Summary of the five energy densities and energy current densities.

Observable	Type/source	Value under a Majorana condition	Conservation and values at $x = a, b$	Use in this thesis
ϱ_E	Energy density associated with $\langle\langle\Psi, \hat{E}\Psi\rangle\rangle$	Real and generally nonzero	Satisfies a continuity equation with j_E when $\dot{S} = 0$ and gives $\int_{\Omega} \varrho_E dx = \text{const.}$	Acceptable.
j_E	Energy current density paired with ϱ_E	Real and generally nonzero	Satisfies $j_E(b, t) = j_E(a, t)$ for all acceptable BCs and characterizes impermeable and permeable BCs	Acceptable quantity that characterizes the BCs.
$\tilde{\varrho}_E$	Real energy density appearing in Eq. (3.9)	Real and generally nonzero	Related to ϱ_E through Eq. (3.9); not the standard tensor component	Comparison density.
T^0_0	Standard energy density from T^μ_ν	Real and generally nonzero	Related to ϱ_E through the alternative rewriting in Eq. (3.11); paired with $\tilde{j}_E \equiv cT^1_0$	Comparison density; conservation depends on the imposed BCs.
$\tilde{j}_E \equiv cT^1_0$	Standard energy current density from T^μ_ν	Real and generally nonzero	Does not always satisfy equality at the ends of the interval; extra BC restrictions are required for $\tilde{j}_E(b, t) = \tilde{j}_E(a, t)$, equivalently $cT^1_0(b, t) = cT^1_0(a, t)$	Limited comparison current.

CHAPTER IV

IMPOSING THE MAJORANA CONDITIONS

This chapter elaborates on the results of Chapter III for the pair of local observables $\{\varrho_E, j_E\}$. These results are the equality $j_E(b, t) = j_E(a, t)$ at the ends of the interval for all acceptable BCs, the on-shell relation $\hat{E}\varrho_E - \hat{p}j_E = (\hat{E}S)\psi^*\psi$, and the conservation of $\int_{\Omega} dx \varrho_E$ when $\dot{S} = 0$. The present chapter shows that, after a Majorana condition is imposed, ϱ_E and j_E become real and nontrivial and are appropriate for characterizing 1D KFGM particles. In contrast, the pair $\{T^0_0, cT^1_0\}$ depends on the imposed BCs and is incomplete; it becomes equally satisfactory only when the relevant boundary contribution vanishes. Furthermore, a three-parameter family of BCs is obtained after imposing a Majorana condition on the general four-parameter family of BCs. This family leads to an explicit expression at $x = a$ and $x = b$ for the acceptable energy current density, from which the confining BCs for 1D KFGM particles are identified. A two-parameter subfamily is further obtained for the confining cases. In addition, the conditions under which cT^1_0 takes equal values at the ends of the interval, and under which the mean value of the energy operator is positive under the stated sufficient assumptions depending on the imposed BCs, are obtained. Within the confining class, only four common types of BCs, namely the Dirichlet, Neumann, and two mixed types of BCs, satisfy these conditions. A one-parameter nonconfining subfamily, including the periodic and antiperiodic cases as typical representatives, also satisfies the corresponding requirements at the ends of the interval. In these cases, the acceptable pair $\{\varrho_E, j_E\}$ and the standard pair $\{T^0_0, cT^1_0\}$ are equally satisfactory for the boundary characterization, although the two current densities remain distinct local observables and differ by a spatial derivative term. For the remaining physically acceptable BCs, only j_E remains reliable for characterizing confinement or nonconfinement; cT^1_0 is reliable

only when its additional boundary term vanishes.

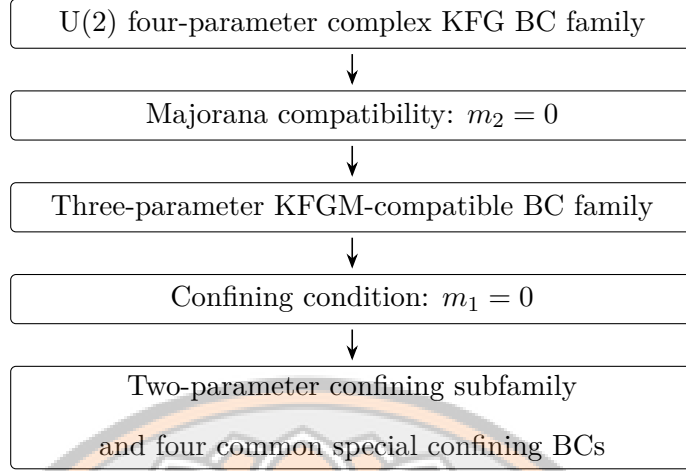


Figure 3 Reduction of the four-parameter $U(2)$ KFG BC family to the three-parameter KFGM-compatible family and, after imposing $m_1 = 0$, to the two-parameter confining subfamily.

4.1 Majorana-compatible BCs

4.1.1 Two-component form, Majorana conditions, and the three-parameter general set of BCs

In the characterization of the one-dimensional KFGM particle, two Majorana conditions must be considered: the standard Majorana condition $\Psi = \Psi^c = \hat{\tau}_1 \Psi^*$, which implies $\psi = \psi^*$, and the nonstandard Majorana condition $\Psi = -\Psi^c = -\hat{\tau}_1 \Psi^*$, which implies $\psi = -\psi^*$. In the FV two-component formalism, charge conjugation acts as complex conjugation followed by a component swap, $\Psi^c \equiv \hat{\tau}_1 \Psi^*$, with $\hat{\tau}_1 = \hat{\sigma}_x$. Hence, the standard condition enforces $\psi \in \mathbb{R}$, whereas the nonstandard one enforces ψ to be purely imaginary. Equivalently, in the latter case one may write $\psi = i\tilde{\psi}$ with $\tilde{\psi} \in \mathbb{R}$, reducing the analysis to the standard situation [5]. In either case, Majorana compatibility reduces the general four-parameter BC family (m_0, m_1, m_2, m_3) to a three-parameter one by forcing $m_2 = 0$. Equivalently, the unitary matrix parametrizing the BCs satisfies $\hat{U}^T = \hat{U}$, and no condition forces

$m_3 = 0$. Throughout this chapter, the standard choice is adopted unless stated otherwise, and we restrict ourselves to the inherited Majorana-compatible BCs ($m_2 = 0$).

When the solutions of the 1D KFG equation satisfy either $\psi = \psi^*$ or $\psi = -\psi^*$, equivalently $\psi = i\tilde{\psi}$ with $\tilde{\psi}$ real, the energy density ϱ_E and the energy current density j_E become real and do not vanish identically; see Eqs. (3.6) and (3.7). In addition, j_E satisfies the condition given in Eq. (3.8). Likewise, $\tilde{\varrho}_E$, T^0_0 , and $\tilde{j}_E$ do not vanish identically either; see Eqs. (3.10), (3.12), and (3.14). However, $\tilde{j}_E$ does not necessarily satisfy the condition given in Eq. (3.16). Consequently, ϱ_E and j_E are the physically appropriate local observables for characterizing a 1D KFGM particle confined to an interval. When $\dot{S} = 0$, they satisfy a continuity equation, and because Eq. (3.8) holds, one obtains the conservation law $\int_{\Omega} dx \varrho_E = \text{const.}$ This establishes ϱ_E as the appropriate energy density in this setting. As will be shown throughout this section, for the 1D KFGM particle the energy current density j_E characterizes as impenetrable precisely those BCs that were already considered impenetrable for a 1D KFG particle; similarly, it characterizes as penetrable precisely those BCs that were already considered penetrable, as expected. By contrast, the energy current density $\tilde{j}_E$ gives only an incomplete description: it succeeds only for some impenetrable and penetrable BCs, and therefore does not capture the full boundary-transport picture for a 1D KFGM particle on a finite interval. In particular, the proper current is j_E , whereas cT^1_0 is reliable only when its boundary contribution cancels.

If one of the two Majorana conditions is imposed on the four-parameter general set of BCs for the solutions Ψ of the 1D FV equation, the set is reduced to the following three-parameter general form, with fewer degrees of freedom:

$$\begin{bmatrix} (\hat{\tau}_3 + i\hat{\tau}_2)(\Psi - i\lambda\Psi_x)(b, t) \\ (\hat{\tau}_3 + i\hat{\tau}_2)(\Psi + i\lambda\Psi_x)(a, t) \end{bmatrix} = \hat{U}_{(4 \times 4)} \begin{bmatrix} (\hat{\tau}_3 + i\hat{\tau}_2)(\Psi + i\lambda\Psi_x)(b, t) \\ (\hat{\tau}_3 + i\hat{\tau}_2)(\Psi - i\lambda\Psi_x)(a, t) \end{bmatrix}, \quad (4.1)$$

where $\lambda \in \mathbb{R}$ and $\hat{U}_{(4 \times 4)}$ denotes the following 4×4 unitary and complex symmetric

matrix:

$$\hat{U}_{(4 \times 4)} = e^{i\mu} \begin{bmatrix} (m_0 - im_3)\hat{1}_2 & -im_1\hat{1}_2 \\ -im_1\hat{1}_2 & (m_0 + im_3)\hat{1}_2 \end{bmatrix}, \quad (4.2)$$

with $\mu \in [0, \pi)$ and real parameters m_0 , m_1 , and m_3 satisfying $(m_0)^2 + (m_1)^2 + (m_3)^2 = 1$. For consistency, the notation follows that of Ref. [5].

4.1.2 Three-parameter general set of BCs in the one-component form

Similarly, the three-parameter general set of BCs for the (ultimately real or purely imaginary) solutions ψ of the 1D KFG equation can be expressed as

$$\begin{bmatrix} \psi(b, t) - i\lambda\psi_x(b, t) \\ \psi(a, t) + i\lambda\psi_x(a, t) \end{bmatrix} = \hat{U}_{(2 \times 2)} \begin{bmatrix} \psi(b, t) + i\lambda\psi_x(b, t) \\ \psi(a, t) - i\lambda\psi_x(a, t) \end{bmatrix}, \quad (4.3)$$

where the 2×2 unitary and complex symmetric matrix $\hat{U}_{(2 \times 2)}$ is given by

$$\hat{U}_{(2 \times 2)} = e^{i\mu} \begin{bmatrix} m_0 - im_3 & -im_1 \\ -im_1 & m_0 + im_3 \end{bmatrix}, \quad (4.4)$$

as explained in Ref. [5]. The general set of BCs presented here is obtained by setting $m_2 = 0$ in the most general set of BCs provided in Eq. (2.13). Imposing either Majorana condition on Eq. (2.13) yields $m_2 = 0$. The algebraic reason is that the Majorana restriction requires the boundary subspace to be compatible with complex conjugation. In the parametrization of Eq. (2.14), this compatibility is expressed by the symmetry of the unitary boundary matrix. Indeed,

$$\hat{U}_{(2 \times 2)}^T - \hat{U}_{(2 \times 2)} = e^{i\mu} \begin{bmatrix} 0 & 2m_2 \\ -2m_2 & 0 \end{bmatrix},$$

therefore the Majorana-compatible condition $\hat{U}_{(2 \times 2)}^T = \hat{U}_{(2 \times 2)}$ gives $m_2 = 0$. Equivalently, because the usual current vanishes identically for $\psi = \pm\psi^*$, the boundary formula in Eq. (2.15) cannot contain a residual antisymmetric m_2 contribution for arbitrary Majorana boundary data. Therefore the four-parameter KFG family in Eqs. (2.13)–(2.14) reduces to the three-parameter KFGM family in Eqs. (4.3)–(4.4).

Furthermore, as discussed following Eq. (3.1), if the quantities $\psi(a, t)$, $\psi_x(a, t)$, $\psi(b, t)$, and $\psi_x(b, t)$ constitute the general set of BCs described by Eq. (4.3), then the quantities $(\hat{E}\psi)(a, t)$, $(\hat{E}\psi_x)(a, t)$, $(\hat{E}\psi)(b, t)$, and $(\hat{E}\psi_x)(b, t)$ also satisfy the same BCs.

4.1.3 General set of BCs acted on by the energy operator

The general set of BCs can also be written as follows:

$$\begin{bmatrix} (\hat{E}\psi)(b, t) - i\lambda(\hat{E}\psi_x)(b, t) \\ (\hat{E}\psi)(a, t) + i\lambda(\hat{E}\psi_x)(a, t) \end{bmatrix} = \hat{U}_{(2 \times 2)} \begin{bmatrix} (\hat{E}\psi)(b, t) + i\lambda(\hat{E}\psi_x)(b, t) \\ (\hat{E}\psi)(a, t) - i\lambda(\hat{E}\psi_x)(a, t) \end{bmatrix}. \quad (4.5)$$

The latter set is obtained by applying the energy operator to both sides of Eq. (4.3).

4.2 Rewriting the general family of BCs

4.2.1 Algebraic manipulation

It is possible to write an explicit expression for j_E , as given in Eq. (3.7), evaluated at the boundaries of the interval. This expression shows similarities to that previously presented in Eq. (2.15) for the usual current j . Specifically, it depends on the parameters characterizing the matrix $\hat{U}_{(2 \times 2)}$, as well as on the values of ψ and $\hat{E}\psi$ at the ends of the interval. To obtain this expression, we first rewrite Eq. (4.3) in transfer-matrix form, solving for the boundary data at $x = b$ in terms of the boundary data at $x = a$. This step follows from straightforward algebraic rearrangements of Eq. (4.3), without explicitly imposing the Majorana constraints $\psi = \psi^*$ or $\psi = -\psi^*$ at this stage.

4.2.2 Rewriting the general set of BCs

Finally, the most general family of BCs compatible with $m_2 = 0$ can be written as

$$\begin{bmatrix} \psi(b, t) \\ \lambda\psi_x(b, t) \end{bmatrix} = \hat{M} \begin{bmatrix} \psi(a, t) \\ \lambda\psi_x(a, t) \end{bmatrix}, \quad (4.6)$$

where the 2×2 matrix $\hat{M}$ is given by

$$\hat{M} = \frac{1}{m_1} \begin{bmatrix} m_3 + \sin(\mu) & -m_0 - \cos(\mu) \\ -m_0 + \cos(\mu) & -m_3 + \sin(\mu) \end{bmatrix}. \quad (4.7)$$

It is clear that $\hat{M}$ is a real matrix with unit determinant, implying that $\hat{M} \in \text{SL}(2, \mathbb{R})$. Here, $\hat{M}$ may be referred to as the boundary transfer matrix, because it maps the boundary values $[\psi(a, t) \ \lambda\psi_x(a, t)]^T$ to $[\psi(b, t) \ \lambda\psi_x(b, t)]^T$. Moreover, the inverse of Eq. (4.7) can be written straightforwardly, with the corresponding inverse matrix obtained by applying the substitutions $m_0 \rightarrow -m_0$, $m_3 \rightarrow -m_3$, and $\cos(\mu) \rightarrow -\cos(\mu)$ to $\hat{M}$.

4.3 Special confining case $m_1 = 0$

The case $m_1 = 0$ is not contained directly in the transfer-matrix form of Eqs. (4.6)–(4.7), because $\hat{M}$ contains the factor $1/m_1$. Nevertheless, the corresponding BCs can be obtained by substituting Eq. (4.7) into Eq. (4.6), multiplying the resulting equation by m_1 , and then setting $m_1 = 0$. This procedure gives two relations that directly link $\psi(a, t)$ with $\lambda\psi_x(a, t)$, namely,

$$(m_3 + \sin(\mu))\psi(a, t) - (m_0 + \cos(\mu))\lambda\psi_x(a, t) = 0, \quad (4.8)$$

and

$$(m_0 - \cos(\mu))\psi(a, t) + (m_3 - \sin(\mu))\lambda\psi_x(a, t) = 0. \quad (4.9)$$

Similarly, applying the same procedure to the inverse form of Eq. (4.6) gives two relations that link $\psi(b, t)$ with $\lambda\psi_x(b, t)$:

$$(m_3 - \sin(\mu))\psi(b, t) - (m_0 + \cos(\mu))\lambda\psi_x(b, t) = 0, \quad (4.10)$$

and

$$(m_0 - \cos(\mu))\psi(b, t) + (m_3 + \sin(\mu))\lambda\psi_x(b, t) = 0. \quad (4.11)$$

Here, $\mu \in [0, \pi)$ and the parameters satisfy $(m_0)^2 + (m_3)^2 = 1$. These four relations generate all BCs with $m_1 = 0$. However, they are not independent: the four relations reduce to two independent relations, one at each end of the interval. Equivalently, the same two-parameter confining subfamily is obtained directly by setting $m_1 = 0$ in Eq. (4.3), or in the matrix $\hat{U}_{(2 \times 2)}$ in Eq. (4.4). Each relation at the end of the interval obtained from Eq. (4.3) is equivalent to the corresponding pair of relations displayed above.

4.4 The rewritten general set of BCs acted on by the energy operator

We differentiate in time the general subfamily of BCs stated in Eq. (4.6), i.e.,

$$\begin{bmatrix} (\hat{E}\psi)(b, t) \\ \lambda(\hat{E}\psi_x)(b, t) \end{bmatrix} = \hat{M} \begin{bmatrix} (\hat{E}\psi)(a, t) \\ \lambda(\hat{E}\psi_x)(a, t) \end{bmatrix}. \quad (4.12)$$

Starting from this matrix relation, we first express $\lambda(\hat{E}\psi_x)(a, t)$ in terms of $(\hat{E}\psi)(a, t)$ and $(\hat{E}\psi)(b, t)$. Next, taking the complex conjugate of the matrix equation in Eq. (4.6), we express $\lambda\psi_x^*(a, t)$ in terms of $\psi^*(a, t)$ and $\psi^*(b, t)$. Then, evaluating the energy current density in Eq. (3.7) at $x = a$ and substituting the preceding expressions leads to

$$j_E(x = a, t) = \frac{i\hbar}{2m} \frac{1}{\lambda} \left(\frac{m_1}{m_0 + \cos \mu} \right) [\psi^*(a, t) (\hat{E}\psi)(b, t) - \psi^*(b, t) (\hat{E}\psi)(a, t)]. \quad (4.13)$$

Owing to Eq. (3.8), the same expression also gives $j_E(x = b, t)$. It is immediate from Eq. (4.13) that setting $m_1 = 0$ yields $j_E(a, t) = j_E(b, t) = 0$. For real or purely imaginary wavefunctions, the condition $j_E(a, t) = j_E(b, t) = 0$ characterizes the confining BCs. This use of j_E is specific to the KFGM setting: for a general complex KFG particle, the usual current j remains the standard boundary-current classifier, while j_E is introduced here because j vanishes identically after the Majorana restriction. Accordingly, all confining BCs follow either from Eq. (4.3) upon

imposing $m_1 = 0$, or equivalently from Eq. (4.6) together with its inverse, namely, from Eqs. (4.8)–(4.11).

4.5 Expectation value of $c\hat{p}$ under Majorana conditions

If the wavefunction is complex, the quantity j_E is indeed complex as well. This is not problematic provided that the spatial integral of j_E remains real. It is straightforward to show that $\int_{\Omega} dx j_E$ is real only under the condition that $\int_{\Omega} dx j = \text{const}$ (see Eq. (3.13)). As discussed earlier, although the local energy density ϱ_E is generally complex for $\psi \in \mathbb{C}$ (due to a purely imaginary contribution), its spatial integral equals $\langle\langle \Psi, \hat{E}\Psi \rangle\rangle$ and reduces to manifestly real bulk terms plus the boundary term $\frac{\hbar}{2mc} \text{Im}[\psi^*(c\hat{p}\psi)]|_a^b$; consequently $\int_{\Omega} \varrho_E dx \in \mathbb{R}$.

Incidentally, the expectation value of the operator $c\hat{p}$ is related to the spatial integral of j_E by

$$\langle\langle \Psi, c\hat{p}\Psi \rangle\rangle = \frac{1}{c} \int_{\Omega} dx j_E - \frac{i}{mc^2} \int_{\Omega} dx \text{Im}[(\hat{E}\psi^*)(c\hat{p}\psi)]. \quad (4.14)$$

This result follows directly from the definition of the scalar product given in Eq. (2.10) together with the definition of the energy current density j_E in Eq. (3.7). Note that while the condition $\int_{\Omega} dx j = \text{const}$ is sufficient to ensure that $\int_{\Omega} dx j_E$ is real, it does not guarantee that $\langle\langle \Psi, c\hat{p}\Psi \rangle\rangle$ is also real (see Eq. (4.14)).

However, when ψ satisfies a Majorana condition, we have

$$\psi = \pm\psi^* \implies (\hat{E}\psi^*)(c\hat{p}\psi) \in \mathbb{R} \implies \int_{\Omega} dx \text{Im}[(\hat{E}\psi^*)(c\hat{p}\psi)] = 0,$$

and therefore

$$\langle\langle \Psi, c\hat{p}\Psi \rangle\rangle = \frac{1}{c} \int_{\Omega} dx j_E. \quad (4.15)$$

Therefore, the expectation value of $c\hat{p}$ is real, because j_E is real in this case.

4.6 Algebraic conditions consistent with $j_E(a, t) = j_E(b, t) = 0$ and $\tilde{j}_E(a, t) = \tilde{j}_E(b, t) = 0$

4.6.1 The condition $[\text{Im}(\psi(c\hat{p}\psi))]_a^b = 0$

At this point, several remarks are in place. The general set of BCs compatible with the relation $[j(x, t)]_a^b = 0$ is given in Eqs. (2.13) and (2.14), under the requirement that the solutions ψ are complex (but not purely imaginary). If these solutions additionally satisfy a Majorana condition, then $[j(x, t)]_a^b = 0$ holds trivially because $j(x, t) = 0$. The general set of BCs in Eqs. (2.13) and (2.14) is likewise compatible with the relation $[j_E(x, t)]_a^b = 0$, allowing solutions ψ that are either real or complex. If ψ satisfies a Majorana condition, then $j_E(x, t)$ becomes real and $m_2 = 0$. As a result, the general BCs in Eqs. (2.13) and (2.14) reduce to those given by Eqs. (4.3) and (4.4), or equivalently, by Eqs. (4.6) and (4.7) together with their inverse forms. Similarly, to determine the BCs compatible with $[\tilde{j}_E(x, t)]_a^b = 0$, it is first necessary to identify the conditions under which $[\text{Im}(\psi(c\hat{p}\psi))]_a^b = 0$ holds (see Eq. (3.15)). If this latter relation is satisfied, then it follows that $\hat{E}(\text{Im}(\psi(c\hat{p}\psi)))_a^b = 0$. Additionally, the mean value of the operator $\hat{E}$ can be positive provided that $S \geq 0$ throughout the interval Ω (see Eq. (3.20)).

We start by writing the algebraic identity

$$\text{Im}(\psi(c\hat{p}\psi)) = -\hbar c \frac{1}{\lambda} \psi(x, t) \lambda \psi_x(x, t) = -\frac{\hbar c}{2} \frac{1}{\lambda} \begin{bmatrix} \psi(x, t) \\ \lambda \psi_x(x, t) \end{bmatrix}^T \hat{\tau}_1 \begin{bmatrix} \psi(x, t) \\ \lambda \psi_x(x, t) \end{bmatrix}, \quad (4.16)$$

where $\hat{\tau}_1 = \hat{\sigma}_x$ is a Pauli matrix. Using the general set of BCs given in Eq. (4.6), the vanishing condition can also be stated explicitly as

$$[\text{Im}(\psi(c\hat{p}\psi))]_a^b = (\text{Im}(\psi(c\hat{p}\psi)))(b, t) - (\text{Im}(\psi(c\hat{p}\psi)))(a, t) = 0. \quad (4.17)$$

4.6.2 Matrix constraints on $\hat{M}$

The mathematical condition that supports Eq. (4.17) is given by the preservation

of the bilinear boundary form. Indeed, the BCs in Eq. (4.6) relate the column vectors at $x = a$ and $x = b$ by

$$\begin{bmatrix} \psi(b, t) \\ \lambda \psi_x(b, t) \end{bmatrix} = \hat{M} \begin{bmatrix} \psi(a, t) \\ \lambda \psi_x(a, t) \end{bmatrix}.$$

Preserving the bilinear quantity associated with $\hat{\tau}_1$ from a to b gives Eq. (4.17) through Eq. (4.16). This preservation condition is

$$\hat{M}^T \hat{\tau}_1 \hat{M} = \hat{\tau}_1. \quad (4.18)$$

If instead the inverse form of the BCs in Eq. (4.6) is considered, the corresponding matrix condition can be written as

$$(\hat{M}^{-1})^T \hat{\tau}_1 \hat{M}^{-1} = \hat{\tau}_1. \quad (4.19)$$

4.6.3 Consequences of the constraints

Recall that the set of BCs given in Eq. (4.6), together with its inverse expression, forms the complete family of BCs when $m_2 = 0$.

By substituting the matrix $\hat{M}$ from Eq. (4.7) into Eq. (4.18), we obtain

$$(m_3 \pm \sin(\mu))(m_0 \mp \cos(\mu)) = 0, \quad (4.20)$$

and

$$(m_0 - \cos(\mu))(m_0 + \cos(\mu)) = 0, \quad (4.21)$$

subject to the constraint $(m_0)^2 + (m_1)^2 + (m_3)^2 = 1$ with $\mu \in [0, \pi)$. Equation (4.21) can also be written as

$$(m_3)^2 - \sin^2(\mu) = -(m_1)^2. \quad (4.22)$$

Likewise, by substituting $\hat{M}^{-1}$ into Eq. (4.19) we obtain

$$(m_3 \pm \sin(\mu))(m_0 \pm \cos(\mu)) = 0, \quad (4.23)$$

and

$$(m_0 - \cos(\mu))(m_0 + \cos(\mu)) = 0, \quad (4.24)$$

Note that Eq. (4.24) coincides with Eq. (4.21), and therefore is equivalent to Eq. (4.22). As a result, the conditions in Eqs. (4.20), (4.21), and (4.23) must all be satisfied in order for Eq. (4.17) to hold.

In the confining case where $m_1 = 0$ (implying $(m_0)^2 + (m_3)^2 = 1$), Eq. (4.22) reduces to

$$(m_3 - \sin(\mu))(m_3 + \sin(\mu)) = 0. \quad (4.25)$$

Thus, Eq. (4.25), together with Eqs. (4.20) and (4.23), must be satisfied by confining BCs that validate the result given in Eq. (4.17).

4.7 Set of confining BCs ($m_1 = 0$)

As previously noted, the most general subfamily of confining BCs can be obtained by setting $m_1 = 0$ in Eq. (4.3). This gives two separate relations, evaluated at $x = a$ and $x = b$, which can be collectively expressed as

$$\begin{bmatrix} 1 - e^{i\mu}(m_0 - im_3) & -i - ie^{i\mu}(m_0 - im_3) \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \psi(b, t) \\ \lambda\psi_x(b, t) \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 1 - e^{i\mu}(m_0 + im_3) & i + ie^{i\mu}(m_0 + im_3) \end{bmatrix} \begin{bmatrix} \psi(a, t) \\ \lambda\psi_x(a, t) \end{bmatrix}. \quad (4.26)$$

Equation (4.26) therefore specifies a two-parameter family, with $\mu \in [0, \pi)$ and $(m_0)^2 + (m_3)^2 = 1$. The same boundary form is preserved after acting with $\hat{E}$: replacing $\psi \mapsto \hat{E}\psi$ and $\psi_x \mapsto \hat{E}\psi_x$ in Eq. (4.26) yields boundary relations of the same form.

Moreover, the two independent relations encoded in Eq. (4.26) are real-linear under the Majorana restriction. To see this for the relation at $x = b$, define $q_b = e^{i\mu}(m_0 - im_3)$ and $z_b = (1 - q_b)/[-i(1 + q_b)]$. Because $(m_0)^2 + (m_3)^2 = 1$, the quantity q_b has unit modulus; hence $q_b^* = q_b^{-1}$. Direct conjugation then gives

$z_b^* = z_b$; hence $z_b \in \mathbb{R}$. Therefore the first row of Eq. (4.26) can be written as $z_b\psi(b, t) + \lambda\psi_x(b, t) = 0$ whenever the denominator is nonzero. The exceptional limiting case gives the corresponding Dirichlet-type relation at that endpoint.

Similarly, for the relation at $x = a$, define $q_a = e^{i\mu}(m_0 + im_3)$ and $z_a = (1 - q_a)/[i(1 + q_a)]$. Again $q_a^* = q_a^{-1}$, and direct conjugation gives $z_a^* = z_a$; hence $z_a \in \mathbb{R}$. Therefore the second row of Eq. (4.26) can be written as $z_a\psi(a, t) + \lambda\psi_x(a, t) = 0$, again apart from the corresponding limiting case. Consequently, the relations at the ends of the interval are compatible with $\psi = \psi^*$ and also with $\psi = -\psi^*$, because the coefficients multiplying ψ and $\lambda\psi_x$ are real.

The relations at the ends of the interval in Eqs. (4.8)–(4.11) are equivalent to the two independent boundary relations obtained from Eq. (4.26) at $x = a$ and $x = b$. Direct substitution shows that any confining BC enforces $j_E(a, t) = j_E(b, t) = 0$. For instance, evaluating Eq. (3.7) at $x = a$ and substituting the expressions for $\lambda\psi_x^*(a, t)$ and $\lambda(\hat{E}\psi_x)(a, t)$ obtained from Eq. (4.26) gives $j_E(a, t) = 0$. By virtue of Eq. (3.8), this implies $j_E(b, t) = 0$ as well. The confining subfamily in Eq. (4.26), together with the subfamily given by Eqs. (4.6)–(4.7) for $m_1 \neq 0$, collectively covers all BCs contained within the three-parameter family in Eq. (4.3).

4.8 A catalog of BCs

4.8.1 Typical confining BCs

As examples of impenetrable (confining) BCs for the 1D KFGM particle, consider the following cases, all characterized by $m_1 = 0$:

$$(i) \quad \begin{cases} \psi(a, t) = \psi(b, t) = 0 \\ (m_0 = -1, m_3 = 0, \mu = 0) \end{cases} \quad (\text{Dirichlet BC})$$

This BC was named in honor of the German mathematician Peter Gustav Lejeune

Dirichlet (1805–1859), who contributed to boundary-value problems [30]. The analysis is restricted to $\mu \in [0, \pi)$; thus, the matrix $\hat{U}_{(2 \times 2)}$ is a one-to-one parameterization of $U(2)$. If $\mu \in [0, \pi]$ had been chosen from the beginning, this BC could also be obtained by taking $m_0 = +1$, $m_3 = 0$ and $\mu = \pi$.

$$(ii) \quad \begin{cases} \lambda \psi_x(a, t) = \lambda \psi_x(b, t) = 0 \\ (m_0 = +1, m_3 = 0, \mu = 0) \end{cases} \quad (\text{Neumann BC})$$

$$(iii) \quad \begin{cases} \psi(a, t) = \lambda \psi_x(b, t) = 0 \\ (m_0 = 0, m_3 = +1, \mu = \frac{\pi}{2}) \end{cases} \quad (\text{Mixed BC})$$

$$(iv) \quad \begin{cases} \lambda \psi_x(a, t) = \psi(b, t) = 0 \\ (m_0 = 0, m_3 = -1, \mu = \frac{\pi}{2}) \end{cases} \quad (\text{Another mixed BC})$$

The Neumann BC was named in honor of the German mathematician Carl Gotfried Neumann (1832–1925), who also contributed to boundary-value problems [31]. This BC specifies the normal derivative $\psi_x(x, t)$ at the ends $x = a$ and $x = b$ of the interval Ω .

The BCs (i)–(iv) satisfy Eqs. (4.20), (4.23), and (4.25); hence,

$[\text{Im}(\psi(c\hat{p}\psi))]|_a^b = 0$. Furthermore, each term in Eq. (4.17) vanishes separately.

Thus, from Eq. (3.15) it follows that

$[\tilde{j}_E]|_a^b = 0$. Additionally, for these four confining BCs, the energy current density $\tilde{j}_E$ defined in Eq. (3.14), namely,

$$\tilde{j}_E = \frac{i\hbar}{m} \frac{1}{\lambda} (\hat{E}\psi)(x, t) \lambda \psi_x(x, t), \quad (4.27)$$

vanishes at the ends of the interval, i.e., $\tilde{j}_E(a, t) = \tilde{j}_E(b, t) = 0$. Furthermore, when applying the Dirichlet BCs $\psi(a = -\infty, t) = \psi(b = +\infty, t) = 0$ for a strictly neutral particle defined on $\Omega = \mathbb{R}$, the energy current density $\tilde{j}_E$ necessarily vanishes at

$x = \pm\infty$. Note that Ref. [9] focused exclusively on the quantity $\tilde{j}_E$.

$$(v) \quad \begin{cases} \psi(a, t) - \lambda\psi_x(a, t) = 0, & \psi(b, t) + \lambda\psi_x(b, t) = 0 \\ (m_0 = +1, m_3 = 0, \mu = \frac{\pi}{2}) \end{cases} \quad (\text{Type of Robin BC})$$

$$(vi) \quad \begin{cases} \psi(a, t) + \lambda\psi_x(a, t) = 0, & \psi(b, t) - \lambda\psi_x(b, t) = 0 \\ (m_0 = -1, m_3 = 0, \mu = \frac{\pi}{2}) \end{cases} \quad (\text{Another Robin-type BC})$$

The Robin BCs were named in honor of the French mathematician Victor Gustave Robin (1855–1897), who also contributed to boundary-value problems [32]. These BCs provide mixed conditions combining the value of the wavefunction $\psi(x, t)$ with its normal derivative $\psi_x(x, t)$ at the ends $x = a$ and $x = b$ of the interval Ω .

The Robin-type confining BCs (v) and (vi) can be viewed as KFG analogs of BCs commonly used in the one-dimensional MIT bag model for hadronic structures. However, these two BCs do not satisfy Eqs. (4.20), (4.23), and (4.25); hence, $[\text{Im}(\psi(c\hat{p}\psi))]_a^b \neq 0$. Consequently, from Eq. (3.15), it follows that $[\tilde{j}_E]_a^b \neq 0$. For BCs (v) and (vi), the energy current density $\tilde{j}_E$ in Eq. (4.27) does not vanish at the walls of the interval, namely, $\tilde{j}_E(a, t) \neq 0$ and $\tilde{j}_E(b, t) \neq 0$.

By contrast, the acceptable energy current density still gives the impenetrability condition, $j_E(a, t) = j_E(b, t) = 0$.

The only confining BCs that satisfy Eq. (4.17) are (i)–(iv). Indeed, from Eq. (4.20) we obtain $m_0 m_3 = \sin(\mu) \cos(\mu)$ and $m_0 \sin(\mu) = m_3 \cos(\mu)$. Similarly, from Eq. (4.23) we obtain $m_0 m_3 = -\sin(\mu) \cos(\mu)$ and $m_0 \sin(\mu) = -m_3 \cos(\mu)$. These imply $m_0 m_3 = 0$, $\sin(\mu) \cos(\mu) = 0$, $m_0 \sin(\mu) = 0$, and $m_3 \cos(\mu) = 0$. Together with $(m_0)^2 = \cos^2(\mu)$ from Eq. (4.21) and $(m_3)^2 = \sin^2(\mu)$ from Eq. (4.25), which ensure $(m_0)^2 + (m_3)^2 = 1$, these conditions lead to exactly four BCs. They are grouped by the value of μ as follows: for $\mu = \pi/2$, one has $m_0 = 0$ and $m_3 = \pm 1$, giving BCs (iii) and (iv); for $\mu = 0$, one has $m_3 = 0$ and $m_0 = \pm 1$, giving BCs (i) and (ii).

4.8.2 Typical nonconfining BCs

Examples of nonconfining (permeable) BCs for the 1D KFGM particle are given by the following cases, all satisfying $m_1 \neq 0$:

$$(vii) \quad \begin{cases} \psi(a, t) = \psi(b, t), & \lambda\psi_x(a, t) = \lambda\psi_x(b, t) \\ (m_0 = 0, m_3 = 0, m_1 = +1, \mu = \frac{\pi}{2}) \end{cases} \quad (\text{Periodic BC})$$

$$(viii) \quad \begin{cases} \psi(a, t) = -\psi(b, t), & \lambda\psi_x(a, t) = -\lambda\psi_x(b, t) \\ (m_0 = 0, m_3 = 0, m_1 = -1, \mu = \frac{\pi}{2}) \end{cases} \quad (\text{Antiperiodic BC})$$

The following subfamily of nonconfining BCs generalizes the periodic and antiperiodic cases:

$$(ix) \quad \begin{cases} \begin{bmatrix} \psi(b, t) \\ \lambda\psi_x(b, t) \end{bmatrix} = \pm \begin{bmatrix} \sin(\mu) & -\cos(\mu) \\ \cos(\mu) & \sin(\mu) \end{bmatrix} \begin{bmatrix} \psi(a, t) \\ \lambda\psi_x(a, t) \end{bmatrix} \\ = \pm e^{-i\hat{\sigma}_y(\frac{\pi}{2}-\mu)} \begin{bmatrix} \psi(a, t) \\ \lambda\psi_x(a, t) \end{bmatrix} \end{cases}$$

Here $m_0 = m_3 = 0$; the upper sign corresponds to $m_1 = +1$, the lower sign to $m_1 = -1$, and $\mu \in [0, \pi)$. Setting $\mu = \pi/2$ yields the periodic BC for $m_1 = +1$ and the antiperiodic BC for $m_1 = -1$. Additionally, choosing $\mu = 0$ leads to the following two BCs:

$$(x) \quad \begin{cases} \psi(a, t) = \pm\lambda\psi_x(b, t), & \psi(b, t) = \mp\lambda\psi_x(a, t) \\ (m_0 = 0, m_3 = 0, \mu = 0, \\ \text{upper sign} \Rightarrow m_1 = +1, \quad \text{lower sign} \Rightarrow m_1 = -1) \end{cases}$$

(Particular mixed BCs)

Among all BCs within the subset (ix), only (vii) and (viii) satisfy Eqs. (4.20), (4.21), and (4.23), because $\mu = \pi/2$ is the unique solution under $m_0 = m_3 = 0$. More generally (see Ref. [5], Eq. (67)), of all nonconfining BCs the only ones that satisfy these same algebraic constraints form the following one-parameter subfamily,

obtained for $m_0 = 0$ and $\mu = \pi/2$:

$$\begin{bmatrix} \psi(b, t) \\ \lambda\psi_x(b, t) \end{bmatrix} = \frac{1}{m_1} \begin{bmatrix} m_3 + 1 & 0 \\ 0 & -m_3 + 1 \end{bmatrix} \begin{bmatrix} \psi(a, t) \\ \lambda\psi_x(a, t) \end{bmatrix}, \quad (4.28)$$

where $(m_1)^2 + (m_3)^2 = 1$ and $m_1 \neq 0$. From the two relations in Eq. (4.20) and the two relations in Eq. (4.23), one obtains $m_0 m_3 = 0$, $\sin(\mu) \cos(\mu) = 0$, $m_0 \sin(\mu) = 0$, and $m_3 \cos(\mu) = 0$. In the present nonconfining case, these relations together with $(m_0)^2 = \cos^2(\mu)$, Eq. (4.21), give $m_0 = 0$ and $\mu = \pi/2$, while m_1 and m_3 remain constrained by $(m_1)^2 + (m_3)^2 = 1$. Substitution of these parameters into Eq. (4.6) gives the subfamily in Eq. (4.28). For every BC in Eq. (4.28), one has $[\text{Im}(\psi(c\hat{p}\psi))]|_a^b = 0$, as in Eq. (4.17); hence $[\tilde{j}_E]|_a^b = 0$, by Eq. (3.16). However, $\text{Im}(\psi(c\hat{p}\psi))$ and $\tilde{j}_E$ are not required to vanish separately at the two endpoints. Thus, for nonconfining BCs outside Eq. (4.28), only j_E remains the generally adequate current for characterizing the penetrability of the interval, since $[j_E]|_a^b = 0$ still holds. The periodic BC (vii) and the antiperiodic BC (viii) are contained in the subfamily in Eq. (4.28).

4.8.3 BCs not suitable for a 1D KFGM particle

As previously discussed, a 1D KFGM particle accepts only BCs satisfying $m_2 = 0$. Examples of BCs that do not meet this requirement—and thus are not suitable for a 1D KFGM particle but remain suitable for a 1D KFG particle where $m_2 \neq 0$ —include:

$$(xi) \quad \begin{cases} \psi(a, t) = \pm i \psi(b, t), & \lambda\psi_x(a, t) = \pm i \lambda\psi_x(b, t) \\ (m_0 = 0, m_1 = 0, m_3 = 0, \mu = \frac{\pi}{2}, \\ \text{upper sign} \Rightarrow m_2 = +1, \text{ lower sign} \Rightarrow m_2 = -1) \end{cases}$$

(Quasiperiodic/quasiantiperiodic BCs)

$$(xii) \quad \begin{cases} \psi(a, t) = \pm i\lambda\psi_x(b, t), & \psi(b, t) = \pm i\lambda\psi_x(a, t) \\ (m_0 = 0, m_1 = 0, m_3 = 0, \mu = 0, \\ \text{upper sign} \Rightarrow m_2 = +1, \quad \text{lower sign} \Rightarrow m_2 = -1) \end{cases} \quad (\text{Quasimixed BCs})$$

The BCs in (xi) and (xii) are complex and nonconfining because $m_2 \neq 0$, which gives $j(b, t) = j(a, t)$. See Appendix G for a table summarizing confining, nonconfining, and unsuitable BCs for a 1D KFGM particle.

4.9 Further constraints and typical solutions

Finally, consider the relationship between the two energy current densities j_E and $\tilde{j}_E$ upon spatial integration. The relation linking these two current densities is given by Eq. (3.13),

$$j_E = \frac{i}{2mc} c\hat{p} [\text{Im}[\psi^*(\hat{E}\psi)]] + \frac{1}{2} \hat{E}j + \tilde{j}_E, \quad (4.29)$$

which also uses the identity $\hat{E} [\text{Im}[\psi^*(c\hat{p}\psi)]] = c\hat{p} [\text{Im}[\psi^*(\hat{E}\psi)]]$.

By explicitly imposing a Majorana condition, i.e., $\psi = \psi^*$ or $\psi = -\psi^*$ (which implies $j = 0$), Eq. (4.29) reduces to

$$j_E = \frac{\hbar}{2m} \frac{\partial}{\partial x} [\text{Im}[\psi(\hat{E}\psi)]] + \tilde{j}_E. \quad (4.30)$$

Integration over the finite interval Ω then gives

$$J_E = \frac{\hbar}{2m} [\text{Im}[\psi(\hat{E}\psi)]]_a^b + \tilde{J}_E, \quad (4.31)$$

where $J_E := \int_{\Omega} dx j_E$ and $\tilde{J}_E := \int_{\Omega} dx \tilde{j}_E$ denote two distinct (integrated) energy currents. If the domain is the entire real line ($\Omega = (-\infty, +\infty)$) and we assume the Dirichlet BC $\psi(a = -\infty, t) = \psi(b = +\infty, t) = 0$, then the boundary term vanishes, eliminating any distinction between J_E and $\tilde{J}_E$. This is the usual assumption in classical field theory that “the fields vanish at infinity,” and it was the only BC considered in Ref. [9].

We now derive algebraic conditions under which BCs are compatible with the boundary term cancellation $[\text{Im}[\psi(\hat{E}\psi)]]|_a^b = 0$. To this end, begin by expressing

$$\text{Im}[\psi(\hat{E}\psi)] = \frac{1}{i} \psi(x, t)(\hat{E}\psi)(x, t) = \frac{1}{2i} \begin{bmatrix} \psi(x, t) \\ \lambda\psi_x(x, t) \end{bmatrix}^T (\hat{1}_2 + \hat{\tau}_3) \begin{bmatrix} (\hat{E}\psi)(x, t) \\ \lambda(\hat{E}\psi_x)(x, t) \end{bmatrix}. \quad (4.32)$$

Using the general family of BCs given in Eqs. (4.6) and (4.12), the matrix condition ensuring that

$$[\text{Im}[\psi(\hat{E}\psi)]]|_a^b = \text{Im}[\psi(\hat{E}\psi)](b, t) - \text{Im}[\psi(\hat{E}\psi)](a, t) = 0 \quad (4.33)$$

is

$$\hat{M}^T(\hat{1}_2 + \hat{\tau}_3)\hat{M} = \hat{1}_2 + \hat{\tau}_3. \quad (4.34)$$

If the inverse expressions of Eqs. (4.6) and (4.12) are used, the matrix condition takes the form

$$(\hat{M}^{-1})^T(\hat{1}_2 + \hat{\tau}_3)\hat{M}^{-1} = \hat{1}_2 + \hat{\tau}_3. \quad (4.35)$$

Substituting the matrix $\hat{M}$ from Eq. (4.7) into Eq. (4.34) yields

$$(m_3 + \sin(\mu))(m_0 + \cos(\mu)) = 0, \quad (4.36)$$

$$(m_3 + \sin(\mu))^2 = (m_1)^2, \quad (4.37)$$

and

$$(m_0 + \cos(\mu))^2 = 0. \quad (4.38)$$

Similarly, substituting $\hat{M}^{-1}$ into Eq. (4.35) leads to

$$(-m_3 + \sin(\mu))(m_0 + \cos(\mu)) = 0, \quad (4.39)$$

$$(-m_3 + \sin(\mu))^2 = (m_1)^2, \quad (4.40)$$

and

$$(m_0 + \cos(\mu))^2 = 0, \quad (4.41)$$

where Eq. (4.41) coincides with Eq. (4.38). These explicit constraint relations are also subject to $(m_0)^2 + (m_1)^2 + (m_3)^2 = 1$ with $\mu \in [0, \pi)$. Accordingly, Eq. (4.33) is satisfied only when Eqs. (4.36)–(4.40) hold simultaneously.

Under these constraints, the Dirichlet BC is the unique confining solution of Eq. (4.33). For $m_1 = 0$, Eqs. (4.37) and (4.40) force $m_3 = 0$ and $\mu = 0$. Then Eqs. (4.36) and (4.39) are automatically satisfied, and Eq. (4.38) fixes $m_0 = -1$, which corresponds precisely to the Dirichlet BC. Hence, among the confining BCs that satisfy $[\text{Im}(\psi(c\hat{p}\psi))]|_a^b = 0$ (Eq. (4.17)), only the Dirichlet BC (i) can also fulfill $[\text{Im}(\psi(\hat{E}\psi))]|_a^b = 0$.

An analogous calculation shows that the nonconfining BCs satisfying $[\text{Im}(\psi(\hat{E}\psi))]|_a^b = 0$ form the following one-parameter family:

$$\begin{bmatrix} \psi(b, t) \\ \lambda\psi_x(b, t) \end{bmatrix} = \pm \begin{bmatrix} 1 & 0 \\ 2\cot(\mu) & 1 \end{bmatrix} \begin{bmatrix} \psi(a, t) \\ \lambda\psi_x(a, t) \end{bmatrix}, \quad \mu \in (0, \pi). \quad (4.42)$$

Indeed, Eq. (4.38) gives $m_0 = -\cos(\mu)$, while Eqs. (4.37) and (4.40) give $m_3 = 0$ and $(m_1)^2 = \sin^2(\mu)$ ($\neq 0$). Consequently, Eqs. (4.36) and (4.39) are automatically satisfied, leading precisely to Eq. (4.42). In addition, among the nonconfining BCs that satisfy $[\text{Im}(\psi(c\hat{p}\psi))]|_a^b = 0$, i.e., within the rotation subfamily (ix), only the periodic (vii) and antiperiodic (viii) BCs can also fulfill $[\text{Im}(\psi(\hat{E}\psi))]|_a^b = 0$, because the rotation subfamily requires $\mu = \pi/2$, and imposing this value in Eq. (4.42) yields precisely these two cases.

CHAPTER V

CONCLUSIONS

5.1 Summary of the main results

This thesis studies a massive first-quantized 1D KFGM particle on a finite interval. The central difficulty is that the usual KFG density-current pair $\{\varrho, j\}$ becomes trivial under the Majorana condition: both ϱ and j vanish for real or purely imaginary KFG wavefunctions. Consequently, j cannot distinguish an impermeable wall from a permeable one. This problem is resolved by using the nontrivial energy current density j_E , together with its energy density ϱ_E .

The FV Hamiltonian $\hat{h}$ was treated as a pseudo self-adjoint operator in the indefinite $\hat{\tau}_3$ -space/Krein space. The acceptable BCs are precisely those that make the boundary term vanish and hence enforce the equality of domains $\mathcal{D}(\hat{h}) = \mathcal{D}(\hat{h}_{\text{adj}})$. This domain condition implies the equality $j_E(a, t) = j_E(b, t)$ at the ends of the interval for all acceptable KFGM BCs. If the Lorentz scalar potential does not explicitly depend on time, the pair $\{\varrho_E, j_E\}$ also gives a conserved global quantity through $\int_{\Omega} \varrho_E dx = \text{const.}$

The Majorana condition reduces the general four-parameter complex KFG BC family to the three-parameter general set of BCs for the 1D KFGM particle by imposing $m_2 = 0$. Within this family, the condition $m_1 = 0$ identifies the impermeable or confining subfamily, for which $j_E(a, t) = j_E(b, t) = 0$. The case $m_1 \neq 0$ gives permeable BCs, for which j_E takes equal values at the two ends of the interval but need not vanish. In this precise sense, j_E is the appropriate energy current density that characterizes the BCs for the 1D KFGM particle.

The standard energy current density $\tilde{j}_E = cT^1_0$ was kept as a comparison current. It is always real, but it is incomplete for BC characterization because the equality

$\tilde{j}_E(b, t) = \tilde{j}_E(a, t)$ requires an additional boundary term cancellation. Only four common confining BCs, namely Dirichlet, Neumann, and two mixed BCs, together with a one-parameter nonconfining family, make the standard pair $\{T^0_0, cT^1_0\}$ equally satisfactory. For all acceptable BCs, only j_E provides the complete characterization of impermeable and permeable BCs, while ρ_E is its associated energy density in the corresponding continuity equation.

5.2 Physical interpretation

The result is not a new condensed-matter or QFT particle model, but a first-quantized way to select physically consistent BCs for a strictly neutral scalar particle on a finite interval. The current j_E measures the relevant energy flow at the ends of the interval. Impermeable BCs force this flow to vanish at the walls, while permeable BCs allow equal values of this flow at the ends of the interval, with the common value not necessarily vanishing, in a manner compatible with the pseudo self-adjoint domain of $\hat{h}$.

Some representative BCs admit familiar physical readings. Dirichlet BCs, $\psi(a, t) = \psi(b, t) = 0$, describe walls at which the one-component wavefunction vanishes, while Neumann BCs, $\psi_x(a, t) = \psi_x(b, t) = 0$, impose vanishing spatial derivative at both walls. Mixed BCs impose one of these restrictions at one end and the other restriction at the opposite end, thereby representing asymmetric confining walls. These BCs are standard members of the pseudo self-adjoint BC catalog for the 1D KFG/FV system [11]. Periodic BCs identify the two ends of the interval by requiring $\psi(b, t) = \psi(a, t)$ and $\psi_x(b, t) = \psi_x(a, t)$; antiperiodic BCs give the analogous identification with opposite signs, $\psi(b, t) = -\psi(a, t)$ and $\psi_x(b, t) = -\psi_x(a, t)$. Robin-type BCs interpolate between value-type and derivative-type restrictions at the walls and therefore provide a flexible way to model partially restrictive boundary behavior [11, 20]. These examples illustrate that the BC

catalog is not merely algebraic: different admissible BCs encode different physical models of the interval walls.

The resulting characterization can serve as input for later studies of boundary QFT, Casimir-type systems, point interactions, and related scalar-field boundary problems, although those applications require additional formalisms.

5.3 Limitations

The analysis is deliberately restricted. First, it is first-quantized; it does not include field quantization, vacuum mode sums, or particle creation. This restriction is consistent with the role of relativistic quantum mechanics described by Grandy: one can use it to examine how far the behavior of stable particles and their interactions can be understood before quantized fields are introduced [37]. Accordingly, the analysis remains within finite interval first-quantized relativistic wave mechanics and does not construct field-theoretic Majorana modes. Second, the model is one-dimensional and based on a finite interval. Third, the Lorentz interaction is a real scalar potential. Fourth, the standard FV variables used here assume that $m \neq 0$; consequently, the massless/CFT limit is not treated in the thesis. Fifth, no full condensed-matter mapping is claimed: Kitaev-chain and topological-superconductor Majorana modes are second-quantized many-body quasiparticles, whereas this work studies a first-quantized scalar KFGM particle.

The thesis also does not provide a full spectral analysis for all acceptable BCs. Spectra and eigenfunctions for particular BCs are useful illustrations, but the main result is the characterization of BCs by the values of j_E at the two ends of the interval. Likewise, no full MIT bag model comparison or complete P , T , C , and PT analysis is attempted, because these constitute separate projects.

5.4 Future directions

Several extensions are natural. A Casimir analysis requires second quantization and vacuum mode summation, not merely the addition of a zeta-function calculation to the present first-quantized derivation. The punctured real line

$\Omega = \mathbb{R} \setminus \{0\} = \mathbb{R}^+ \cup \mathbb{R}^-$ is a natural continuation of the interval analysis, where $a \rightarrow 0^+$ and $b \rightarrow 0^-$, but a full point-interaction comparison with delta-type potentials requires a separate treatment. A genuine second-quantized formulation could study mode decompositions, vacuum energy, and particle creation.

A higher-dimensional extension is also nontrivial. In $(3 + 1)$ dimensions, BCs at the ends of the interval become surface BCs, the finite-dimensional boundary matrix structure becomes more complicated, and the flux characterization must be reformulated on the boundary of a spatial region. Finally, the massless limit requires a generalized FV/CFFV formalism because the standard FV variables contain factors singular at $m = 0$. These topics therefore remain outside the scope of the present thesis.



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APPENDIX A DEMONSTRATION OF EQ. (2.3)

Recall the definition of the formal generalized adjoint of the Hamiltonian operator:

$$\hat{h}_{\text{adj}} \equiv \hat{\tau}_3 \hat{h}^\dagger \hat{\tau}_3. \quad (\text{A1})$$

Substituting the Hamiltonian in Eq. (2.1) into the latter expression, namely,

$$\hat{h}_{\text{adj}} = \hat{\tau}_3 \left(\frac{\hat{p}^2}{2m} (\hat{\tau}_3 + i\hat{\tau}_2) + mc^2 \hat{\tau}_3 + S(\hat{\tau}_3 + i\hat{\tau}_2) \right)^\dagger \hat{\tau}_3, \quad (\text{A2})$$

we obtain

$$\hat{h}_{\text{adj}} = \hat{\tau}_3 \left(\frac{\hat{p}^2}{2m} (\hat{\tau}_3 - i\hat{\tau}_2) + mc^2 \hat{\tau}_3 + S(\hat{\tau}_3 - i\hat{\tau}_2) \right) \hat{\tau}_3. \quad (\text{A3})$$

Rewriting the latter expression by positioning the Pauli matrices properly in Eq. (A3), that is,

$$\hat{h}_{\text{adj}} = \hat{\tau}_3 \frac{\hat{p}^2}{2m} (\hat{\tau}_3 - i\hat{\tau}_2) \hat{\tau}_3 + \hat{\tau}_3 mc^2 \hat{\tau}_3 \hat{\tau}_3 + \hat{\tau}_3 S(\hat{\tau}_3 - i\hat{\tau}_2) \hat{\tau}_3, \quad (\text{A4})$$

we can finally write

$$\hat{h}_{\text{adj}} = \frac{\hat{p}^2}{2m} (\hat{\tau}_3 + i\hat{\tau}_2) + mc^2 \hat{\tau}_3 + S(\hat{\tau}_3 + i\hat{\tau}_2). \quad (\text{A5})$$

Thus, the action of $\hat{h}_{\text{adj}}$ is the same as that of $\hat{h}$.

APPENDIX B DEMONSTRATION OF EQ. (2.4)

Recall the definition of the formal generalized adjoint of the Hamiltonian operator:

$$\hat{h}_{\text{adj}} = \hat{\tau}_3 \hat{h}^\dagger \hat{\tau}_3. \quad (\text{B1})$$

Using the definition of the inner product given in Eq. (2.5), i.e.,

$$\langle\langle \hat{h}_{\text{adj}} \Psi, \Phi \rangle\rangle = \int_{\Omega} dx (\hat{\tau}_3 \hat{h}^\dagger \hat{\tau}_3 \Psi)^\dagger \hat{\tau}_3 \Phi, \quad (\text{B2})$$

and developing the integrand in the latter integral, we can write

$$\langle\langle \hat{h}_{\text{adj}} \Psi, \Phi \rangle\rangle = \int_{\Omega} dx \Psi^\dagger \hat{\tau}_3 \hat{h} \hat{\tau}_3 \Phi. \quad (\text{B3})$$

Thus,

$$\langle\langle \hat{h}_{\text{adj}} \Psi, \Phi \rangle\rangle = \int_{\Omega} dx \Psi^\dagger \hat{\tau}_3 \hat{h} \Phi. \quad (\text{B4})$$

The latter integral is $\langle\langle \Psi, \hat{h} \Phi \rangle\rangle$, namely,

$$\langle\langle \hat{h}_{\text{adj}} \Psi, \Phi \rangle\rangle = \langle\langle \Psi, \hat{h} \Phi \rangle\rangle. \quad (\text{B5})$$

This is precisely Eq. (2.4).

APPENDIX C PSEUDO-HERMITICITY AND ITS IMPLICATIONS

C.1 The mean value of $\hat{h}$ in the state Ψ

Equation (2.7) is given by

$$\langle\langle \hat{h}\Psi, \Phi \rangle\rangle = \langle\langle \Psi, \hat{h}\Phi \rangle\rangle. \quad (C1)$$

Setting $\Phi = \Psi$ gives

$$\langle\langle \hat{h}\Psi, \Psi \rangle\rangle = \langle\langle \Psi, \hat{h}\Psi \rangle\rangle. \quad (C2)$$

Using the property $\langle\langle \Psi, \Phi \rangle\rangle = \langle\langle \Phi, \Psi \rangle\rangle^*$, we can write the left-hand side of Eq. (C2) as follows:

$$\langle\langle \hat{h}\Psi, \Psi \rangle\rangle = \langle\langle \Psi, \hat{h}\Psi \rangle\rangle^*. \quad (C3)$$

This confirms that

$$\langle\langle \Psi, \hat{h}\Psi \rangle\rangle = \langle\langle \Psi, \hat{h}\Psi \rangle\rangle^*. \quad (C4)$$

The latter result establishes that $\langle\langle \Psi, \hat{h}\Psi \rangle\rangle \equiv \langle\hat{h}\rangle_\Psi$ is real. Because $\hat{h}\Psi = \hat{E}\Psi$ on-shell, $\langle\langle \Psi, \hat{h}\Psi \rangle\rangle = \langle\langle \Psi, \hat{E}\Psi \rangle\rangle$, so the on-shell energy expectation value is real.

C.2 Reality of the eigenvalues of the Hamiltonian operator

The mean value of the Hamiltonian is defined as

$$\langle\langle \hat{h} \rangle\rangle_\Psi \equiv \langle\langle \Psi, \hat{h}\Psi \rangle\rangle \in \mathbb{R}. \quad (C5)$$

On-shell, $\langle\langle \Psi, \hat{h}\Psi \rangle\rangle = \langle\langle \Psi, \hat{E}\Psi \rangle\rangle \in \mathbb{R}$. For an eigenstate satisfying $\hat{h}\Psi = E\Psi$, we obtain

$$\langle\langle \Psi, \hat{h}\Psi \rangle\rangle = \langle\langle \Psi, E\Psi \rangle\rangle, \quad (C6)$$

that is,

$$\langle\langle \Psi, \hat{h}\Psi \rangle\rangle = E\langle\langle \Psi, \Psi \rangle\rangle. \quad (C7)$$

Because $\langle\langle \Psi, \hat{h}\Psi \rangle\rangle$ is real and $\langle\langle \Psi, \Psi \rangle\rangle \in \mathbb{R}$, it follows that E is also real.

C.3 Orthogonality of eigenfunctions of $\hat{h}$ with different eigenvalues

Writing the eigenvalue equations $\hat{h}\Psi_1 = E_1\Psi_1$ and $\hat{h}\Psi_2 = E_2\Psi_2$, with $E_1 \neq E_2$, leads to the relations

$$\langle\langle \Psi_1, \hat{h}\Psi_2 \rangle\rangle = \langle\langle \Psi_1, E_2\Psi_2 \rangle\rangle = E_2\langle\langle \Psi_1, \Psi_2 \rangle\rangle \quad (\text{C8})$$

and

$$\langle\langle \Psi_1, \hat{h}\Psi_2 \rangle\rangle = \langle\langle \hat{h}\Psi_1, \Psi_2 \rangle\rangle = E_1\langle\langle \Psi_1, \Psi_2 \rangle\rangle. \quad (\text{C9})$$

From Eqs. (C8) and (C9), we obtain

$$(E_2 - E_1)\langle\langle \Psi_1, \Psi_2 \rangle\rangle = 0. \quad (\text{C10})$$

Because $E_1 \neq E_2$, it follows that $\langle\langle \Psi_1, \Psi_2 \rangle\rangle = 0$, which confirms that Ψ_1 and Ψ_2 are pseudo-orthogonal. Thus, as a consequence of Eq. (2.7), i.e., $\hat{h} = \hat{h}_{\text{adj}}$, we obtain properties that are analogous to those satisfied by self-adjoint operators in the usual sense.

APPENDIX D EXAMPLE IN WHICH THE DOMAINS OF THE HAMILTONIAN AND ITS GENERALIZED HERMITIAN CONJUGATE ARE DIFFERENT

The boundary term in Eq. (2.6) is given by

$$\text{B.T.} = -\frac{\hbar^2}{2m} \frac{1}{2} \left[((\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi - ((\hat{\tau}_3 + i\hat{\tau}_2)\Psi)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi_x \right] \Big|_a^b, \quad (\text{D1})$$

where $\Psi \in \mathcal{D}(\hat{h}_{\text{adj}})$ and $\Phi \in \mathcal{D}(\hat{h})$. Here, $[f]_a^b \equiv f(b, t) - f(a, t)$, and $\Psi_x \equiv \partial\Psi/\partial x$, etc.

Neglecting the constant term $-\frac{\hbar^2}{2m} \frac{1}{2}$ in Eq. (D1) permits us to write the following expression:

$$\text{B.T.} = \left[((\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi - ((\hat{\tau}_3 + i\hat{\tau}_2)\Psi)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi_x \right] \Big|_a^b. \quad (\text{D2})$$

Defining $\hat{A} \equiv \hat{\tau}_3 + i\hat{\tau}_2$, the expression becomes

$$\text{B.T.} = \left[(\hat{A}\Psi_x)^\dagger \hat{A}\Phi - (\hat{A}\Psi)^\dagger \hat{A}\Phi_x \right] \Big|_a^b. \quad (\text{D3})$$

Further simplification yields the following boundary expression, with the time dependence displayed explicitly.

$$\begin{aligned} \text{B.T.} = & \left[(\hat{A}\Psi_x)^\dagger(b, t) \hat{A}\Phi(b, t) - (\hat{A}\Psi)^\dagger(b, t) \hat{A}\Phi_x(b, t) \right] \\ & - \left[(\hat{A}\Psi_x)^\dagger(a, t) \hat{A}\Phi(a, t) - (\hat{A}\Psi)^\dagger(a, t) \hat{A}\Phi_x(a, t) \right]. \end{aligned} \quad (\text{D4})$$

To ensure that $\text{B.T.} = 0$, the following BCs are imposed on $\Phi \in \mathcal{D}(\hat{h})$:

$$\begin{aligned} (\hat{A}\Phi)(a, t) &= (\hat{A}\Phi)(b, t) = 0, \\ (\hat{A}\Phi_x)(a, t) &= (\hat{A}\Phi_x)(b, t) = 0. \end{aligned} \quad \} \in \mathcal{D}(\hat{h}). \quad (\text{D5})$$

With these BCs, $\text{B.T.} = 0$ is obtained. However, it is not necessary for any BCs to be imposed on $\Psi \in \mathcal{D}(\hat{h}_{\text{adj}})$. As a consequence, $\mathcal{D}(\hat{h}) \subsetneq \mathcal{D}(\hat{h}_{\text{adj}})$. This relation is illustrated below:

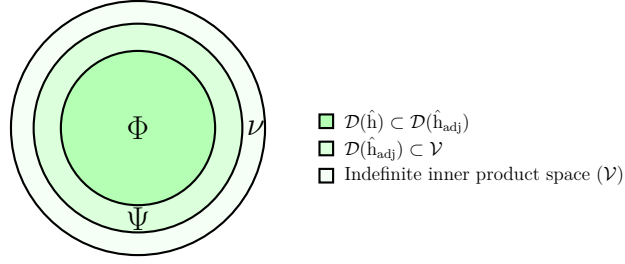


Figure 4 Indefinite inner product space with domains.

APPENDIX E EXAMPLE IN WHICH THE DOMAINS OF THE HAMILTONIAN AND ITS GENERALIZED HERMITIAN CONJUGATE ARE EQUAL

To demonstrate that the equality $\mathcal{D}(\hat{h}_{\text{adj}}) = \mathcal{D}(\hat{h})$ can also be realized, we can follow the procedure in Ref. [11] to equalize the domains. Thus, we start from the following relation:

$$\langle\langle \Psi, \hat{h}\Phi \rangle\rangle = \langle\langle \hat{h}_{\text{adj}}\Psi, \Phi \rangle\rangle + f[\Psi, \Phi]. \quad (\text{E1})$$

The boundary term for $f[\Psi, \Phi]$ is given by

$$f[\Psi, \Phi] = \frac{\hbar^2}{2m} \frac{1}{2} \left[((\hat{\tau}_3 + i\hat{\tau}_2)\Psi_x)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi - ((\hat{\tau}_3 + i\hat{\tau}_2)\Psi)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi_x \right] \Big|_a^b. \quad (\text{E2})$$

Using the relations

$$\phi_1 + \phi_2 = \phi \quad \text{and} \quad \psi_1 + \psi_2 = \psi, \quad (\text{E3})$$

and recalling that

$$\Phi = [\phi_1 \ \phi_2]^\text{T}, \quad \Psi = [\psi_1 \ \psi_2]^\text{T},$$

the boundary term must be zero and can be rewritten as follows:

$$f[\Psi, \Phi] = \frac{\hbar^2}{2m} [\psi_x^* \phi - \psi^* \phi_x] \Big|_a^b. \quad (\text{E4})$$

First, let us rewrite the boundary term with a parameter λ for dimensional consistency:

$$\begin{aligned}\lambda \frac{2m}{\hbar^2} f[\Psi, \Phi] &= [\phi \lambda \psi_x^* - \psi^* \lambda \phi_x] \Big|_a^b \\ &= [\phi(b, t) \lambda \psi_x^*(b, t) - \psi^*(b, t) \lambda \phi_x(b, t)] \\ &\quad - [\phi(a, t) \lambda \psi_x^*(a, t) - \psi^*(a, t) \lambda \phi_x(a, t)] = 0.\end{aligned}\tag{E5}$$

Using the following identity for complex numbers z_1, z_2, z_3, z_4 :

$$z_1 z_2^* - z_3^* z_4 = \frac{i}{2} [(z_1 + i z_4)(z_3 + i z_2)^* - (z_1 - i z_4)(z_3 - i z_2)^*], \tag{E6}$$

the result in Eq. (E5) takes the form

$$\begin{aligned}\lambda \frac{2m}{\hbar^2} f[\Psi, \Phi] &= \frac{i}{2} \begin{bmatrix} \psi(b, t) + i \lambda \psi_x(b, t) \\ \psi(a, t) - i \lambda \psi_x(a, t) \end{bmatrix}^\dagger \begin{bmatrix} \phi(b, t) + i \lambda \phi_x(b, t) \\ \phi(a, t) - i \lambda \phi_x(a, t) \end{bmatrix} \\ &\quad - \frac{i}{2} \begin{bmatrix} \psi(b, t) - i \lambda \psi_x(b, t) \\ \psi(a, t) + i \lambda \psi_x(a, t) \end{bmatrix}^\dagger \begin{bmatrix} \phi(b, t) - i \lambda \phi_x(b, t) \\ \phi(a, t) + i \lambda \phi_x(a, t) \end{bmatrix} = 0.\end{aligned}\tag{E7}$$

We impose the following general set of BCs for the one-component wavefunction ϕ related to $\Phi \in \mathcal{D}(\hat{h})$:

$$\begin{bmatrix} \phi(b, t) + i \lambda \phi_x(b, t) \\ \phi(a, t) - i \lambda \phi_x(a, t) \end{bmatrix} = \hat{N} \begin{bmatrix} \phi(b, t) - i \lambda \phi_x(b, t) \\ \phi(a, t) + i \lambda \phi_x(a, t) \end{bmatrix}, \tag{E8}$$

where $\hat{N}$ is an arbitrary complex matrix. Substituting Eq. (E8) into Eq. (E7), we obtain the following set of BCs for the one-component wavefunction ψ related to $\Psi \in \mathcal{D}(\hat{h}_{\text{adj}})$:

$$\begin{bmatrix} \psi(b, t) - i \lambda \psi_x(b, t) \\ \psi(a, t) + i \lambda \psi_x(a, t) \end{bmatrix} = \hat{N}^\dagger \begin{bmatrix} \psi(b, t) + i \lambda \psi_x(b, t) \\ \psi(a, t) - i \lambda \psi_x(a, t) \end{bmatrix}. \tag{E9}$$

However, ψ must satisfy the same BC as ϕ , namely,

$$\begin{bmatrix} \psi(b, t) + i \lambda \psi_x(b, t) \\ \psi(a, t) - i \lambda \psi_x(a, t) \end{bmatrix} = \hat{N} \begin{bmatrix} \psi(b, t) - i \lambda \psi_x(b, t) \\ \psi(a, t) + i \lambda \psi_x(a, t) \end{bmatrix}. \tag{E10}$$

Substituting Eq. (E10) into Eq. (E9), we obtain the following relation:

$$\begin{bmatrix} \psi(b, t) + i\lambda\psi_x(b, t) \\ \psi(a, t) - i\lambda\psi_x(a, t) \end{bmatrix} = \hat{N}\hat{N}^\dagger \begin{bmatrix} \psi(b, t) + i\lambda\psi_x(b, t) \\ \psi(a, t) - i\lambda\psi_x(a, t) \end{bmatrix}. \quad (\text{E11})$$

This implies that $\hat{N}$ must be a unitary matrix, i.e., $\hat{N}\hat{N}^\dagger = \hat{1}$. Therefore, the most general set of BCs for the function ϕ related to $\Phi \in \mathcal{D}(\hat{h})$ can be written as follows:

$$\begin{bmatrix} \phi(b, t) - i\lambda\phi_x(b, t) \\ \phi(a, t) + i\lambda\phi_x(a, t) \end{bmatrix} = \hat{U} \begin{bmatrix} \phi(b, t) + i\lambda\phi_x(b, t) \\ \phi(a, t) - i\lambda\phi_x(a, t) \end{bmatrix}, \quad (\text{E12a})$$

and the most general set of BCs for the function ψ related to $\Psi \in \mathcal{D}(\hat{h}_{\text{adj}})$ can be written as follows:

$$\begin{bmatrix} \psi(b, t) - i\lambda\psi_x(b, t) \\ \psi(a, t) + i\lambda\psi_x(a, t) \end{bmatrix} = \hat{U} \begin{bmatrix} \psi(b, t) + i\lambda\psi_x(b, t) \\ \psi(a, t) - i\lambda\psi_x(a, t) \end{bmatrix}, \quad (\text{E12b})$$

where $\hat{U} = \hat{N}^{-1}$ is unitary. Because the BCs are the same for both domains, it has been algebraically demonstrated that $\mathcal{D}(\hat{h}_{\text{adj}}) = \mathcal{D}(\hat{h})$, and consequently $\hat{h} = \hat{h}_{\text{adj}}$, making $\hat{h}$ a pseudo self-adjoint operator, as illustrated below:

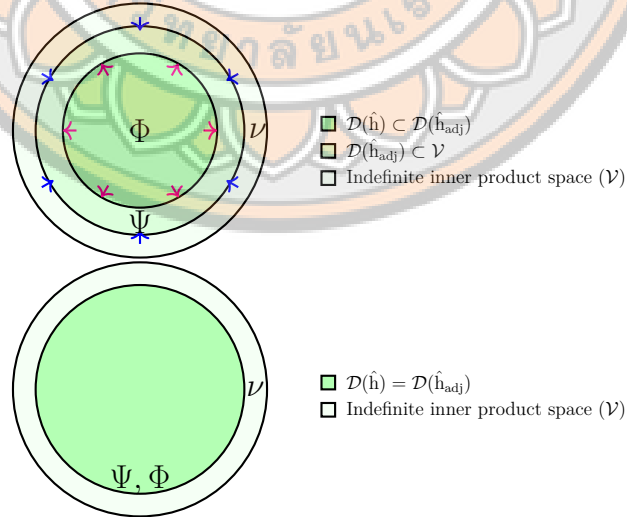


Figure 5 Illustration of the equalization of domains. (a) Initial stage with unequal domains for $\hat{h}$ and $\hat{h}_{\text{adj}}$. (b) Final stage where $\mathcal{D}(\hat{h}) = \mathcal{D}(\hat{h}_{\text{adj}})$.

APPENDIX F STANDARD ENERGY-MOMENTUM TENSOR AND ENERGY CURRENT CONSTRUCTIONS IN (1 + 1) DIMENSIONS

F.1 Lagrangian density and Euler-Lagrange equations

The covariant one-component Lagrangian density used for the standard KFG equation with a real Lorentz scalar interaction $S = S(x, t)$ is

$$\mathcal{L} = \frac{\hbar^2}{2m} \left[g^{\mu\nu} (\partial_\mu \psi^*) (\partial_\nu \psi) - \frac{m^2 c^2}{\hbar^2} \psi^* \psi - \frac{2mS}{\hbar^2} \psi^* \psi \right], \quad (\text{F1})$$

where $\mu, \nu, \dots = 0, 1$, $g^{\mu\nu} = \text{diag}(1, -1)$, $\partial_0 = \partial/\partial(ct)$, and $\partial_1 = \partial/\partial x$, as usual [16]. The fields ψ and ψ^* are treated as independent fields in the Euler-Lagrange calculation. Thus

$$\partial_\alpha \left[\frac{\partial \mathcal{L}}{\partial(\partial_\alpha \psi)} \right] - \frac{\partial \mathcal{L}}{\partial \psi} = 0, \quad \partial_\alpha \left[\frac{\partial \mathcal{L}}{\partial(\partial_\alpha \psi^*)} \right] - \frac{\partial \mathcal{L}}{\partial \psi^*} = 0. \quad (\text{F2})$$

For the first equation in Eq. (F2),

$$\frac{\partial \mathcal{L}}{\partial(\partial_\alpha \psi)} = \frac{\hbar^2}{2m} g^{\mu\alpha} \partial_\mu \psi^*, \quad \frac{\partial \mathcal{L}}{\partial \psi} = -\frac{\hbar^2}{2m} \left[\frac{m^2 c^2}{\hbar^2} \psi^* + \frac{2mS}{\hbar^2} \psi^* \right], \quad (\text{F3})$$

which gives

$$\frac{\hbar^2}{2m} \left[g^{\mu\alpha} \partial_\alpha \partial_\mu \psi^* + \frac{m^2 c^2}{\hbar^2} \psi^* + \frac{2mS}{\hbar^2} \psi^* \right] = 0. \quad (\text{F4})$$

Similarly, the second equation in Eq. (F2) gives

$$\frac{\hbar^2}{2m} \left[g^{\mu\alpha} \partial_\alpha \partial_\mu \psi + \frac{m^2 c^2}{\hbar^2} \psi + \frac{2mS}{\hbar^2} \psi \right] = 0. \quad (\text{F5})$$

Multiplying Eq. (F5) by $-2mc^2$ and using $i\hbar c \partial_0 = \hat{E}$ and $-i\hbar \partial_1 = \hat{p}$ gives

$$[\hat{E}^2 - (c\hat{p})^2 - (mc^2)^2 - 2mc^2 S] \psi = 0. \quad (\text{F6})$$

Thus the scalar interaction used in this appendix is the same scalar interaction used in the main text.

F.2 A direct FV Lagrangian density

This subsection gives a derivation of the FV equations from a first-order Lagrangian density for a real Lorentz scalar interaction $S = S(x, t)$. The mass is assumed to be nonzero, $m \neq 0$, which ensures the equivalence between the standard KFG and FV formulations. When $S = 0$, equivalently when the Lorentz scalar interaction is absent, the construction reduces to the standard interaction-free FV formulation of the spin-zero KFG equation, as presented, for example, in Greiner's treatment of the FV representation, especially in Example 1.7 of Section 1.8 [16]. A related FV Lagrangian construction was also given by Darewych for the $\lambda(\varphi^*\varphi)^2$ field theory [38]. The present construction is simpler: it contains only a real-valued Lorentz scalar interaction S , not a quartic self-interaction. The derivation below keeps S arbitrary, real, and not necessarily independent of time.

F.2.1 FV-adjoint row field and independent variables

The FV-adjoint row field is $\bar{\Psi}$, namely,

$$\bar{\Psi} \equiv \Psi^\dagger \hat{\tau}_3, \quad \text{where} \quad \Psi = \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} \quad \text{and} \quad \bar{\Psi} = [\psi_1^* \quad -\psi_2^*]. \quad (\text{F7})$$

The two fields Ψ and $\bar{\Psi}$ are treated as independent variational fields in the Euler-Lagrange variation.

F.2.2 Zero scalar interaction and total-derivative rearrangement

It is useful first to record how the row-field Lagrangian density is obtained from the interaction-free FV Lagrangian density. When the Lorentz scalar interaction is absent, $S = 0$, one may start from the Lagrangian density

$$\mathcal{L}_{0,\Psi} = \bar{\Psi} \hat{E} \Psi - \frac{\hbar^2}{2m} (\partial_x \bar{\Psi})(\hat{\tau}_3 + i\hat{\tau}_2)(\partial_x \Psi) - mc^2 \bar{\Psi} \hat{\tau}_3 \Psi, \quad \hat{E} \Psi = i\hbar \partial_t \Psi. \quad (\text{F8})$$

The time-derivative term in Eq. (F8) satisfies the product-rule identity for the FV

row and column fields,

$$\hat{E}(\bar{\Psi}\Psi) = (\hat{E}\bar{\Psi})\Psi + \bar{\Psi}(\hat{E}\Psi), \quad \hat{E} = i\hbar\partial_t$$

Therefore,

$$\begin{aligned} \bar{\Psi}(\hat{E}\Psi) &= \hat{E}(\bar{\Psi}\Psi) - (\hat{E}\bar{\Psi})\Psi \\ &= i\hbar\partial_t(\bar{\Psi}\Psi) - i\hbar(\partial_t\bar{\Psi})\Psi. \end{aligned} \quad (F9)$$

Accordingly, up to the total time derivative $i\hbar\partial_t(\bar{\Psi}\Psi)$, the interaction-free Lagrangian density can be represented in the row-field form

$$\mathcal{L}_{0,\bar{\Psi}} = -i\hbar(\partial_t\bar{\Psi})\Psi - \frac{\hbar^2}{2m}(\partial_x\bar{\Psi})(\hat{\tau}_3 + i\hat{\tau}_2)(\partial_x\Psi) - mc^2\bar{\Psi}\hat{\tau}_3\Psi. \quad (F10)$$

The Lorentz scalar interaction is included in the Lagrangian density by adding the term

$$-\bar{\Psi}(\hat{\tau}_3 + i\hat{\tau}_2)S\Psi. \quad (F11)$$

F.2.3 Row-field variation and the column FV equation

We use the following Lagrangian density when the independent variational variables associated with the row field are $\bar{\Psi}$, $\partial_t\bar{\Psi}$, and $\partial_x\bar{\Psi}$:

$$\mathcal{L}_{\bar{\Psi}} = -i\hbar(\partial_t\bar{\Psi})\Psi - \frac{\hbar^2}{2m}(\partial_x\bar{\Psi})(\hat{\tau}_3 + i\hat{\tau}_2)(\partial_x\Psi) - mc^2\bar{\Psi}\hat{\tau}_3\Psi - \bar{\Psi}(\hat{\tau}_3 + i\hat{\tau}_2)S\Psi. \quad (F12)$$

The Euler-Lagrange equation associated with the row field $\bar{\Psi}$ is written as

$$\partial_t\left[\frac{\partial\mathcal{L}_{\bar{\Psi}}}{\partial(\partial_t\bar{\Psi})}\right] + \partial_x\left[\frac{\partial\mathcal{L}_{\bar{\Psi}}}{\partial(\partial_x\bar{\Psi})}\right] - \frac{\partial\mathcal{L}_{\bar{\Psi}}}{\partial\bar{\Psi}} = 0. \quad (F13)$$

The required derivatives of the Lagrangian density are

$$\begin{aligned} \frac{\partial\mathcal{L}_{\bar{\Psi}}}{\partial(\partial_t\bar{\Psi})} &= -i\hbar\Psi, & \partial_t\left[\frac{\partial\mathcal{L}_{\bar{\Psi}}}{\partial(\partial_t\bar{\Psi})}\right] &= -i\hbar\partial_t\Psi, \\ \frac{\partial\mathcal{L}_{\bar{\Psi}}}{\partial(\partial_x\bar{\Psi})} &= -\frac{\hbar^2}{2m}(\hat{\tau}_3 + i\hat{\tau}_2)\partial_x\Psi, & \partial_x\left[\frac{\partial\mathcal{L}_{\bar{\Psi}}}{\partial(\partial_x\bar{\Psi})}\right] &= -\frac{\hbar^2}{2m}(\hat{\tau}_3 + i\hat{\tau}_2)\partial_x^2\Psi, \\ \frac{\partial\mathcal{L}_{\bar{\Psi}}}{\partial\bar{\Psi}} &= -mc^2\hat{\tau}_3\Psi - (\hat{\tau}_3 + i\hat{\tau}_2)S\Psi. \end{aligned} \quad (F14)$$

Substitution of the derivative relations in Eq. (F14) into the Euler-Lagrange equation in Eq. (F13) gives

$$-i\hbar \partial_t \Psi - \frac{\hbar^2}{2m}(\hat{\tau}_3 + i\hat{\tau}_2)\partial_x^2 \Psi + mc^2 \hat{\tau}_3 \Psi + (\hat{\tau}_3 + i\hat{\tau}_2)S\Psi = 0. \quad (\text{F15})$$

Using $\hat{p} = -i\hbar \partial_x$ and $\hat{E} = i\hbar \partial_t$, the equation can be written in operator form as

$$\left[(\hat{\tau}_3 + i\hat{\tau}_2) \frac{\hat{p}^2}{2m} + mc^2 \hat{\tau}_3 + (\hat{\tau}_3 + i\hat{\tau}_2)S \right] \Psi = \hat{E}\Psi. \quad (\text{F16})$$

Therefore, the corresponding FV Hamiltonian is

$$\hat{h} = (\hat{\tau}_3 + i\hat{\tau}_2) \frac{\hat{p}^2}{2m} + mc^2 \hat{\tau}_3 + (\hat{\tau}_3 + i\hat{\tau}_2)S, \quad \hat{h}\Psi = \hat{E}\Psi. \quad (\text{F17})$$

Thus, the Euler-Lagrange equation associated with the row field $\bar{\Psi}$ yields the FV equation for the column field Ψ .

F.2.4 Column-field variation and the FV-adjoint row equation

We use the following Lagrangian density when the independent variational variables associated with the column field are Ψ , $\partial_t \Psi$, and $\partial_x \Psi$:

$$\mathcal{L}_\Psi = i\hbar \bar{\Psi}(\partial_t \Psi) - \frac{\hbar^2}{2m}(\partial_x \bar{\Psi})(\hat{\tau}_3 + i\hat{\tau}_2)(\partial_x \Psi) - mc^2 \bar{\Psi} \hat{\tau}_3 \Psi - \bar{\Psi}(\hat{\tau}_3 + i\hat{\tau}_2)S\Psi. \quad (\text{F18})$$

The two Lagrangian densities in Eqs. (F12) and (F18) differ only by the total time derivative already identified in Eq. (F9):

$$\mathcal{L}_\Psi = i\hbar \partial_t(\bar{\Psi}\Psi) + \mathcal{L}_{\bar{\Psi}}. \quad (\text{F18a})$$

This is the standard classical-field-theory use of a total derivative: two Lagrangian densities that differ by a total derivative yield the same Euler-Lagrange equations under the usual fixed-boundary variations.

The Euler-Lagrange equation associated with the column field Ψ is

$$\partial_t \left[\frac{\partial \mathcal{L}_\Psi}{\partial(\partial_t \Psi)} \right] + \partial_x \left[\frac{\partial \mathcal{L}_\Psi}{\partial(\partial_x \Psi)} \right] - \frac{\partial \mathcal{L}_\Psi}{\partial \Psi} = 0. \quad (\text{F19})$$

The required derivatives of the Lagrangian density are

$$\begin{aligned}\frac{\partial \mathcal{L}_\Psi}{\partial(\partial_t \Psi)} &= i\hbar \bar{\Psi}, & \partial_t \left[\frac{\partial \mathcal{L}_\Psi}{\partial(\partial_t \Psi)} \right] &= i\hbar \partial_t \bar{\Psi}, \\ \frac{\partial \mathcal{L}_\Psi}{\partial(\partial_x \Psi)} &= -\frac{\hbar^2}{2m} (\partial_x \bar{\Psi})(\hat{\tau}_3 + i\hat{\tau}_2), & \partial_x \left[\frac{\partial \mathcal{L}_\Psi}{\partial(\partial_x \Psi)} \right] &= -\frac{\hbar^2}{2m} (\partial_x^2 \bar{\Psi})(\hat{\tau}_3 + i\hat{\tau}_2), \\ \frac{\partial \mathcal{L}_\Psi}{\partial \Psi} &= -mc^2 \bar{\Psi} \hat{\tau}_3 - \bar{\Psi}(\hat{\tau}_3 + i\hat{\tau}_2)S.\end{aligned}\quad (\text{F20})$$

Substitution of the derivative relations in Eq. (F20) into the Euler-Lagrange equation in Eq. (F19) gives

$$i\hbar \partial_t \bar{\Psi} - \frac{\hbar^2}{2m} (\partial_x^2 \bar{\Psi})(\hat{\tau}_3 + i\hat{\tau}_2) + mc^2 \bar{\Psi} \hat{\tau}_3 + \bar{\Psi}(\hat{\tau}_3 + i\hat{\tau}_2)S = 0. \quad (\text{F21})$$

Thus, the Euler-Lagrange equation associated with the column field Ψ yields the equation for the FV-adjoint row field $\bar{\Psi}$. This equation is the row-field counterpart of the standard column-field FV equation.

F.2.5 Recovery of the row-field equation by Hermitian conjugation

The row-field equation in Eq. (F21) is also recovered from the column-field equation. Taking the Hermitian conjugate of Eq. (F16) and using $S = S^*$ gives

$$-\frac{\hbar^2}{2m} (\partial_x^2 \Psi^\dagger)(\hat{\tau}_3 - i\hat{\tau}_2) + mc^2 \Psi^\dagger \hat{\tau}_3 + \Psi^\dagger(\hat{\tau}_3 - i\hat{\tau}_2)S = -i\hbar \partial_t \Psi^\dagger. \quad (\text{F22})$$

This coordinate-space derivative form makes explicit that the second spatial derivative acts on the row field $\Psi^\dagger$. Using $\Psi^\dagger = \bar{\Psi} \hat{\tau}_3$, $\partial_t \Psi^\dagger = (\partial_t \bar{\Psi}) \hat{\tau}_3$, $\partial_x^2 \Psi^\dagger = (\partial_x^2 \bar{\Psi}) \hat{\tau}_3$, and

$$\hat{\tau}_3(\hat{\tau}_3 - i\hat{\tau}_2) = (\hat{\tau}_3 + i\hat{\tau}_2)\hat{\tau}_3, \quad \hat{\tau}_3^2 = \hat{1}_2, \quad (\text{F23})$$

one has

$$\begin{aligned}(\partial_x^2 \Psi^\dagger)(\hat{\tau}_3 - i\hat{\tau}_2) &= (\partial_x^2 \bar{\Psi}) \hat{\tau}_3 (\hat{\tau}_3 - i\hat{\tau}_2) \\ &= (\partial_x^2 \bar{\Psi})(\hat{\tau}_3 + i\hat{\tau}_2) \hat{\tau}_3, \\ \Psi^\dagger \hat{\tau}_3 &= \bar{\Psi} \hat{\tau}_3^2 = \bar{\Psi}, \\ \Psi^\dagger(\hat{\tau}_3 - i\hat{\tau}_2)S &= \bar{\Psi} \hat{\tau}_3 (\hat{\tau}_3 - i\hat{\tau}_2)S \\ &= \bar{\Psi}(\hat{\tau}_3 + i\hat{\tau}_2) \hat{\tau}_3 S.\end{aligned}$$

Eq. (F22) becomes

$$-\frac{\hbar^2}{2m}(\partial_x^2 \bar{\Psi})(\hat{\tau}_3 + i\hat{\tau}_2)\hat{\tau}_3 + mc^2 \bar{\Psi} + \bar{\Psi}(\hat{\tau}_3 + i\hat{\tau}_2)\hat{\tau}_3 S = -i\hbar (\partial_t \bar{\Psi})\hat{\tau}_3. \quad (\text{F24})$$

Right-multiplying Eq. (F24) by $\hat{\tau}_3$ and using that the real-valued scalar interaction S , viewed as a multiplication operator, commutes with the Pauli matrices gives

$$-\frac{\hbar^2}{2m}(\partial_x^2 \bar{\Psi})(\hat{\tau}_3 + i\hat{\tau}_2) + mc^2 \bar{\Psi}\hat{\tau}_3 + \bar{\Psi}(\hat{\tau}_3 + i\hat{\tau}_2)S = -i\hbar \partial_t \bar{\Psi}. \quad (\text{F25})$$

Moving the right-hand side of Eq. (F25) to the left gives precisely Eq. (F21). The two first-order Lagrangian densities therefore give the same FV column equation and the corresponding FV-adjoint row-field equation; for the present derivation, this establishes their equivalence at the level of the Euler-Lagrange equations.

F.3 Standard energy-momentum tensor and its components

The usual energy-momentum tensor is [16]

$$\begin{aligned} T^\nu_\mu &= (\partial_\mu \psi) \frac{\partial \mathcal{L}}{\partial (\partial_\nu \psi)} + (\partial_\mu \psi^*) \frac{\partial \mathcal{L}}{\partial (\partial_\nu \psi^*)} - \mathcal{L} g_\mu^\nu \\ &= \frac{\hbar^2}{2m} [(\partial^\nu \psi^*)(\partial_\mu \psi) + (\partial_\mu \psi^*)(\partial^\nu \psi)] - \mathcal{L} g_\mu^\nu. \end{aligned} \quad (\text{F26})$$

The component needed later is obtained directly from Eq. (F26):

$$T^1_1 = \frac{1}{2mc^2} [(\hat{E}\psi^*)(\hat{E}\psi) + (c\hat{p}\psi^*)(c\hat{p}\psi) + (mc^2)^2 \psi^* \psi + 2mc^2 S \psi^* \psi]. \quad (\text{F27})$$

F.4 Divergence identity and conservation statements for T^μ_ν

The pair $\{T^0_0, cT^1_0\}$ satisfies $\partial_\mu T^\mu_0 = (\partial_0 S)\psi^* \psi$; likewise, the pair $\{T^0_1, cT^1_1\}$ satisfies $\partial_\mu T^\mu_1 = (\partial_1 S)\psi^* \psi$. Combining these two relations yields

$$\partial_\mu T^\mu_\nu = (\partial_\nu S)\psi^* \psi. \quad (\text{F28})$$

When $\partial_0 S = 0$, the local equation $\partial_\mu T^\mu_0 = 0$ holds. The corresponding global conservation statement $\int_\Omega dx T^0_0 = \text{const}$ additionally requires the boundary relation $[cT^1_0]_a^b = 0$. Thus, this conservation statement is BC-dependent.

F.5 Two-vector current and an associated tensor

The standard conserved two-current is

$$j^\mu = j^\mu(x, t) = \frac{i\hbar}{2m} [\psi^*(\partial^\mu \psi) - (\partial^\mu \psi^*)\psi], \quad (\text{F29})$$

where $j^0 = c\rho$ and $j^1 = j$. Its continuity equation is $\partial_\mu j^\mu = 0$ [16].

Define the second-rank Lorentz tensor

$$K^\mu{}_\nu = K^\mu{}_\nu(x, t) = \frac{i\hbar}{2m} [\psi^*(\partial^\mu (i\hbar \partial_\nu \psi)) - (\partial^\mu \psi^*)(i\hbar \partial_\nu \psi)]. \quad (\text{F30})$$

This object may be regarded as an unconventional energy-momentum tensor. In particular,

$$K^\mu{}_\nu = T^\mu{}_\nu + \mathcal{L} g^\mu{}_\nu - \frac{\hbar^2}{2m} \partial_\nu (\psi^*(\partial^\mu \psi)). \quad (\text{F31})$$

F.6 Divergence identities and conservation laws for $K^\mu{}_\nu$

Using Eqs. (F1), (F4), and (F5), one obtains

$$\partial_\mu K^\mu{}_\nu = \partial_\mu T^\mu{}_\nu. \quad (\text{F32})$$

Together with Eq. (F28), this gives

$$\partial_\mu K^\mu{}_\nu = (\partial_\nu S) \psi^* \psi. \quad (\text{F33})$$

Thus $\partial_\mu K^\mu{}_0 = 0$ whenever $\partial_0 S = 0$. In this case, $K^0{}_0 = \rho_E$ and $K^1{}_0 = j_E/c$, which gives

$$\int_\Omega dx K^0{}_0 = \int_\Omega dx \rho_E = \langle\langle \Psi, \hat{E} \Psi \rangle\rangle = \langle\langle \Psi, \hat{h} \Psi \rangle\rangle = \text{const} \quad (\text{F34})$$

provided the boundary relation $[cK^1{}_0]_a^b = [j_E]_a^b = 0$ is satisfied. In the main text this boundary relation follows from the pseudo self-adjointness of $\hat{h}$ for the admissible BCs.

APPENDIX G TABULATED BC CATALOG

The BCs discussed in Chapter IV are summarized in Table 5.

Table 5 Catalog of BCs and their parameter values for 1D KFG and KFGM particles.

Case	BCs	Parameter values	Classification
(i) Dirichlet	$\psi(a, t) = \psi(b, t) = 0$	$m_0 = -1, \quad m_1 = 0, \quad m_2 = 0,$ $m_3 = 0, \quad \text{and} \quad \mu = 0$	Confining
(ii) Neumann	$\lambda\psi_x(a, t) = \lambda\psi_x(b, t) = 0$	$m_0 = +1, \quad m_1 = 0, \quad m_2 = 0,$ $m_3 = 0, \quad \text{and} \quad \mu = 0$	Confining
(iii) Mixed	$\psi(a, t) = 0, \quad \lambda\psi_x(b, t) = 0$	$m_0 = 0, \quad m_1 = 0, \quad m_2 = 0,$ $m_3 = +1, \quad \text{and} \quad \mu = \frac{\pi}{2}$	Confining
(iv) Mixed	$\lambda\psi_x(a, t) = 0, \quad \psi(b, t) = 0$	$m_0 = 0, \quad m_1 = 0, \quad m_2 = 0,$ $m_3 = -1, \quad \text{and} \quad \mu = \frac{\pi}{2}$	Confining
(v) Robin	$\psi(a, t) - \lambda\psi_x(a, t) = 0, \quad \psi(b, t) + \lambda\psi_x(b, t) = 0$	$m_0 = +1, \quad m_1 = 0, \quad m_2 = 0,$ $m_3 = 0, \quad \text{and} \quad \mu = \frac{\pi}{2}$	Confining
(vi) Robin	$\psi(a, t) + \lambda\psi_x(a, t) = 0, \quad \psi(b, t) - \lambda\psi_x(b, t) = 0$	$m_0 = -1, \quad m_1 = 0, \quad m_2 = 0,$ $m_3 = 0, \quad \text{and} \quad \mu = \frac{\pi}{2}$	Confining
(vii) Periodic	$\psi(a, t) = \psi(b, t), \quad \lambda\psi_x(a, t) = \lambda\psi_x(b, t)$	$m_0 = 0, \quad m_1 = +1, \quad m_2 = 0,$ $m_3 = 0, \quad \text{and} \quad \mu = \frac{\pi}{2}$	Nonconfining
(viii) Antiperiodic	$\psi(a, t) = -\psi(b, t), \quad \lambda\psi_x(a, t) = -\lambda\psi_x(b, t)$	$m_0 = 0, \quad m_1 = -1, \quad m_2 = 0,$ $m_3 = 0, \quad \text{and} \quad \mu = \frac{\pi}{2}$	Nonconfining
(ix) Generalized	$\begin{bmatrix} \psi(b, t) \\ \lambda\psi_x(b, t) \end{bmatrix} = \pm e^{-i\sigma_y(\frac{\pi}{2}-\mu)} \begin{bmatrix} \psi(a, t) \\ \lambda\psi_x(a, t) \end{bmatrix}$	$m_0 = 0, \quad m_1 = \pm 1, \quad m_2 = 0,$ $m_3 = 0, \quad \text{and} \quad \mu \in [0, \pi)$	Nonconfining
(x) Mixed-like	$\psi(a, t) = \pm \lambda\psi_x(b, t), \quad \psi(b, t) = \mp \lambda\psi_x(a, t)$	$m_0 = 0, \quad m_1 = \pm 1, \quad m_2 = 0,$ $m_3 = 0, \quad \text{and} \quad \mu = 0$	Nonconfining
(xi) Quasiperiodic	$\psi(a, t) = \pm i\psi(b, t), \quad \lambda\psi_x(a, t) = \pm i\lambda\psi_x(b, t)$	$m_0 = 0, \quad m_1 = 0,$ $m_2 = \pm 1, \quad \text{and} \quad m_3 = 0$	Not for KFGM
(xii) Quasimixed	$\psi(a, t) = \pm i\lambda\psi_x(b, t), \quad \psi(b, t) = \pm i\lambda\psi_x(a, t)$	$m_0 = 0, \quad m_1 = 0,$ $m_2 = \pm 1, \quad \text{and} \quad m_3 = 0$	Not for KFGM