

Interior-boundary conditions for Schrödinger operators on codimension-1 boundaries

Roderich Tumulka 

Mathematisches Institut, Eberhard-Karls-Universität, Auf der Morgenstelle 10,
72076 Tübingen, Germany

E-mail: roderich.tumulka@uni-tuebingen.de

Received 19 September 2019, revised 25 February 2020

Accepted for publication 27 February 2020

Published 24 March 2020



Abstract

Interior-boundary conditions (IBCs) are boundary conditions on wave functions for Schrödinger equations that allow that probability can flow into (and thus be lost at) a boundary of configuration space while getting added in another part of configuration space. IBCs are of particular interest because they allow for defining Hamiltonians involving particle creation and annihilation (as used in quantum field theories) without the need for renormalization or ultraviolet cut-off. For those Hamiltonians, the relevant boundary has codimension 3. In this paper, we develop (what we conjecture is) the general form of IBCs for the Laplacian operator (or Schrödinger operators), but we focus on the simpler case of boundaries with codimension 1.

Keywords: regularization of quantum field theory, Laplacian operator, particle creation, probability current

1. Introduction

Interior-boundary conditions (IBCs) are a type of boundary condition for wave functions in Schrödinger equations that allows the loss of probability at a boundary ∂Q due to flux into ∂Q while at the same time the probability gets added in another part of configuration space Q . In contrast, ordinary boundary conditions (such as Dirichlet or Neumann boundary conditions) reflect all waves that reach ∂Q , with the consequence that no probability can get lost at ∂Q . IBCs come up in particular in the context of theories with particle creation and annihilation, in which probability needs to get shifted from the n -particle sector of configuration space to the $n + 1$ -particle sector and vice versa [1–6]. IBCs have attracted interest recently for providing

Hamiltonians with particle creation without the need for renormalization or ultraviolet cut-off [7–10]. For a gentle introduction to IBCs, see [11]. Other recent works about IBCs include [12–14].

Our goal in this paper is to develop the general form of an IBC that conserves probability (and thus can lead to a self-adjoint Hamiltonian) for Schrödinger operators (i.e., non-relativistic Hamiltonians whose kinetic part is the negative Laplacian) for a boundary of codimension 1. This form is similar to certain IBCs on codimension-3 boundaries considered in [5, 7, 8]. IBCs for the Dirac equation with codimension-1 boundaries are studied in [15]. Particular such IBCs are used in a model of particle creation in one space dimension, involving a codimension-1 boundary, that is studied in [16]. Preliminary considerations in the direction of this paper were described in [6].

The IBC we propose, see (26), should be the most general in the following sense. We do not consider boundary conditions that will be reflecting for some components of ψ and IBCs for others, but focus on pure IBCs. Moreover, we do not consider conditions that force amounts of probability that have flown into the boundary to reappear out of other parts of the boundary; rather, we focus on the case that all probability lost at the boundary reappears in the interior of configuration space. On the basis of our attempts to set up IBCs, we conjecture that (26) is the general form, and in particular that an IBC for a self-adjoint Hamiltonian can involve derivatives normal but not tangential to the boundary.

Codimension-1 boundaries form a natural framework for considering boundary conditions, including IBCs, although applications often have codimension-3 boundaries. To put things into perspective, we mention that in the application to particle creation, the configuration space consists of configurations of a variable number of particles,

$$\mathcal{Q} = \bigcup_{n=0}^{\infty} \mathcal{Q}_n = \bigcup_{n=0}^{\infty} (\mathbb{R}^{nd} \setminus \Delta_n), \quad (1)$$

where n means the particle number, d the dimension of physical space, and Δ_n the set of collision configurations,

$$\Delta_n = \{(x_1, \dots, x_n) \in \mathbb{R}^{nd} : x_i = x_j \text{ for some } i \neq j\}. \quad (2)$$

The boundary $\partial\mathcal{Q}$ is then $\cup_n \Delta_n$, and the IBC relates values (or limits) of ψ on Δ_n to values of ψ on \mathcal{Q}_{n-1} , the $n-1$ -particle sector of \mathcal{Q} . In this case, the codimension of the boundary is d , so the physical case has codimension 3. Still, in spherical relative coordinates, the boundary corresponds to $r = 0$, which in coordinates is a surface of codimension 1, and this allows us to carry over some considerations for codimension 1 to the case of codimension 3.

This paper is organized as follows. In section 2, we begin by discussing a simple example. After that, we turn to the general case: the configuration and Hilbert space are set up in section 3, the IBC and Hamiltonian are written down in section 4, and the conservation of probability is verified in section 5. In section 6, we apply the IBC to an unusual kind of ultraviolet cut-off, in which the electron is smeared out not over a ball but over a sphere. In section 7, we summarize.

2. Simple example

We begin with a special case that features many elements of the general discussion that will follow. Let the configuration space $\mathcal{Q} = \mathcal{Q}^{(1)} \cup \mathcal{Q}^{(2)}$ be the union of $\mathcal{Q}^{(1)} = \mathbb{R}^{d-1}$ (where d is any natural number, not related to the dimension of physical space) and a half-space $\mathcal{Q}^{(2)} = \{(x_1, \dots, x_d) \in \mathbb{R}^d : x_d \geq 0\}$. The boundary $\partial\mathcal{Q} = \partial\mathcal{Q}^{(2)} = \{(x_1, \dots, x_d) \in \mathbb{R}^d : x_d = 0\}$

has codimension 1. A volume measure μ on \mathcal{Q} is defined by

$$\mu(S) = \text{vol}_{d-1}(S \cap \mathcal{Q}^{(1)}) + \text{vol}_d(S \cap \mathcal{Q}^{(2)}). \quad (3)$$

Wave functions are complex-valued functions on \mathcal{Q} belonging to

$$\mathcal{H} = L^2(\mathcal{Q}, \mathbb{C}, \mu) = L^2(\mathcal{Q}^{(1)}) \oplus L^2(\mathcal{Q}^{(2)}) \quad (4)$$

The IBC demands that for every $q \in \mathbb{R}^{d-1}$,

$$(\alpha(q) + \beta(q)\partial_d)\psi(q, 0) = \frac{2m}{\hbar^2}\psi(q), \quad (5)$$

where α and β are functions $\mathbb{R}^{d-1} \rightarrow \mathbb{C}$, and ∂_d means the partial derivative with respect to the last coordinate in $\mathcal{Q}^{(2)}$. The Hamiltonian is defined by

$$H\psi(q) = -\frac{\hbar^2}{2m}\Delta\psi(q) + V(q)\psi(q) + (\gamma(q) + \delta(q)\partial_d)\psi(q, 0) \quad (6)$$

$$H\psi(q, q_d) = -\frac{\hbar^2}{2m}\Delta\psi(q, q_d) + V(q, q_d)\psi(q, q_d) \quad (7)$$

for any $q \in \mathbb{R}^{d-1}$ and any $q_d > 0$. Here, $V: \mathcal{Q} \rightarrow \mathbb{R}$ is a potential function, and the coefficients γ and δ (not to be confused with a Dirac delta function) are functions $\mathbb{R}^{d-1} \rightarrow \mathbb{C}$ required to satisfy the conditions

$$\alpha(q)^* \gamma(q) \in \mathbb{R} \quad (8)$$

$$\beta(q)^* \delta(q) \in \mathbb{R} \quad (9)$$

$$\alpha(q)^* \delta(q) - \gamma(q)^* \beta(q) = -1 \quad (10)$$

at every $q \in \mathbb{R}^{d-1}$. Thus, of the 4 complex (or 8 real) degrees of freedom in the choice of coefficients $\alpha, \beta, \gamma, \delta$ at every q , only 4 real degrees of freedom can actually be chosen freely, while the others are determined by the conditions (8)–(10). A slightly more restricted choice of IBCs was considered in [[11], equation (25)]. Analogous IBCs for codimension-3 boundaries with coefficients satisfying the same relations (8)–(10) were considered in [5], ([7], remark 5), ([8], section 4). However, at codimension-3 boundaries, ψ diverges like $1/r$ at the boundary, where r is the distance from the bounda; in contrast, ψ stays bounded at codimension-1 boundaries.

We now verify the conservation of probability on the non-rigorous level. From the Schrödinger equation for the Hamiltonian H , we obtain that for every $q \in \mathbb{R}^{d-1}$ and $q_d > 0$,

$$\frac{\partial |\psi(q)|^2}{\partial t} = -\text{div} j(q) + \frac{2}{\hbar} \text{Im} [\psi(q)^* (\gamma(q) + \delta(q)\partial_d)\psi(q, 0)] \quad (11)$$

$$\frac{\partial |\psi(q, q_d)|^2}{\partial t} = -\text{div} j(q, q_d), \quad (12)$$

where j means the usual probability current in either $\mathcal{Q}^{(1)}$ or $\mathcal{Q}^{(2)}$ and div the divergence. For each $q \in \mathbb{R}^{d-1}$, the last term in (11) can be written, by virtue of the IBC (5), as

$$\begin{aligned}
& \frac{2}{\hbar} \text{Im} \left[\frac{\hbar^2}{2m} (\alpha(q)^* + \beta(q)^* \partial_d) \psi(q, 0)^* (\gamma(q) + \delta(q) \partial_d) \psi(q, 0) \right] \\
&= \frac{\hbar}{m} \text{Im} [\psi(q, 0)^* \alpha(q)^* \gamma(q) \psi(q, 0)] \\
&\quad + \frac{\hbar}{m} \text{Im} [\psi(q, 0)^* \alpha(q)^* \delta(q) \partial_d \psi(q, 0)] \\
&\quad - \frac{\hbar}{m} \text{Im} [\psi(q, 0)^* \gamma(q)^* \beta(q) \partial_d \psi(q, 0)] \\
&\quad + \frac{\hbar}{m} \text{Im} [\partial_d \psi(q, 0)^* \beta(q)^* \delta(q) \partial_d \psi(q, 0)] ,
\end{aligned} \tag{13}$$

where the first and the last term vanish by virtue of (8) and (9). What remains is

$$\frac{\hbar}{m} \text{Im} [\psi(q, 0)^* (\alpha(q)^* \delta(q) - \gamma(q)^* \beta(q)) \partial_d \psi(q, 0)] , \tag{14}$$

which agrees, by virtue of (10), with

$$-\frac{\hbar}{m} \text{Im} [\psi(q, 0)^* \partial_d \psi(q, 0)] = -j_d(q, 0) , \tag{15}$$

i.e., the negative of the last component of j on $\partial Q^{(2)}$. Thus, the gain in $Q^{(1)}$ compensates the loss in $Q^{(2)}$, so that $\|\psi\|^2 = \int_Q |\psi(q)|^2 \mu(dq)$ is conserved.

After this simple example, we now turn to the general discussion of IBCs on codimension-1 boundaries.

3. General setting

We take the configuration space Q to be a finite or countable union of disjoint manifolds with boundary, $Q = \cup_n Q^{(n)}$. (By definition, in a manifold with boundary, a neighborhood of an interior point looks like a piece of \mathbb{R}^d , while a neighborhood of a boundary point looks like a piece of a half-space in \mathbb{R}^d . In particular, the boundary has codimension 1, i.e., dimension $d - 1$. The boundary may be empty.) We write $\partial Q^{(n)}$ for the boundary of $Q^{(n)}$, $\partial Q = \cup_n \partial Q^{(n)}$, and $Q^\circ = Q \setminus \partial Q$ for the interior of Q . We take Q to be equipped with a Riemann metric g_{ij} , which also defines a volume measure $\mu^{(n)}$ on $Q^{(n)}$, and thus a measure μ on Q ,

$$\mu(S) = \sum_n \mu^{(n)}(S \cap Q^{(n)}) . \tag{16}$$

Likewise, the metric defines a surface area measure λ on ∂Q .

Wave functions can be complex-valued functions on Q . However, we can also be more general and allow cross-sections of vector bundles. Readers unfamiliar with vector bundles may ignore this further generality and think of complex-valued wave functions. So, for every n , let $E^{(n)}$ be a *Hermitian vector bundle* over $Q^{(n)}$ of finite rank (dimension of the fiber spaces)

$$r_n = r(q) = \dim_{\mathbb{C}} E_q^{(n)} , \tag{17}$$

i.e., a complex vector bundle equipped with a positive definite Hermitian inner product $(\cdot, \cdot)_q$ in every fiber $E_q^{(n)}$, $q \in Q^{(n)}$, and a metric connection (i.e., a connection relative to which the inner product is parallel, or, equivalently, a connection such that the parallel transport it defines along any path from q to q' is a unitary isomorphism $E_q^{(n)} \rightarrow E_{q'}^{(n)}$). We write E for $\cup_n E^{(n)}$ and E_q

for $E_q^{(n)}$ if $q \in \mathcal{Q}^{(n)}$. The wave function will be a cross-section of E , i.e., a mapping $\psi: \mathcal{Q} \rightarrow E$ such that $\psi(q) \in E_q$ for every $q \in \mathcal{Q}$.

The Hilbert space $\mathcal{H} = L^2(\mathcal{Q}, E, \mu)$ consists of the square-integrable cross-sections of E and is equipped with the inner product

$$\langle \psi | \phi \rangle = \int_{\mathcal{Q}} \mu(dq) (\psi(q), \phi(q))_q. \quad (18)$$

Note that $\int_{\mathcal{Q}}$ means the same as $\sum_n \int_{\mathcal{Q}^{(n)}}$, and that $\mathcal{H} = \oplus_n L^2(\mathcal{Q}^{(n)}, E^{(n)}, \mu^{(n)})$.

4. IBC and Hamiltonian

The IBC will be so constructed that the amount of probability per time that flows out of the boundary at $q' \in \partial\mathcal{Q}$ gets added to $|\psi|^2$ at an interior point

$$q = f(q') \quad (19)$$

in a different sector, $f: \partial\mathcal{Q} \rightarrow \mathcal{Q}^\circ$. We suppose that

$$r(f(q)) \leq r(q) \quad (20)$$

(recall that $r(q) = \dim_{\mathbb{C}} E_q$) and further that the derivative of f has full rank, i.e., that the image of f in $\mathcal{Q}^{(n)}$ does not have lower dimension than $\mathcal{Q}^{(n)}$; in particular, if $q' \in \partial\mathcal{Q}^{(n')}$ and $q = f(q') \in \mathcal{Q}^{(n)}$ then $\dim \mathcal{Q}^{(n)} \leq \dim \partial\mathcal{Q}^{(n')} = \dim \mathcal{Q}^{(n')} - 1$. Since many boundary points q' can be mapped to the same interior point q , the set of which will be denoted

$$f^{-1}(q) = \{q' \in \partial\mathcal{Q}: f(q') = q\}, \quad (21)$$

we will need to make use of a measure over $f^{-1}(q)$. The appropriate (unnormalized) measure for our purpose is

$$\nu_q(\cdot) = \text{weak-} \lim_{dq \rightarrow \{q\}} \frac{\lambda(\cdot \cap f^{-1}(dq))}{\mu(dq)}, \quad (22)$$

or, equivalently, the measure characterized by

$$\int_{\mathcal{Q}} \mu(dq) \nu_q(M \cap f^{-1}(q)) = \lambda(M) \quad (23)$$

for any $M \subseteq \partial\mathcal{Q}$. For example, if $S = f^{-1}(q) \cap \partial\mathcal{Q}^{(n')}$ is a submanifold of $\partial\mathcal{Q}^{(n')}$ of dimension k and $\partial\mathcal{Q}^{(n')}$ has dimension ℓ , then the density of ν_q relative to the volume measure arising from the Riemann metric on S is

$$\left| \frac{\det(g_{\partial\mathcal{Q}^{(n')}}(e_i, e_j))_{i,j \leq \ell}}{\det(g_S(e_i, e_j))_{i,j \leq k} \det(g_{\mathcal{Q}^{(n)}}(df(e_i), df(e_j)))_{k < i, j \leq \ell}} \right|^{1/2}, \quad (24)$$

where $df: T_q \partial\mathcal{Q} \rightarrow T_q \mathcal{Q}$ is the derivative (tangent mapping) of f , and e_i are any linearly independent vectors in $T_q \partial\mathcal{Q}$ with the first k in $T_q S$; the quantity (24) does not depend on the choice

of e_i .¹ In particular, if $f^{-1}(q)$ is a finite or countable set (say, f is a local diffeomorphism), then for any $q' \in f^{-1}(q)$,

$$\nu_q(\{q'\}) = \lim_{dq' \rightarrow \{q'\}} \frac{\lambda(dq')}{\mu(f(dq'))} = \left| \det \left(g_{\mathcal{Q}(n)} \left(df(e_i), df(e_j) \right) \right)_{i,j \leq \ell} \right|^{-1/2} \quad (25)$$

for any orthonormal basis $\{e_i\}$ of the tangent space $T_{q'}\partial\mathcal{Q}$.

We now set up the Hamiltonian and IBC. We may include a potential, either as a function $V: \mathcal{Q} \rightarrow \mathbb{R}$ or more generally as a cross-section of $E \otimes E^*$ that is pointwise self-adjoint; here, E_q^* denotes the dual space of E_q , so an element $V(q)$ of $E_q \otimes E_q^*$ corresponds to an endomorphism $E_q \rightarrow E_q$ that we also denote by $V(q)$, and V being pointwise self-adjoint means that $V(q)$ is self-adjoint on E_q relative to $(\cdot)_q$.

To formulate the IBC, we need an auxiliary Hermitian vector bundle F on $\partial\mathcal{Q}$ such that $\dim_{\mathbb{C}} F_q = r(q) - r(f(q))$. (For example, if q is an n -particle configuration and $f(q)$ an $n-1$ -particle configuration, and if E_q is a spin space of dimension 2^n and $\dim E_{f(q)} = 2^{n-1}$, then the auxiliary space F_q will have 2^{n-1} dimensions and serve the purpose of us having as many equations in the IBC as $\psi(q)$ has components, and keeping track of those components that are set to 0 by the IBC.) The IBC demands that for every boundary point q ,

$$(\alpha(q) + \beta(q)\partial_n) \psi(q) = \frac{2}{\hbar^2} \iota \psi(f(q)), \quad (26)$$

where $\alpha(q)$ and $\beta(q)$ are given complex-linear mappings $E_q \rightarrow E_{f(q)} \oplus F_q$ (where \oplus means orthogonal sum), ι is the inclusion $E_{f(q)} \rightarrow E_{f(q)} \oplus F_q$, $\iota(\chi) = \chi \oplus 0$, and ∂_n means the normal derivative, i.e., the directional covariant derivative in the inward normal direction to the boundary at q (normal in terms of the Riemann metric g_{ij}).² Note that the IBC (26) consists of $r(q)$ equations, which is the number of components of $\psi(q)$. Of the mappings $\alpha(q)$ and $\beta(q)$ we require that

$$[\alpha(q)|\beta(q)] \quad \text{has full rank } r(q), \quad (27)$$

where the notation $[\alpha(q)|\beta(q)]$ (indicating the juxtaposition of two matrices) means the mapping $E_q \oplus E_q \rightarrow E_{f(q)} \oplus F_q$ that maps $\chi \oplus \phi$ to $\alpha(q)\chi + \beta(q)\phi$.

The Hamiltonian is, for any interior point q :

$$H\psi(q) = -\frac{\hbar^2}{2} \Delta \psi(q) + V(q)\psi(q) + \int_{f^{-1}(q)} \nu_q(dq') (\gamma(q') + \delta(q')\partial_n) \psi(q'). \quad (28)$$

Here, Δ is the Laplace operator associated with the Riemannian metric of \mathcal{Q} and the connection of E (see, e.g., [17] for a detailed definition), and the coefficients $\gamma(q')$ and $\delta(q')$ are given

¹ Alternatively, ν_q can be expressed as a differential form $\hat{\nu}_q$ of maximal degree on S , $\hat{\nu}_q(q')(v_1, \dots, v_k) = \hat{\lambda}(q')(v_1, \dots, v_k, e_1, \dots, e_\ell)$ for any $q' \in S$ and $v_1, \dots, v_k \in T_{q'}S$, where $\hat{\lambda}$ is the differential form corresponding to the measure λ (i.e., the Riemannian volume form on $\partial\mathcal{Q}^{(n)}$), and the e_i are any vectors such that $df(e_1), \dots, df(e_\ell)$ is an orthonormal basis of $T_q\mathcal{Q}$.

² With the form (26) we assume that all components of $\psi(f(q))$ occur in the IBC. One could set up more general boundary conditions by using only some components of $\psi(f(q))$ or a certain projection of $\psi(f(q))$. Such a variant would amount to a kind of combination of a reflecting boundary condition and an interior-boundary condition and will not be considered here.

complex-linear mappings $E_{q'} \rightarrow E_{f(q')}$. The functions $\alpha, \beta, \gamma, \delta$ are required to satisfy at every $q \in \partial\mathcal{Q}$ the conditions

$$\alpha(q)^\dagger \iota \gamma(q) : E_q \rightarrow E_q \quad \text{is self-adjoint relative to } (\cdot, \cdot)_q \quad (29)$$

$$\beta(q)^\dagger \iota \delta(q) : E_q \rightarrow E_q \quad \text{is self-adjoint relative to } (\cdot, \cdot)_q \quad (30)$$

$$\alpha(q)^\dagger \iota \delta(q) - \gamma(q)^\dagger P_{E_{f(q)}} \beta(q) = -I_{E_q}, \quad (31)$$

where I_{E_q} means the identity operator on E_q , $P_{E_{f(q)}}$ the projection $E_{f(q)} \oplus F_q \rightarrow E_{f(q)}$, and S^\dagger means, for any linear mapping $S : X \rightarrow Y$ between spaces with inner products, the adjoint mapping $Y \rightarrow X$, i.e.,

$$(\chi, S^\dagger \phi)_X = (S\chi, \phi)_Y \quad (32)$$

for any $\chi \in X$ and $\phi \in Y$.

We think of the masses as incorporated into the metric g_{ij} , as in, e.g.,

$$ds^2 = m_1 dx_1^2 + m_1 dy_1^2 + m_1 dz_1^2 + m_2 dx_2^2 + m_2 dy_2^2 + m_2 dz_2^2 \quad (33)$$

for two particles of different mass in Euclidean space (see [17] for further discussion). Then the mass need not be put into the prefactor of the Laplacian (in the Hamiltonian H as in (28) above) or the gradient (in the current j as in (36) below)³.

This completes the definition of the Hamiltonian.

5. Conservation of probability

Here is a formal (non-rigorous) derivation of the conservation of $|\psi|^2$, i.e., a check of self-adjointness of H on the non-rigorous level. By $|\psi|^2$, we mean $|\psi(q)|^2 = (\psi(q), \psi(q))_q$, which is the density relative to μ of the probability distribution in \mathcal{Q} associated with $\psi \in \mathcal{H}$ with $\|\psi\| = 1$. It evolves in general according to the balance equation

$$\frac{\partial |\psi(q)|^2}{\partial t} = \frac{2}{\hbar} \text{Im}(\psi(q), H\psi(q))_q. \quad (34)$$

It is known (e.g., [17]) that for $H = -\frac{\hbar^2}{2}\Delta$ in a Hermitian vector bundle over a Riemannian manifold,

$$\frac{2}{\hbar} \text{Im}(\psi(q), H\psi(q))_q = -\text{div } j(q) \quad (35)$$

with the probability current vector field

$$j(q) = \hbar \text{Im}(\psi(q), \nabla \psi(q))_q \quad (36)$$

³ This convention has the possibly undesirable consequence that, when different sectors correspond to different particle number, the Riemannian volume μ is weighted in different sectors with different powers of the mass (such as m^{3n}); however, this can easily be compensated by reweighting $\psi^{(n)}$ by a factor of $m^{-3n/2}$, which in turn requires, if $f(q)$ contains one particle less than q , a further factor of $m^{-3/2}$ in $\alpha, \beta, \gamma, \delta$.

on \mathcal{Q} . Here, $\text{div } j$ denotes the divergence of the vector field j ; in coordinates, $\text{div } j = \sum_a D_a j^a$, where D_a is the covariant derivative operator arising from the Riemann metric on \mathcal{Q} . The gradient $\nabla \psi$ is the E -valued vector field obtained from the E -valued 1-form that is the covariant derivative of ψ by ‘raising the index’ using the Riemann metric.

Now for the Hamiltonian (28), the balance equation (34) becomes

$$\frac{\partial |\psi(q)|^2}{\partial t} = -\text{div } j(q) + \int_{f^{-1}(q)} \nu_q(dq') \frac{2}{\hbar} \text{Im}(\psi(q), [\gamma(q') + \delta(q') \partial_n] \psi(q'))_q. \quad (37)$$

For each q' , the integrand can be written, by virtue of the IBC (26), as

$$\begin{aligned} & \frac{2}{\hbar} \text{Im} \left(\frac{\hbar^2}{2} P_{E_q} [\alpha(q') + \beta(q') \partial_n] \psi(q'), [\gamma(q') + \delta(q') \partial_n] \psi(q') \right)_q \\ &= \hbar \text{Im}(\psi(q'), \alpha(q')^\dagger \iota \gamma(q') \psi(q'))_{q'} \\ &+ \hbar \text{Im}(\psi(q'), \alpha(q')^\dagger \iota \delta(q') \partial_n \psi(q'))_{q'} \\ &- \hbar \text{Im}(\psi(q'), \gamma(q')^\dagger P_{E_q} \beta(q') \partial_n \psi(q'))_{q'} \\ &+ \hbar \text{Im}(\partial_n \psi(q'), \beta(q')^\dagger \iota \delta(q') \partial_n \psi(q'))_{q'}, \end{aligned} \quad (38)$$

where the first and the last term vanish by virtue of (29) and (30). What remains is

$$\hbar \text{Im}(\psi(q'), [\alpha(q')^\dagger \iota \delta(q') - \gamma(q')^\dagger P_{E_q} \beta(q')] \partial_n \psi(q'))_{q'}, \quad (39)$$

which agrees, by virtue of (31), with

$$-\hbar \text{Im}(\psi(q'), \partial_n \psi(q'))_{q'} = -j_n(q'), \quad (40)$$

where $j_n(q')$ means the component of $j(q')$ normal to the boundary, or

$$j_n = f^i n^j g_{ij} \quad (41)$$

with n the inward-pointing unit normal vector to the boundary. Thus, in total,

$$\frac{\partial |\psi(q)|^2}{\partial t} = -\text{div } j(q) - \int_{f^{-1}(q)} \nu_q(dq') j_n(q'). \quad (42)$$

Now, if $j_n(q') < 0$ then $-j_n(q') \lambda(dq') dt$ is the amount of $|\psi|^2$ weight lost in the sector containing q' due to current into the boundary region dq' around q' within duration dt . Likewise, if $j_n(q') > 0$ then $j_n(q') \lambda(dq') dt$ is the amount of $|\psi|^2$ weight *gained* in the sector containing q' due to current coming from dq' within duration dt . That is, $j_n(q') \lambda(dq') dt$ is the net gain, positive or negative. Now the second term on the right-hand side of (42) represents a gain in the amount of $|\psi|^2$ weight (while the $\text{div } j$ term represents transport of $|\psi|^2$ weight within one sector); in fact, the gain in the region dq around q within duration dt is

$$-\mu(dq) dt \int_{f^{-1}(q)} \nu_q(dq') j_n(q') = -dt \int_{f^{-1}(dq)} \lambda(dq') j_n(q'). \quad (43)$$

Thus, the net gain in dq exactly compensates the net loss in $f^{-1}(dq)$, and $\|\psi\|^2 = \int_{\mathcal{Q}} |\psi(q)|^2 \mu(dq)$ is conserved.

Equation (42) can be regarded as a transport equation for the $|\psi|^2$ weight, with two types of transport: continuous motion within a sector of \mathcal{Q} , and transport between sectors of \mathcal{Q} (either from q' to $f(q')$ or from $f(q')$ to q'). Equation (42) actually is a probability transport equation for the $|\psi|^2$ -distributed stochastic process in \mathcal{Q} described in [18].

It also seems clear from the above derivation of (42) that the conditions (29), (30), and (31) cannot be weakened within our scheme without losing (42) and thus the self-adjointness of H . (Except that (29)–(31) may fail on a λ -null set of boundary configurations, or $\alpha, \beta, \gamma, \delta$ may be undefined on such a set.) After all, if $\psi(q')$ and $\partial_n \psi(q')$ can be chosen independently, then the only way in which can always be equal to (40) is if (29), (30), and (31) are true. Now $\psi(q')$ and $\partial_n \psi(q')$ can be chosen independently by appropriate choice of initial data for ψ —despite the IBC (26), which can be satisfied by appropriate choice of $\psi(f(q'))$. To be sure, (42) can be true for all ψ satisfying the IBC also if the integrals in (37) and (42) agree while the integrands are not equal. For example, this happens when $\gamma = 0 = \delta$ (so (31) is violated), $f^{-1}(q)$ contains two boundary points, say q' and q'' , and the loss at q' always compensates the gain at q'' and vice versa (e.g., if $j_n(q') = -j_n(q'')$ and $\nu_q(\{q'\}) = \nu_q(\{q''\})$). However, such possibilities lie outside our scheme, according to which the weight lost at q' is added to $f(q')$, and will not be considered here.

6. Application: cut-off radius

IBCs on a codimension-1 boundary can be used for implementing an unusual kind of UV cut-off, in which the source is smeared out, but not over a ball but over a sphere of small radius $\rho > 0$.

For the sake of definiteness, let us consider a model quantum field theory in \mathbb{R}^3 with two kinds of particles, called x -particles and y -particles in the following, in which x -particles can emit and absorb y -particles. Suppose there is only one x -particle, which is fixed at the origin, whereas the y -particles are non-relativistic spinless bosons of mass m_y and can move in \mathbb{R}^3 ; the model is adapted from the ‘scalar field model’ in ([19], chapter 12) and the Nelson model [20], and is called ‘Model 2’ in [7]. The configuration space is $\mathcal{Q} = \bigcup_{n=0}^{\infty} \mathbb{R}^{3n}$.

Let us turn to the cut-off. While an x -particle smeared out over a ball can emit and absorb y -particles anywhere within that ball, an x -particle smeared out over a sphere can only emit and absorb y -particles at a distance from its center that is exactly ρ . That is, a y -particle gets absorbed as soon as it reaches distance ρ from an x -particle, and gets created on the sphere of radius ρ . We exclude the possibility that any y -particle is ever closer than ρ to the x -particle. This kind of UV cut-off was first described, as far as we know, in [6]; we will call it a ‘ ρ -cut-off’ in the following.

When we apply this cut-off to the aforementioned model, the configuration space becomes

$$\mathcal{Q} = \bigcup_{n=0}^{\infty} \{(\mathbf{y}_1, \dots, \mathbf{y}_n) \in \mathbb{R}^{3n} : |\mathbf{y}_j| \geq \rho \quad \forall j\}, \quad (44)$$

whose boundary

$$\partial \mathcal{Q} = \{(\mathbf{y}_1, \dots, \mathbf{y}_n) \in \mathcal{Q} : |\mathbf{y}_j| = \rho \quad \text{for some } j\} \quad (45)$$

has codimension 1 almost everywhere. The Hilbert space \mathcal{H} is the subspace of $L^2(\mathcal{Q})$ of functions that are permutation invariant on each sector. Let B_ρ denote the open ρ -ball around the origin, $B_\rho = \{\mathbf{y} \in \mathbb{R}^3 : |\mathbf{y}| < \rho\}$. We will write y^n for a configuration of $n y$ -particles, $y^n = (\mathbf{y}_1, \dots, \mathbf{y}_n)$.

The IBC of Dirichlet type demands the following: for every $\omega \in \mathbb{S}^2$, $n \in \{0, 1, 2, \dots\}$, $y^n \in (\mathbb{R}^3 \setminus B_\rho)^n$,

$$\psi^{(n+1)}(y^n, \rho\omega) = -\frac{gm_y}{2\pi\hbar^2\rho\sqrt{n+1}}\psi^{(n)}(y^n). \quad (46)$$

The associated Hamiltonian is defined by

$$\begin{aligned} (H\psi)^{(n)}(y^n) &= -\frac{\hbar^2}{2m_y} \sum_{j=1}^n \nabla_{y_j}^2 \psi^{(n)}(y^n) + nE_0 \psi^{(n)}(y^n) \\ &\quad + \frac{g\sqrt{n+1}}{4\pi} \int_{\mathbb{S}^2} d^2\omega \left. \frac{\partial}{\partial r} \right|_{r=\rho} (r\psi^{(n+1)}(y^n, r\omega)) \end{aligned} \quad (47)$$

at any $y^n \in \mathcal{Q} \setminus \partial\mathcal{Q}$.

In the language of sections 3–5, $g_{ij} = m_y \delta_{ij}$, $f(y^n) = y^n \setminus B_\rho$, the Hermitian vector bundle E is the trivial rank-1 bundle $E = \mathcal{Q} \times \mathbb{C}$, μ is the volume as in (16),

$$\partial\mathcal{Q}^{(n)} = \bigcup_{j=1}^n (\mathbb{R}^3 \setminus B_\rho)^{j-1} \times \mathbb{S}_\rho^2 \times (\mathbb{R}^3 \setminus B_\rho)^{n-j}, \quad (48)$$

λ is locally $\text{vol}_{3(j-1)} \times \text{area} \times \text{vol}_{3(n-j)}$,

$$f^{-1}(y^n) = \bigcup_{j=1}^n \{(y_1, \dots, y_{j-1}, \rho\omega, y_j, \dots, y_n) : \omega \in \mathbb{S}^2\}, \quad (49)$$

$\nu_{y^n}(d^2\omega) = \rho^2 d^2\omega$ on any of the n spheres in (49), and

$$\alpha(y^n) = -4\pi\rho\sqrt{n+1}/gm_y \quad (50)$$

$$\beta(y^n) = 0 \quad (51)$$

$$\gamma(y^n) = 0 \quad (52)$$

$$\delta(y^n) = gm_y/4\pi\rho\sqrt{n+1}. \quad (53)$$

7. Summary

We have formulated a general version of IBCs in the non-relativistic case for boundaries of codimension 1, along with the appropriate additional term in the Hamiltonian. This formulation applies also to configuration spaces that are Riemannian manifolds with boundary, to spinor-valued wave functions, and to spin spaces that form a vector bundle. We have presented a calculation verifying that total probability is conserved. We have argued that this is the most general form of IBC unless we allow that probability lost in some part of the boundary comes out of another part of the boundary. It would be of interest to have rigorous results showing that this form of IBC is the most general one, and that it defines a self-adjoint Hamiltonian. A similar study for the Dirac equation can be found in [15]. As an example, we have described a model of particle creation from a source that is neither a point nor a ball but a sphere.

Conflict of interests

The author has no conflict of interests.

ORCID iDs

Roderich Tumulka  <https://orcid.org/0000-0001-5075-9929>

References

- [1] Landau L and Peierls R 1930 Quantenelektrodynamik im Konfigurationsraum *Z. Phys.* **62** 188–200
Landau L and Peierls R 1997 English translation: quantum electrodynamics in configuration space *Selected Scientific Papers of Sir Rudolf Peierls With Commentary* ed R H Dalitz and R Peierls (Singapore: World Scientific) pp 71–82 (Engl transl.)
- [2] Moshinsky M 1951 Boundary conditions for the description of nuclear reactions *Phys. Rev.* **81** 347–52
- [3] Moshinsky M 1951 Boundary conditions and time-dependent states *Phys. Rev.* **84** 525–32
- [4] Thomas L E 1984 Multiparticle Schrödinger Hamiltonians with point interactions *Phys. Rev.D* **30** 1233–7
- [5] Yafaev D R 1992 On a zero-range interaction of a quantum particle with the vacuum *J. Phys. A: Math. Gen.* **25** 963–78
- [6] Georgii H-O and Tumulka R 2004 Some jump processes in quantum field theory *Interacting Stochastic Systems* ed J-D Deuschel and A Greven (Berlin: Springer) pp 55–73 (arXiv:0312326)
- [7] Teufel S and Tumulka R 2020 Hamiltonians without ultraviolet divergence for quantum field theories *Quantum Stud.: Math. Found.* <https://doi.org/10.1007/s40509-020-00223-9>
- [8] Lampart J, Schmidt J, Teufel S and Tumulka R 2018 Particle creation at a point source by means of interior-boundary conditions *Math. Phys. Anal. Geom.* **21** 12
- [9] Lampart J and Schmidt J 2019 On Nelson-type Hamiltonians and abstract boundary conditions *Commun. Math. Phys.* **376** 629–63
- [10] Lampart J 2019 A nonrelativistic quantum field theory with point interactions in three dimensions *Ann. Henri Poincaré* **20** 3509–41
- [11] Teufel S and Tumulka R 2016 Avoiding ultraviolet divergence by means of interior-boundary conditions *Quantum Mathematical Physics—A Bridge between Mathematics and Physics* ed F Finster, J Kleiner, C Röken and J Tolksdorf (Basel: Birkhäuser) pp 293–311 (arXiv:1506.00497)
- [12] Keppeler S and Sieber M 2016 Particle creation and annihilation at interior boundaries: one-dimensional models *J. Phys. A: Math. Theor.* **49** 125204
- [13] Schmidt J and Tumulka R 2019 Complex charges, time reversal asymmetry, and interior-boundary conditions in quantum field theory *J. Phys. A: Math. Theor.* **52** 115301
- [14] Schmidt J 2019 On a direct description of pseudorelativistic Nelson Hamiltonians *J. Math. Phys.* **60** 102303
- [15] Schmidt J, Teufel S and Tumulka R 2019 Interior-boundary conditions for many-body Dirac operators and codimension-1 boundaries *J. Phys. A: Math. Theor.* **52** 295202
- [16] Lienert M and Nickel L 2020 Multi-time formulation of particle creation and annihilation via interior-boundary conditions *Rev. Math. Phys.* **32** 2050004
- [17] Dürr D, Goldstein S, Taylor J, Tumulka R and Zanghì N 2007 Quantum mechanics in multiply-connected spaces *J. Phys. A: Math. Theor.* **40** 2997–3031
- [18] Dürr D, Goldstein S, Teufel S, Tumulka R and Zanghì N 2019 Bohmian trajectories for Hamiltonians with interior-boundary conditions *J. Stat. Phys.* <https://doi.org/10.1007/s10955-019-02335-y>
- [19] Schweber S 1961 *An Introduction to Relativistic Quantum Field Theory* (New York: Harper and Row)
- [20] Nelson E 1964 Interaction of nonrelativistic particles with a quantized scalar field *J. Math. Phys.* **5** 1190–7