Majorana Fermions in a Box

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July 29, 2016

Abstract

Majorana fermion dynamics may arise at the edge of Kitaev wires or superconductors. Alternatively, it can be engineered by using trapped ions or ultracold atoms in an optical lattice as quantum simulators. This motivates the theoretical study of Majorana fermions confined to a finite volume, whose boundary conditions are characterized by self-adjoint extension parameters. While the boundary conditions for Dirac fermions in $(1+1)$-d are characterized by a 1-parameter family, $\lambda = -\lambda^*$, of self-adjoint extensions, for Majorana fermions λ is restricted to $\pm i$. Based on this result, we compute the frequency spectrum of Majorana fermions confined to a 1-d interval. The boundary conditions for Dirac fermions confined to a 3-d region of space are characterized by a 4-parameter family of self-adjoint extensions, which is reduced to two distinct 1-parameter families for Majorana fermions. We also consider the problems related to the quantum mechanical interpretation of the Majorana equation as a single-particle equation and we relate the equation to a relativistic Schrödinger equation that does not suffer from these problems.

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1 Introduction

Majorana fermions [1] result from Dirac fermions [2] by imposing a reality condition on the Dirac spinor [3]. As a result, Majorana fermions are neutral and are their own antiparticles. In the minimal version of the standard model of particle physics, neutrinos are electrically neutral left-handed Weyl fermions [4] charged under the electroweak $SU(2)_L \times U(1)_Y$ gauge symmetry. In this case, no renormalizable neutrino mass terms exist, and thus, in this minimal theoretical framework, neutrinos are massless particles. Since the observation of neutrino oscillations, it is known that neutrinos indeed must have a small non-zero mass. When one extends the standard model by introducing additional right-handed neutrino fields, one can construct gauge invariant Dirac mass terms which involve the Higgs field and give rise to non-zero neutrino masses via the Higgs mechanism of electroweak symmetry breaking. Gauge invariance then requires that the right-handed neutrino fields are neutral under all gauge interactions. This in turn implies that one can also construct gauge invariant renormalizable Majorana mass terms which do not involve the Higgs field and thus give rise to neutrino masses, unrelated to the energy scale of electroweak symmetry breaking. Since the right-handed component does not participate in the electroweak or strong gauge interactions, Majorana neutrinos are extremely weakly interacting. In particular, like any neutrino they easily penetrate even dense materials and can thus not be confined in any container. Still, in some extensions of the standard model with extra spatial dimensions, neutrinos may be confined to finite regions of the extra-dimensional space.

The confinement of Majorana neutrinos in finite regions of space is a more important issue in condensed matter physics. In particular, Majorana fermions, which may emerge as edge modes of Kitaev wires [5] or of superconductors [6], have been discussed in the context of topological quantum computation [7–12]. Majorana fermions may also arise in engineered systems, such as ultracold atoms in optical lattices or ion traps [13–15]. We take these systems as a motivation to investigate the Majorana equation, restricted to a finite region in space, using the theory of self-adjoint extensions [16, 17]. In previous work, we have analyzed the Schrödinger, Pauli, and Dirac equations in a similar manner [18, 19]. For example, the perfectly reflecting wall of a box that confines nonrelativistic Schrödinger particles without spin is characterized by a single self-adjoint extension parameter. The most general boundary condition for relativistic Dirac fermions (which generalizes the boundary conditions of the MIT bag model [20–22]) is characterized by a 4-parameter family of self-adjoint extension parameters [18]. As we will show, imposing the Majorana reality condition on the corresponding Dirac spinor restricts the admissible values of the self-adjoint extension parameters. We then study the Majorana equation both in $(1+1)$ and in $(3+1)$ dimensions, with confining spatial boundary conditions.

The rest of this paper is organized as follows. In Section 2 we investigate the Majorana equation in $(1+1)$ dimensions, review its symmetries, and relate it to a relativistic Schrödinger-type equation with a consistent quantum mechanical single-particle interpretation. In Section 3 we study the self-adjoint extension parameters that characterize a perfectly reflecting boundary. The Majorana equation is then solved for a particle confined to a finite interval. In Section 4 we extend these investigations to $(3 + 1)$ dimensions by reviewing the Majorana equation and its symmetries, and by again constructing an equivalent relativistic Schrödinger-type equation. In Section 5 we construct a family of self-adjoint extensions for $(3+1)$-d Majorana fermions, confined to a finite region of space. Finally, Section 6 contains our conclusions.

2 Majorana Fermions in $(1 + 1)$ Dimensions

In this section we investigate the Majorana equation in $(1 + 1)$ dimensions. In particular, we review its symmetry properties and investigate some problems related to its quantum mechanical interpretation as a single-particle equation.

2.1 The Majorana equation in $(1 + 1)$ dimensions

Let us first consider the Dirac equation in $(1 + 1)$ dimensions

$$i\partial_t\Psi(x,t) = (\alpha pc + \beta Mc^2)\Psi(x,t), \quad \Psi(x,t) = \begin{pmatrix} \psi_1(x,t) \\ \psi_2(x,t) \end{pmatrix},$$
$$\alpha = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.1}$$

Here M is the fermion mass, c is the velocity of light, and we have put $\hbar = 1$. A consistent choice of the γ-matrices is provided in the Dirac basis

$$\gamma^0 = \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \gamma^1 = \gamma^0\alpha = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{2.2}$$

where the space-time metric is given by $g_{\mu\nu} = \mathrm{diag}(1, -1)$. Alternatively, we can use a Majorana basis

$$\widetilde{\gamma}^0 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \widetilde{\gamma}^1 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \tag{2.3}$$

in which the $\widetilde{\gamma}$-matrices have purely imaginary entries. The Dirac and the Majorana basis are related by the unitary transformation

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix}, \quad \gamma^\mu = U\widetilde{\gamma}^\mu U^\dagger, \quad \Psi(x,t) = U\widetilde{\Psi}(x,t). \tag{2.4}$$

In the Majorana basis, the Dirac equation is consistent with imposing the reality condition $\widetilde{\Psi}(x,t)^* = \widetilde{\Psi}(x,t)$. In the Dirac basis, the Majorana condition takes the form

$$\begin{aligned}
\Psi(x,t) &= U\widetilde{\Psi}(x,t) = U\widetilde{\Psi}(x,t)^* = U[U^\dagger\Psi(x,t)]^* = UU^T\Psi(x,t)^* \\
&= \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix}\begin{pmatrix} 1 & i \\ -i & -1 \end{pmatrix}\Psi(x,t)^* = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}\begin{pmatrix} \psi_1(x,t)^* \\ \psi_2(x,t)^* \end{pmatrix} \Rightarrow \\
\psi_1(x,t) &= i\psi_2(x,t)^*, \quad \psi_2(x,t) = i\psi_1(x,t)^*. \qquad (2.5)
\end{aligned}$$

Introducing $\psi(x,t) = \psi_1(x,t)$ the 2-component Dirac equation reduces to the 1-component Majorana equation

$$\begin{aligned}
&i\partial_t\begin{pmatrix} \psi(x,t) \\ i\psi(x,t)^* \end{pmatrix} = (\alpha pc + \beta Mc^2)\begin{pmatrix} \psi(x,t) \\ i\psi(x,t)^* \end{pmatrix} \Rightarrow \\
&i\partial_t\psi(x,t) = Mc^2\psi(x,t) + c\partial_x\psi(x,t)^*. \qquad (2.6)
\end{aligned}$$

Here we have used $p = -i\partial_x$. Unlike for the Schrödinger or Dirac equation, the right-hand side of the Majorana equation involves both $\psi(x,t)$ and $\psi(x,t)^*$. As a consequence, it can not be interpreted as an ordinary quantum mechanical Hamiltonian acting on a wave function $\psi(x,t)$. In any case, a quantum mechanical single-particle interpretation is problematical already for the Dirac equation. Putting this caveat aside, one can still use the Dirac Hamiltonian as well as other quantum mechanical operators of the Dirac theory, acting on constrained Majorana wave functions, to define expectation values for Majorana fermions. For the expectation value of the energy one then obtains

$$\begin{aligned}
\langle H\rangle &= \int dx\,(\psi^*, -i\psi)\,\big(\alpha pc + \beta Mc^2\big)\begin{pmatrix} \psi \\ i\psi^* \end{pmatrix} \\
&= \int dx\,(\psi^*, -i\psi)\begin{pmatrix} Mc^2 & -ic\partial_x \\ -ic\partial_x & Mc^2 \end{pmatrix}\begin{pmatrix} \psi \\ i\psi^* \end{pmatrix} \\
&= \int dx\,(\psi^*, -i\psi)\begin{pmatrix} Mc^2\psi + c\partial_x\psi^* \\ -ic\partial_x\psi - iMc^2\psi^* \end{pmatrix} \\
&= \int dx\,(\psi^* i\partial_t\psi + \psi i\partial_t\psi^*) = i\partial_t\int dx\ |\psi|^2 = 0. \qquad (2.7)
\end{aligned}$$

In the last step we have used the Majorana equation. As we will see in the next subsection, the total "probability" $2\int dx\ |\psi|^2$ is indeed conserved. As a consequence, the energy expectation value of a Majorana fermion state, evaluated with the Dirac Hamiltonian, always vanishes. The same is true for the momentum operator

$$\begin{aligned}
\langle p\rangle &= \int dx\,(\psi^*, -i\psi)\,(-i\partial_x)\begin{pmatrix} \psi \\ i\psi^* \end{pmatrix} \\
&= \int dx\,(-i\psi^*\partial_x\psi - i\psi\partial_x\psi^*) = -i\int dx\ \partial_x|\psi|^2 = 0. \qquad (2.8)
\end{aligned}$$

Here we have used partial integration and we have assumed that the wave function vanishes at spatial infinity. The expectation values of energy and momentum vanish because a Majorana fermion is an equal weight superposition of positive and negative energy and momentum states. As a consequence, the solutions of the Majorana equation do not include stationary energy eigenstates with a unique (positive or negative) energy.

2.2 Conserved "probability" current

The Majorana equation is not invariant against multiplication of $\psi(x,t)$ by an arbitrary $U(1)$ phase, but only against a change of sign. As a result, fermion number is conserved only modulo 2. Interestingly, the Majorana equation still inherits the conserved current of the Dirac equation,

$$\begin{aligned} j^\mu(x,t) &= \overline{\Psi}(x,t)\gamma^\mu\Psi(x,t) \ \Rightarrow \\ \rho(x,t) &= \overline{\Psi}(x,t)\gamma^0\Psi(x,t) = \Psi(x,t)^\dagger\Psi(x,t) = |\psi_1(x,t)|^2 + |\psi_2(x,t)|^2, \\ j(x,t) &= c\overline{\Psi}(x,t)\gamma^1\Psi(x,t) = c\Psi(x,t)^\dagger\gamma^0\gamma^1\Psi(x,t) = c\Psi(x,t)^\dagger\alpha\Psi(x,t) \\ &= c\left[\psi_1(x,t)^*\psi_2(x,t) + \psi_2(x,t)^*\psi_1(x,t)\right], \end{aligned} \tag{2.9}$$

which, after imposing the Majorana condition eq.(2.5), takes the form

$$\rho(x,t) = 2|\psi(x,t)|^2, \quad j(x,t) = ic\left[\psi(x,t)^{*2} - \psi(x,t)^2\right]. \tag{2.10}$$

Indeed, by using the Majorana equation (2.6), we obtain

$$\begin{aligned} \partial_t\rho(x,t) + \partial_x j(x,t) &= 2\left[\psi(x,t)^*\partial_t\psi(x,t) + \psi(x,t)\partial_t\psi(x,t)^*\right] \\ &+ 2ic\left[\psi(x,t)^*\partial_x\psi(x,t)^* - \psi(x,t)\partial_x\psi(x,t)\right] \\ &= -2i\psi(x,t)^*\left[Mc^2\psi(x,t) + c\partial_x\psi(x,t)^*\right] \\ &+ 2i\psi(x,t)\left[Mc^2\psi(x,t)^* + c\partial_x\psi(x,t)\right] \\ &+ 2ic\left[\psi(x,t)^*\partial_x\psi(x,t)^* - \psi(x,t)\partial_x\psi(x,t)\right] = 0. \end{aligned} \tag{2.11}$$

Although, just like for the Dirac equation, a quantum mechanical single-particle interpretation of the Majorana equation is problematical, and despite the fact that Majorana fermion number is conserved only modulo 2, the continuity equation implies that the total "probability"

$$\int dx\ \rho(x,t) = 2\int dx\ |\psi(x,t)|^2 = 1 \tag{2.12}$$

is conserved.

2.3 Lorentz invariance

Let us consider a Lorentz boost

$$x' = \frac{x - vt}{\sqrt{1 - v^2/c^2}}, \quad ct' = \frac{ct - \frac{v}{c}x}{\sqrt{1 - v^2/c^2}} \Rightarrow$$
$$\begin{pmatrix} ct' \\ x' \end{pmatrix} = \gamma \begin{pmatrix} 1 & -\beta \\ -\beta & 1 \end{pmatrix} \begin{pmatrix} ct \\ x \end{pmatrix}, \quad \beta = \frac{v}{c}, \quad \gamma = \frac{1}{\sqrt{1 - v^2/c^2}} = \cosh\theta \Rightarrow$$
$$\begin{pmatrix} ct' \\ x' \end{pmatrix} = \Lambda^{-1} \begin{pmatrix} ct \\ x \end{pmatrix}, \quad \Lambda = \begin{pmatrix} \cosh\theta & \sinh\theta \\ \sinh\theta & \cosh\theta \end{pmatrix}. \tag{2.13}$$

Under Lorentz boosts a Dirac spinor transforms as

$$\Psi'(x,t) = \begin{pmatrix} \cosh\frac{\theta}{2} & \sinh\frac{\theta}{2} \\ \sinh\frac{\theta}{2} & \cosh\frac{\theta}{2} \end{pmatrix} \Psi(x',t'). \tag{2.14}$$

For a Majorana spinor this implies

$$\psi'(x,t) = \cosh\frac{\theta}{2}\ \psi(x',t') + i\sinh\frac{\theta}{2}\ \psi(x',t')^*. \tag{2.15}$$

It is straightforward to show that the Majorana equation is indeed invariant under this transformation.

2.4 Parity, time-reversal, and charge conjugation

Let us now consider the discrete symmetries P, T, and C for Majorana fermions in one spatial dimension. For a Dirac fermion, the parity transformation P takes the form

$$^P\Psi(x,t) = \gamma^0\Psi(-x,t) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \Psi(-x,t) \Rightarrow$$
$$^P\psi_1(x,t) = \psi_1(-x,t), \quad ^P\psi_2(x,t) = -\psi_2(-x,t). \tag{2.16}$$

This is inconsistent with the Majorana condition $\psi_2(x,t) = i\psi_1(x,t)^*$. However, combining the Dirac parity operation with a $U(1)$ phase multiplication by i (which alone is not a symmetry of the Majorana equation) we obtain the Majorana parity transformation

$$^P\psi(x,t) = i\psi(-x,t), \tag{2.17}$$

which indeed leaves the Majorana equation invariant

$$\begin{aligned} i\partial_t\ ^P\psi(x,t) &= -\partial_t\psi(-x,t) = iMc^2\psi(-x,t) + ic\partial_{-x}\psi(-x,t)^* \\ &= Mc^2 i\psi(-x,t) + c\partial_x[i\psi(-x,t)]^* \\ &= Mc^2\ ^P\psi(x,t) + c\partial_x\ ^P\psi(x,t)^*. \end{aligned} \tag{2.18}$$

As one would expect, under P the probability and current densities transform as

$$\begin{aligned} {}^P\rho(x,t) &= 2|{}^P\psi(x,t)|^2 = 2|i\psi(-x,t)|^2 = \rho(-x,t), \\ {}^Pj(x,t) &= ic\left[{}^P\psi(x,t)^{*2} - {}^P\psi(x,t)^2\right] \\ &= ic\left[-\psi(-x,t)^{*2} + \psi(-x,t)^2\right] = -j(-x,t). \end{aligned} \tag{2.19}$$

For a Majorana fermion, we define time-reversal as

$${}^T\psi(x,t) = \psi(x,-t)^*, \tag{2.20}$$

which again leaves the Majorana equation invariant

$$\begin{aligned} i\partial_t\, {}^T\psi(x,t) &= i\partial_t\psi(x,-t)^* = -i\partial_{-t}\psi(x,-t)^* \\ &= Mc^2\psi(x,-t)^* + c\partial_x\psi(x,-t) \\ &= Mc^2\, {}^T\psi(x,t) + c\partial_x\, {}^T\psi(x,t)^*. \end{aligned} \tag{2.21}$$

Under time-reversal the probability and current densities transform as

$$\begin{aligned} {}^T\rho(x,t) &= 2|{}^T\psi(x,t)|^2 = 2|\psi(x,-t)^*|^2 = \rho(x,-t), \\ {}^Tj(x,t) &= ic\left[{}^T\psi(x,t)^{*2} - {}^T\psi(x,t)^2\right] = ic\left[\psi(x,-t)^2 - \psi(x,-t)^{*2}\right] \\ &= -j(x,-t). \end{aligned} \tag{2.22}$$

Finally, let us consider charge conjugation C, which for a Dirac fermion takes the form

$${}^C\Psi(x,t) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \Psi(x,t)^* \;\Rightarrow\; {}^C\psi_1(x,t) = i\psi_2(x,t)^*, \quad {}^C\psi_2(x,t) = i\psi_1(x,t)^*. \tag{2.23}$$

As it should, this implies that a Majorana fermion is C-invariant

$${}^C\psi(x,t) = \psi(x,t). \tag{2.24}$$

2.5 Propagation of wave packets

By inserting the plane wave ansatz

$$\psi(x,t) = A\exp(i(kx-\omega t)) + B\exp(-i(kx-\omega t)), \tag{2.25}$$

into the Majorana equation (2.6) one obtains

$$\omega = \sqrt{(Mc^2)^2 + k^2c^2}, \quad B = iA^*\frac{\omega - Mc^2}{kc}, \tag{2.26}$$

such that the most general wave packet solution of the Majorana equation is given by

$$\psi(x,t) = \int dk \left[A(k) \exp(i(kx - \omega t)) + iA(k)^* \frac{\omega - Mc^2}{kc} \exp(-i(kx - \omega t)) \right]. \tag{2.27}$$

The normalization condition, inherited from the Dirac equation, then takes the form

$$\langle \Psi | \Psi \rangle = \int dx \, (\psi^*, -i\psi) \begin{pmatrix} \psi \\ i\psi^* \end{pmatrix} = 2 \int dx \, |\psi|^2 = \frac{2}{\pi} \int dk \, |A(k)|^2 \frac{\omega(\omega - Mc^2)}{k^2 c^2}. \tag{2.28}$$

We have seen that the expectation values of energy and momentum vanish because a Majorana fermion is its own antiparticle. Let us now calculate the expectation value of the velocity operator

$$v = \partial_k \omega = \frac{kc^2}{\omega}, \tag{2.29}$$

which takes the form

$$\langle v \rangle(t) = \frac{2}{\pi} \int dk \, |A(k)|^2 \frac{\omega - Mc^2}{k} = \langle v \rangle(0), \tag{2.30}$$

and hence is time-independent. It is straightforward but somewhat tedious to calculate the expectation value of the position operator and one obtains

$$\begin{aligned}
\langle x \rangle(t) &= \langle x \rangle(0) + \langle v \rangle(0) t \\
&+ \frac{1}{2\pi} \Re \int dk \, A(-k) A(k) \frac{Mc}{\omega k^2} (\omega - Mc^2) \left[\exp(-2i\omega t) - 1 \right] \\
\langle x \rangle(0) &= \frac{1}{2\pi} \Re \int dk \, A(-k) A(k) \frac{Mc}{\omega k^2} (\omega - Mc^2) \\
&+ \frac{1}{\pi} \Im \int dk \, A(k) \partial_k A(k)^* \frac{\omega(\omega + Mc^2)}{k^2 c^2}.
\end{aligned} \tag{2.31}$$

The oscillatory contribution to $\langle x \rangle(t)$ involving $\exp(-2i\omega t)$ is reminiscent of "Zitterbewegung". This term is not present for the propagation of wave packets following the nonrelativistic free particle Schrödinger equation for which $\langle x \rangle(t) = \langle x \rangle(0) + \langle v \rangle(0) t$ [24].

2.6 Relation of the Majorana equation to a relativistic Schrödinger equation

As we discussed before, it is well known that a quantum mechanical single-particle interpretation of the Dirac or Majorana equation is problematical. The right-hand side of the Majorana equation cannot even be viewed as a quantum mechanical

Hamiltonian acting on a wave function, because it involves both ψ and ψ^*. Let us map ψ to a Schrödinger-type wave function

$$\Phi(x,t) = \psi(x,t) + i\frac{\sqrt{(Mc^2)^2 + p^2c^2} - Mc^2}{pc}\psi(x,t)^*, \quad p = -i\partial_x, \tag{2.32}$$

which obeys

$$\begin{aligned}
i\partial_t\Phi(x,t) &= i\partial_t\psi(x,t) + i\frac{\sqrt{(Mc^2)^2 + p^2c^2} - Mc^2}{pc} i\partial_t\psi(x,t)^* \\
&= Mc^2\psi(x,t) + c\partial_x\psi(x,t)^* \\
&- i\frac{\sqrt{(Mc^2)^2 + p^2c^2} - Mc^2}{pc}\left[Mc^2\psi(x,t)^* + c\partial_x\psi(x,t)\right] \\
&= \sqrt{(Mc^2)^2 + p^2c^2}\left[\psi(x,t) + i\frac{\sqrt{(Mc^2)^2 + p^2c^2} - Mc^2}{pc}\psi(x,t)^*\right] \\
&= \sqrt{(Mc^2)^2 + p^2c^2}\ \Phi(x,t).
\end{aligned} \tag{2.33}$$

Remarkably, Φ obeys a relativistic Schrödinger equation with only positive energy states. In particular, the equation for Φ has a consistent quantum mechanical single-particle interpretation, with $\sqrt{(Mc^2)^2 + p^2c^2}$ playing the role of the Hamiltonian. In the context of point-particle relativistic quantum mechanics it is no problem that this Hamiltonian is nonlocal (i.e. is contains derivatives of arbitrary order).

Interestingly, while the Majorana equation allows only a sign change of ψ, the relativistic Schrödinger equation allows global $U(1)$ phase changes

$${}^\alpha\Phi(x,t) = \exp(i\alpha)\Phi(x,t), \tag{2.34}$$

which give rise to a nonlocal conserved probability current that was constructed in [23]. This current is not directly related to the conserved local Majorana current of eq.(2.10). One can invert the relation between ψ and Φ to obtain

$$\psi(x,t) = \frac{1}{2\sqrt{(Mc^2)^2 + p^2c^2}}\left[\left(\sqrt{(Mc^2)^2 + p^2c^2} + Mc^2\right)\Phi(x,t) + ipc\ \Phi(x,t)^*\right]. \tag{2.35}$$

The simple $U(1)$ symmetry of eq.(2.34) then turns into the complicated nonlocal transformation

$$\begin{aligned}
{}^\alpha\psi(x,t) &= \frac{1}{2\sqrt{(Mc^2)^2 + p^2c^2}}\left[\left(\sqrt{(Mc^2)^2 + p^2c^2} + Mc^2\right)\ {}^\alpha\Phi(x,t) + ipc\ {}^\alpha\Phi(x,t)^*\right] \\
&= \frac{1}{2\sqrt{(Mc^2)^2 + p^2c^2}}\left[\left(\sqrt{(Mc^2)^2 + p^2c^2} + Mc^2\right)\exp(i\alpha)\Phi(x,t)\right. \\
&+ \left. ipc\exp(-i\alpha)\Phi(x,t)^*\right].
\end{aligned} \tag{2.36}$$

Similarly, the simple Lorentz transformation for a Majorana spinor of eq.(2.15) turns into a complicated nonlocal transformation rule for Φ, which is not very illuminating in the present context but may be interesting to study in more details in the framework of relativistic quantum mechanics of free particles (in contrast to quantum field theory) [25].

The Schrödinger-type wave function Φ inherits its P and T symmetry properties from the Majorana "wave function" ψ

$$
\begin{aligned}
{}^P\Phi(x,t) &= {}^P\psi(x,t) + i\frac{\sqrt{(Mc^2)^2 + p^2c^2} - Mc^2}{pc}\, {}^P\psi(x,t)^* \\
&= i\psi(-x,t) + \frac{\sqrt{(Mc^2)^2 + p^2c^2} - Mc^2}{pc}\, \psi(-x,t)^* = i\Phi(-x,t), \\
{}^T\Phi(x,t) &= {}^T\psi(x,t) + i\frac{\sqrt{(Mc^2)^2 + p^2c^2} - Mc^2}{pc}\, {}^T\psi(x,t)^* \\
&= \psi(x,-t)^* + i\frac{\sqrt{(Mc^2)^2 + p^2c^2} - Mc^2}{pc}\, \psi(x,-t) = \Phi(x,-t)^*. \qquad (2.37)
\end{aligned}
$$

The introduction of Φ and its corresponding relativistic Schrödinger equation may provide a consistent quantum mechanical single-particle interpretation of the Majorana equation. Based on this, one could evaluate new expectation values. For example, when evaluated with Φ (rather than with the Dirac spinor Ψ that obeys the Majorana condition), one would obtain $\langle x\rangle(t) = \langle x\rangle(0) + \langle v\rangle(0)t$ without any additional contribution from "Zitterbewegung", such as the one in eq.(2.31). While this is interesting, it is not the subject of the current paper. Here we stay with the original Majorana equation by imposing the Majorana condition on a Dirac spinor, and accept the problems of its quantum mechanical interpretation as a single-particle equation.

3 Majorana Fermions Confined to an Interval

In this section we investigate Majorana fermions in a 1-dimensional box. In particular, we study the self-adjoint extension parameters that characterize a perfectly reflecting boundary condition and we solve the Majorana equation for a particle confined to an interval.

3.1 Perfectly Reflecting Walls for Majorana Fermions

It is well known to the experts, but only rarely emphasized in quantum mechanics textbooks, that a quantum mechanical wave function need not necessarily vanish at a perfectly reflecting wall [18, 26–28]. In fact, the most general perfectly reflecting Robin boundary condition is characterized by a self-adjoint extension parameter

$\gamma \in \mathbb{R}$ and takes the form $\gamma\Psi(0) + \partial_x \Psi(0) = 0$. The standard textbook boundary condition $\Psi(0) = 0$ then corresponds to the special case $\gamma = \infty$. The general Robin boundary condition ensures that the nonrelativistic probability current vanishes at the boundary. This implies that no probability is leaking out of the box. More than this is not required for a consistent unitary quantum mechanical evolution.

Let us begin by studying the $(1+1)$-d Dirac equation on the positive x-axis with a perfectly reflecting boundary at $x = 0$ [18]. In order to investigate the Hermiticity of the Dirac Hamiltonian, we consider

$$\begin{aligned}\langle \chi | H | \Psi \rangle &= \int_0^\infty dx\ \chi(x)^\dagger \left[-c\alpha i \partial_x + \beta m c^2 \right] \Psi(x) \\ &= \int_0^\infty dx\ \left\{ \left[-c\alpha i \partial_x + \beta m c^2 \right] \chi(x) \right\}^\dagger \Psi(x) - ic\chi(0)^\dagger \alpha \Psi(0) \\ &= \langle \Psi | H | \chi \rangle^* - ic\chi(0)^\dagger \alpha \Psi(0), \end{aligned} \tag{3.1}$$

which leads to the Hermiticity condition

$$\chi(0)^\dagger \alpha \Psi(0) = 0. \tag{3.2}$$

We now introduce the self-adjoint extension condition

$$\psi_2(0) = \lambda \psi_1(0), \quad \lambda \in \mathbb{C}, \tag{3.3}$$

which reduces eq.(3.2) to

$$\chi(0)^\dagger \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Psi(0) = \left[\chi_1(0)^* \lambda + \chi_2(0)^* \right] \psi_1(0) = 0 \ \Rightarrow\ \chi_2(0) = -\lambda^* \chi_1(0). \tag{3.4}$$

In order for H to be self-adjoint, the domains of H and $H^\dagger$ must coincide, i.e. $D(H) = D(H^\dagger)$. To achieve this, one must request

$$\lambda = -\lambda^*, \tag{3.5}$$

i.e. λ must be purely imaginary. Hence, for Dirac fermions in 1-d there is a 1-parameter family of self-adjoint extensions that characterizes a perfectly reflecting wall. The self-adjointness condition eq.(3.3) implies

$$\begin{aligned} j(0) &= c\Psi(0)^\dagger \alpha \Psi(0) = c\Psi(0)^\dagger \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Psi(0) = c \left[\psi_1(0)^* \psi_2(0) + \psi_2(0)^* \psi_1(0) \right] \\ &= c \left[\psi_1(0)^* \lambda \psi_1(0) + \psi_1(0)^* \lambda^* \psi_1(0) \right] = 0. \end{aligned} \tag{3.6}$$

Hence, as in the nonrelativistic case, the current $j(0)$ vanishes at the perfectly reflecting wall.

Majorana fermions obey the additional constraint $\psi_2 = i\psi_1^*$, such that

$$\lambda \psi_1(0) = \psi_2(0) = i\psi_1(0)^* \ \Rightarrow\ |\lambda| = 1 \ \Rightarrow\ \lambda = \pm i. \tag{3.7}$$

Hence, Majorana fermions admit only two discrete self-adjoint extensions, no longer a continuous 1-parameter family.

3.2 Majorana fermion in a 1-d box

Let us consider a 1-d box $x \in [-L/2, L/2]$ endowed with perfectly reflecting boundary conditions. For Majorana fermions this means

$$s_+\psi(L/2) = \psi(L/2)^*, \quad s_-\psi(-L/2) = \psi(-L/2)^*, \quad s_+, s_- = \pm 1. \tag{3.8}$$

In order to maintain parity symmetry, we demand that the parity transformed field also obeys the boundary condition

$$s_+ \, {}^P\psi(L/2) = {}^P\psi(L/2)^* \Rightarrow s_+ i\psi(-L/2) = [i\psi(-L/2)]^* = -i\psi(-L/2)^* \Rightarrow$$
$$s_- = -s_+. \tag{3.9}$$

We now make the ansatz

$$\begin{aligned}\psi(x,t) &= A\exp(i(kx-\omega t)) + iA^*\frac{\omega - Mc^2}{kc}\exp(-i(kx-\omega t)) \\ &+ B\exp(i(-kx-\omega t)) - iB^*\frac{\omega - Mc^2}{kc}\exp(-i(-kx-\omega t)),\end{aligned} \tag{3.10}$$

with $\omega = \sqrt{(Mc^2)^2 + k^2c^2}$. Imposing the boundary conditions of eq.(3.8) then implies

$$B = A\exp(ikL)\frac{\omega - Mc^2 - is_+kc}{\omega - Mc^2 + is_+kc}, \quad B = A\exp(-ikL)\frac{\omega - Mc^2 - is_-kc}{\omega - Mc^2 + is_-kc}. \tag{3.11}$$

If we choose parity-violating boundary conditions with $s_- = s_+$, this implies

$$\exp(ikL) = \pm 1 \Rightarrow k = \frac{\pi}{L}n, \quad n \in \mathbb{Z}, \tag{3.12}$$

which is equivalent to the nonrelativistic momentum quantization condition for the standard box boundary condition $\Psi(\pm L/2) = 0$. On the other hand, using parity-symmetric boundary conditions with $s_- = -s_+$, one obtains the quantization condition

$$\exp(ikL) = \pm\frac{\omega - Mc^2 + is_+kc}{\omega - Mc^2 - is_+kc}. \tag{3.13}$$

Let us first consider the massless limit $M = 0$, $\omega = |k|c$, such that

$$\exp(ikL) = \pm\frac{\omega - Mc^2 + is_+kc}{\omega - Mc^2 - is_+kc} = \pm\frac{|k|c + is_+kc}{|k|c - is_+kc} = \pm i \Rightarrow k = \frac{\pi}{L}\left(n + \frac{1}{2}\right), \; n \in \mathbb{Z}. \tag{3.14}$$

This solution also applies to massive fermions in the high-energy limit $\omega \gg Mc^2$. In the nonrelativistic limit, on the other hand, we obtain

$$\exp(ikL) = \pm\frac{\frac{k^2}{2M} + is_+kc}{\frac{k^2}{2M} - is_+kc} = \pm\frac{k + 2is_+Mc}{k - 2is_+Mc}. \tag{3.15}$$

In the low-energy limit $\frac{k^2}{2M} \ll Mc^2$ this again leads to

$$\exp(ikL) = \pm 1 \;\Rightarrow\; k = \frac{\pi}{L} n, \quad n \in \mathbb{Z}, \tag{3.16}$$

It should be noted that the discrete k-values resulting from the quantization conditions as well as the corresponding discrete frequencies $\omega = \sqrt{(Mc^2)^2 + k^2c^2}$ do not yield stationary energy eigenstates. This is because the solution of eq.(3.10) is again a superposition of states with positive and negative energy $\pm\omega$.

4 Majorana Fermions in $(3+1)$ Dimensions

In this section we extend our previous considerations from $(1+1)$ to $(3+1)$ dimensions. We again consider the Majorana equation and its symmetries as well as a mapping to a relativistic Schrödinger equation.

4.1 The Majorana equation in $(3+1)$ dimensions

We start out with the Dirac equation in $(3+1)$ dimensions

$$i\partial_t \Psi(\vec{x},t)(\vec{\alpha}\cdot\vec{p}c + \beta Mc^2)\Psi(\vec{x},t), \quad \Psi(x,t) = \begin{pmatrix} \psi_1(x,t) \\ \psi_2(x,t) \\ \psi_3(x,t) \\ \psi_4(x,t) \end{pmatrix},$$
$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}. \tag{4.1}$$

For the γ-matrices we choose the Dirac basis

$$\gamma^0 = \beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}, \quad \gamma^i = \gamma^0\alpha^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}, \tag{4.2}$$

using the space-time metric $g_{\mu\nu} = \mathrm{diag}(1,-1,-1,-1)$. Next, we consider the Majorana basis

$$\widetilde{\gamma}^0 = \begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix}, \widetilde{\gamma}^1 = \begin{pmatrix} i\sigma^1 & 0 \\ 0 & i\sigma^1 \end{pmatrix}, \widetilde{\gamma}^2 = \begin{pmatrix} 0 & \sigma^2 \\ -\sigma^2 & 0 \end{pmatrix}, \widetilde{\gamma}^3 = \begin{pmatrix} i\sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix}, \tag{4.3}$$

in which the $\widetilde{\gamma}$ matrices again have purely imaginary entries. In this basis, the Majorana condition takes the simple form

$$\widetilde{\Psi}(\vec{x},t) = \widetilde{\Psi}(\vec{x},t)^*. \tag{4.4}$$

The Dirac and the Majorana basis are now related by the unitary transformation

$$U = \frac{1}{2}\left(\begin{array}{cccc} 1 & -1 & -i & -i \\ 1 & 1 & i & -i \\ i & i & 1 & -1 \\ -i & i & 1 & 1 \end{array}\right), \quad \gamma^\mu = U\widetilde{\gamma}^\mu U^\dagger, \quad \Psi(x,t) = U\widetilde{\Psi}(x,t). \tag{4.5}$$

In the Dirac basis, the Majorana condition reads

$$\begin{aligned} \Psi(\vec{x},t) &= U\widetilde{\Psi}(x,t) = U\widetilde{\Psi}(\vec{x},t)^* = U[U^\dagger\Psi(\vec{x},t)]^* = UU^T\Psi(\vec{x},t)^* \\ &= \frac{1}{4}\left(\begin{array}{cccc} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{array}\right)\left(\begin{array}{c} \psi_1(\vec{x},t)^* \\ \psi_2(\vec{x},t)^* \\ \psi_3(\vec{x},t)^* \\ \psi_4(\vec{x},t)^* \end{array}\right) \Rightarrow \\ \psi_3(\vec{x},t) &= i\psi_2(\vec{x},t)^*, \quad \psi_4(\vec{x},t) = -i\psi_1(\vec{x},t)^*. \end{aligned} \tag{4.6}$$

Introducing the two-component Majorana spinor

$$\psi(\vec{x},t) = \left(\begin{array}{c} \psi_1(\vec{x},t) \\ \psi_2(\vec{x},t) \end{array}\right), \tag{4.7}$$

the 4-component Dirac equation reduces to the 2-component Majorana equation

$$\begin{aligned} & i\partial_t \left(\begin{array}{c} \psi_1(\vec{x},t) \\ \psi_2(\vec{x},t) \\ i\psi_2(\vec{x},t)^* \\ -i\psi_1(\vec{x},t) \end{array}\right) = \left(\vec{\alpha}\cdot\vec{p}c + \beta Mc^2\right)\left(\begin{array}{c} \psi_1(\vec{x},t) \\ \psi_2(\vec{x},t) \\ i\psi_2(\vec{x},t)^* \\ -i\psi_1(\vec{x},t) \end{array}\right) \Rightarrow \\ & i\partial_t\psi(x,t) = Mc^2\psi(x,t) - c\vec{\sigma}\cdot\vec{p}\sigma^2\psi(x,t)^*. \end{aligned} \tag{4.8}$$

4.2 Conserved current

Again, the Majorana equation inherits the conserved current of the Dirac equation,

$$\begin{aligned} j^\mu(\vec{x},t) &= \overline{\Psi}(\vec{x},t)\gamma^\mu\Psi(\vec{x},t) \Rightarrow \\ \rho(\vec{x},t) &= \overline{\Psi}(\vec{x},t)\gamma^0\Psi(\vec{x},t) = \Psi(\vec{x},t)^\dagger\Psi(\vec{x},t), \\ \vec{j}(\vec{x},t) &= c\overline{\Psi}(\vec{x},t)\vec{\gamma}\Psi(\vec{x},t) = c\Psi(\vec{x},t)^\dagger\gamma^0\vec{\gamma}\Psi(\vec{x},t) = c\Psi(\vec{x},t)^\dagger\vec{\alpha}\Psi(\vec{x},t). \end{aligned} \tag{4.9}$$

By imposing the Majorana condition eq.(2.5), the charge and current densities take the form

$$\rho(\vec{x},t) = 2\psi(\vec{x},t)^\dagger\psi(\vec{x},t), \quad \vec{j}(\vec{x},t) = -c\psi(\vec{x},t)^\dagger\vec{\sigma}\sigma^2\psi(\vec{x},t)^* - c\psi(\vec{x},t)^T\sigma^2\vec{\sigma}\psi(\vec{x},t). \tag{4.10}$$

By using the Majorana equation (2.6) it is again straightforward to verify the continuity equation

$$\partial_t\rho(\vec{x},t) + \vec{\nabla}\cdot\vec{j}(\vec{x},t) = 0. \tag{4.11}$$

4.3 Lorentz invariance, parity, time-reversal, and charge conjugation

Just as in $(1 + 1)$ dimensions, it is straightforward to show that the $(3 + 1)$-d Majorana condition eq.(4.6) is again Lorentz covariant. Let us also consider the discrete symmetries P, T, and C for $(3 + 1)$-d Majorana fermions. For a Dirac fermion field $\Psi(\vec{x}, t)$, parity P corresponds to $\gamma^0\Psi(-\vec{x}, t)$. This transformation is again incompatible with the Majorana condition, but can be combined with a $U(1)$ phase multiplication by i, such that

$$
\begin{aligned}
&{}^P\Psi(\vec{x}, t) = i\gamma^0\Psi(-\vec{x}, t) = i\begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}\Psi(-\vec{x}, t) \;\Rightarrow \\
&{}^P\psi_1(\vec{x}, t) = i\psi_1(-\vec{x}, t), \quad {}^P\psi_2(\vec{x}, t) = i\psi_2(-\vec{x}, t), \\
&{}^P\psi_3(\vec{x}, t) = -i\psi_3(-\vec{x}, t), \quad {}^P\psi_2(\vec{x}, t) = -i\psi_4(-\vec{x}, t).
\end{aligned} \tag{4.12}
$$

Hence, for a $(3 + 1)$-d Majorana fermion parity takes the form

$$
{}^P\psi(\vec{x}, t) = \begin{pmatrix} {}^P\psi_1(\vec{x}, t) \\ {}^P\psi_2(\vec{x}, t) \end{pmatrix} = \begin{pmatrix} i\ \psi_1(-\vec{x}, t) \\ i\psi_2(-\vec{x}, t) \end{pmatrix} = i\psi(-\vec{x}, t). \tag{4.13}
$$

This transformation is consistent with the Majorana condition because

$$
\begin{aligned}
{}^P\psi_3(\vec{x}, t) &= -i\psi_3(-\vec{x}, t) = \psi_2(-\vec{x}, t)^* = i\ {}^P\psi_2(\vec{x}, t)^*, \\
{}^P\psi_4(\vec{x}, t) &= -i\psi_4(-\vec{x}, t) = -\psi_1(-\vec{x}, t)^* = -i\ {}^P\psi_1(\vec{x}, t)^*,
\end{aligned} \tag{4.14}
$$

and it indeed leaves the Majorana equation invariant. This is straightforward to show using

$$
\sigma^2(\vec{\sigma} \cdot \vec{p})^*\sigma^2 = -\sigma^2\vec{\sigma}^*\sigma^2 \cdot \vec{p} = \vec{\sigma} \cdot \vec{p}. \tag{4.15}
$$

For a Dirac fermion in $(3 + 1)$-d time-reversal takes the form

$$
{}^T\Psi(\vec{x}, t) = \begin{pmatrix} \sigma^2 & 0 \\ 0 & \sigma^2 \end{pmatrix}\Psi(\vec{x}, -t)^*. \tag{4.16}
$$

For a Majorana spinor this implies

$$
{}^T\psi(\vec{x}, t) = \sigma^2\psi(\vec{x}, -t)^*. \tag{4.17}
$$

It is again straightforward to check that this transformation leaves the Majorana equation invariant.

Finally, let us consider charge conjugation C, which for a $(3+1)$-d Dirac fermion takes the form

$$
{}^C\Psi(\vec{x}, t) = \begin{pmatrix} 0 & \sigma^2 \\ -\sigma^2 & 0 \end{pmatrix}\Psi(\vec{x}, t)^*. \tag{4.18}
$$

This implies that a Majorana fermion is indeed C-invariant

$$
{}^C\psi(\vec{x}, t) = \psi(\vec{x}, t). \tag{4.19}
$$

4.4 Relation of the $(3+1)$-d Majorana equation to a relativistic Schrödinger equation

Let us also consider the relation of the $(3+1)$-d Majorana equation to a relativistic Schrödinger equation. In this case we construct

$$\Phi(\vec{x},t) = \psi(\vec{x},t) - \frac{\vec{\sigma}\cdot\vec{p}c\sigma^2}{\sqrt{(Mc^2)^2+p^2c^2}+Mc^2}\psi(\vec{x},t)^*, \quad \vec{p} = -i\vec{\nabla}. \tag{4.20}$$

It is straightforward to show that, just as in $(1+1)$-d, $\Phi(\vec{x},t)$ obeys the relativistic Schrödinger-type equation

$$i\partial_t\Phi(\vec{x},t) = \sqrt{(Mc^2)^2+p^2c^2}\ \Phi(\vec{x},t). \tag{4.21}$$

In this case, $\Phi(\vec{x},t)$ is a 2-component spinor, which enjoys a global $U(2)$ symmetry

$${}^{\Omega}\Phi(\vec{x},t) = \Omega\Phi(\vec{x},t), \quad \Omega \in U(2). \tag{4.22}$$

This symmetry is not manifest in the Majorana equation. In fact, the $U(2)$ symmetry is like an internal "flavor" symmetry, while the two components of the original Majorana spinor are related by space-time rotations. Again, we can invert the relation between ψ and Φ

$$\psi(\vec{x},t) = \frac{1}{2\sqrt{(Mc^2)^2+p^2c^2}}\left[\left(\sqrt{(Mc^2)^2+p^2c^2}+Mc^2\right)\Phi(\vec{x},t) - \vec{\sigma}\cdot\vec{p}c\sigma^2\Phi(\vec{x},t)^*\right]. \tag{4.23}$$

The $U(2)$ symmetry of eq.(4.22) then turns into the nonlocal transformation

$$\begin{aligned} {}^{\Omega}\psi(\vec{x},t) &= \frac{1}{2\sqrt{(Mc^2)^2+p^2c^2}}\left[\left(\sqrt{(Mc^2)^2+p^2c^2}+Mc^2\right)\ {}^{\Omega}\Phi(\vec{x},t)\right. \\ &- \left.\vec{\sigma}\cdot\vec{p}c\sigma^2\ {}^{\Omega}\Phi(\vec{x},t)^*\right] \\ &= \frac{1}{2\sqrt{(Mc^2)^2+p^2c^2}}\left[\left(\sqrt{(Mc^2)^2+p^2c^2}+Mc^2\right)\Omega\Phi(\vec{x},t)\right. \\ &- \left.\vec{\sigma}\cdot\vec{p}c\sigma^2\Omega^*\Phi(\vec{x},t)^*\right] \end{aligned} \tag{4.24}$$

Just as in $(1+1)$-d, Lorentz invariance, which is manifest in the Majorana equation, is represented by a complicated nonlinear transformation of the Schrödinger-type wave function Φ, which inherits its P and T symmetry properties from the

Majorana "wave function" ψ

$$\begin{aligned}
{}^P\Phi(\vec{x},t) &= {}^P\psi(\vec{x},t) - \frac{\vec{\sigma}\cdot\vec{p}c\sigma^2}{\sqrt{(Mc^2)^2+p^2c^2}+Mc^2}\psi(\vec{x},t)^* \\
&= i\psi(-\vec{x},t) + i\frac{\vec{\sigma}\cdot\vec{p}c\sigma^2}{\sqrt{(Mc^2)^2+p^2c^2}+Mc^2}\psi(-\vec{x},t)^* = i\Phi(-\vec{x},t), \\
{}^T\Phi(\vec{x},t) &= {}^T\psi(\vec{x},t) - \frac{\vec{\sigma}\cdot\vec{p}c\sigma^2}{\sqrt{(Mc^2)^2+p^2c^2}+Mc^2}\,{}^T\psi(\vec{x},t)^* \\
&= \sigma^2\psi(\vec{x},-t)^* + \frac{\vec{\sigma}\cdot\vec{p}c\sigma^2}{\sqrt{(Mc^2)^2+p^2c^2}+Mc^2}\sigma^2\psi(\vec{x},-t) \\
&= \sigma^2\Phi(x,-t)^*. \qquad (4.25)
\end{aligned}$$

5 Perfectly Reflecting Walls for (3+1)-d Majorana Fermions

In this section we study the self-adjoint extension parameters that characterize a perfectly reflecting boundary condition for $(3+1)$-d Majorana fermions. Let us first consider Dirac fermions confined to a finite 3-d spatial domain Ω [18]. In order to investigate the Hermiticity of the Hamiltonian we consider

$$\begin{aligned}
\langle\chi|H|\Psi\rangle &= \int_\Omega d^3x\ \chi(\vec{x})^\dagger\left[\vec{\alpha}\cdot\vec{p}c+\beta Mc^2\right]\Psi(\vec{x}) \\
&= \int_\Omega d^3x\ \chi(\vec{x})^\dagger\left[\vec{\alpha}\cdot\left(-i\vec{\nabla}\right)c+\beta Mc^2\right]\Psi(\vec{x}) \\
&= \int_\Omega d^3x\ \left\{\left[\vec{\alpha}\cdot\left(-i\vec{\nabla}\right)c+\beta Mc^2\right]\chi(\vec{x})\right\}^\dagger\Psi(\vec{x}) \\
&- ic\int_{\partial\Omega} d\vec{n}\cdot\chi(\vec{x})^\dagger\vec{\alpha}\Psi(\vec{x}) \\
&= \langle\Psi|H|\chi\rangle^* - ic\int_{\partial\Omega} d\vec{n}\cdot\chi(\vec{x})^\dagger\vec{\alpha}\Psi(\vec{x}), \qquad (5.1)
\end{aligned}$$

which thus leads to the Hermiticity condition

$$\chi(\vec{x})^\dagger\vec{n}(\vec{x})\cdot\vec{\alpha}\Psi(\vec{x}) = 0, \quad \vec{x}\in\partial\Omega. \qquad (5.2)$$

Here $\vec{n}(\vec{x})$ is the unit-vector normal to the boundary $\partial\Omega$. Next we introduce the self-adjoint extension condition

$$\left(\begin{array}{c}\Psi_3(\vec{x})\\ \Psi_4(\vec{x})\end{array}\right) = \lambda(\vec{x})\left(\begin{array}{c}\Psi_1(\vec{x})\\ \Psi_2(\vec{x})\end{array}\right), \quad \lambda(\vec{x})\in GL(2,\mathbb{C}), \quad \vec{x}\in\partial\Omega, \qquad (5.3)$$

which turns eq.(5.2) to

$$\chi(\vec{x})^\dagger \left(\begin{array}{cc} 0 & \vec{n}(\vec{x}) \cdot \vec{\sigma} \\ \vec{n}(\vec{x}) \cdot \vec{\sigma} & 0 \end{array} \right) \Psi(\vec{x}) =$$
$$[(\chi_1(\vec{x})^*, \chi_2(\vec{x})^*)\, \vec{n}(\vec{x}) \cdot \vec{\sigma} \lambda(\vec{x}) + (\chi_3(\vec{x})^*, \chi_4(\vec{x})^*)\, \vec{n}(\vec{x}) \cdot \vec{\sigma}] \left(\begin{array}{c} \Psi_1(\vec{x}) \\ \Psi_2(\vec{x}) \end{array} \right) = 0 \ \Rightarrow$$
$$\left(\begin{array}{c} \chi_3(\vec{x}) \\ \chi_4(\vec{x}) \end{array} \right) = -\vec{n}(\vec{x}) \cdot \vec{\sigma} \lambda(\vec{x})^\dagger \vec{n}(\vec{x}) \cdot \vec{\sigma} \left(\begin{array}{c} \chi_1(\vec{x}) \\ \chi_2(\vec{x}) \end{array} \right), \tag{5.4}$$

In order to guarantee self-adjointness of H, i.e. the equality of the domains $D(H) = D(H^\dagger)$, we demand

$$\lambda(\vec{x}) = -\vec{n}(\vec{x}) \cdot \vec{\sigma} \lambda(\vec{x})^\dagger \vec{n}(\vec{x}) \cdot \vec{\sigma} \ \Rightarrow \ \vec{n}(\vec{x}) \cdot \vec{\sigma} \lambda(\vec{x}) = - \left[\vec{n}(\vec{x}) \cdot \vec{\sigma} \lambda(\vec{x})\right]^\dagger. \tag{5.5}$$

Hence, $\vec{n}(\vec{x}) \cdot \vec{\sigma} \lambda(\vec{x})$ is anti-Hermitean. For Dirac fermions, there is thus a 4-parameter family of self-adjoint extensions that characterizes a perfectly reflecting wall. In the MIT bag model [20–22], the boundary condition was chosen as $\lambda(\vec{x}) = i\vec{n}(\vec{x}) \cdot \vec{\sigma}$. This maintains spatial rotation invariance around the normal $\vec{n}(\vec{x})$ on the boundary, but is not the most general choice.

Let us now impose the Majorana condition eq.(4.6), which implies

$$\lambda(\vec{x}) \left(\begin{array}{c} \Psi_1(\vec{x},t) \\ \Psi_2(\vec{x},t) \end{array} \right) = \left(\begin{array}{c} \Psi_3(\vec{x},t) \\ \Psi_4(\vec{x},t) \end{array} \right) = -\sigma^2 \left(\begin{array}{c} \Psi_1(\vec{x},t)^* \\ \Psi_2(\vec{x},t)^* \end{array} \right) \ \Rightarrow$$
$$\lambda(\vec{x})^* \left(\begin{array}{c} \Psi_1(\vec{x},t)^* \\ \Psi_2(\vec{x},t)^* \end{array} \right) = \sigma^2 \left(\begin{array}{c} \Psi_1(\vec{x},t) \\ \Psi_2(\vec{x},t) \end{array} \right) \ \Rightarrow$$
$$\lambda(\vec{x}) \sigma^2 \lambda(\vec{x})^* \left(\begin{array}{c} \Psi_1(\vec{x},t)^* \\ \Psi_2(\vec{x},t)^* \end{array} \right) = \lambda(\vec{x}) \left(\begin{array}{c} \Psi_1(\vec{x},t)^* \\ \Psi_2(\vec{x},t)^* \end{array} \right) = -\sigma^2 \left(\begin{array}{c} \Psi_1(\vec{x},t)^* \\ \Psi_2(\vec{x},t)^* \end{array} \right) \tag{5.6}$$

In order to be consistent with the Majorana condition eq.(4.6), the matrix $\lambda(\vec{x})$ of self-adjoint extension parameters must hence obey

$$\lambda(\vec{x}) \sigma^2 \lambda(\vec{x})^* = -\sigma^2. \tag{5.7}$$

How does this constraint affect the original 4-parameter family of self-adjoint extensions? In order to answer this question, let us perform a unitary transformation $V(\vec{x}) \in SU(2)$ that diagonalizes $\vec{n}(\vec{x}) \cdot \vec{\sigma}$, i.e.

$$V(\vec{x}) \vec{n}(\vec{x}) \cdot \vec{\sigma} V(\vec{x})^\dagger = \sigma^3, \quad V(\vec{x}) \lambda(\vec{x}) V(\vec{x})^\dagger = \lambda(\vec{x})' \ \Rightarrow$$
$$\sigma^3 \lambda(\vec{x})' = - \left[\sigma^3 \lambda(\vec{x})'\right]^\dagger, \quad \lambda(\vec{x})' \sigma^2 \lambda(\vec{x})'^* = -\sigma^2. \tag{5.8}$$

First of all, we make the ansatz

$$\lambda(\vec{x})' = \lambda_0(\vec{x})' + \vec{\lambda}(\vec{x})' \cdot \vec{\sigma}, \quad \lambda_0(\vec{x})', \lambda_i(\vec{x})' \in \mathbb{C}. \tag{5.9}$$

The condition

$$\sigma^3 \lambda(\vec{x})' = - \left[\sigma^3 \lambda(\vec{x})'\right]^\dagger, \tag{5.10}$$

then implies

$$\lambda_0(\vec{x})' = -\lambda_0(\vec{x})'^*, \quad \lambda_1(\vec{x})' = \lambda_1(\vec{x})'^*, \quad \lambda_2(\vec{x})' = \lambda_2(\vec{x})'^*, \quad \lambda_3(\vec{x})' = -\lambda_3(\vec{x})'^*, \tag{5.11}$$

which indeed represents a 4-parameter family of self-adjoint extensions. The additional relation

$$\lambda(\vec{x})'\sigma^2\lambda(\vec{x})'^* = -\sigma^2, \tag{5.12}$$

can be satisfied in two different ways. First, we assume that $\lambda_1(\vec{x})' = \lambda_2(\vec{x})' = 0$. In that case, eq.(5.12) implies

$$\lambda_0(\vec{x})'^2 - \lambda_3(\vec{x})'^2 = 1, \tag{5.13}$$

which reduces the original 4-parameter family for Dirac fermions to a 1-parameter family of self-adjoint extensions for Majorana fermions. Alternatively, we may assume that $\lambda_0(\vec{x})' = \lambda_3(\vec{x})' = 0$. In that case, eq.(5.12) implies

$$\lambda_1(\vec{x})'^2 + \lambda_2(\vec{x})'^2 = 1, \tag{5.14}$$

which corresponds to another 1-parameter family of self-adjoint extensions. Hence, we conclude that the boundary conditions for Majorana fermions confined to a finite 3-d spatial volume are characterized by two distinct 1-parameter families of self-adjoint extensions.

6 Conclusions

Motivated by the edge modes of Kitaev wires or superconductors, as well as by engineered quantum systems of ultracold atoms or trapped ions that can be used as quantum simulators, we have investigated Majorana fermions confined to a 1-d interval or to a 3-d finite volume. This required an understanding of the self-adjoint extension parameters that characterize the most general perfectly reflecting boundary conditions. In contrast to (1 + 1)-d Dirac fermions, whose hard wall boundary conditions are described by a continuous 1-parameter family of self-adjoint extension parameters, there are only two discrete types of wall boundary conditions for (1 + 1)-d Majorana fermions. In three spatial dimensions, on the other hand, the most general perfectly reflecting wall boundary condition for Dirac fermions is characterized by a 4-parameter family of self-adjoint extension parameters, while the corresponding boundary condition for Majorana fermions is characterized by two different families of self-adjoint extensions, each with only a single parameter. Based on these results, one can derive the features of engineered systems of Majorana fermions in a variety of confining spatial geometries, which we did here explicitly for a 1-d interval. In addition, we have mapped the Majorana equation in one and three spatial dimensions to an equivalent nonlocal relativistic Schrödinger-type equation, whose quantum mechanical interpretation as a single-particle equation is not problematical.

Acknowledgments

This publication was made possible by the NPRP grant # NPRP 5 - 261-1-054 from the Qatar National Research Fund (a member of the Qatar Foundation). The statements made herein are solely the responsibility of the authors.

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