From a Particle in a Box to the Uncertainty Relation in a Quantum Dot and to Reflecting Walls for Relativistic Fermions

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Abstract

We consider a 1-parameter family of self-adjoint extensions of the Hamiltonian for a particle confined to a finite interval with perfectly reflecting boundary conditions. In some cases, one obtains negative energy states which seems to violate the Heisenberg uncertainty relation. We use this as a motivation to derive a generalized uncertainty relation valid for an arbitrarily shaped quantum dot with general perfectly reflecting walls in $d$ dimensions. In addition, a general uncertainty relation for non-Hermitean operators is derived and applied to the non-Hermitean momentum operator in a quantum dot. We also consider minimal uncertainty wave packets in this situation, and we prove that the spectrum depends monotonically on the self-adjoint extension parameter. In addition, we construct the most general boundary conditions for semiconductor heterostructures such as quantum dots, quantum wires, and quantum wells, which are characterized by a 4-parameter family of self-adjoint extensions. Finally, we consider perfectly reflecting boundary conditions for relativistic fermions confined to a finite volume or localized on a domain wall, which are characterized by a 1-parameter family of self-adjoint extensions in the $(1 + 1)$-d and $(2 + 1)$-d cases, and by a 4-parameter family in the $(3 + 1)$-d and $(4 + 1)$-d cases.
1 Introduction

The subtle differences between Hermiticity and self-adjointness of quantum mechanical operators, which were first understood by von Neumann [1], are rarely emphasized in quantum mechanics textbooks. This already affects the elementary textbook problem of a particle in a box [2]. Almost exclusively, the students are taught to set the wave function to zero at the boundary, in order to ensure its continuity. However, it is sufficient to guarantee that no probability leaks outside the box, i.e. that the probability current (but not necessarily the wave function itself) vanishes at the boundary. The resulting most general perfectly reflecting boundary condition contains a real-valued parameter that characterizes a family of self-adjoint extensions of the quantum mechanical Hamiltonian. In general, the wave function then does not go to zero at the boundary, and consequently the probability density to find the particle directly at the wall does not vanish. This is consistent with classical intuition of a ball bouncing off a perfectly reflecting wall.

While the self-adjoint extensions of the Hamiltonian are certainly known to the experts, in the beginning of this paper we introduce them in a pedagogical manner, since they, unfortunately, seem not to constitute common knowledge in quantum mechanics. When re-doing the standard textbook problem of a particle in a box, we will find states of negative energy for a particle with only kinetic energy. Such states seem to violate the Heisenberg uncertainty relation. In order to clarify this issue we then derive a generalized uncertainty relation valid for a particle confined to an arbitrarily shaped region with general perfectly reflecting walls in $d$ dimensions. This situation is relevant in the context of quantum dots. The most general perfectly reflecting boundary condition ensures that the component of the current normal to the reflecting surface must vanish. Again there is a 1-parameter family of self-adjoint extensions. The real-valued parameter that characterizes the boundary condition is a material-specific constant whose value could be determined experimentally for actual quantum dots. In particular, this parameter enters the generalized uncertainty relation. We also consider minimal uncertainty wave packets in a general quantum dot. Interestingly, when the self-adjoint extension parameter vanishes, a constant wave function of zero energy has $\Delta p = 0$ and saturates the generalized uncertainty relation. While the purpose of our paper is to some extent pedagogical, to the best of our knowledge the generalized uncertainty relation for quantum dots has not been derived before. Perfectly reflecting boundary conditions for relativistic fermions have been investigated in the context of the MIT bag model [3–5]. Here we construct the most general boundary condition for relativistic Dirac fermions, which is characterized by a 1-parameter family of self-adjoint extensions in the $(1 + 1)$-d case, and by a 4-parameter family in the $(3 + 1)$-d case. Finally, we extend the discussion to domain wall fermions in $(2 + 1)$-d and $(4 + 1)$-d space-times.

The paper is organized as follows. In section 2 we discuss a particle confined to a finite interval with general perfectly reflecting boundary conditions, and we
derive the corresponding generalized uncertainty relation. In section 3 this relation is extended to an arbitrarily shaped quantum dot with perfectly reflecting walls in \(d\) dimensions. We also derive a general uncertainty relation for non-Hermitean operators and apply it to the non-Hermitean momentum operator. In addition, we construct the corresponding most general minimal uncertainty wave packet, and we prove that the spectrum varies monotonically with the self-adjoint extension parameter. We also construct the most general boundary conditions for semiconductor heterostructures. In section 4, we extend the discussion to relativistic Dirac fermions in \((1 + 1)\)-d and \((3 + 1)\)-d, and in section 5 to domain wall fermions in \((2 + 1)\)-d and \((4 + 1)\)-d space-times. Finally, section 6 contains our conclusions.

## 2 Particle in a 1-d Box with General Perfectly Reflecting Walls

Let us consider a particle of mass \(m\) moving in the 1-d interval \(\Omega = [-L/2, L/2]\). This problem has been discussed in the context of self-adjoint extensions in [2]. Other examples of quantum mechanical problems involving the theory of self-adjoint extensions are discussed, for example, in [3]. We use natural units in which \(\hbar = 1\). For simplicity, we restrict the Hamiltonian to the kinetic energy operator

\[
H = \frac{p^2}{2m} = -\frac{1}{2m} \partial_x^2. \tag{2.1}
\]

The wave function \(\Psi(x, t)\) gives rise to the probability current density

\[
j(x, t) = \frac{1}{2m} \left[ \Psi(x, t) \overline{\partial_x \Psi(x, t)} - \partial_x \Psi(x, t) \overline{\Psi(x, t)} \right], \tag{2.2}
\]

which together with the probability density \(\rho(x, t) = |\Psi(x, t)|^2\) obeys the continuity equation

\[
\partial_t \rho(x, t) + \partial_x j(x, t) = 0. \tag{2.3}
\]

In the following discussion, we can ignore the time-dependence of the wave function and simplify the notation to \(\Psi(x)\).

### 2.1 Spatial Boundary Conditions

In order to guarantee probability conservation, one must demand that the probability current vanishes at the boundary, i.e.

\[
j(L/2) = j(-L/2) = 0. \tag{2.4}
\]

The most general local boundary condition that implies this takes the form

\[
\gamma(x)\Psi(x) + \partial_x \Psi(x) = 0, \quad x = \pm L/2. \tag{2.5}
\]
Indeed, one then obtains
\[ j(x) = \frac{1}{2m} [ -\Psi(x)^* \gamma(x) \Psi(x) + \gamma(x)^* \Psi(x)^* \Psi(x) ] = 0 \Rightarrow \gamma(x) \in \mathbb{R}, \quad x = \pm L/2. \] (2.6)

The two real-valued parameters \( \gamma(L/2) \) and \( \gamma(-L/2) \) characterize a 1-parameter family of self-adjoint extensions of the Hamiltonian at each of the two ends of the interval \( \Omega \). In order not to break parity via the boundary conditions, we restrict ourselves to
\[ \gamma(L/2) = -\gamma(-L/2) = \gamma \in \mathbb{R}, \] (2.7)
such that
\[ \gamma \Psi(L/2) + \partial_x \Psi(L/2) = 0, \quad -\gamma \Psi(-L/2) + \partial_x \Psi(-L/2) = 0. \] (2.8)

### 2.2 Self-Adjointness of the Hamiltonian

In order to investigate whether the Hamiltonian is indeed self-adjoint when the wave functions obey the boundary conditions eq.(2.8), we now consider

\[ \langle \Psi | H | \chi \rangle = -\frac{1}{2m} \int_{-L/2}^{L/2} dx \, \chi(x)^* \partial_x^2 \Psi(x) \]
\[ = \frac{1}{2m} \int_{-L/2}^{L/2} dx \, \partial_x \chi(x)^* \partial_x \Psi(x) - \frac{1}{2m} [ \chi(x)^* \partial_x \Psi(x) ]_{-L/2}^{L/2} \]
\[ = \frac{1}{2m} \int_{-L/2}^{L/2} dx \, \partial_x^2 \chi(x)^* \Psi(x) + \frac{1}{2m} [ \partial_x \chi(x)^* \Psi(x) - \chi(x)^* \partial_x \Psi(x) ]_{-L/2}^{L/2} \]
\[ = \langle \chi | H \chi \rangle^* + \frac{1}{2m} [ \partial_x \chi(x)^* \Psi(x) - \chi(x)^* \partial_x \Psi(x) ]_{-L/2}^{L/2}. \] (2.9)

The Hamiltonian is Hermitean (or symmetric in mathematical parlance) if
\[ \langle \chi | H | \Psi \rangle = \langle H^\dagger \chi | \Psi \rangle = \langle H \chi | \Psi \rangle = \langle \Psi | H \chi \rangle^*, \] (2.10)
which is indeed the case if
\[ [ \partial_x \chi(x)^* \Psi(x) - \chi(x)^* \partial_x \Psi(x) ]_{-L/2}^{L/2} = 0. \] (2.11)

The domain \( D(H) \) of the Hamiltonian contains the at least twice-differentiable square-integrable wave functions \( \Psi(x) \) that obey the boundary condition eq.(2.8). Using that condition, eq.(2.11) reduces to
\[ \Psi(L/2) [ \partial_x \chi(L/2)^* + \gamma \chi(L/2)^* ] - \Psi(-L/2) [ \partial_x \chi(-L/2)^* - \gamma \chi(-L/2)^* ] = 0. \] (2.12)
Since \( \Psi(L/2) \) and \( \Psi(-L/2) \) can take arbitrary values, the Hamiltonian is Hermitean if
\[ \gamma \chi(L/2) + \partial_x \chi(L/2) = 0, \quad -\gamma \chi(-L/2) + \partial_x \chi(-L/2) = 0, \] (2.13)
i.e. if the wave function $\chi(x)$ also obeys the boundary condition eq. (2.8). Imposing this boundary condition also on $\chi(x)$ implies that the domain of $H^\dagger$ coincides with the domain of $H$, $D(H^\dagger) = D(H)$. Since $H$ is indeed Hermitian when both $\Psi(x)$ and $\chi(x)$ obey eq. (2.8), and since, in addition, $D(H^\dagger) = D(H)$, the Hamiltonian is, in fact, self-adjoint.

It should be noted that there is even a 4-parameter family of self-adjoint extensions of $H$. Here we have encountered only two parameters, $\gamma(L/2)$ and $\gamma(-L/2)$, which we have reduced to one parameter $\gamma$ by demanding parity symmetry. The other two parameters of the 4-parameter family of self-adjoint extensions relate the values of the wave function and its derivative at $x = L/2$ to the corresponding values at $x = -L/2$. Such a boundary condition violates locality and is thus not physically meaningful in the present context.

### 2.3 Non-Hermiticity of the Momentum Operator

In order to investigate whether the momentum operator $p = -i\partial_x$ is self-adjoint or at least Hermitean, let us also consider

\[
\langle \chi | p | \Psi \rangle = -i \int_{-L/2}^{L/2} dx \chi(x)^\ast \partial_x \Psi(x)
\]

\[
= i \int_{-L/2}^{L/2} dx \partial_x \chi(x)^\ast \Psi(x) - i [\chi(x)^\ast \Psi(x)]_{-L/2}^{L/2}
\]

\[
= \langle \Psi | p | \chi \rangle^\ast - i [\chi(x)^\ast \Psi(x)]_{-L/2}^{L/2}.
\]  

(2.14)

Hence, $p$ would be Hermitean only if

\[
\chi(L/2)^\ast \Psi(L/2) = \chi(-L/2)^\ast \Psi(-L/2).
\]  

(2.15)

There is no reason why this should be the case when $\Psi(x)$ and $\chi(x)$ obey the boundary condition eq. (2.8). Hence, in the domain $D(H)$ of the Hamiltonian, the momentum operator $p$ is not even Hermitean, and thus certainly not self-adjoint.

The only self-adjoint extension of the momentum operator on a finite interval results from the boundary condition

\[
\Psi(L/2) = \lambda \Psi(-L/2), \quad \lambda \in \mathbb{C}.
\]  

(2.16)

Inserting this relation in eq. (2.15), we obtain

\[
\chi(L/2)^\ast \lambda \Psi(-L/2) = \chi(-L/2)^\ast \Psi(-L/2) \Rightarrow \chi(L/2) = \frac{1}{\lambda^\ast} \chi(-L/2).
\]  

(2.17)

If $\Psi(x)$ obeys eq. (2.16) and $\chi(x)$ obeys eq. (2.17) the operator $p$ is Hermitean (i.e. symmetric). The domain $D(p)$ contains those at least once-differentiable square-integrable wave functions $\Psi(x)$ that obey eq. (2.16). The domain $D(p^\dagger)$, on the
other hand, contains the corresponding wave functions $\chi(x)$ that obey eq. (2.17). The operator $p$ is self-adjoint only if $D(p) = D(p^\dagger)$ which implies

$$\lambda = \frac{1}{\lambda^*} \Rightarrow \lambda = \exp(i\theta) \Rightarrow$$

$$\Psi(L/2) = \exp(i\theta)\Psi(-L/2), \quad \chi(L/2) = \exp(i\theta)\chi(-L/2). \quad (2.18)$$

Hence, the momentum operator is self-adjoint only if the probability density is a periodic function, i.e. $\rho(L/2) = |\Psi(L/2)|^2 = |\Psi(-L/2)|^2 = \rho(-L/2)$. Since non-local periodic boundary conditions make no physical sense in the present context, and since the wave functions in the domain of the self-adjoint Hamiltonian obey the boundary condition eq. (2.8), but not eq. (2.18), in this case the momentum operator is neither Hermitean nor self-adjoint. Hence, we must conclude that, in the present context, momentum is not a physical observable. This indeed makes sense for a particle that is confined to a finite region of space. After all, a momentum measurement would put the particle in a momentum eigenstate, which also exists outside the box and would therefore require infinite energy. An alternative point of view is taken in [8, 9] where the infinite potential in the energetically forbidden region is approached as a limit of a large but finite potential.

### 2.4 Energy Spectrum and Energy Eigenstates

Let us now consider the energy eigenstates and the corresponding energy eigenvalues for the particle in a box with general reflecting boundary conditions parameterized by $\gamma$. First, we consider positive energy states of even parity, i.e.

$$\Psi_n(x) = A \cos(k_n x), \quad E_n = \frac{k_n^2}{2m}, \quad n = 0, 2, 4, \ldots, \infty. \quad (2.19)$$

The boundary condition eq. (2.8) then implies

$$\gamma \cos(k_n L/2) - k_n \sin(k_n L/2) = 0 \Rightarrow \frac{\gamma}{k_n} = \tan(k_n L/2). \quad (2.20)$$

Interestingly, for $\gamma = 0$ there is a zero-energy solution with $k_n = 0$ and a constant wave function $\Psi_0(x) = \sqrt{1/L}$.

Similarly, the positive energy states of odd parity take the form

$$\Psi_n(x) = A \sin(k_n x), \quad E_n = \frac{k_n^2}{2m}, \quad n = 1, 3, 5, \ldots, \infty, \quad (2.21)$$

and must obey

$$\gamma \sin(k_n L/2) + k_n \cos(k_n L/2) = 0 \Rightarrow \frac{\gamma}{k_n} = -\cot(k_n L/2). \quad (2.22)$$
In this case, a zero-energy solution exists for $\gamma = -2/L$ with the wave function
$\Psi_1(x) = \sqrt{\frac{12}{L^3}} x$. While this solution emerges from $\Psi_1(x) = A \sin(k_1 x)$ in the
limit $\gamma \to -2/L$, it also follows directly from the zero-energy Schrödinger equation
$\partial_x^2 \Psi(x) = 0$, and the boundary condition $(-2/L) \Psi(L/2) + \partial_x \Psi(L/2) = 0$.

Next, let us consider eigenstates of negative energy and even parity. In that case,
the wave function takes the form
$\Psi_0(x) = A \cosh(\kappa x), \ E_0 = -\frac{\kappa^2}{2m}$, \hspace{1cm} (2.23)
and must obey
$\gamma \cosh(\kappa L/2) + \kappa \sinh(\kappa L/2) = 0 \Rightarrow \frac{\gamma}{\kappa} = -\tanh(\kappa L/2)$.
(2.24)
Again, for $\gamma = 0$ one recovers the zero-energy state $\Psi_0(x) = \sqrt{1/L}$.

Finally, we consider the negative energy eigenstates with odd parity, i.e.
$\Psi_1(x) = A \sinh(\kappa x), \ E_1 = -\frac{\kappa^2}{2m}$, \hspace{1cm} (2.25)
which must obey
$\gamma \sinh(\kappa L/2) + \kappa \cosh(\kappa L/2) = 0 \Rightarrow \frac{\gamma}{\kappa} = -\coth(\kappa L/2)$.
(2.26)
In this case, for $\gamma = -2/L$ we recover the zero-energy eigenstate $\Psi_1(x) = \sqrt{12/L^3} x$.

The spectrum as a function of $\gamma$ as well as the corresponding wave functions
are illustrated in figure 1. For $\gamma = \infty$, we recover the standard textbook case with
$\Psi(L/2) = \Psi(-L/2) = 0$. In that case, the energy spectrum takes the familiar form
$E_n(\gamma \to \infty) = \frac{\pi^2(n + 1)^2}{2mL^2}, \ n = 0, 1, 2, \ldots, \infty$. \hspace{1cm} (2.27)
As $\gamma$ decreases to zero, the energy eigenvalues decrease such that
$E_n(\gamma = 0) = \frac{\pi^2 n^2}{2mL^2}, \ n = 0, 1, 2, \ldots, \infty$. \hspace{1cm} (2.28)
For $-2/L < \gamma < 0$ there is one negative energy state, and for $\gamma < -2/L$ there are
even two negative energy states, which reach negative infinite energies in the limit
$\gamma \to -\infty$, i.e.
$E_{0,1}(\gamma \to -\infty) \to -\frac{\gamma^2}{2m} \to -\infty$. \hspace{1cm} (2.29)
In the limit $\gamma \to -\infty$, the wave functions of the negative energy states reduce to
$\delta$-function-like structures localized at the boundaries. The rest of the spectrum is
exactly as in the standard textbook case (i.e. $\gamma = \infty$), namely
$E_n(\gamma \to -\infty) = \frac{\pi^2(n - 1)^2}{2mL^2}, \ n = 2, 3, 4, \ldots, \infty$. \hspace{1cm} (2.30)
Figure 1: Top panel: Energy spectrum of a particle in a 1-d box as a function of the self-adjoint extension parameter $\gamma$. The $x$-value represents $\arctan(\gamma L/2) \in [-\pi/2, \pi/2]$, which corresponds to $\gamma \in [-\infty, \infty]$. The $y$-value represents the energies $E_n$ (with $n = 0, 1, 2, 3, 4$) in units of $\pi^2/(2mL^2)$. Bottom panel: The wave functions $\Psi_n(x)$, $x \in [-L/2, L/2]$, (with $n = 0, 1, 2, 3$), for $\gamma = -\infty, -\frac{L}{2}, 0, \infty$. The sharp peaks in the $n = 0$ and $n = 1$ states at $\gamma = -\infty$ represent $\delta$-function-type wave functions of negative infinite energy localized at the boundaries. Except for these states, the energies and wave functions at $\gamma = -\infty$ are the same as those at $\gamma = \infty$. 
The existence of negative energy states is somewhat counter-intuitive. In particular, since the boundary conditions are perfectly reflecting, one may expect that the particle cannot bind to the wall. However, quantum mechanics does indeed allow the existence of walls which are perfectly reflecting for positive energy states and, at the same time, “sticky” for negative energy states. Since negative energy states have \( E = \langle p^2 / 2m \rangle < 0 \), they seem to violate the Heisenberg uncertainty relation \( \Delta x \Delta p \geq \frac{1}{2} \). Obviously, any state confined to the box has \( \Delta x \leq L / 2 \). Hence, the Heisenberg uncertainty relation seems to suggest that \( \Delta p \geq 1 / L \), which would be in conflict with \( \langle p^2 \rangle < 0 \). To resolve this puzzle, one must realize that the Heisenberg uncertainty relation was derived for an infinite volume, and thus needs to be reconsidered in a finite box with perfectly reflecting boundary conditions.

2.5 Uncertainty Relation for a 1-d Box with Perfectly Reflecting Boundary Conditions

Let us derive a variant of the Heisenberg uncertainty relation, taking into account the boundary condition eq. (2.8). We follow the standard procedure by constructing the non-negative integral

\[
I = \int_{-L/2}^{L/2} dx \left| \partial_x \Psi(x) + \alpha x \Psi(x) + \beta \Psi(x) \right|^2 \geq 0. \tag{2.31}
\]

Here \( \alpha \in \mathbb{R} \) and \( \beta = \beta_r + i\beta_i \in \mathbb{C} \) are parameters to be varied in order to minimize \( I \) and thus derive the most stringent inequality. Using partial integration as well as the boundary condition eq. (2.8), it is straightforward to obtain

\[
I = \langle p^2 \rangle - \alpha + \beta_r^2 + \beta_i^2 + \alpha^2 \langle x^2 \rangle + 2\alpha \beta_r \langle x \rangle + 2\beta_i \overline{p} + \alpha a - b + \beta_r c, \tag{2.32}
\]

where we have introduced

\[
a = \frac{L}{2} [\rho(L/2) + \rho(-L/2)], \]
\[
b = \gamma [\rho(L/2 + \rho(-L/2)], \]
\[
c = \rho(L/2) - \rho(-L/2), \quad \rho(\pm L/2) = |\Psi(\pm L/2)|^2. \tag{2.33}
\]

We have also defined

\[
\overline{p} = \mathbb{R} \int_{-L/2}^{L/2} dx \, \Psi(x)^* (-i\partial_x) \Psi(x). \tag{2.34}
\]

If \( p = -i\partial_x \) were a self-adjoint operator, \( \overline{p} \) would simply be the momentum expectation value. However, since \( p \) is not self-adjoint in this case, the corresponding expectation value is in general complex. In particular, \( \overline{p} \) is not the expectation value of any observable associated with a self-adjoint operator.
By varying $\alpha$, $\beta_r$, and $\beta_i$ in order to minimize $I$, one obtains

\[
\begin{align*}
\frac{\partial I}{\partial \alpha} &= -1 + 2\alpha\langle x^2 \rangle + 2\beta_r\langle x \rangle + a = 0, \\
\frac{\partial I}{\partial \beta_r} &= 2\beta_r + 2\alpha\langle x \rangle + c = 0 \Rightarrow \beta_r = -\alpha\langle x \rangle - \frac{c}{2}, \\
\frac{\partial I}{\partial \beta_i} &= 2\beta_i + 2\bar{p} = 0 \Rightarrow \beta_i = -\bar{p},
\end{align*}
\]

which implies

\[
\alpha = \frac{1 + c\langle x \rangle - a}{2(\Delta x)^2}, \quad (\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = \langle (x - \langle x \rangle)^2 \rangle. \quad (2.36)
\]

Inserting these results for $\alpha$, $\beta_r$, and $\beta_i$ back into the expression for $I$, eq. (2.32), one obtains

\[
I = \langle p^2 \rangle - \bar{p}^2 - \left(\frac{1 + c\langle x \rangle - a}{2\Delta x}\right)^2 - b - \frac{c^2}{4} \geq 0, \quad (2.37)
\]

which implies the generalized uncertainty relation

\[
\langle p^2 \rangle \geq \bar{p}^2 + \left(\frac{1 + c\langle x \rangle - a}{2\Delta x}\right)^2 + b + \frac{c^2}{4}. \quad (2.38)
\]

In the infinite volume limit, the wave function vanishes at infinity, such that $a = b = c = 0$. Furthermore, the momentum operator would then be self-adjoint with $\langle p \rangle = \bar{p}$. Hence, in the infinite volume limit, the inequality (2.38) reduces to the standard Heisenberg uncertainty relation

\[
\langle p^2 \rangle \geq \langle p \rangle^2 + \left(\frac{1}{2\Delta x}\right)^2 \Rightarrow \Delta x\Delta p \geq \frac{1}{2}, \quad (\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2 = \langle (p - \langle p \rangle)^2 \rangle. \quad (2.39)
\]

Interestingly, thanks to time-reversal invariance, the eigenfunctions of the particle in the 1-d box are real-valued and thus $\bar{p} = 0$. Since $H = p^2/2m$, for energy eigenstates the generalized uncertainty relation takes the form

\[
2mE_n = \langle p^2 \rangle \geq \left(\frac{1 + c\langle x \rangle - a}{2\Delta x}\right)^2 + b + \frac{c^2}{4}. \quad (2.40)
\]

The zero-energy eigenstate $\Psi_0(x) = \sqrt{1/L}$ for $\gamma = 0$ has $a = 1$, $b = c = 0$, such that the uncertainty relation reduces to $2mE_0 \geq 0$, which is indeed satisfied as an equality. This means that this state represents a minimal uncertainty wave packet. The zero-energy state $\Psi_1(x) = \sqrt{12/L^2} x$ for $\gamma = -2/L$, on the other hand, has $a = 3$, $b = -12/L^2$, $c = 0$, as well as $\Delta x = \sqrt{3/20} L$, such that the inequality reduces to $2mE_1 \geq -16/(3L^2)$, which is again satisfied, but not saturated as an equality. Hence, in this case, the state does not represent a minimal uncertainty wave packet.
2.6 Constructing a Wall with $\gamma < \infty$

It is interesting to ask whether perfectly reflecting walls with $\gamma < \infty$ are just a mathematical curiosity or whether they can also be constructed physically. Of course, it is clear that, independent of the value of $\gamma$, a perfectly reflecting wall is always a mathematical idealization. Any real wall will eventually be penetrable if it is hit by a sufficiently energetic particle. In this context it may be interesting to mention the MIT bag model [3–5], in which quarks are confined by restricting them to a finite region of space with perfectly reflecting boundary conditions. While this model is quite successful in modeling the confinement of quarks, in the fundamental QCD theory confinement does not arise through perfectly reflecting walls but through confining strings. When a dynamical QCD string connects a very energetic quark-anti-quark pair, the string can break by the dynamical creation of further quark-anti-quark pairs. Since perfectly reflecting walls do not even exist in the confining theory of the strong force, they certainly do not exist in condensed matter either. However, when low-energy particles hit a very high energy barrier, it acts effectively like a reflecting wall. In this sense, the self-adjoint extension parameter $\gamma$ can be viewed as a low-energy parameter that characterizes the reflection properties of a very high energy barrier.

Since $\gamma$ appears as a natural mathematical parameter characterizing a perfectly reflecting wall, there is no reason to expect that it cannot be physically realized. To show this explicitly, we now construct a wall with an arbitrary value of $\gamma$ as a limit of square-well potentials. Let us consider the potential illustrated in figure 2, which consists of a perfectly reflecting wall at $x = 0$ with the standard textbook value $\gamma = \infty$, and a very narrow and very deep square-well potential of size $\epsilon > 0$ and depth $-V_0 < 0$ next to it. The wave function then takes the form

$$\Psi(x) = A \sin(qx), \quad 0 \leq x \leq \epsilon, \quad E = \frac{q^2}{2m} - V_0.$$  \hspace{1cm} (2.41)

For $x \geq \epsilon$, the wave function is determined by enforcing continuity of the wave function itself and its derivative at $x = \epsilon$. When $\epsilon \to 0$, we can determine the resulting value of $\gamma$ from

$$-\gamma \Psi(\epsilon) + \partial_x \Psi(\epsilon) = 0 \quad \Rightarrow \quad \gamma = q \cot(q\epsilon).$$  \hspace{1cm} (2.42)

In order to keep $\gamma$ fixed as $\epsilon \to 0$, we must hence let $q$ go to infinity such that

$$q = \frac{\pi}{2\epsilon} - \frac{2}{\pi \gamma}.$$  \hspace{1cm} (2.43)

For all states of finite energy $E$, this is achieved by sending $V_0 = q^2/2m \to \infty$, in such a way that

$$V_0 = \frac{1}{2m} \left( \frac{\pi}{2\epsilon} - \frac{2}{\pi \gamma} \right)^2.$$  \hspace{1cm} (2.44)

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1We like to thank F. Niedermayer for suggesting this construction.
Figure 2: A deep and narrow square-well potential \( V(x) \) with depth \(-V_0 \to -\infty\) and width \( \epsilon \to 0\) mimics a boundary with non-standard self-adjoint extension parameter \( \gamma < \infty \). The wave function \( \Psi(x) \) and its first derivative are continuous at \( x = \epsilon \). In the example shown here, \( \gamma < 0 \), such that a bound state is localized at the boundary.

It goes without saying that a perfectly reflecting wall with an arbitrary value of \( \gamma \) can also be constructed in many other ways, for example, by using an attractive \( \delta \)-function potential next to the wall.

## 2.7 Experimental Determination of \( \gamma \)

It is natural to ask how one can determine the value of \( \gamma \) for some perfectly reflecting wall that can be investigated experimentally. For example, for a planar homogeneous perfectly reflecting wall, the material-specific parameter \( \gamma \) can be determined from the scattering phase shift \( \delta(k) \) of an incident plane wave that propagates perpendicular to the surface. Assuming that the incident wave propagates in the negative \( x \)-direction in the region \( x > 0 \), and scatters off a perfectly reflecting wall at \( x = 0 \), the wave function takes the form

\[
\Psi(x) = \exp(-ikx) + R \exp(ikx), \quad x \geq 0. \tag{2.45}
\]

Imposing the boundary condition

\[
- \gamma \Psi(0) + \partial_x \Psi(0) = 0, \tag{2.46}
\]
one obtains
\[-\gamma(1 + R) - ik(1 - R) = 0 \Rightarrow R = \exp(i\delta(k)) = \frac{\gamma + ik}{\gamma - ik}. \quad (2.47)\]

Hence, by measuring the phase shift
\[\delta(k) = 2\arctan(k/\gamma) + \pi, \quad (2.48)\]
one can determine the material-specific self-adjoint extension parameter $\gamma$.

3 Uncertainty Relation for a Quantum Dot with General Perfectly Reflecting Boundary Conditions

In this section we consider an arbitrarily shaped $d$-dimensional region $\Omega$ with general perfectly reflecting walls at the boundary $\partial\Omega$. This may be viewed as a model for a quantum dot, in which electrons are confined inside a finite region of space. As illustrated in figure 3, $\Omega$ may have multiple disconnected boundaries. For a mathematical exposition of boundary value problems for operator differential equations we refer to [10]. Let us consider the Hamiltonian
\[H = \frac{\hat{p}^2}{2m} + V(\vec{x}) = -\frac{1}{2m}\Delta + V(\vec{x}), \quad (3.1)\]
where $V(\vec{x})$ is a non-singular potential. In $d$ dimensions, the continuity equation for local probability conservation takes the form
\[\partial_t \rho(\vec{x}, t) + \vec{\nabla} \cdot \vec{j}(\vec{x}, t) = 0, \quad (3.2)\]
with the probability density and current density given by
\[\rho(\vec{x}, t) = |\Psi(\vec{x}, t)|^2, \quad \vec{j}(\vec{x}, t) = \frac{1}{2mi} \left[ \Psi(\vec{x}, t)\Psi^*(\vec{x}, t) - \Psi^*(\vec{x}, t)\Psi(\vec{x}, t) \right]. \quad (3.3)\]
Again, in the following discussion the time-dependence is not essential and we simplify the notation to $\Psi(\vec{x})$.

3.1 Spatial Boundary Conditions

As in the 1-d case, we demand that no probability may leak outside the region $\Omega$. This is ensured by requiring that the component of the probability current density normal to the surface vanishes, i.e.
\[\vec{n}(\vec{x}) \cdot \vec{j}(\vec{x}) = 0, \quad \vec{x} \in \partial\Omega, \quad (3.4)\]
Figure 3: A region $\Omega$ of a quantum dot with two disconnected boundaries $\partial \Omega$. The shaded region is energetically forbidden. The vector $\vec{n}$ is normal to the boundary.

where $\vec{n}(\vec{x})$ is the unit-vector normal to the surface $\partial \Omega$ at the point $\vec{x}$. The most general local boundary condition that ensures this takes the form

$$\gamma(\vec{x})\Psi(\vec{x}) + \vec{n}(\vec{x}) \cdot \vec{\nabla}\Psi(\vec{x}) = 0, \quad x \in \partial \Omega,$$  
(3.5)

and one then indeed obtains

$$\vec{n}(\vec{x}) \cdot \vec{j}(\vec{x}) = \frac{1}{2mi} [ -\Psi(\vec{x})^* \gamma(\vec{x})\Psi(\vec{x},t) + \gamma(\vec{x})^* \Psi(\vec{x},t)^* \Psi(\vec{x},t) ] = 0, \quad \vec{x} \in \partial \Omega,$$  
(3.6)

which again implies $\gamma(\vec{x}) \in \mathbb{R}$. In general $\gamma(\vec{x})$ will depend on the position $\vec{x} \in \partial \Omega$ on the boundary. In a real system such as a quantum dot, $\gamma(\vec{x})$ is a material-specific parameter, to be determined experimentally.
3.2 Self-Adjointness of the Hamiltonian

Let us again convince ourselves that the Hamiltonian endowed with the boundary condition eq.(3.5) is indeed self-adjoint. For this purpose, we consider

\[
\langle \chi | H | \Psi \rangle = \int_{\Omega} \! d^d x \, \chi(\vec{x})^* \left[ -\frac{1}{2m} \Delta + V(\vec{x}) \right] \Psi(\vec{x})
\]

\[- \frac{1}{2m} \int_{\partial \Omega} d\vec{n} \cdot \chi(\vec{x})^* \vec{\nabla} \Psi(\vec{x})
\]

\[
= \int_{\Omega} \! d^d x \left\{ -\frac{1}{2m} \Delta + V(\vec{x}) \right\} \chi(\vec{x})^* \Psi(\vec{x})
\]

\[+ \frac{1}{2m} \int_{\partial \Omega} d\vec{n} \cdot \left[ \vec{\nabla} \chi(\vec{x})^* \Psi(\vec{x}) - \chi(\vec{x})^* \vec{\nabla} \Psi(\vec{x}) \right]
\]

\[= \langle \Psi | H | \chi \rangle^* + \frac{1}{2m} \int_{\partial \Omega} d\vec{n} \cdot \left[ \vec{\nabla} \chi(\vec{x})^* \Psi(\vec{x}) - \chi(\vec{x})^* \vec{\nabla} \Psi(\vec{x}) \right]. \quad (3.7)
\]

Hence, the Hamiltonian is Hermitean if

\[
\int_{\partial \Omega} d\vec{n} \cdot \left[ \vec{\nabla} \chi(\vec{x})^* \Psi(\vec{x}) - \chi(\vec{x})^* \vec{\nabla} \Psi(\vec{x}) \right] = 0. \quad (3.8)
\]

Using the boundary condition eq.(3.5), the integral in eq.(3.8) reduces to

\[
\int_{\partial \Omega} d^{d-1} \vec{x} \left[ \vec{n}(\vec{x}) \cdot \vec{\nabla} \chi(\vec{x})^* + \gamma(\vec{x}) \chi(\vec{x})^* \right] \Psi(\vec{x}) = 0. \quad (3.9)
\]

Since \( \Psi(\vec{x}) \) itself can take arbitrary values at the boundary, the Hermiticity of \( H \) requires that

\[
\vec{n}(\vec{x}) \cdot \vec{\nabla} \chi(\vec{x}) + \gamma(\vec{x}) \chi(\vec{x}) = 0. \quad (3.10)
\]

For \( \gamma(\vec{x}) \in \mathbb{R} \), this is again the boundary condition of eq.(3.5), which ensures that \( D(H^\dagger) = D(H) \), such that \( H \) is indeed self-adjoint. In complete analogy to the 1-d case, it is easy to convince oneself that the momentum operator \( \vec{p} = -i \vec{\nabla} \) is not even Hermitean in the domain \( D(H) \) of the Hamiltonian, which contains those twice-differentiable and square-integrable wave functions that obey the boundary condition eq.(3.5).

3.3 Generalized Uncertainty Relation

Mathematical investigations of generalized uncertainty relations can be found, for example, in \([11, 12]\). In this subsection, we derive a generalized uncertainty relation
for an arbitrarily shaped quantum dot in $d$ dimensions, by considering the non-negative integral

$$I = \int_{\Omega} d^d x \left| \nabla \Psi(\vec{x}) + \alpha \vec{x} \Psi(\vec{x}) + \vec{\beta} \Psi(\vec{x}) \right|^2 \geq 0.$$  

(3.11)

Again, $\alpha \in \mathbb{R}$ and $\vec{\beta} = \vec{\beta}_r + i \vec{\beta}_i \in \mathbb{C}^d$ are parameters to be varied in order to minimize $I$. Using the boundary condition eq. (3.5) after performing some partial integrations, one finds

$$I = \langle \vec{p}^2 \rangle - \alpha d + \vec{\beta}_r^2 + \vec{\beta}_i^2 + \alpha^2 \langle \vec{x}^2 \rangle + 2 \alpha \vec{\beta}_r \cdot \langle \vec{x} \rangle + 2 \vec{\beta}_i \cdot \vec{p} + \alpha \langle \vec{n} \cdot \vec{x} \rangle - \langle \gamma \rangle + \vec{\beta}_r \cdot \langle \vec{n} \rangle.$$

(3.12)

Here we have defined

$$\langle \vec{n} \cdot \vec{x} \rangle = \int_{\partial \Omega} d\vec{n} \cdot \vec{x} \rho(\vec{x}),$$

$$\langle \gamma \rangle = \int_{\partial \Omega} d^{d-1} x \, \gamma(\vec{x}) \rho(\vec{x}),$$

$$\langle \vec{n} \rangle = \int_{\partial \Omega} d\vec{n} \, \rho(\vec{x}), \quad \rho(\vec{x}) = |\Psi(\vec{x})|^2.$$  

(3.13)

In analogy to the 1-d case, we have also introduced

$$\vec{p} = \mathcal{R} \int_{\Omega} d^d x \, \Psi(\vec{x})^*(-i\nabla) \Psi(\vec{x}).$$

(3.14)

If $\vec{p} = -i\nabla$ had been a self-adjoint operator, $\vec{p}$ would be the momentum expectation value. However, in this case, $\vec{p}$ is again not the expectation value of any observable physical quantity.

By varying $\alpha$, $\vec{\beta}_r$, and $\vec{\beta}_i$, one obtains

$$\frac{\partial I}{\partial \alpha} = -d + 2\alpha \langle \vec{x}^2 \rangle + 2 \vec{\beta}_r \cdot \langle \vec{x} \rangle + \langle \vec{n} \cdot \vec{x} \rangle = 0,$$

$$\frac{\partial I}{\partial \vec{\beta}_r^j} = 2 \vec{\beta}_r^j + 2\alpha \langle x^j \rangle + \langle n^j \rangle = 0 \Rightarrow \vec{\beta}_r = -\alpha \langle \vec{x} \rangle - \frac{\langle \vec{n} \rangle}{2},$$

$$\frac{\partial I}{\partial \vec{\beta}_i^j} = 2 \vec{\beta}_i^j + 2\vec{p}^j = 0 \Rightarrow \vec{\beta}_i = -\vec{p},$$

(3.15)

which then implies

$$\alpha = \frac{d + \langle \vec{n} \cdot \vec{x} \rangle - \langle \vec{n} \cdot \vec{x} \rangle}{2(\Delta x)^2}, \quad (\Delta x)^2 = \langle \vec{x}^2 \rangle - \langle \vec{x} \rangle^2 = ((\vec{x} - \langle \vec{x} \rangle)^2).$$

(3.16)

Again, by inserting the results for $\alpha$, $\vec{\beta}_r$, and $\vec{\beta}_i$ back into eq. (3.12), one obtains

$$I = \langle \vec{p}^2 \rangle - \frac{\vec{p}^2}{4} - \left( \frac{d + \langle \vec{n} \cdot \vec{x} \rangle - \langle \vec{n} \cdot \vec{x} \rangle}{2\Delta x} \right)^2 - \langle \gamma \rangle - \frac{\langle \vec{n} \rangle^2}{4} \geq 0,$$

(3.17)
which finally implies the generalized uncertainty relation

\[ \langle \vec{p}^2 \rangle \geq \vec{p}^2 + \left( \frac{d + \langle \vec{n} \cdot \langle \vec{x} \rangle - \langle \vec{n} \cdot \vec{x} \rangle}{2 \Delta x} \right)^2 + \langle \gamma \rangle + \frac{\langle \vec{n} \rangle^2}{4}. \]  

(3.18)

It is not obvious that eq. (3.18) is invariant under a spatial translation \( \vec{x} \to \vec{x}' = \vec{x} + \vec{d} \). While \( \langle \vec{p}^2 \rangle, \vec{p}, \Delta x, \langle \gamma \rangle, \) and \( \langle \vec{n} \rangle \) are translation invariant by construction, \( \langle \vec{x} \rangle \) and \( \langle \vec{n} \cdot \vec{x} \rangle \) are not. It is thus reassuring to realize that the combination

\[ \langle \vec{n} \rangle \cdot \langle \vec{x}' \rangle - \langle \vec{n} \cdot \vec{x}' \rangle = \langle \vec{n} \rangle \cdot (\langle \vec{x} \rangle + \vec{d}) - \langle \vec{n} \cdot \vec{x} \rangle = \langle \vec{n} \rangle \cdot \langle \vec{x} \rangle - \langle \vec{n} \cdot \vec{x} \rangle, \]  

(3.19)

that enters the generalized uncertainty relation is indeed translation invariant.

All quantities entering the uncertainty relation, except \( \vec{p} \), are directly related to physically observable quantities. However, since the momentum is not a self-adjoint operator and hence not observable in a finite volume, despite the fact that it is mathematically completely well-defined, the quantity \( \vec{p} \) seems not to be physically measurable. In that case, the question arises how the generalized uncertainty relation should be interpreted physically. Since momentum cannot even be measured inside a quantum dot, \( (\Delta p)^2 = \langle \vec{p}^2 \rangle - \vec{p}^2 \) can obviously not be interpreted as the uncertainty of momentum. Still, \( \langle \vec{p}^2 \rangle \) determines the energy of an eigenstate of the free particle Hamiltonian with \( V(\vec{x}) = 0 \). Since time-reversal invariance guarantees that energy eigenstates have real-valued wave functions, for those states we know that \( \vec{p} = 0 \). In that case, the generalized uncertainty relation reduces to

\[ 2mE_n = \langle \vec{p}^2 \rangle \geq \left( \frac{d + \langle \vec{n} \cdot \langle \vec{x} \rangle - \langle \vec{n} \cdot \vec{x} \rangle}{2 \Delta x} \right)^2 + \langle \gamma \rangle + \frac{\langle \vec{n} \rangle^2}{4}, \]  

(3.20)

which indeed contains measurable physical quantities only.

3.4 General Uncertainty Relation for non-Hermitean Operators

For two general self-adjoint operators \( A \) and \( B \), the uncertainty relation is sometimes quoted as \( \Delta A \Delta B \geq \frac{1}{2} \langle [A, B] \rangle \). However, a more stringent form of the inequality is given by

\[ \Delta A \Delta B \geq |\langle \tilde{A} \tilde{B} \rangle| = |\langle AB \rangle - \langle A \rangle \langle B \rangle|, \quad \tilde{A} = A - \langle A \rangle, \quad \tilde{B} = B - \langle B \rangle. \]  

(3.21)

In the case discussed before, the momentum operator is not even Hermitean. Hence, the question arises, how the uncertainty relation looks like for a general pair of non-Hermitean operators \( A \neq A^\dagger \) and \( B \neq B^\dagger \). In that case, it is natural to define

\[ (\Delta A)^2 = \langle \tilde{A} \Psi | \tilde{A} \Psi \rangle = \langle \tilde{A}^\dagger \tilde{A} \rangle = \langle A^\dagger A \rangle - \langle A^\dagger \rangle \langle A \rangle = \langle A^\dagger A \rangle - |\langle A \rangle|^2 \geq 0. \]  

(3.22)
Here we have used $\langle A^\dagger \rangle = \langle A \rangle^*$. Using the Schwarz inequality, we then obtain

$$
(\Delta A)^2 (\Delta B)^2 = \langle \tilde{A} \Psi | \tilde{A} \Psi \rangle \langle \tilde{B} \Psi | \tilde{B} \Psi \rangle \\
\geq |\langle \tilde{A} \Psi | \tilde{B} \Psi \rangle|^2 = |\tilde{A}^\dagger \tilde{B}|^2 = |\langle A^\dagger B \rangle - \langle A^\dagger \rangle \langle B \rangle|^2,
$$

such that

$$
\Delta A \Delta B \geq |\langle A^\dagger B \rangle - \langle A^\dagger \rangle \langle B \rangle|.
$$

(3.23)

Let us compare the general uncertainty relation (3.24) for non-Hermitian operators with the generalized uncertainty relation (3.18) that we obtained for a particle confined to the region $\Omega$. In that case, we can identify $A$ with the self-adjoint operator $\vec{x}$ and $B$ with the non-Hermitian operator $\vec{p} = -i\vec{\nabla}$. The uncertainty of the momentum is then given by

$$
(\Delta p)^2 = \langle \vec{p}^2 \rangle - \langle \gamma \rangle.
$$

(3.25)

Since $\vec{p}^\dagger \neq \vec{p}$, in this case, $\vec{p}^\dagger \cdot \vec{p} \neq \vec{p}^2$. In particular, we obtain

$$
\langle \vec{p}^\dagger \cdot \vec{p} \rangle = \langle \vec{p} \Psi | \vec{p} \Psi \rangle = \int_{\Omega} d^d x \vec{\nabla} \Psi(\vec{x})^* \cdot \vec{\nabla} \Psi(\vec{x}) \\
= -\int_{\Omega} d^d x \Psi(\vec{x})^* \Delta \Psi(\vec{x}) + \int_{\partial \Omega} d\vec{n} \cdot \Psi(\vec{x})^* \vec{\nabla} \Psi(\vec{x}) \\
= \langle \vec{p}^2 \rangle - \int_{\partial \Omega} d^{d-1} x \gamma(\vec{x}) \Psi(\vec{x})^* \Psi(\vec{x}) = \langle \vec{p}^2 \rangle - \langle \gamma \rangle.
$$

(3.26)

Furthermore, decomposing $\langle \vec{p} \rangle$ into real and imaginary parts, we find

$$
\langle \vec{p} \rangle = \Re \int_{\Omega} d^d x \Psi(\vec{x})^* (-i\vec{\nabla}) \Psi(\vec{x}) + i \Im \int_{\Omega} d^d x \Psi(\vec{x})^* (-i\vec{\nabla}) \Psi(\vec{x}) = \overrightarrow{p} - \frac{i}{2} \langle \overrightarrow{n} \rangle.
$$

(3.27)

Here we have used

$$
\Im \int_{\Omega} d^d x \Psi(\vec{x})^* (-i\vec{\nabla}) \Psi(\vec{x}) = \frac{1}{2i} \int_{\Omega} d^d x \left[ \Psi(\vec{x})^* (-i\vec{\nabla}) \Psi(\vec{x}) - \Psi(\vec{x}) (i\vec{\nabla}) \Psi(\vec{x})^* \right] \\
= -\frac{1}{2} \int_{\partial \Omega} d\vec{n} \cdot \Psi(\vec{x})^* \Psi(\vec{x}) = -\frac{1}{2} \langle \overrightarrow{n} \rangle,
$$

(3.28)

and hence we obtain

$$
(\Delta p)^2 = \langle \vec{p}^2 \rangle - \langle \gamma \rangle - \overrightarrow{p}^2 - \langle \overrightarrow{n} \rangle^2.
$$

(3.29)

The generalized uncertainty relation (3.18) can thus be rewritten as

$$
\Delta x \Delta p \geq \frac{1}{2} |d + \langle \overrightarrow{n} \rangle \cdot \langle \vec{x} \rangle - \langle \overrightarrow{n} \cdot \vec{x} \rangle|.
$$

(3.30)

On the other hand, in this case the general uncertainty relation for non-Hermitian operators (3.24) takes the form

$$
\Delta x \Delta p \geq |\langle \vec{x} \cdot \vec{p} \rangle - \langle \vec{x} \rangle \cdot \langle \vec{p} \rangle|.
$$

(3.31)
Introducing \( \vec{x} \cdot \vec{p} = \Re \langle \vec{x} \cdot \vec{p} \rangle \) and using
\[
\mathcal{I} \langle \vec{x} \cdot \vec{p} \rangle = \frac{1}{2} \int_Ω d^d\vec{x} \Psi(\vec{x})^\ast (i\vec{n} \cdot \vec{x}) \Psi(\vec{x}) + \frac{i}{2} (d - \langle \vec{n} \cdot \vec{x} \rangle + \langle \vec{n} \rangle \cdot \langle \vec{x} \rangle),
\]
(3.32)
one obtains
\[
\langle \vec{x} \cdot \vec{p} \rangle - \langle \vec{x} \rangle \cdot \langle \vec{p} \rangle = \vec{x} - \langle \vec{x} \rangle \cdot \vec{p} + \frac{i}{2} (d - \langle \vec{n} \cdot \vec{x} \rangle + \langle \vec{n} \rangle \cdot \langle \vec{x} \rangle),
\]
(3.33)
such that
\[
\Delta x \Delta p \geq \sqrt{(\vec{x} - \langle \vec{x} \rangle \cdot \vec{p})^2 + \frac{1}{4} (d - \langle \vec{n} \cdot \vec{x} \rangle + \langle \vec{n} \rangle \cdot \langle \vec{x} \rangle)^2}.
\]
(3.34)
Hence, unless \( \vec{x} \cdot \vec{p} = \langle \vec{x} \rangle \cdot \vec{p} \), the general uncertainty relation for non-Hermitean operators (3.24) is more stringent than the generalized uncertainty relation (3.18).

Since energy eigenstates have a real-valued wave function, for them \( \vec{x} \cdot \vec{p} = 0 \) and \( \vec{p} = 0 \), such that both inequalities are then equivalent.

### 3.5 Minimal Uncertainty Wave Packets

It is interesting to ask which wave functions saturate the generalized uncertainty relation (3.18), and thus satisfy it as an equality. First of all, when \( \gamma(\vec{x}) = 0 \) everywhere at the boundary, the constant wave function \( \Psi(\vec{x}) = 1/\sqrt{V} \), where \( V \) is the volume of \( \Omega \), is an energy eigenstate of zero energy. In that case, we obtain \( \vec{p} = 0 \), \( \langle \gamma \rangle = 0 \), as well as
\[
\langle \vec{n} \cdot \vec{x} \rangle = \frac{1}{V} \int_{\partial Ω} d\vec{n} \cdot \vec{x} = \frac{1}{V} \int_Ω d^d\vec{x} \vec{n} \cdot \vec{x} = d,
\]
\[
\langle \vec{n} \rangle = \frac{1}{V} \int_{\partial Ω} d\vec{n} = \frac{1}{V} \int_Ω d^d\vec{x} \vec{n} \cdot 1 = 0,
\]
(3.35)
such that the inequality (3.18) then reduces to \( 2mE = \langle \vec{p}^2 \rangle \geq 0 \). Hence, the zero-energy state indeed saturates the inequality. In this sense, it can be viewed as a state of minimal uncertainty. Of course, one should not forget that, since in this case momentum is not even a physical observable, \( \langle \vec{p}^2 \rangle \) cannot be interpreted as the uncertainty of a momentum measurement.

Are there other minimal uncertainty wave packets beyond the zero-energy state with a constant wave function that exists for \( \gamma(\vec{x}) = 0 \)? It is clear by construction,
that the inequality (3.18) can be saturated only if the integrand in eq. (3.11) vanishes, i.e. if
\[ \vec{\nabla} \Psi(\vec{x}) + \alpha \vec{x} \Psi(\vec{x}) + \vec{\beta} \Psi(\vec{x}) = 0. \] (3.36)

Using the boundary condition eq. (3.5), for points \( \vec{x} \in \partial \Omega \) this implies
\[ \left(-\gamma(\vec{x}) + \alpha \vec{n}(\vec{x}) \cdot \vec{x} + \vec{n}(\vec{x}) \cdot \vec{\beta}\right) \Psi(\vec{x}) = 0 \Rightarrow \gamma(\vec{x}) = \vec{n}(\vec{x}) \cdot (\alpha \vec{x} + \vec{\beta}). \] (3.37)

Since \( \gamma(\vec{x}) \in \mathbb{R} \), we must further demand \( \vec{\beta} = -\vec{p} = 0 \). This implies that \( \gamma(\vec{x}) \) must have a very peculiar form at the boundary, which will generically not be the case. Thus, in general, there are no minimal uncertainty wave packets in a finite volume. In the bulk eq. (3.36) is satisfied just by the standard Gaussian wave packet
\[ \Psi(\vec{x}) = A \exp \left(-\frac{\alpha}{2} \vec{x}^2 - \vec{\beta} \cdot \vec{x}\right), \] (3.38)

which is known to saturate the Heisenberg uncertainty relation in the infinite volume. We then also have
\[ \alpha = \frac{d + \langle \vec{n} \rangle \cdot \langle \vec{x} \rangle - \langle \vec{n} \cdot \vec{x} \rangle}{2(\Delta x)^2}, \quad \vec{\beta} = -\alpha \langle \vec{x} \rangle - \frac{\langle \vec{n} \rangle}{2}, \] (3.39)
such that \( \gamma(\vec{x}) \) must satisfy
\[ \gamma(\vec{x}) = \vec{n}(\vec{x}) \cdot \left(\alpha(\vec{x} - \langle \vec{x} \rangle) - \frac{\langle \vec{n} \rangle}{2}\right) \Rightarrow \langle \gamma \rangle = \alpha(\langle \vec{n} \cdot \vec{x} \rangle - \langle \vec{n} \cdot \langle \vec{x} \rangle \rangle - \frac{\langle \vec{n} \rangle^2}{2}. \] (3.40)

Only if \( \gamma(\vec{x}) \) happens to be such that the Gaussian wave packet automatically satisfies the boundary condition, it remains a minimal uncertainty wave packet in the finite volume.

### 3.6 \( \gamma \)-Dependence of the Energy Spectrum

In this subsection we assume that \( \gamma(\vec{x}) = \gamma \in \mathbb{R} \) is a constant independent of the position \( \vec{x} \in \partial \Omega \) on the boundary. We then ask how the energy spectrum changes with \( \gamma \). A similar calculation for the Dirac operator in a relativistic field theory was performed in [13]. Let us introduce the energy eigenvalues \( E_n \) and the corresponding wave functions \( \Psi_n(\vec{x}) \), i.e.
\[ H \Psi_n(\vec{x}) = \left(-\frac{1}{2m} \Delta + V(\vec{x})\right) \Psi_n(\vec{x}) = E_n \Psi_n(\vec{x}). \] (3.41)

Both \( E_n \) and \( \Psi_n(\vec{x}) \) depend on \( \gamma \) via the boundary condition
\[ \gamma \Psi_n(\vec{x}) + \vec{n}(\vec{x}) \cdot \vec{\nabla} \Psi_n(\vec{x}) = 0, \quad \vec{x} \in \partial \Omega. \] (3.42)

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The $\gamma$-dependence of the energy spectrum follows from

\[
\partial_\gamma E_n = \partial_\gamma \int_{\Omega} d^d x \, \Psi_n(\vec{x})^* H \Psi_n(\vec{x})
\]

\[
= \int_{\Omega} d^d x \, \left[ \partial_\gamma \Psi_n(\vec{x})^* H \Psi_n(\vec{x}) + \Psi_n(\vec{x})^* H \partial_\gamma \Psi_n(\vec{x}) \right]
\]

\[
+ \frac{1}{2m} \int_{\partial\Omega} d\vec{n} \cdot \left[ \nabla \Psi_n(\vec{x})^* \partial_\gamma \Psi_n(\vec{x}) - \Psi_n(\vec{x})^* \nabla \partial_\gamma \Psi_n(\vec{x}) \right]
\]

\[
= E_n \partial_\gamma \int_{\Omega} d^d x \, \Psi_n(\vec{x})^* \Psi_n(\vec{x})
\]

\[
+ \frac{1}{2m} \int_{\partial\Omega} d^{d-1} x \, \left[ -\gamma \Psi_n(\vec{x})^* \partial_\gamma \Psi_n(\vec{x}) + \Psi_n(\vec{x})^* \partial_\gamma (\gamma \Psi_n(\vec{x})) \right]
\]

\[
= \frac{1}{2m} \int_{\partial\Omega} d^{d-1} x \, \Psi_n(\vec{x})^* \Psi_n(\vec{x}) = \frac{1}{2m} \int_{\partial\Omega} d^{d-1} x \, \rho_n(\vec{x}) \geq 0, \quad (3.43)
\]

which shows that the spectrum is monotonically rising with $\gamma$.

Indeed, in the 1-d case, the spectrum illustrated in figure 1 is monotonic in $\gamma$. In that case, eq. (3.43) reduces to

\[
\partial_\gamma E_n = \frac{1}{2m} \left[ \rho_n(L/2) + \rho_n(-L/2) \right]. \quad (3.44)
\]

Let us explicitly verify this equation for the positive energy eigenstates of even parity

\[
\Psi_n(x) = A \cos(k_n x), \quad E_n = \frac{k_n^2}{2m}, \quad \frac{\gamma}{k_n} = \tan \frac{k_n L}{2}. \quad (3.45)
\]

In this case, one obtains

\[
\partial_\gamma E_n = \frac{k_n \partial_\gamma k_n}{m} = \frac{2k_n \cos^2(k_n L/2)}{m[k_n L + \sin(k_n L)]}, \quad (3.46)
\]

as well as

\[
\rho_n(L/2) + \rho_n(-L/2) = 2|A|^2 \cos^2 \frac{k_n L}{2}. \quad (3.47)
\]

The normalization condition for the wave function implies

\[
|A|^2 \int_{-L/2}^{L/2} dx \, \cos^2 \frac{k_n L}{2} = |A|^2 \frac{1}{2k_n} \left( k_n L + \sin(k_n L) \right) = 1, \quad (3.48)
\]

such that indeed

\[
\frac{1}{2m} \left[ \rho_n(L/2) + \rho_n(-L/2) \right] = \frac{2k_n}{m[k_n L + \sin(k_n L)]} \cos^2 \frac{k_n L}{2} = \partial_\gamma E_n. \quad (3.49)
\]

It is straightforward to repeat this check for states of odd parity or negative energy.
3.7 General Boundary Conditions for Heterostructures

Semiconductor heterostructures such as quantum dots, quantum wires, and quantum wells are separated into regions with different effective electron masses \[14\]. Until now we have considered quantum dots consisting of a single region isolated from an energetically forbidden environment. In this subsection, we construct the most general condition at the boundary \( \partial \Omega \) separating two regions, \( \Omega_I \) and \( \Omega_{II} \) as illustrated in figure 4, with different effective electron masses \( m_I \) and \( m_{II} \). In the two regions the Hamiltonian is then given by

\[
H_I = \frac{\hat{p}_I^2}{2m_I} + V_I(x), \quad H_{II} = \frac{\hat{p}_{II}^2}{2m_{II}} + V_{II}(x). \tag{3.50}
\]

Figure 4: Two regions \( \Omega_I \) and \( \Omega_{II} \) in a quantum heterostructure are separated by a boundary \( \partial \Omega \) with the unit-vector \( \vec{n} \) normal to the surface. An electron may have different effective masses \( m_I \) and \( m_{II} \) in the two regions.
For points at the boundary $\partial \Omega$, the Hermiticity condition takes the form

$$
\vec{n}(\vec{x}) \cdot \frac{1}{2m_1} \left[ \chi_1(\vec{x})^{\ast} \vec{\nabla} \Psi_1(\vec{x}) - \vec{\nabla} \chi_1(\vec{x})^{\ast} \Psi_1(\vec{x}) \right] = 
\vec{n}(\vec{x}) \cdot \frac{1}{2m_\Pi} \left[ \chi_\Pi(\vec{x})^{\ast} \vec{\nabla} \Psi_\Pi(\vec{x}) - \vec{\nabla} \chi_\Pi(\vec{x})^{\ast} \Psi_\Pi(\vec{x}) \right].
$$

(3.51)

The self-adjointness condition can now be expressed as

$$
\left( \frac{\Psi_1(\vec{x})}{\vec{n}(\vec{x}) \cdot \vec{\nabla} \Psi_1(\vec{x})} \right) = \Gamma(\vec{x}) \left( \frac{\Psi_\Pi(\vec{x})}{\vec{n}(\vec{x}) \cdot \vec{\nabla} \Psi_\Pi(\vec{x})} \right), \quad \Gamma(\vec{x}) \in GL(2, \mathbb{C}),
$$

(3.52)

which turns the Hermiticity condition eq. (3.51) into

$$
\begin{bmatrix}
\Gamma_{21}(\vec{x}) \chi_1(\vec{x})^{\ast} - \Gamma_{11}(\vec{x}) & \frac{1}{2m_1} \vec{n}(\vec{x}) \cdot \vec{\nabla} \chi_1(\vec{x})^{\ast} + \frac{1}{2m_\Pi} \vec{n}(\vec{x}) \cdot \vec{\nabla} \chi_\Pi(\vec{x})^{\ast} \\
\Gamma_{22}(\vec{x}) \chi_1(\vec{x})^{\ast} - \Gamma_{12}(\vec{x}) & \frac{1}{2m_1} \vec{n}(\vec{x}) \cdot \vec{\nabla} \chi_1(\vec{x})^{\ast} - \chi_\Pi(\vec{x})^{\ast}
\end{bmatrix}
\Psi_\Pi(\vec{x}) + 
\begin{bmatrix}
\Gamma_{21}(\vec{x}) \chi_1(\vec{x})^{\ast} - \Gamma_{11}(\vec{x}) & \frac{1}{2m_1} \vec{n}(\vec{x}) \cdot \vec{\nabla} \chi_1(\vec{x})^{\ast} + \frac{1}{2m_\Pi} \vec{n}(\vec{x}) \cdot \vec{\nabla} \chi_\Pi(\vec{x})^{\ast} \\
\Gamma_{22}(\vec{x}) \chi_1(\vec{x})^{\ast} - \Gamma_{12}(\vec{x}) & \frac{1}{2m_1} \vec{n}(\vec{x}) \cdot \vec{\nabla} \chi_1(\vec{x})^{\ast} - \chi_\Pi(\vec{x})^{\ast}
\end{bmatrix}
\frac{1}{2m_\Pi} \vec{n}(\vec{x}) \cdot \vec{\nabla} \Psi_\Pi(\vec{x}) = 0.
$$

(3.53)

In order to satisfy this relation we must thus demand

$$
\left( \frac{\chi_\Pi(\vec{x})}{\vec{n}(\vec{x}) \cdot \vec{\nabla} \chi_\Pi(\vec{x})} \right) = \left( \begin{array}{cc}
\Gamma_{22}(\vec{x})^{\ast} & -\Gamma_{12}(\vec{x})^{\ast} \\
-\Gamma_{21}(\vec{x})^{\ast} & \Gamma_{11}(\vec{x})^{\ast}
\end{array} \right)
\left( \frac{\chi_1(\vec{x})}{\vec{n}(\vec{x}) \cdot \vec{\nabla} \chi_1(\vec{x})} \right).
$$

(3.54)

Self-adjointness requires equality of the domains, $D(H^\dagger) = D(H)$, which thus implies

$$
\Gamma(\vec{x})^{-1} = \frac{1}{\Gamma_{11}(\vec{x}) \Gamma_{22}(\vec{x}) - \Gamma_{12}(\vec{x}) \Gamma_{21}(\vec{x})}
\begin{bmatrix}
\Gamma_{22}(\vec{x})^{\ast} & -\Gamma_{12}(\vec{x})^{\ast} \\
-\Gamma_{21}(\vec{x})^{\ast} & \Gamma_{11}(\vec{x})^{\ast}
\end{bmatrix}
\begin{bmatrix}
\Gamma_{22}(\vec{x}) & -\Gamma_{12}(\vec{x}) \\
-\Gamma_{21}(\vec{x}) & \Gamma_{11}(\vec{x})
\end{bmatrix}
\Gamma(\vec{x}) = 
\begin{bmatrix}
\Gamma_{22}(\vec{x})^{\ast} & -\Gamma_{12}(\vec{x})^{\ast} \\
-\Gamma_{21}(\vec{x})^{\ast} & \Gamma_{11}(\vec{x})^{\ast}
\end{bmatrix}.
$$

(3.55)

This condition is satisfied by a 4-parameter family of self-adjoint extensions which satisfy

$$
\Gamma_{ij}(\vec{x}) \in \exp(i\theta(\vec{x})) \mathbb{R}, \quad \Gamma_{11}(\vec{x}) \Gamma_{22}(\vec{x}) - \Gamma_{12}(\vec{x}) \Gamma_{21}(\vec{x}) = \exp(2i\theta(\vec{x})),
$$

(3.56)

i.e. $\Gamma(\vec{x})$ is real with determinant 1, up to an overall phase $\exp(i\theta(\vec{x}))$.

Using this form of $\Gamma(\vec{x})$, it is straightforward to show that self-adjointness implies
probability current conservation, i.e.

\[
\mathbf{i} \mathbf{n}(\mathbf{x}) \cdot \mathbf{j}_1(\mathbf{x}) = \mathbf{n}(\mathbf{x}) \cdot \left( \frac{1}{2m_{\Pi}} \left[ \Psi_I(\mathbf{x})^* \nabla \Psi_I(\mathbf{x}) - \nabla \Psi_I(\mathbf{x})^* \Psi_I(\mathbf{x}) \right] \right)
\]

\[
= \mathbf{n}(\mathbf{x}) \cdot \left( \frac{1}{2m_{\Pi}} \nabla \Psi_{\Pi}(\mathbf{x})^* \Psi_{\Pi}(\mathbf{x}) \left[ \Gamma_{11}(\mathbf{x})^* \Gamma_{22}(\mathbf{x}) - \Gamma_{21}(\mathbf{x})^* \Gamma_{12}(\mathbf{x}) \right] \right)
\]

\[
+ \mathbf{n}(\mathbf{x}) \cdot \left( \frac{1}{2m_{\Pi}} \nabla \Psi_{\Pi}(\mathbf{x})^* \Psi_{\Pi}(\mathbf{x}) \left[ \Gamma_{12}(\mathbf{x})^* \Gamma_{21}(\mathbf{x}) - \Gamma_{22}(\mathbf{x})^* \Gamma_{11}(\mathbf{x}) \right] \right)
\]

\[
+ |\Psi_{\Pi}(\mathbf{x})|^2 \left[ \Gamma_{11}(\mathbf{x})^* \Gamma_{21}(\mathbf{x}) - \Gamma_{21}(\mathbf{x})^* \Gamma_{11}(\mathbf{x}) \right]
\]

\[
+ \left| \mathbf{n}(\mathbf{x}) \cdot \left( \frac{1}{2m_{\Pi}} \nabla \Psi_{\Pi}(\mathbf{x})^* \Psi_{\Pi}(\mathbf{x}) \right) \right|^2 \left[ \Gamma_{12}(\mathbf{x})^* \Gamma_{22}(\mathbf{x}) - \Gamma_{22}(\mathbf{x})^* \Gamma_{12}(\mathbf{x}) \right]
\]

\[
= \mathbf{n}(\mathbf{x}) \cdot \left( \frac{1}{2m_{\Pi}} \left[ \Psi_{\Pi}(\mathbf{x})^* \nabla \Psi_{\Pi}(\mathbf{x}) - \nabla \Psi_{\Pi}(\mathbf{x})^* \Psi_{\Pi}(\mathbf{x}) \right] \right)
\]

\[
= \mathbf{i} \mathbf{n}(\mathbf{x}) \cdot \mathbf{j}_{\Pi}(\mathbf{x}). \tag{3.57}
\]

Here we have used again that \( \Gamma(\mathbf{x}) \) is real with determinant 1 up to the overall phase \( \exp(i\theta(\mathbf{x})) \), which implies

\[
\Gamma_{11}(\mathbf{x})^* \Gamma_{22}(\mathbf{x}) - \Gamma_{21}(\mathbf{x})^* \Gamma_{12}(\mathbf{x}) = 1,
\]

\[
\Gamma_{12}(\mathbf{x})^* \Gamma_{21}(\mathbf{x}) - \Gamma_{22}(\mathbf{x})^* \Gamma_{11}(\mathbf{x}) = -1,
\]

\[
\Gamma_{11}(\mathbf{x})^* \Gamma_{21}(\mathbf{x}) - \Gamma_{21}(\mathbf{x})^* \Gamma_{11}(\mathbf{x}) = 0,
\]

\[
\Gamma_{12}(\mathbf{x})^* \Gamma_{22}(\mathbf{x}) - \Gamma_{22}(\mathbf{x})^* \Gamma_{12}(\mathbf{x}) = 0. \tag{3.58}
\]

### 4 Reflecting Walls for Relativistic Fermions

In this section we consider perfectly reflecting boundary conditions for relativistic fermions. Such boundary conditions have been introduced in the MIT bag model to mimic the confinement of quarks and gluons inside hadrons. Here we construct the most general perfectly reflecting boundary conditions for relativistic Dirac fermions both in one and in three spatial dimensions, as well as for the resulting non-relativistic fermions described by the Pauli equation.

#### 4.1 Reflecting Boundary Conditions for 1-d Dirac Fermions

General boundary conditions for a Dirac particle in a box have been investigated in [15]. Here we consider a Dirac fermion moving on the positive \( x \)-axis with a perfectly reflecting wall at \( x = 0 \). The corresponding free particle Hamiltonian is then given by

\[
H = \alpha pc + \beta mc^2, \quad \alpha = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4.1}
\]
The Hamiltonian acts on a 2-component spinor $\Psi(x,t)$, and the corresponding continuity equation
\[ \partial_t \rho(x,t) + \partial_x j(x,t) = 0, \] (4.2)
is satisfied by
\[ \rho(x,t) = \Psi(x,t)\dagger\Psi(x,t), \quad j(x,t) = c\Psi(x,t)\dagger\alpha\Psi(x,t). \] (4.3)

Let us investigate the Hermiticity of the Hamiltonian on the positive $x$-axis
\[ \langle \chi | H | \Psi \rangle = \int_0^\infty dx \, \chi(x)\dagger \left[ -\alpha c i \partial_x + \beta mc^2 \right] \Psi(x) \]
\[ = \int_0^\infty dx \left\{ \left[ -\alpha c i \partial_x + \beta mc^2 \right] \chi(x) \right\}\dagger \Psi(x) - ic\chi(0)\dagger\alpha\Psi(0) \]
\[ = \langle \Psi | H | \chi \rangle^* - ic\chi(0)\dagger\alpha\Psi(0), \] (4.4)
which thus leads to the Hermiticity condition
\[ \chi(0)\dagger\alpha\Psi(0) = 0. \] (4.5)

We now introduce the self-adjoint extension condition
\[ \Psi_2(0) = \lambda \Psi_1(0), \quad \lambda \in \mathbb{C}, \] (4.6)
which reduces eq.(4.5) to
\[ \chi(0)\dagger \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Psi(0) = [\chi_1(0)^*\lambda + \chi_2(0)^*] \Psi_1(0) = 0 \Rightarrow \chi_2(0) = -\lambda^*\chi_1(0). \] (4.7)

In order to guarantee self-adjointness of $H$, i.e. $D(H) = D(H^\dagger)$, we must request
\[ \lambda = -\lambda^*, \] (4.8)
i.e. $\lambda$ must be purely imaginary. For 1-d Dirac fermions, there is thus a 1-parameter family of self-adjoint extensions that characterizes a perfectly reflecting wall. The self-adjointness condition eq.(4.6) implies
\[ j(0) = c\Psi(0)\dagger\alpha\Psi(0) = c\Psi(0)\dagger \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Psi(0) = c [\Psi_1(0)^*\Psi_2(0) + \Psi_2(0)^*\Psi_1(0)] \]
\[ = c [\Psi_1(0)^*\lambda\Psi_1(0) + \Psi_1(0)^*\lambda^*\Psi_1(0)] = 0. \] (4.9)

In the chiral limit, $m = 0$, not only the vector current but also the axial current is conserved. In the basis we have chosen, the $\gamma$-matrices take the form
\[ \gamma^0 = \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \gamma^1 = \gamma^0\alpha = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \gamma^3 = \gamma^0\gamma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \] (4.10)
Thus the axial charge density and the axial current density are given by
\[
\rho_A(x, t) = \Psi(x, t) \gamma^3 \Psi(x, t),
\]
\[
j_A(x, t) = c \Psi(x, t) \gamma^0 \gamma^1 \gamma^3 \Psi(x, t) = c \Psi(x, t) \gamma^3 \Psi(x, t).
\] (4.11)
Indeed, it is easy to convince oneself that \( \partial_t \rho_A(x, t) + \partial_x j_A(x, t) = 0 \) in the chiral limit \( m = 0 \). Let us now consider the axial current at the boundary \( x = 0 \)
\[
j_A(0) = c \left| \Psi_1(0) \right|^2 + \left| \Psi_2(0) \right|^2 = c \left( 1 + \left| \lambda \right|^2 \right) \left| \Psi_1(0) \right|^2 \geq 0.
\] (4.12)
Since in general \( \Psi_1(0) \neq 0 \), the axial current does not vanish at the boundary. Hence, chiral symmetry is explicitly broken by the most general perfectly reflecting boundary condition. It is well-known that this is indeed the case for the boundary condition in the MIT bag model [3–5]. Only in the chiral bag model the axial current is conserved because it is carried by a pion field outside the bag [16, 17].

It is interesting to ask how the self-adjoint extension parameter \( \lambda \) in the relativistic case is related to the parameter \( \gamma \) in the non-relativistic limit, in which
\[
\Psi_2(x) = \frac{p}{2mc} \Psi_1(x) = \frac{1}{2mci} \partial_x \Psi_1(x).
\] (4.13)
Inserting this relation in the relativistic current,
\[
j(x) = c \Psi(x) \gamma^3 \Psi(x) = c \left[ \Psi_1(x)^* \Psi_2(x) + \Psi_2(x)^* \Psi_1(x) \right]
\]
\[
= \frac{1}{2mci} \left[ \Psi_1(x)^* \partial_x \Psi_1(x) - \partial_x \Psi_1(x)^* \Psi_1(x) \right],
\] (4.14)
we indeed recover the non-relativistic current of eq.(2.2). In the non-relativistic limit, the relativistic self-adjointness condition eq.(4.6) takes the form
\[
\frac{1}{2mci} \partial_x \Psi_1(0) = \lambda \Psi_1(0) \Rightarrow -2mci \lambda \Psi_1(0) + \partial_x \Psi_1(0) = 0.
\] (4.15)
Hence, the non-relativistic self-adjoint extension parameter of eq.(2.46) can be identified as
\[
\gamma = -2mci \lambda,
\] (4.16)
which is indeed real because \( \lambda \) is purely imaginary.

### 4.2 Reflecting Boundary Conditions for 3-d Dirac Fermions

Let us now consider Dirac fermions coupled to an external static electromagnetic field and confined to a finite domain \( \Omega \). The corresponding Hamiltonian then takes the form
\[
H = \bar{\alpha} \cdot \left( \gamma^5 \gamma^0 \gamma^1 \gamma^2 \gamma^3 \gamma^5 \right) + \beta mc^2 - e \Phi(x) = -i \bar{\alpha} \cdot \nabla c + \beta mc^2 - e \Phi(x),
\]
\[
\bar{\alpha} = \left( \begin{array}{cc} 0 & \sigma & 0 \\ \sigma & 0 & 0 \end{array} \right), \quad \beta = \left( \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right).
\] (4.17)
Here $\mathbb{1}$ and $\mathbb{0}$ are the $2 \times 2$ unit- and zero-matrix, and $\sigma$ is the vector of Pauli matrices, while $\Phi(\vec{x})$ and $\vec{A}(\vec{x})$ are the scalar and vector potential, and $e$ is the electric charge. The covariant derivative is given by

$$ \vec{D} = \vec{\nabla} + i \frac{e}{c} \vec{A}(\vec{x}). $$

(4.18)

The Dirac Hamiltonian acts on a 4-component spinor $\Psi(\vec{x}, t)$. In this case, the continuity equation

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

(4.19)

is satisfied by

$$ \rho(\vec{x}, t) = \Psi(\vec{x}, t)^\dagger \Psi(\vec{x}, t), \quad \vec{j}(\vec{x}, t) = e \Psi(\vec{x}, t)^\dagger \vec{A}(\vec{x}). $$

(4.20)

Under time-independent gauge transformations, the gauge fields as well as the Dirac spinor transform as

$$ ^\varphi \Phi(\vec{x}) = \Phi(\vec{x}), \quad ^\varphi \vec{A}(\vec{x}) = \vec{A}(\vec{x}) - \vec{\nabla} \varphi(\vec{x}), \quad ^\varphi \Psi(\vec{x}) = \exp \left( i \frac{e}{c} \varphi(\vec{x}) \right) \Psi(\vec{x}). $$

(4.21)

In order to investigate the Hermiticity of the Hamiltonian in the finite spatial domain $\Omega$, we consider

$$ \langle \chi | H | \Psi \rangle = \int_\Omega d^3 x \chi(\vec{x})^\dagger \left[ \vec{\alpha} \cdot \left( -ic \vec{\nabla} + e \vec{A}(\vec{x}) \right) + \beta mc^2 - e\Phi(\vec{x}) \right] \Psi(\vec{x}) $$

$$ = \int_\Omega d^3 x \left\{ \vec{\alpha} \cdot \left( -ic \vec{\nabla} + e \vec{A}(\vec{x}) \right) + \beta mc^2 - e\Phi(\vec{x}) \right\}^\dagger \chi(\vec{x}) + ic \int_{\partial \Omega} d\vec{n} \cdot \chi(\vec{x})^\dagger \vec{\alpha} \Psi(\vec{x}) $$

$$ = \langle \Psi | H | \chi \rangle^* - ic \int_{\partial \Omega} d\vec{n} \cdot \chi(\vec{x})^\dagger \vec{\alpha} \Psi(\vec{x}), $$

(4.22)

which thus leads to the Hermiticity condition

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

(4.23)

We now introduce the self-adjoint extension condition

$$ \begin{pmatrix} \Psi_3(\vec{x}) \\ \Psi_4(\vec{x}) \end{pmatrix} = \lambda(\vec{x}) \begin{pmatrix} \Psi_1(\vec{x}) \\ \Psi_2(\vec{x}) \end{pmatrix}, \quad \lambda(\vec{x}) \in GL(2, \mathbb{C}), \quad \vec{x} \in \partial \Omega, $$

(4.24)

which reduces eq.(4.23) to

$$ \chi(\vec{x})^\dagger \begin{pmatrix} 0 & \vec{n}(\vec{x}) \cdot \vec{\sigma} \\ \vec{n}(\vec{x}) \cdot \vec{\sigma} & 0 \end{pmatrix} \Psi(\vec{x}) = $$

$$ \left[ (\chi_1(\vec{x})^*, \chi_2(\vec{x})^*) \vec{n}(\vec{x}) \cdot \vec{\alpha} \lambda(\vec{x}) + (\chi_3(\vec{x})^*, \chi_4(\vec{x})^*) \vec{n}(\vec{x}) \cdot \vec{\sigma} \right] \begin{pmatrix} \Psi_1(\vec{x}) \\ \Psi_2(\vec{x}) \end{pmatrix} = 0 \Rightarrow $$

$$ \begin{pmatrix} \chi_3(\vec{x}) \\ \chi_4(\vec{x}) \end{pmatrix} = -\vec{n}(\vec{x}) \cdot \vec{\sigma} \lambda(\vec{x})^\dagger \vec{n}(\vec{x}) \cdot \vec{\sigma} \begin{pmatrix} \chi_1(\vec{x}) \\ \chi_2(\vec{x}) \end{pmatrix}, $$

(4.25)
In order to guarantee self-adjointness of $H$, i.e. $D(H) = D(H^\dagger)$, we now demand
\[ \lambda(\vec{x}) = -\vec{n}(\vec{x}) \cdot \bar{\sigma} \lambda(\vec{x}) \vec{n}(\vec{x}) \cdot \bar{\sigma} \Rightarrow \vec{n}(\vec{x}) \cdot \bar{\sigma} \lambda(\vec{x}) = -[\vec{n}(\vec{x}) \cdot \bar{\sigma} \lambda(\vec{x})]^\dagger. \] (4.26)
Hence, $\vec{n}(\vec{x}) \cdot \bar{\sigma} \lambda(\vec{x})$ is anti-Hermitean. For Dirac fermions, there is thus a 4-parameter family of self-adjoint extensions that characterizes a perfectly reflecting wall. It is important to note that the self-adjointness condition eq. (4.24) is gauge covariant and implies
\[ \vec{n}(\vec{x}) \cdot \vec{j}(\vec{x}) = c \Psi(\vec{x})^\dagger \begin{pmatrix} 0 & \vec{n}(\vec{x}) \cdot \bar{\sigma} \\ \vec{n}(\vec{x}) \cdot \bar{\sigma} & 0 \end{pmatrix} \Psi(\vec{x}) = \\
= c \left[ (\Psi_1(\vec{x})^*, \Psi_2(\vec{x})^*) \vec{n}(\vec{x}) \cdot \bar{\sigma} \lambda(\vec{x}) + (\Psi_3(\vec{x})^*, \Psi_4(\vec{x})^*) \vec{n}(\vec{x}) \cdot \bar{\sigma} \right] \begin{pmatrix} \Psi_1(\vec{x}) \\ \Psi_2(\vec{x}) \end{pmatrix} \\
= c (\Psi_1(\vec{x})^*, \Psi_2(\vec{x})^*) \left[ \vec{n}(\vec{x}) \cdot \bar{\sigma} \lambda(\vec{x}) + \lambda(\vec{x})^\dagger \vec{n}(\vec{x}) \cdot \bar{\sigma} \right] \begin{pmatrix} \Psi_1(\vec{x}) \\ \Psi_2(\vec{x}) \end{pmatrix} = 0. \] (4.27)

Let us again consider the chiral limit $m = 0$, in which the axial current is also conserved. The $\gamma$-matrices now take the form
\[ \gamma^0 = \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \bar{\gamma} = \gamma^0 \bar{\alpha} = \begin{pmatrix} 0 & \bar{\sigma} \\ -\bar{\sigma} & 0 \end{pmatrix}, \quad \gamma^5 = i \gamma^0 \gamma^1 \gamma^2 \gamma^3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \] (4.28)
Hence the axial charge density and the axial current density are given by
\[ \rho_A(\vec{x}, t) = \Psi(\vec{x}, t)^\dagger \gamma^5 \Psi(\vec{x}, t), \]
\[ \vec{j}_A(\vec{x}, t) = c \Psi(\vec{x}, t)^\dagger \gamma^0 \vec{\gamma}^5 \Psi(\vec{x}, t) = -c \Psi(\vec{x}, t)^\dagger \begin{pmatrix} \bar{\sigma} & 0 \\ 0 & \bar{\sigma} \end{pmatrix} \Psi(\vec{x}, t), \] (4.29)
such that the axial current at the boundary is
\[ \vec{n}(\vec{x}) \cdot \vec{j}_A(\vec{x}) = -c \Psi(\vec{x})^\dagger \begin{pmatrix} \vec{n}(\vec{x}) \cdot \bar{\sigma} & 0 \\ 0 & \vec{n}(\vec{x}) \cdot \bar{\sigma} \end{pmatrix} \Psi(\vec{x}) = \\
= -c (\Psi_1(\vec{x})^*, \Psi_2(\vec{x})^*) \left[ \vec{n}(\vec{x}) \cdot \bar{\sigma} + \lambda(\vec{x})^\dagger \vec{n}(\vec{x}) \cdot \bar{\sigma} \lambda(\vec{x}) \right] \begin{pmatrix} \Psi_1(\vec{x}) \\ \Psi_2(\vec{x}) \end{pmatrix}. \] (4.30)
As in the 1-d case, in general, the axial current does not vanish at the boundary. Hence, chiral symmetry is again explicitly broken by the most general perfectly reflecting boundary condition.

### 4.3 Reflecting Boundary Conditions in the Non-relativistic Limit

In the non-relativistic limit, the lower components of the Dirac spinor are given by
\[ \begin{pmatrix} \Psi_3(\vec{x}) \\ \Psi_4(\vec{x}) \end{pmatrix} = \frac{\bar{\sigma} \cdot (\vec{p}c + e\vec{A}(\vec{x}))}{2mc^2} \begin{pmatrix} \Psi_1(\vec{x}) \\ \Psi_2(\vec{x}) \end{pmatrix} = \frac{1}{2mc} \bar{\sigma} \cdot \vec{D} \Psi(\vec{x}), \] (4.31)
with the 2-component Pauli spinor
\[ \Psi(\vec{x}) = \begin{pmatrix} \Psi_1(\vec{x}) \\ \Psi_2(\vec{x}) \end{pmatrix}. \] (4.32)

The Dirac equation then reduces to the Pauli equation. Expanding up to the leading Zeemann term, but neglecting the higher order spin-orbit coupling and Darwin terms, the Hamiltonian entering the Pauli equation takes the form
\[ H = mc^2 + \left( \vec{p}c + e\vec{A}(\vec{x}) \right)^2 - e\Phi(\vec{x}) + \mu\vec{\sigma} \cdot \vec{B}(\vec{x}), \] (4.33)

where \( \vec{B}(\vec{x}) = \vec{\nabla} \times \vec{A}(\vec{x}) \) is the magnetic field and \( \mu = e/2mc \) is the magnetic moment of the fermion.

Using eq.(4.31), the relativistic current reduces to
\[ \vec{j}(\vec{x}) = \begin{pmatrix} \Psi_1(\vec{x})^*, \Psi_2(\vec{x})^*, \Psi_3(\vec{x})^*, \Psi_4(\vec{x})^* \end{pmatrix} \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \begin{pmatrix} \Psi_1(\vec{x}) \\ \Psi_2(\vec{x}) \\ \Psi_3(\vec{x}) \\ \Psi_4(\vec{x}) \end{pmatrix} \]
\[ = \frac{1}{2mi} \left[ \Psi(\vec{x})^\dagger \vec{D} \Psi(\vec{x}) - (\vec{D} \Psi(\vec{x}))^\dagger \Psi(\vec{x}) \right] \\
- \frac{1}{2m} \left[ \Psi(\vec{x}, t)^\dagger \vec{\sigma} \times \vec{D} \Psi(\vec{x}, t) - (\vec{D} \Psi(\vec{x}, t))^\dagger \times \vec{\sigma} \Psi(\vec{x}, t) \right] \\
+ \frac{1}{2m} \vec{\nabla} \times \left[ \Psi(\vec{x}, t)^\dagger \vec{\sigma} \Psi(\vec{x}, t) \right]. \] (4.34)

As a curl, the spin term entering the current is automatically divergenceless. In this case, the continuity equation
\[ \partial_t \rho(\vec{x}, t) + \vec{\nabla} \cdot \vec{j}(\vec{x}, t) = 0, \] (4.35)
is satisfied with the probability density \( \rho(\vec{x}, t) = \Psi(\vec{x}, t)^\dagger \Psi(\vec{x}, t) \).

Introducing the gauge covariant boundary condition
\[ \gamma(\vec{x}) \Psi(\vec{x}) + \vec{n}(\vec{x}) \cdot \left[ \vec{D} \Psi(\vec{x}) - i\vec{\sigma} \times \vec{D} \Psi(\vec{x}) \right] = 0, \quad \gamma(\vec{x}) \in GL(2, \mathbb{C}), \quad \vec{x} \in \partial \Omega, \] (4.36)
we obtain
\[ \vec{n}(\vec{x}) \cdot \vec{j}(\vec{x}) = \frac{1}{2mi} \left[ \Psi(\vec{x})^\dagger \vec{n}(\vec{x}) \cdot \vec{D} \Psi(\vec{x}) - (\vec{n}(\vec{x}) \cdot \vec{D} \Psi(\vec{x}))^\dagger \Psi(\vec{x}) \right] \\
- \frac{1}{2m} \left[ \Psi(\vec{x}, t)^\dagger \vec{n} \cdot \left( \vec{\sigma} \times \vec{D} \Psi(\vec{x}, t) \right) - \vec{n} \cdot \left( (\vec{D} \Psi(\vec{x}, t))^\dagger \times \vec{\sigma} \right) \Psi(\vec{x}, t) \right] \\
+ \frac{1}{2mi} \left[ -\Psi(\vec{x})^\dagger \gamma(\vec{x}) \Psi(\vec{x}) + \Psi(\vec{x})^\dagger \gamma(\vec{x})^\dagger \Psi(\vec{x}) \right] = 0, \] (4.37)
which immediately implies
\[ \gamma(\vec{x})^\dagger = \gamma(\vec{x}). \]  
(4.38)

Hence, again there is a 4-parameter family of self-adjoint extensions, now parameterized by a 2 \times 2 Hermitean matrix.

In complete analogy to the previous cases, by partial integration one arrives at the Hermiticity condition for the Pauli Hamiltonian of eq.(4.33)
\[ \int_{\partial \Omega} d\vec{n} \cdot \left[ (\vec{D}\chi(\vec{x}))^\dagger \Psi(\vec{x}) - \chi(\vec{x})^\dagger \vec{D}\Psi(\vec{x}) \right] = 0. \]  
(4.39)

One also readily derives
\[ (\vec{D}\chi(\vec{x}))^\dagger \times \vec{\sigma} \Psi(\vec{x}) - \chi(\vec{x})^\dagger \vec{\sigma} \times \vec{D}\Psi(\vec{x}) = \vec{\nabla} \times \left( \chi(\vec{x})^\dagger \vec{\sigma} \Psi(\vec{x}) \right). \]  
(4.40)

Using Stoke’s theorem as well as \( \partial(\partial \Omega) = \emptyset \), (i.e. the boundary of a boundary is an empty set), one then obtains
\[ \int_{\partial \Omega} d\vec{n} \cdot \left[ (\vec{D}\chi(\vec{x}) - i\vec{\sigma} \times \vec{D}\chi(\vec{x}))^\dagger \Psi(\vec{x}) - \chi(\vec{x})^\dagger \left( \vec{D}\Psi(\vec{x}) - i\vec{\sigma} \times \vec{D}\Psi(\vec{x}) \right) \right] = 0, \]  
(4.41)

such that the Hermiticity condition eq.(4.39) may be rewritten as
\[ \int_{\partial \Omega} d\vec{n} \cdot \left[ (\vec{D}\chi(\vec{x}) - i\vec{\sigma} \times \vec{D}\chi(\vec{x}))^\dagger \Psi(\vec{x}) - \chi(\vec{x})^\dagger \left( \vec{D}\Psi(\vec{x}) - i\vec{\sigma} \times \vec{D}\Psi(\vec{x}) \right) \right] = 0. \]  
(4.42)

Using the self-adjointness condition eq.(4.36), this relation reduces to
\[ \int_{\partial \Omega} d^2x \left[ \chi(\vec{x})^\dagger \gamma(\vec{x}) \Psi(\vec{x}) - \chi(\vec{x})^\dagger \gamma(\vec{x}) \Psi(\vec{x}) \right] = 0, \]  
(4.43)

which is indeed satisfied because \( \gamma(\vec{x}) \) is Hermitean.

It is again interesting to ask how the Hermitean matrix \( \gamma(\vec{x}) \) emerges from the matrix \( \lambda(\vec{x}) \) in the non-relativistic limit. Noting that the self-adjointness condition eq.(4.36) can also be expressed as
\[ \gamma(\vec{x}) \Psi(\vec{x}) + \vec{n}(\vec{x}) \cdot \vec{\sigma} \cdot \vec{D}\Psi(\vec{x}) = \gamma(\vec{x}) \Psi(\vec{x}) + 2mc i\vec{n}(\vec{x}) \cdot \vec{\sigma} \lambda(\vec{x}) \Psi(\vec{x}) = 0, \]  
(4.44)

one immediately identifies
\[ \gamma(\vec{x}) = -2mc i\vec{n}(\vec{x}) \cdot \vec{\sigma} \lambda(\vec{x}). \]  
(4.45)

Since \( \vec{n}(\vec{x}) \cdot \vec{\sigma} \lambda(\vec{x}) \) is anti-Hermitean, the resulting matrix \( \gamma(\vec{x}) \) is indeed Hermitean.
5 Domain Wall Fermions

Using Shamir’s variant [18] of Kaplan’s domain wall fermions [19], let us imagine that our world has an additional hidden spatial dimension and that we live very near a perfectly reflecting flat domain wall. For simplicity, we first explore this idea in (2 + 1)-d and then extend it to (4 + 1)-d. Since there is no notion of chirality in odd space-time dimensions, it is natural to consider massive Dirac fermions.

5.1 Domain Wall Boundary Conditions in (2 + 1)-d

Let us consider fermions moving freely along the $x_1$-direction and localized near a perfectly reflecting wall located at $x_3 = 0$ at very small positive values of $x_3$. We denote the two spatial coordinates by $x_1$ and $x_3$, while time is denoted by $x_0$. We would reserve $x_2$ for Euclidean time which, however, does not play a role in the present paper. Starting from the $\gamma$-matrices of eq.(4.10), it is more convenient to change to a chiral basis by performing the unitary transformation

$$\tilde{\gamma}^0 = U\gamma^0 U^\dagger = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tilde{\gamma}^1 = U\gamma^1 U^\dagger = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

$$\tilde{\gamma}^3 = U\gamma^3 U^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = U^\dagger,$$

$$\tilde{\alpha} = \tilde{\gamma}^0\gamma^1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \tilde{\beta} = \tilde{\gamma}^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tilde{\alpha}^3 = -i\tilde{\gamma}^0\tilde{\gamma}^3 = i\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (5.1)$$

The domain wall fermion Hamiltonian then takes the form

$$H = \tilde{\alpha}pc + \tilde{\beta}mc^2 + \tilde{\alpha}^3p_3c = \tilde{\alpha}pc + \tilde{\beta}mc^2 - i\tilde{\alpha}^3c\partial_3, \quad (5.2)$$

and the 3-component of the current is given by

$$j^3(x_1, x_3) = ec\Psi(x_1, x_3)^\dagger\tilde{\alpha}^3\Psi(x_1, x_3)
= ic(\Psi_R(x_1, x_3)^*, \Psi_L(x_1, x_3)^*)(\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix})(\begin{pmatrix} \Psi_R(x_1, x_3) \\ \Psi_L(x_1, x_3) \end{pmatrix}). \quad (5.3)$$

In complete analogy to the cases discussed before, the Hermiticity condition then reads

$$(\chi_R(x_1, 0)^*, \chi_L(x_1, 0)^*)(\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix})(\begin{pmatrix} \Psi_R(x_1, 0) \\ \Psi_L(x_1, 0) \end{pmatrix}) = 0. \quad (5.4)$$

Introducing the self-adjointness condition

$$\Psi_R(x_1, 0) = \eta\Psi_L(x_1, 0), \quad (5.5)$$
the Hermiticity condition turns into

\[
(\chi_R(x_1, 0)^* - \chi_L(x_1, 0)^* \eta) \Psi_L(x_1, 0) = 0 \Rightarrow \chi_R(x_1, 0) = \eta^* \chi_L(x_1, 0).
\]  

(5.6)

Thus, in order to ensure \(D(H^\dagger) = D(H)\) and hence self-adjointness, we must demand

\[
\eta = \eta* \in \mathbb{R}.
\]  

(5.7)

Since the boundary condition eq.(5.5) couples left- and right-handed components, which transform differently under the \((1 + 1)\)-d Lorentz group, it explicitly breaks \((1 + 1)\)-d Lorentz invariance (unless \(\eta = 0\) or \(\pm \infty\)).

The Dirac equation takes the form

\[
\begin{pmatrix}
 pc & mc^2 + c\partial_3 \\
 mc^2 - c\partial_3 & -pc
\end{pmatrix}
\begin{pmatrix}
 \Psi_R(x_1, x_3) \\
 \Psi_L(x_1, x_3)
\end{pmatrix}
= E
\begin{pmatrix}
 \Psi_R(x_1, x_3) \\
 \Psi_L(x_1, x_3)
\end{pmatrix}.
\]  

(5.8)

Inserting the ansatz

\[
\Psi_R(x_1, x_3) = A_R \exp(ipx_1) \exp(-\kappa x_3), \quad \Psi_L(x_1, x_3) = A_L \exp(ipx_1) \exp(-\kappa x_3),
\]  

(5.9)

for a state localized on the domain wall, the Dirac equation reduces to

\[
\begin{pmatrix}
 pc & mc^2 - c\kappa \\
 mc^2 + c\kappa & -pc
\end{pmatrix}
\begin{pmatrix}
 A_R \\
 A_L
\end{pmatrix}
= E
\begin{pmatrix}
 A_R \\
 A_L
\end{pmatrix}.
\]  

(5.10)

Imposing the boundary condition eq.(5.5), one then obtains

\[
E = \frac{2\eta}{1 + \eta^2} mc^2 - \frac{1 - \eta^2}{1 + \eta^2} pc, \quad c\kappa = \frac{1 - \eta^2}{1 + \eta^2} mc^2 + \frac{2\eta}{1 + \eta^2} pc.
\]  

(5.11)

This is the energy-momentum dispersion relation of a fermion moving with the speed

\[
v = \left| \frac{1 - \eta^2}{1 + \eta^2} \right| c \leq c,
\]  

(5.12)

and coupled to a chemical potential

\[
\mu = \frac{2\eta}{1 + \eta^2} mc^2.
\]  

(5.13)

Only for \(\eta = 0\) or \(\pm \infty\), one obtains \(v = c\) and \(\mu = 0\), as a consequence of \((1 + 1)\)-d Lorentz invariance. It is important to note that normalizability of the state localized on the domain wall requires \(\kappa > 0\), which restricts the allowed range of \(p\). Only for \(\eta = 0\) or \(\pm \infty\), there is no restriction and one obtains a relativistic massless left-handed domain wall fermion with \(E = -pc\). This means that particles (i.e. positive energy states) are left-moving (\(p < 0\)) while anti-particles are right-moving.
5.2 Domain Wall Boundary Condition in \( (4 + 1) \)-d

Let us now consider domain wall fermions in \((4 + 1)\)-d localized near a perfectly reflecting wall located at \(x_5 = 0\) at very small positive values of \(x_5\). We denote the four spatial coordinates by \(x_1, x_2, x_3\) and \(x_5\), reserving \(x_4\) for Euclidean time. In this case, the \(\gamma\)-matrices are given by eq.(4.28). Again, it is useful to change to a chiral basis

\[
\tilde{\gamma}^0 = U \gamma^0 U^\dagger = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tilde{\gamma} = U \gamma U^\dagger = \begin{pmatrix} 0 & -\vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix},
\]

\[
\tilde{\gamma}^5 = U \gamma^5 U^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = U^\dagger,
\]

\[
\tilde{\alpha} = \tilde{\gamma}^0 \tilde{\gamma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & -\vec{\sigma} \end{pmatrix}, \quad \tilde{\beta} = \tilde{\gamma}^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tilde{\alpha}^5 = -i \tilde{\gamma}^0 \tilde{\gamma}^5 = i \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.
\]

The domain wall fermion Hamiltonian is now given by

\[
H = \tilde{\alpha} \cdot \vec{p} c + \tilde{\beta} m c^2 + \tilde{\alpha}^5 p_5 c = \tilde{\alpha} \cdot \vec{p} c + \tilde{\beta} m c^2 - i \tilde{\alpha}^5 c \partial_5,
\]

and the 5-component of the current takes the form

\[
J^5(\vec{x}, x_5) = e \Psi(\vec{x}, x_5)^\dagger \tilde{\alpha}^5 \Psi(\vec{x}, x_5)
\]

\[
= ic \begin{pmatrix} \Psi_R(\vec{x}, x_5)^\dagger, \Psi_L(\vec{x}, x_5)^\dagger \end{pmatrix} \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix} \begin{pmatrix} \Psi_R(\vec{x}, x_5) \\ \Psi_L(\vec{x}, x_5) \end{pmatrix},
\]

where \(\Psi_R(\vec{x}, x_5)\) and \(\Psi_L(\vec{x}, x_5)\) are 2-component Weyl spinors. The Hermiticity condition now reads

\[
(\chi_R(\vec{x}, 0)^\dagger, \chi_L(\vec{x}, 0)^\dagger) \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix} \begin{pmatrix} \Psi_R(\vec{x}, 0) \\ \Psi_L(\vec{x}, 0) \end{pmatrix} = 0,
\]

and the self-adjointness condition takes the form

\[
\Psi_R(\vec{x}, 0) = \eta \Psi_L(\vec{x}, 0), \quad \eta \in GL(2, \mathbb{C}).
\]

Inserting this in the Hermiticity condition eq.(5.17), one obtains

\[
(\chi_R(\vec{x}, 0)^\dagger - \chi_L(\vec{x}, 0)^\dagger \eta) \Psi_L(\vec{x}, 0) = 0 \Rightarrow \chi_R(\vec{x}, 0) = \eta^\dagger \chi_L(\vec{x}, 0).
\]

In order to ensure \(D(H^\dagger) = D(H)\), we must hence demand

\[
\eta = \eta^\dagger = \eta_0 \mathbb{I} + \vec{\eta} \cdot \vec{\sigma}.
\]

In this case, there is a 4-parameter family of self-adjoint extensions. For general \(\eta\), the boundary condition explicitly breaks \((3 + 1)\)-d Lorentz invariance, and for \(\eta \neq 0\) it even breaks 3-d spatial rotation invariance.
The Dirac equation now takes the form
\[
\begin{pmatrix}
\sigma \cdot \vec{p} c & mc^2 + c\partial_5 \\
mc^2 - c\partial_5 & -\sigma \cdot \vec{p} c
\end{pmatrix}
\begin{pmatrix}
\Psi_R(\vec{x}, x_5) \\
\Psi_L(\vec{x}, x_5)
\end{pmatrix}
= E
\begin{pmatrix}
\Psi_R(\vec{x}, x_5) \\
\Psi_L(\vec{x}, x_5)
\end{pmatrix}.
\]
(5.21)

In analogy to the (2 + 1)-d case, we make the ansatz
\[
\Psi_R(\vec{x}, x_5) = A_R \exp(i\vec{p} \cdot \vec{x}) \exp(-\kappa x_5),
\Psi_L(\vec{x}, x_5) = A_L \exp(i\vec{p} \cdot \vec{x}) \exp(-\kappa x_5),
\]
which reduces the Dirac equation to
\[
\begin{pmatrix}
\sigma_3 |\vec{p}| c & mc^2 - c\kappa \\
mc^2 + c\kappa & -\sigma_3 |\vec{p}| c
\end{pmatrix}
\begin{pmatrix}
A_R' \\
A_L'
\end{pmatrix}
= E \begin{pmatrix}
A_R' \\
A_L'
\end{pmatrix}.
\]
(5.23)

Here we have performed a unitary transformation $U(\vec{p})$ to diagonalize $\sigma \cdot \vec{p}$, i.e.
\[
U(\vec{p})\sigma \cdot \vec{p} U(\vec{p})^\dagger = |\vec{p}|\sigma_3, \quad A_R' = U(\vec{p}) A_R, \quad A_L' = U(\vec{p}) A_L.
\]
(5.24)

For simplicity, we now restrict ourselves to the rotation invariant case $\vec{\eta} = 0$, such that the boundary condition reduces to $A_R' = \eta_0 A_L'$ with $\eta_0 \in \mathbb{R}$. One then obtains
\[
E = \frac{2\eta_0}{1 + \eta_0^2} mc^2 \pm \frac{1 - \eta_0^2}{1 + \eta_0^2} |\vec{p}| c, \quad c\kappa = \frac{1 - \eta_0^2}{1 + \eta_0^2} mc^2 \pm \frac{2\eta_0}{1 + \eta_0^2} |\vec{p}| c.
\]
(5.25)

Again, this is the dispersion relation of a massless fermion moving with the speed
\[
v = \left| \frac{1 - \eta_0^2}{1 + \eta_0^2} \right| c \leq c,
\]
and coupled to a chemical potential
\[
\mu = \frac{2\eta_0}{1 + \eta_0^2} mc^2.
\]
(5.27)

The normalizability of the domain wall state requires $\kappa > 0$ which again implies restrictions on $\vec{p}$. Only for $\eta_0 = 0$ or $\pm \infty$ there is no restriction and one obtains a relativistic massless left-handed domain wall fermion with $E = |\vec{p}| c$.

6 Conclusions

While the results presented here are easy to derive, they seem not to constitute common knowledge in quantum mechanics. The theory of self-adjoint extensions is not only mathematically elegant, but also physically relevant. Therefore, we hope that our paper contributes to changing the view on elementary textbook problems such as the particle in a box. While it may not be appropriate to discuss the most general reflecting boundary condition in a first encounter with the Schrödinger
equation, one might at least point out that other boundary conditions are possible as well.

Since the main purpose of this paper is of conceptual nature, we have not made an attempt to determine the value of the self-adjoint extension parameter $\gamma$ for actual quantum dots. In typical cases, $\gamma$ may be very large, so that the wave function practically vanishes at the boundary. However, there may be specific situations that lead to much smaller values of $\gamma$ and thus to quantitatively or even qualitatively different behavior, such as bound states localized at the wall of a quantum dot. It would certainly be interesting to investigate this in more detail. As a special case of the general uncertainty relation for non-Hermitean operators, we have derived a generalized uncertainty relation for the self-adjoint position and the non-Hermitean momentum operator in a quantum dot. Interestingly, additional boundary terms enter this relation. In particular, negative energy states, which may seem to be inconsistent with the uncertainty relation, are in perfect agreement with the generalized relation. Minimal uncertainty wave packets, which saturate the corresponding inequality and satisfy it as an equality, have been constructed as well. They are standard Gaussian wave packets, but require very special boundary conditions and thus generically do not exist. If the self-adjoint extension parameter $\gamma(\vec{x})$ vanishes everywhere at the boundary, a constant wave function plays the role of a minimal uncertainty wave packet. Furthermore, we have shown that the spectrum depends monotonically on the self-adjoint extension parameter $\gamma$.

We have also applied the theory of self-adjoint extensions to theories of relativistic fermions described by the Dirac equation. In $(1+1)$ and $(3+1)$ dimensions, we have considered the most general perfectly reflecting boundary condition as a generalization of the one used in the MIT bag model. All these boundary conditions necessarily explicitly break chiral symmetry. This can be avoided in the chiral bag model were the axial current is carried by a pion field outside the bag. We have also discussed generalized domain wall fermion boundary conditions both in $(2+1)$ and in $(4+1)$ dimensions. The most general perfectly reflecting boundary condition explicitly breaks $(1+1)$-d or $(3+1)$-d Lorentz invariance or even 3-d spatial rotation invariance. A relativistic massless chiral fermion arises only for a particular choice of the self-adjoint extension parameters. For other values of the self-adjoint extension parameters, one obtains a fermion at non-zero chemical potential, with a linear energy-momentum dispersion relation, however, with a speed $v < c$.

We conclude this paper by expressing our hope that it may contribute to emphasizing the sometimes subtle differences between Hermiticity and self-adjointness also in the teaching of quantum mechanics.
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