Boundary Conditions for Quantum Mechanics on the Discretized Half Line

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1. **Self-adjoint extensions**: Schrodinger quantum mechanics on the half line
2. **Polymer quantization**: quantum gravity and the value of being discrete
3. **Analogue of self-adjoint extensions for polymer quantization on the discretized half line**
4. **Results and conclusions**
Quantum Mechanics on the Half Line

- Useful and sometimes necessary to do QM on $(0, \infty)$.
- The boundary (at $x = 0$ w.l.o.g) can be location of singularity in potential (e.g., coulomb potential) or impenetrable wall (e.g., bouncing ball).
- The form of Hamiltonian determines what conditions if any on wave function at boundary allow unitary time evolution.
- In the real world, this is always an approximation (regulation); quantum gravity may be the exception.
General Procedure

Find deficiency indices \( n_\pm \) which give the dimension of space of normalizable solutions: \( \hat{H} \psi = \pm i \psi \)

1. \( n_+ = 0 = n_- \rightarrow \) essentially self-adjoint
2. \( n_+ = n_- \neq 0 \) has \( U(n_+) \)-parameter family of self-adjoint extensions
3. \( n_+ \neq n_- \), you’re ”toast”, non-self-adjoint and no self-adjoint extensions
Example: Free Particle with Infinite Reflecting Potential

Short version (verified by above analysis):

▶ $\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$

▶ Unitary evolution:

$$\frac{d\langle \psi(t)|\chi(t) \rangle}{dt} = 0 \rightarrow \int_0^\infty \partial_x (\psi^* \partial_x \chi - \partial_x \psi^* \chi) = 0 \quad (1)$$

▶ This is satisfied provide ALL STATES (i.e. $\psi$ and $\chi$ satisfy: $\psi(0) + L\partial_x \psi(0) = 0$, with same $L$ real, or infinity.

▶ $L = 0$ is Dirichlet, $L = \infty$ is Neumann.
Need to find normalizable wave functions that satisfy free particle Schrödinger equation with given bc’s for particular choice of $L$:

- **Scattering solutions:**
  \[
  \psi(x) = A \left( e^{-ikx} - \frac{1 - iLk}{1 + iLk} e^{ikx} \right) \quad E_k = \frac{k^2}{2m} > 0
  \]

- **Physically:** arbitrary complex phase change on reflection $\rightarrow$ parameter periodic.

- **Reflection coefficient** $R = \left| \frac{1 + iLk}{1 - iLk} \right|^2 = 1 \rightarrow$ perfectly reflecting

- **Surprise:** Bound State exists for $L > 0$

  \[
  \psi(x) = \sqrt{\frac{2}{|L|}} e^{-x/|L|} \quad E = -\frac{\hbar^2}{2mL^2}
  \]
Coulomb Potential \((l = 0 \text{ Hydrogen Atom})\)


\[
\hat{H} u(r) = -\frac{\hbar^2}{2M} \frac{\partial^2 u(r)}{\partial r^2} - \frac{\lambda}{r} u(r) \quad u(r) = rR(r)
\]

- There exists a parameter family of self-adjoint extensions, parametrized by \(L\), say.
- \(L = 0\) (Dirichlet) gives usual Bohr spectrum
- For \(0 < L << a_0\), there is an extra very low-lying bound state, \(E_0 \sim 1/L^2 << -13.6\text{eV}\)
- Physical answer from experiment: \(E_0 = -13.6\text{eV} \rightarrow L = 0\)
- From purely mathematical perspective, all are equally valid, and in principle no guidance from \(l \neq 0\).
Why Dirichlet?

For most physical applications (e.g., hydrogen atom, bouncing balls) nature prefers Dirichlet. Reason:

- We know the potential at the origin is not really infinite.
- There must exist some effective regular potential that doesn’t require self-adjoint extensions → unique spectrum
- **BUT:** We don’t know the form of regular (i.e., microscopic) potential, so are we back to square one.
- Do we really need to solve QED to get reliable prediction for hydrogen atom, or bouncing ball for that matter?

**ANSWER** (for Schrödinger quantum mechanics):

*Dirchlet generic* see Walton ’10, references therein
Quantum Gravity and the Discrete Half Line

- Classical General Relativity predicts the existence of singularities (black holes, cosmology)
- Mini-superspace models \(\rightarrow\) quantum mechanics on the half line
- Loop quantum gravity (and perhaps common sense) suggests that space (and possibly time) are not necessarily continuous and smooth to arbitrary small scales
- One concrete realization of this is **Polymer Quantization**
- Note that: PQ is a viable quantization scheme on its own and is unitarily inequivalent to Schrodinger quantization
Polymer Quantization

- Real line given discrete topology $\rightarrow$ momentum operator $p = -\hbar \frac{d}{dx}$ doesn’t exist.
- Can still use a basis of position eigenstates $\hat{x}|x\rangle = x|x\rangle$, such that $\langle x|x'\rangle = \delta_{x,x'}$, i.e. normalizable.
- One can also define discrete (as opposed to infinitesimal) translation operators: and the family of translation operators $\{\hat{U}_\mu | \mu \in \mathcal{R}\}$ is defined as in Schrödinger quantization by

$$ (\hat{U}_\mu \psi)(x) := \psi(x + \mu). \quad (2) $$
For fixed $\mu$ one can define a momentum operator, and kinetic operator as:

$$\hat{p} := \frac{1}{2i\mu}(\hat{U}_\mu - \hat{U}_\mu^\dagger),$$  \hspace{1cm} (3)

$$\hat{T} := \hat{p}^2 = \frac{1}{\tilde{\mu}^2}(2 - \hat{U}_{\tilde{\mu}} - \hat{U}_{\tilde{\mu}}^\dagger).$$  \hspace{1cm} (4)

Can now restrict to a basis of states $|m\mu\rangle$ $m = 0, \pm 1, \pm 2...$

Then $\psi = \sum_m c_m |m\mu\rangle$, with inner product

$$\left(\psi^{(1)}, \psi^{(2)}\right) = \sum_m \overline{c_m^{(1)}} c_m^{(2)}$$

The action of $\hat{H}$ now reads

$$(\hat{H}c)_m = \frac{2c_m - c_{m+1} - c_{m-1}}{\tilde{\mu}^2} + V(m\tilde{\mu})c_m.$$  \hspace{1cm} (5)

$\rightarrow$ Quantum Mechanics on a Lattice
Key Questions:

- Are there analogues of different self-adjoint extensions/boundary conditions in PQ?
- How are they implemented (not completely trivial)
- Is Dirichlet still somehow generic?
### General Method

**Inner product:** \((d, c) = \sum_{m=1}^{\infty} \overline{d_m} c_m\).

**Hamiltonian:**

\[
(\hat{H}_\alpha c)_m := \begin{cases} 
2c_m - c_{m+1} - c_{m-1} + V(m\tilde{\mu})c_m & \text{for } m > 1; \\
\frac{(2 - \alpha)c_1 - c_2}{\tilde{\mu}^2} + V(\tilde{\mu})c_1 & \text{for } m = 1.
\end{cases}
\]  

(6)

**Key observation:** \((\hat{H}_\alpha c)_m\) is consistent with \((\hat{H}c)_m\) (5) for \(m \geq 1\) assuming the presence of a fictitious lattice point at \(m = 0\) such that

\[c_0 = \alpha c_1\]  

(7)

**NOTE:**
- \(\alpha \in \mathcal{R}\) is lattice counterpart of the continuum theory self-adjoint extension parameter \(L\).
- \(\alpha = 0\) is continuum Dirichlet, with boundary at \(m = 0\),
- \(\alpha = \pm 1\) are, resp., continuum Neumann and Dirichlet, with boundary half-way between \(m = 0\) and \(m = 1\).
Example: Free Particle on Discretized Half Line

Recall Hamiltonian:

\[ \begin{align*}
\text{for } m > 1 & \quad 2c_m - c_{m+1} - c_{m-1} = \tilde{\mu}^2 E \\
\text{for } m = 1 & \quad \frac{(2 - \alpha)c_1 - c_2}{\tilde{\mu}^2} = \tilde{\mu}^2 E \rightarrow c_0 = \alpha c_1
\end{align*} \]

General solution to (8)

\[ c_m = (X_{\pm})^m \]

where

\[ X_{\pm} = (1 - \tilde{\mu}^2 E/4) \pm \sqrt{(1 - \tilde{\mu}^2 E/4)^2 - 1} \]

Scattering states: in energy band \( 0 \leq E \leq 4/\tilde{\mu}^2 \). Define \( \sin^2(\frac{\theta}{2}) \equiv \tilde{\mu}^2 E/4 \).

Then BC’s at \( m = 1 \) require

\[ \tilde{c}_m = \sin(m\theta_E + \delta(\alpha)) \quad \text{with} \quad \sin(\delta) = \alpha \sin(\theta_E + \delta) \]
Free Particle (cont’d)

- **Bound State**: for $|\alpha| > 1$ there is a normalizable bound state:
  \[
  c_m = \alpha^{-m}, \quad \tilde{\mu}^2 E = (2 - \alpha - \alpha^{-1})
  \]  
  which satisfies both (8) and (9).

- **Continuum Limit**:
  Define: $L_p = \frac{\tilde{\mu}}{1 - \alpha} \rightarrow \alpha = 1 - \frac{\tilde{\mu}}{L_p}$
  then:
  \[
  \psi(x) := c_{x/\tilde{\mu}} = \left(1 - \frac{\tilde{\mu}}{L_p}\right)^{x/\tilde{\mu}} = e^{-x/L_p} + O(\tilde{\mu}),
  \]
  (14)

- **Note**: This requires keeping $L_p(\tilde{\mu}, \alpha)$ fixed while taking $\tilde{\mu} \to 0$
  i.e. fine tuning
Results and Conclusions

- We have constructed a one-parameter family of polymer quantization Hamiltonians on the half-line, and calculated spectra for the following systems:
  - Free particle
  - Coulomb potential
  - Scale invariant potential
  - Black hole throat quantization

- Analogous to one-parameter of Robin boundary conditions in Schrodinger quantization.

- To recover full set of Robin conditions must fine tune polymer parameter wrt extension parameter when taking continuum limit.

Moral: Polymer quantization worth further investigation.

Dirichlet boundary conditions are generic on the discrete half line.
Self Adjoint Extensions


Robin BC's in Schrodinger Quantum Mechanics


Polymer Quantization


Self-Adjoint Extensions in Polymer Quantization