Case Study of the Momentum Operator

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I. INTRODUCTION

In this review paper, I focus mainly on how to see if one can construct a *specific operator* for a *given domain.* This is a lost art as many books take the existence of meaningful physical operators on a Hilbert space for granted. If I had to categorize this paper it would go under *Mathematical quantum mechanics.* The modern mathematical toolkit explaining quantum mechanics is *Functional analysis.* Therefore before starting to read this paper, I would request the reader to familiarize themselves with the most important basic facts of Functional analysis needed for Quantum mechanics. One can read this in [Szekeres] or even better [Background read] (This is a link of some lecture notes I have uploaded online, they are password protected as they are not mine and I don't want to publicly post some notes that don't belong to me. The password can be found along with the link in the bibliography). The paper could be somewhat difficult to read for someone who is not familiar with basics of *Functional analysis.* If you feel this please leave a comment on the abstract post so we can take this matter to *Prof. Bloomfield*

II. OPERATORS

Hilbert spaces are what coordinate systems or phase space are to classical mechanics. In order to construct an entire physical system we needs the concept of *function* or *observable.*

Definition II.1 (***Operator***)**.** Let A and B be two normed spaces. An **operator** $\mathcal{T}$ is a linear map $\mathcal{T} : A \to B$.

Remark II.1. In most of the linear algebra courses it is assumed that the concept of *continuity* is well-defined. This is true in the case when A is assumed to be finite dimensional. The reason for this is that all norm's are equivalent in finite dimensional vector spaces. This is not true in infinite dimensional vector spaces.. In order to understand the concept of continuity in infinite dimensional vector spaces like $L^2\left(\mathbb{R}^N\right)$ which is one of the most fundamental Hilbert space in Quantum mechanics. We need to understand the idea of a *bounded operator* before we talk about continuity.

Definition II.2 (***Bounded Operator***)**.** Let $(V, \|.\|_V)$ be a normed space and $(W, \|.\|_W)$ be a Banach space. A linear operator $A : V \to W$ is called *bounded* if $\forall\, f \in V \setminus \{0\}$,

$$\sup_{f \in V} \frac{\|Af\|_W}{\|f\|_V} < \infty \tag{II.1}$$

another definition is,
If $\exists\, C \in \mathbb{R}$ with $\forall\, \boldsymbol{x} \in H$

$$\|A\boldsymbol{x}\|_W \leq C \|\boldsymbol{x}\|_V \tag{II.2}$$

Lemma II.1. *An operator $\mathcal{T} : A \to B$ is called **continuous** iff it is bounded.*

Definition II.3. We denote H' to be the set of continuous operators from $H \to \mathbb{C}$. Also, we denote $\mathcal{B}(H)$ to be the set of continuous operators from $H \to H$. Basically a map $\mathcal{T} \in H'$ is a continuous bounded map $T : H \to \mathbb{C}$. Also, a map $A \in \mathcal{B}(H)$ is a continuous bounded map $A : H \to H$.

Definition II.4 (***Unbounded operator***)**.** An operator which is not bounded is an unbounded operator.

The most frequently used in physics is the $L^2\left(\mathbb{R}^3\right)$ which is the space of square-integrable functions. The most important operators up-to a multiplicative constant are

1. The *position operat*or

$$\hat{\boldsymbol{x}} : L^2\left(\mathbb{R}^3\right) \to L^2\left(\mathbb{R}^3\right) \tag{II.3}$$
$$\hat{x}\psi \mapsto \boldsymbol{x}\psi \tag{II.4}$$

2. The momentum operator

$$\hat{\boldsymbol{p}} : L^2\left(\mathbb{R}^3\right) \to L^2\left(\mathbb{R}^3\right) \tag{II.5}$$
$$\hat{\boldsymbol{p}}\psi \mapsto \frac{\hbar}{i}\nabla\psi \tag{II.6}$$

These operators are not well defined on the entire *Hilbert space* and even on the subspace where they are well defined, they are not bounded. As this paper focuses on the study of the momentum operator. The momentum operator is just the derivative operator with some finite multiplicative constant (we have an imaginary number so the concept of finite seems vague, what we mean is that the real and imaginary part of it is finite). The finite multiplicative constant will not matter if we have an unbounded operator. One can easily using basic analysis techniques prove that the derivative operator D is an unbounded operator. We know from basic real analysis that D is a *linear* operator.

Consider the following the derivative operator defined abstractly in the following way :

$$D : C^1_{\mathbb{C}}[0,1] \to C^0_{\mathbb{C}}[0,1] \qquad \text{(II.7)}$$
$$f \mapsto f'$$

We will now show that this operator is indeed unbounded. The momentum operator is defined on a subset of $C^1_{\mathbb{C}}$ with additional structure. If we prove that this operator is unbounded on such a big space, then we can later use this result claiming that the momentum operator is unbounded.

Proposition II.1. *The operator D defined in (II.7) is unbounded.*

Proof. Can be found in literature [Szekeres, Hall]. Not extremely necessary right now. □

III. SELF ADJOINT AND ESSENTIALLY SELF-ADJOINT OPERATORS

Definition III.1 (***Densely defined linear operator***)**.** A linear map or operator $\mathcal{T} : \mathcal{D}_{\mathcal{T}} \to \mathcal{H}$ is said to be **densely defined** if $\mathcal{D}_{\mathcal{T}}$ is a *dense set* in $\mathcal{H}$, i.e.

$$\forall \varepsilon > 0 : \forall \psi \in \mathcal{H} : \exists \varphi \in \mathcal{D}_{\mathcal{T}} : \|\varphi - \psi\| < \varepsilon \qquad \text{(III.1)}$$

Remark III.1. Equivalently we can say, if $\overline{\mathcal{D}_{\mathcal{T}}} = \mathcal{H}$ then we have a densely defined operator. Essentially, $\forall \psi \in \mathcal{H} : \exists \{\varphi_n\}_{n\in\mathbb{N}} \in \mathcal{D}_{\mathcal{T}} : \{\varphi_n\} \longrightarrow_{n\to\infty} \psi$.

Definition III.2 (***Adjoint operator***)**.** Let $\mathcal{T} : \mathcal{D}_{\mathcal{T}} \to \mathcal{H}$ be a *densely* defined operator on $\mathcal{H}$. The **adjoint** of $\mathcal{T}$ is the operator $\mathcal{T}^* : \mathcal{D}_{\mathcal{T}^*} \to \mathcal{H}$ defined by $\mathcal{T}$ if
$\mathcal{D}_{\mathcal{T}^*} := \{\psi \in \mathcal{H} | \exists \eta \in \mathcal{H} : \forall \varphi \in \mathcal{D}_{\mathcal{T}} : \langle \psi \mid \mathcal{T}\varphi\rangle = \langle \eta \mid \varphi\rangle\}$ and $\mathcal{T}^*\psi := \eta$ is true.

Let us use the definition above to prove a trivial property of the *adjoint.*

Proposition III.1. *The adjoint operator $\mathcal{T}^* : \mathcal{D}_{\mathcal{T}^*} \to \mathcal{H}$ is well defined.*

Proof. Let $\psi \in \mathcal{H}$ and let $\eta, \tilde{\eta} \in \mathcal{H}$ be such that

$$\forall \varphi \ \in \ \mathcal{D}_{\mathcal{T}}$$
$$\langle \psi \mid \mathcal{T}\varphi\rangle = \langle \eta \mid \varphi\rangle \text{ and } \langle \psi \mid \mathcal{T}\varphi\rangle = \langle \tilde{\eta} \mid \varphi\rangle$$

Then $\forall \varphi \in \mathcal{D}_{\mathcal{T}}$,

$$\begin{aligned} \langle \eta - \tilde{\eta} \mid \varphi\rangle &= \langle \eta \mid \varphi\rangle - \langle \tilde{\eta} \mid \varphi\rangle \\ &= \langle \psi \mid \mathcal{T}\varphi\rangle - \langle \psi \mid \mathcal{T}\varphi\rangle = 0 \qquad \text{(III.2)} \\ \langle \eta \mid \varphi\rangle &= \langle \tilde{\eta} \mid \varphi\rangle \\ \eta &= \tilde{\eta} \qquad \text{(III.3)} \end{aligned}$$

In the last step we use positive-definiteness. □

Definition III.3 (***Kernel and Range of a Linear operator***)**.** The definitions of *kernel and range* are the same that one knows from their elementary linear algebra course.

- $\ker(\mathcal{T}) := \{\varphi \in \mathcal{D}_{\mathcal{T}} | \mathcal{T}\varphi = 0\}$
- $\operatorname{ran}(\mathcal{T}) := \{\mathcal{T}\varphi | \varphi \in \mathcal{D}_{\mathcal{T}}\}$

The range is also known as the *image* and $\operatorname{im}(\mathcal{T})$ is an alternative notation.

Definition III.4 (***Invertible operator***)**.** An operator $\mathcal{T}$ is called **invertible** if,

$$\exists \text{an operator } : \mathcal{O} \text{such that } \mathcal{T} \circ \mathcal{O} = \mathrm{id}_{\mathcal{H}} \mathcal{O} \circ \mathcal{T} = \mathrm{id}_{\mathcal{D}_{\mathcal{T}}}$$

An operator is **invertible** iff

1. $\ker(\mathcal{T}) = \{0\}$
2. $\overline{\operatorname{ran}(\mathcal{T})} = \mathcal{H}$

Proposition III.2. *Let $\mathcal{T}$ be a densely defined operator. Then $\ker(\mathcal{T}^*) = ran(\mathcal{T})^{\perp}$.*

Proof. Let $\psi \in \ker(\mathcal{T}^*) \iff \mathcal{T}\psi = 0$, then

$$\forall \varphi \in \mathcal{D}_{\mathcal{T}} : \langle \psi \mid \mathcal{T}\varphi\rangle = \langle \mathcal{T}^*\psi \mid \varphi\rangle = 0 \Rightarrow \psi \in \operatorname{ran}(\mathcal{T})^{\perp}$$

□

Definition III.5 (***Extension of an operator***)**.** Let $\mathcal{T}$ and $\widetilde{\mathcal{T}}$ be operators defined in the following way

$$\mathcal{T} : \mathcal{D}_{\mathcal{T}} \to \mathcal{H} \qquad \text{(III.4)}$$
$$\widetilde{\mathcal{T}} : \mathcal{D}_{\widetilde{\mathcal{T}}} \to \mathcal{H} \qquad \text{(III.5)}$$

We say that $\widetilde{\mathcal{T}}$ is an **extension** of $\mathcal{T}$ i.e. $\mathcal{T} \subseteq \widetilde{\mathcal{T}}$ if

1. $\mathcal{D}_{\mathcal{T}} \subseteq \mathcal{D}_{\widetilde{\mathcal{T}}}$
2. $\forall \varphi \in \mathcal{D}_{\mathcal{T}} \Rightarrow \mathcal{T}\varphi = \widetilde{\mathcal{T}}\varphi$

Proposition III.3. *Let $\mathcal{T}, \widetilde{\mathcal{T}}$ be densely defined operators. If $\mathcal{T} \subseteq \widetilde{\mathcal{T}}$ then $\widetilde{\mathcal{T}}^* \subseteq \mathcal{T}^*$*

Proof. Let $\psi \in \mathcal{D}_{\widetilde{\mathcal{T}}^*}$. Then $\exists \eta \in \mathcal{H}$ such that $\forall \beta \in \mathcal{D}_{\mathcal{T}}$: $\left\langle \psi | \widetilde{\mathcal{T}}\beta \right\rangle = \langle \eta | \beta\rangle$ where $\eta := \widetilde{\mathcal{T}}^*\psi$

In the above line we just redefined what we know. Now we will use some more facts to prove our proposition.

Particularly, as $\mathcal{T} \subseteq \widetilde{\mathcal{T}}$ we have $\mathcal{D}_{\mathcal{T}} \subseteq \mathcal{D}_{\widetilde{\mathcal{T}}}$ and then

$$\forall \alpha \in \mathcal{D}_{\mathcal{T}} \subseteq \mathcal{D}_{\widetilde{\mathcal{T}}} : \left\langle \psi | \widetilde{\mathcal{T}}\alpha \right\rangle = \langle \psi | \mathcal{T}\alpha\rangle = \langle \eta | \alpha\rangle \qquad \text{(III.6)}$$

Therefore $\psi \in \mathcal{D}_{\mathcal{T}^*}$ and hence $\mathcal{D}_{\widetilde{\mathcal{T}}^*} \subseteq \mathcal{D}_{\mathcal{T}^*}$ □

A. Adjoint of a Symmetric operator

Definition III.6 (***Symmetric operator***)**.** A *densely defined operator* $\mathcal{T}:\mathcal{D}_{\mathcal{T}}\to\mathcal{H}$ is called **symmetric** if

$$\forall\,\alpha,\beta\in\mathcal{D}_{\mathcal{T}}\Rightarrow\langle\alpha|\mathcal{T}\beta\rangle$$

Remark III.2. Let us address the big elephant in the mathematical notions related to quantum mechanics. What are these *so called Hermitian operators and what do they have to do with symmetric or self-adjointness?* In a lot of Physics literature, these symmetric operators are referred to as *Hermitian operators.* However, many times the notion of *Hermitian* is associated with the notion of self-adjointness. Statements like *Observables in quantum mechanics correspond to Hermitian operators* are incorrect as *Hermitian* corresponds to symmetric operators and not self-adjointness. On the other hand, if one decides to use Hermitian as a synonym of self-adjoint, then it is not true that all symmetric operators are *Hermitian.* We can avoid this confusion by completely erasing the word Hermitian and instead just using *symmetric* and *self-adjoint* operator.

Lemma III.1. *If $\mathcal{T}$ is symmetric, then $\mathcal{T}\subseteq\mathcal{T}^*$.*

Proof. Let $\psi\in\mathcal{D}_{\mathcal{T}}$ and let $\eta\equiv\mathcal{T}\psi$. Then by symmetry we have

$$\forall\,\alpha\in\mathcal{D}_{\mathcal{T}}:\langle\psi|\mathcal{T}\alpha\rangle=\langle\mathcal{T}\psi|\alpha\rangle=\langle\eta|\alpha\rangle$$

This means $\psi\in\mathcal{D}_{\mathcal{T}^*}$. Hence, $\mathcal{D}_{\mathcal{T}}\subseteq\mathcal{D}_{\mathcal{T}^*}$ and $\mathcal{T}^*\psi\equiv\eta=\mathcal{T}\psi$. □

Definition III.7 (***Self adjoint operator***)**.** A *densely defined operator* $\mathcal{T}:\mathcal{D}_{\mathcal{T}}\to\mathcal{H}$ is called *self-adjoint* if $\mathcal{T}=\mathcal{T}^*$. We are comparing operators, so this means the following must be true if the equality must hold

1. $\mathcal{D}_{\mathcal{T}}=\mathcal{D}_{\mathcal{T}^*}$
2. $\forall\,\varphi\in\mathcal{D}_{\mathcal{T}}:\mathcal{T}\varphi=\mathcal{T}^*\varphi$

Corollary III.1. *A self-adjoint operator is maximal with respect to the self-adjoint extension.*

Proof. Let $\mathcal{T},\widetilde{\mathcal{T}}$ be self-adjoint operators and suppose $\mathcal{T}\subseteq\widetilde{\mathcal{T}}$. Then we have

$$\mathcal{T}\subseteq\widetilde{\mathcal{T}}=\widetilde{\mathcal{T}}^*\subseteq\mathcal{T}^*=\mathcal{T}$$

and hence $\widetilde{\mathcal{T}}=\mathcal{T}$. □

Remark III.3. As a fact, self-adjoint operators are maximal even with respect to symmetric extension. The difference will be $\widetilde{\mathcal{T}}\subseteq\widetilde{\mathcal{T}}^*$ instead of $\widetilde{\mathcal{T}}\subseteq\widetilde{\mathcal{T}}^*$.

B. Closability, closure, closedness of an operator

Definition III.8 (***Closable operator***)**.**
A *densely defined operator* $\mathcal{T}$ is called **closeable** if it's *adjoint* $\mathcal{T}^*$ is also *densely defined*

Definition III.9 (***Closure of an operator***)**.**
The **closure** of a *closable operator* $\mathcal{T}$ is

$$\overline{\mathcal{T}}\equiv\mathcal{T}^{**}=(\mathcal{T}^*)^*$$

where the *over-line* denotes closure.

Definition III.10 (***Closed operator***)**.**
An *operator* $\mathcal{T}$ is called **closed** if

$$\mathcal{T}=\overline{\mathcal{T}}$$

Proposition III.4. *A symmetric operator is necessarily closable.*

Proof. Let $\mathcal{T}$ be a symmetric operator. Then, $\mathcal{T}\subseteq\mathcal{T}^*$ and $\mathcal{D}_{\mathcal{T}}\subseteq\mathcal{D}_{\mathcal{T}^*}$. Symmetric operators by definition are densely defined. Hence

$$\mathcal{H}=\overline{\mathcal{D}_{\mathcal{T}}}\subseteq\overline{\mathcal{D}_{\mathcal{T}^*}}\subseteq\mathcal{H}$$

which concludes the fact that the adjoint of a symmetric operator is also densely defined. Hence, $\mathcal{T}$ is **closable** if it is symmetric. □

C. Essentially Self Adjoint operators

Definition III.11 (***Essentially self-adjoint operator***)**.** A *symmetric* operator $\mathcal{T}$ is called **essentially self-adjoint** if $\overline{\mathcal{T}}$ is self-adjoint.

Remark III.4. The condition for *essentially-self adjointness* is a weaker condition than self-adjointness i.e if an operator is self-adjoint it is implied that it is also essentially self adjoint. The other way is not true in general.

Proof. $\mathcal{T}=\mathcal{T}^*\Rightarrow\mathcal{T}^*=\mathcal{T}^{**}\Rightarrow\mathcal{T}^{**}=\mathcal{T}^{***}\Rightarrow\overline{\mathcal{T}}=\overline{\mathcal{T}}^*$ □

Theorem III.1. *If $\mathcal{T}$ is essentially self-adjoint, then there exists a unique self-adjoint extension of $\mathcal{T}$, namely $\overline{\mathcal{T}}$.*

Proof. This theorem is the essence of essentially self-adjoint operators. So we will go through the proof here, □

1. $\mathcal{T}$ is symmetric $\Rightarrow\mathcal{T}$ is closable $\Rightarrow\overline{\mathcal{T}}$ exists

2. $\mathcal{T}\subseteq\overline{\mathcal{T}}=\mathcal{T}^{**}$ is known. Hence, $\overline{\mathcal{T}}$ is an extension of $\mathcal{T}$.

3. The only thing that remains to be shown is that $\overline{\mathcal{T}}$ is the *unique* self-adjoint extension.

IV. CASE STUDY OF THE MOMENTUM OPERATOR

In this section we will exclusively talk about the momentum operator in quantum mechanics in the language we built in the previous sections. Let us define the momentum operator precisely.

Definition IV.1 (***Momentum operator***)**.** The momentum operator on the j'th coordinate (in the operator language described above) is defined as follows

$$\hat{\mathcal{P}}_j : \mathcal{D}_{\mathcal{P}} \to L^2(\mathbb{R}) \tag{IV.1}$$
$$\psi \mapsto -i\hbar\partial_j\psi \tag{IV.2}$$
$$\psi \mapsto -i\psi' \tag{IV.3}$$

We will use the last equation from above indefinite times. We use $\hbar = 1$.

Remark IV.1. This is one of the most commonly found definition of the momentum operator in quantum mechanics. In the previous sections whenever we are talking about operators which are self-adjoint or have some other property, we have assumed them to be densely defined. If an operator needs to be explicitly defined, along with the map we also need to define it's domain. This is something that is always exclusively skipped in most of the quantum mechanics texts.

A. Absolutely continuous functions and Sobolev spaces

In some of the calculations in this section we will be needing a few more definitions. Let us take a moment to define them before proceeding. More precisely we will be needing the following relation between *Continuous functions* $\mathcal{C}^1$, *absolutely continuous functions* $\mathcal{AC}$ *and Sobolev spaces* $\mathscr{H}^1$

$$\mathcal{C}^1([a,b]) \subseteq \mathscr{H}^1([a,b]) \subseteq \mathcal{AC}([a,b]) \tag{IV.4}$$

Definition IV.2 (***Absolutely continuous spaces*** **(**$\mathcal{AC}$**)**)**.** Let us define a function $\psi : [a,b] \to \mathbb{C}$. ψ is *absolutely continuous i.e.* $\psi \in \mathcal{AC}$ *if* $\exists\, \rho \in [a,b] \to \mathbb{C}$ *integrable* (Lebesgue integrable) such that

$$\psi(x) = \psi(a) + \int_a^x \rho(y)\, y$$

where ρ is the derivative of ψ almost everywhere (a.e), i.e $\rho =_{\text{a.e}} \psi'$.

$$\mathcal{AC}([a,b]) \equiv \left\{\psi \in L^2(\mathbb{R}) \mid \psi \text{ is absolutely continuous}\right\} \tag{IV.5}$$

Definition IV.3 (***Sobolev space***)**.** The Sobolev space is defined by the following set

$$\mathscr{H}([a,b]) \equiv \left\{\psi \in \mathcal{AC}([a,b]) \mid \psi' \in L^2(\mathbb{R})\right\} \tag{IV.6}$$

Momentum operator on a Compact interval v/s on a Circle

In this section we will try defining our momentum operator precisely on a compact interval and on a circle. We do this so we can analyze the properties of this operator by looking at spaces that are one dimensional but not $\mathbb{R}$ itself. In both the cases we will define our Hilbert space to be $\mathcal{H} \equiv L^2([0, 2\pi])$.

Let us try to define *reasonable* domains for the momentum operators on both these intervals by eyeballing the situation:

- On a *compact interval*

$$\mathcal{D}_{\mathcal{P}} \equiv \left\{\psi \in \mathcal{C}^1([0,2\pi]) \mid \psi(0) = 0 = \psi(2\pi)\right\} \tag{IV.7}$$

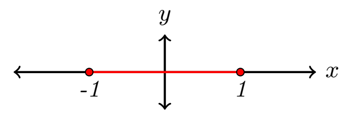

Figure IV.1. Compact interval from $x = -1$ to $x = 1$

- On a *circle*

$$\mathcal{D}_{\mathcal{P}} \equiv \left\{\psi \in \mathcal{C}^1([0,2\pi]) \mid \psi(0) = \psi(2\pi)\right\} \tag{IV.8}$$

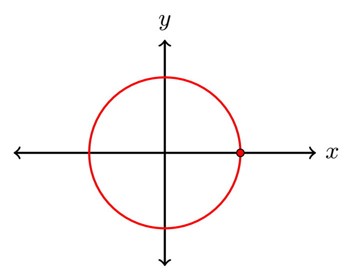

Figure IV.2. Unit circle

These look like reasonable guesses but we need to actually check if the $\hat{\mathcal{P}}_j$ defined on these domains are self-adjoint or not (It turns out that neither of them are self-adjoint). This is the main goal of this review paper - *understanding the procedure of formulating a momentum operator on some Hilbert space.*

B. Momentum operator on a *Compact interval*

We consider the interval $\mathcal{I} = [0, 2\pi]$ with the operator defined as follows (we will take $\hbar = 1$ i.e. use Planck units for convenience). Let us rewrite the momentum operator

$$\hat{\mathcal{P}}_j : \mathcal{D}_{\mathcal{P}} \to L^2\left([0,2\pi]\right) \tag{IV.9}$$
$$\psi \mapsto -i\psi' \tag{IV.10}$$
$$\psi' = \frac{\partial \psi}{\partial x_j} \tag{IV.11}$$

The main goal of this part is to check if $\hat{\mathcal{P}}_j$ defined as above is self adjoint with respect to our domain $\mathcal{I}$. Let us do this one step at a time and formulate an algorithm to do this eventually :

1. *Step I : Is $\hat{\mathcal{P}}_j$ symmetric?*

We need to check if our operator is symmetric because it is a necessary condition for self-adjointness. We check if the operator is self-adjoint by checking if, $\forall\, \psi, \varphi \in \mathcal{D}_{\mathcal{P}}$

$$\left\langle \psi | \hat{\mathcal{P}}_j \varphi \right\rangle = \left\langle \hat{\mathcal{P}}_j \psi | \varphi \right\rangle \tag{IV.12}$$

Let us explicitly compute this to check. We will be using integration by parts $\left(\int u\, dv = uv - \int v\, du\right)$ which is a common technique for such computations.

$$\begin{aligned} -i\int_0^{2\pi} dx_j\, \overline{\psi\left(x_j\right)}\, \varphi'\left(x_j\right) &= \int_0^{2\pi} dx_j \overline{\left(-i\right)\psi'\left(x_j\right)}\, \varphi\left(x_j\right) \\ &= i\int_0^{2\pi} dx_j \overline{\psi'\left(x_j\right)}\, \varphi\left(x_j\right) \\ &= i[\left(\overline{\psi\left(x_j\right)}\varphi\left(x_j\right)\right)\Big|_0^{2\pi} \\ &\quad - \int_0^{2\pi} dx_j\, \varphi'\left(x_j\right)\overline{\psi\left(x_j\right)}] \end{aligned} \tag{IV.13}$$

We need to be careful with the boundary term. We know that $\psi, \varphi \in \mathcal{D}_{\mathcal{P}}$ and hence $\psi(0) = \varphi(0) = \psi(2\pi) = \varphi(2\pi) = 0$. Using this in the above condition we get the following

$$\begin{aligned} \left\langle \psi | \hat{\mathcal{P}}_j \varphi \right\rangle &= 0 - i\int_0^{2\pi} \varphi'\left(x_j\right)\overline{\psi\left(x_j\right)}\, dx_j \\ &= \left\langle \hat{\mathcal{P}}_j \psi | \varphi \right\rangle \end{aligned} \tag{IV.14}$$

Hence, proving that $\hat{\mathcal{P}}_j$ is symmetric indeed.

2. *Step II : Is $\hat{\mathcal{P}}_j$ self adjoint?*

To check this, we need to calculate the adjoint of $\hat{\mathcal{P}}_j$ and see if it coincides with the original operator. As we recall, when we are comparing the equality between two *operators* we need to make sure that their domains match along with their actions on the elements of these domains.

Let us start with something that we know - $\hat{\mathcal{P}}_j$ is symmetric and by using lemma(III.1), we can say

$$\hat{\mathcal{P}}_j \subseteq \hat{\mathcal{P}}_j^* \to \hat{\mathcal{P}}_j^* \text{ is an extension of } \hat{\mathcal{P}}_j$$

Let $\psi \in \mathcal{D}_{\mathcal{P}^*}$ then we have to show that

$$\exists\, \eta \in L^2\left(R\right) : \forall\, \varphi \in \mathcal{D}_{\mathcal{P}} : \left\langle \psi | \hat{\mathcal{P}}_j \varphi \right\rangle = \left\langle \eta | \varphi \right\rangle \tag{IV.15}$$

The above condition is equivalent to showing

$$\int_0^{2\pi} dx_j\, \overline{\psi\left(x_j\right)}\left(-i\right)\varphi'\left(x_j\right) = \int_0^{2\pi} dx_j\, \overline{\eta\left(x_j\right)}\varphi\left(x_j\right) \tag{IV.16}$$

With a loose argument we can always find a function $N : [a,b] \to \mathbb{C}$ such that $\eta =_{\text{ae}} N'$. Using this we will rewrite the above equation as

$$\begin{aligned} \int_0^{2\pi} dx_j\, \overline{\psi\left(x_j\right)}\left(-i\right)\varphi'\left(x_j\right) &= \int_0^{2\pi} \overline{\eta\left(x_j\right)}\varphi\left(x_j\right) \\ &= \int_0^{2\pi} dx_j\, \overline{N'\left(x_j\right)}\varphi\left(x_j\right) \end{aligned}$$

$$\int_0^{2\pi} dx_j \left(\overline{\psi\left(x_j\right)}\left(-i\right)\varphi'\left(x_j\right)\right) = -\int_0^{2\pi} \overline{N'\left(x\right)}\varphi'\left(x_j\right) dx_j + \left[\overline{N\left(x_j\right)}\varphi\left(x_j\right)\right]\Big|_0^{2\pi}$$

$$\int_0^{2\pi} dx_j \left[\overline{\psi\left(x_j\right)}\left(-i\right)\varphi'\left(x_j\right) + \overline{N'\left(x\right)}\varphi'\left(x_j\right)\right] = 0 \tag{IV.17}$$

$$-i\int_0^{2\pi} \left(\varphi'\left(x_j\right)\overline{\left(\psi\left(x_j\right) - iN\left(x_j\right)\right)}\right) dx_j = 0 \tag{IV.18}$$

$$\left\langle \psi\left(x_j\right) - iN\left(x_j\right) | \varphi'\left(x_j\right) \right\rangle = 0 \tag{IV.19}$$

From this last statement we can conclude that $\psi\left(x_j\right) - iN\left(x_j\right) \in \left\{\varphi' | \varphi \in \mathcal{D}_{\mathcal{P}}\right\}^{\perp}$ where $\perp$ means the orthogonal complement.

We can make two observations at this point :

1.
$$\left\{\varphi'\left(x_j\right) \mid \varphi \in \mathcal{D}_{\mathcal{P}}\right\} = \left\{\xi \in \mathcal{C}^0\left(\mathcal{I}\right) \mid \int_0^{2\pi} \xi\left(x_j\right) dx_j = 0\right\}$$

Proof. We will prove equality of the sets by proving LHS $\subseteq$ RHS and LHS $\supseteq$ RHS simultaneously :

$(\subseteq)$

Let $\varphi' \in \left\{\varphi'\left(x_j\right) \mid \varphi \in \mathcal{D}_{\mathcal{P}}\right\}$. Let $\varphi' = \xi$,

$$\begin{aligned} \int_0^{2\pi} \xi\, dx_j &= \int_0^{2\pi} \varphi'\, dx_j = \left[\varphi'\left(x_j\right)\right]\big|_0^{2\pi} = 0 \\ &\Rightarrow \varphi'\left(x_j\right) \in \left\{\xi \in \mathcal{C}^0\left(\mathcal{I}\right) \mid \int_0^{2\pi} \xi\left(x_j\right) dx_j = 0\right\} \end{aligned}$$

(⊇)

Let $\xi \in \left\{\xi \in \mathcal{C}^0(\mathcal{I}) \mid \int_0^{2\pi} \xi(x_j)\, dx_j = 0\right\}$. This implies

$$\begin{aligned}\varphi_\xi(x_j) = \int_0^{\pi} \xi(y)\, dy \Rightarrow \varphi_\xi \in \mathcal{C}^1 \\ \Rightarrow \varphi_\xi(0) = 0 = \varphi_\xi(2\pi) \\ \Rightarrow \varphi_\xi \in \{\varphi'(x_j) \mid \varphi \in \mathcal{D}_\mathcal{P}\}\end{aligned}$$

Together with (⊆) and (⊇) we can conclude the proof. □

2. $\overline{\{\varphi'(x_j) | \varphi(x_j) \in \mathcal{D}_\mathcal{P}\}} = \{1\}^\perp$ where 1 is the constant function.

Proof. We can write

$$\int_0^{2\pi} \xi(x)\, dx = 0 \Rightarrow \langle 1|\xi\rangle = 0$$

Using this and the proof from above we can effectively say

$$\left\{\xi \in \overline{\mathcal{C}^0(\mathcal{I})} \mid \langle 1|\xi\rangle = 0\right\} = \{1\}^\perp$$

□

We can now proceed the following way

$$\begin{aligned}\psi - iN \in \{\varphi'(x_j) \mid \varphi \in \mathcal{D}_\mathcal{P}\}^\perp &= \overline{\{\varphi'(x_j) \mid \varphi \in \mathcal{D}_\mathcal{P}\}^\perp} \\ \hookrightarrow \left(\{\varphi'(x_j) \mid \varphi \in \mathcal{D}_\mathcal{P}\}^\perp\right)^{\perp\perp} &= \left(\{\varphi'(x_j) \mid \varphi \in \mathcal{D}_\mathcal{P}\}^{\perp\perp}\right)^\perp \\ \hookrightarrow \overline{\{\varphi'(x_j) \mid \varphi \in \mathcal{D}_\mathcal{P}\}}^\perp &= \left(\{1\}^\perp\right)^\perp = \{1\}^{\perp\perp} \\ \hookrightarrow \overline{\{1\}} &= \{C : [a,b] \to \mathbb{C} \\ &\quad \mid x \mapsto \text{Constant}\}\end{aligned}$$

Hence we say $\psi(x_j) - iN(x_j) = \text{Constant} \Rightarrow \psi(x_j) = \text{Constant} + iN(x_j)$ and we use the fact that $N(x_j) \in \mathcal{AC}$ to say

$$\psi(x_j) \in \mathcal{AC}$$

Thus, $\psi \in \mathcal{D}_{\mathcal{P}^*} \Rightarrow \psi(x_j) \in \mathcal{AC}(\mathcal{I}) \Rightarrow \mathcal{D}_{\mathcal{P}^*} \subseteq \mathcal{AC}(\mathcal{I})$

What we need is $\hat{\mathcal{P}}_j^* : \mathcal{D}_{\mathcal{P}^*} \to L^2(\mathbb{R})$ which requires $-i\psi'(x_j) \in L^2(\mathbb{R})$

$$\begin{aligned}\psi(x_j) \in \mathscr{H}^1(\mathcal{I}) \\ \Rightarrow \mathcal{D}_{\mathcal{P}^*} \subseteq \mathscr{H}^1(\mathcal{I})\end{aligned}$$

So, as expected we get

$$\begin{aligned}\hat{\mathcal{P}}_j \subseteq \hat{\mathcal{P}}_j^* \\ \Rightarrow \mathcal{D}_\mathcal{P} \subseteq \mathcal{D}_{\mathcal{P}^*}\end{aligned}$$

$\hat{\mathcal{P}}_j$ was defined on $\mathcal{C}^1$ with boundary conditions and $\hat{\mathcal{P}}_j^*$ was defined on $\mathscr{H}^1$

$$\Rightarrow \hat{\mathcal{P}}_j \subsetneq \hat{\mathcal{P}}_j^*$$

Hence, $\hat{\mathcal{P}}_j$ is not self adjoint. This *problem* can goes further ahead and can be dealt with the notion of Essentially self adjointness.

So, we showed that $\hat{\mathcal{P}}_j$ is not self-adjoint. It could be *essentially self-adjoint?* We recall that essentially self-adjoint means the *closure (double adjoint)* of $\hat{\mathcal{P}}_j$ is self-adjoint. If we could prove this then it works in our favor, Why? Because we have theorem saying, If the closure is self-adjoint, then the closure is the unique self-adjoint extension. In this case, we just take the closure instead of the original operator and we will have a self-adjoint operator.

3. *Step III: Calculate the closure $\hat{\mathcal{P}}_j^{**}$ of $\hat{\mathcal{P}}_j$*

We know that $\hat{\mathcal{P}}_j$ is symmetric and from one of the theorem we proved earlier : $\hat{\mathcal{P}}_j \subseteq \hat{\mathcal{P}}_j^{**} \subseteq \hat{\mathcal{P}}_j^*$. We also know from previous section that $\hat{\mathcal{P}}_j^{**}$ is also symmetric.

Let $\psi \in \mathcal{D}_{\mathcal{P}^{**}}$ then $\forall\ \varphi \in \mathcal{D}_{\mathcal{P}^*}$: $\left\langle \psi|\hat{\mathcal{P}}_j\varphi\right\rangle = \left\langle \hat{\mathcal{P}}_j^{**}\psi|\varphi\right\rangle$.

Now we use a standard trick from the book using the fact : $\hat{\mathcal{P}}_j^{**} \subseteq \hat{\mathcal{P}}_j$ which means $\mathcal{D}_{\mathcal{P}^{**}} \subseteq \mathcal{D}_{\mathcal{P}^*}$ and $\hat{\mathcal{P}}_j^{**}\psi = \hat{\mathcal{P}}_j^*\psi$. The above two lines give us the equality

$$\left\langle \psi|\hat{\mathcal{P}}_j\varphi\right\rangle = \left\langle \hat{\mathcal{P}}_j^{**}\psi|\varphi\right\rangle = \left\langle \hat{\mathcal{P}}_j^*\psi|\varphi\right\rangle \tag{IV.20}$$

Thus, $\forall\, \psi \in \mathcal{D}_{\mathcal{P}^{**}}$ and $\forall\, \varphi \in \mathcal{D}_{\mathcal{P}^*}$ we have

$$\begin{aligned}\left\langle \psi|\hat{\mathcal{P}}_j^*\varphi\right\rangle &= \int_0^{2\pi} \overline{\psi(x)}\,(-i)\,\varphi'(x)\, dx \\ \left\langle \hat{\mathcal{P}}_j^*\psi|\varphi\right\rangle &= \int_0^{2\pi} \overline{(-i)\psi'(x)}\varphi(x)\, dx\end{aligned}$$

The left hand side of both the equations are the same and hence we get

$$\begin{aligned}\int_0^{2\pi} \overline{\psi(x)}\,(-i)\,\varphi'(x)\, dx &= i\int_0^{2\pi} \overline{\psi(x)}\varphi(x)\, dx \\ -i\int_0^{2\pi} \overline{\psi(x)}\varphi'(x)\, dx &= i\left[\overline{\psi(x)}\varphi(x)|_0^{2\pi} - \int_0^{2\pi} \overline{\psi(x)}\varphi'(x)\, dx\right] \\ 0 &= i\left[\overline{\psi(x)}\varphi(x)\right]_0^{2\pi} \\ 0 &= \overline{\psi(2\pi)}\varphi(2\pi) - \overline{\psi(0)}\varphi(0)\end{aligned}$$

We know nothing about φ at the endpoints 0 and 2π as $\varphi \in \mathscr{H}^1(I)$ (Sobolev space). Hence, $\overline{\psi(2\pi)} = \overline{\psi(0)} = 0$ in order to satisfy the equation above. This condition precisely means that $\psi \in \mathcal{D}_{\mathcal{P}^{**}}$. This gives is

$$\begin{aligned}\psi &\in \{\theta \in \mathcal{D}_{\mathcal{P}^*} | \psi(2\pi) = 0 = \psi(0)\} \\ &= \left\{\theta \in \mathscr{H}^1(I) | \psi(2\pi) = 0 = \psi(0)\right\}\end{aligned}$$

Hence, we can conclude that

$$\mathcal{D}_{\mathcal{P}^{**}} = \left\{\theta \in \mathscr{H}^1(I) | \psi(2\pi) = 0 = \psi(0)\right\}$$

At this point if one summarizes the definitions of the operators $\hat{\mathcal{P}}_j, \hat{\mathcal{P}}_j^*, \hat{\mathcal{P}}_j^{**}$ (don't forget their domain) one will believe that $\hat{\mathcal{P}}_j$ is neither self-adjoint nor essentially self-adjoint. This in particular is not good as this means one cannot compute a meaningful momentum operator on an interval. This problem is solved by calculating the defect indices of the operators and is beyond the scope of this paper. In the next example, this problem does not arise and a much more meaningful result is concluded quite early.

C. Momentum operator on a *Circle*

Let us begin by first stating our operator and domain like always.

$$\begin{aligned} \hat{\mathcal{P}}_j &: \mathcal{D}_{\mathcal{P}} \to L^2(I) \\ &: \psi \mapsto (-i)\,\psi' \\ \mathcal{D}_{\mathcal{P}} &\equiv \left\{\psi \in \mathcal{C}^1 | \psi(0) = \psi(2\pi)\right\} \end{aligned}$$

We can note that $\left(\hat{\mathcal{P}}_j\right)_{\text{Interval}} \subsetneq \left(\hat{\mathcal{P}}_j\right)_{\text{Circle}}$ as $\psi(2\pi) = 0 = \psi(0)$ is a stronger condition than $\psi(2\pi) = \psi(0)$. Hence we say momentum on the circle is an extension of the momentum operator on a interval. In this section whenever we write $\hat{\mathcal{P}}_j$ without specifying whether it is on the circle or interval, we will assume that it is $\left(\hat{\mathcal{P}}_j\right)_{\text{Circle}}$. Same applies to similar notations like $\hat{\mathcal{P}}_j^*, \mathcal{D}_{\mathcal{P}}$,etc.

1. Step I : Is $\hat{\mathcal{P}}_j$ symmetric?

We won't go through the calculations again. Using the algorithm from momentum on an interval one can effectively check that this is true. One of the major differences being that $[\psi\varphi]_0^{2\pi} = 0$ because of different boundary conditions.

2. Step II : Calculate the adjoint $\hat{\mathcal{P}}_j^*$

We will use the fact $\left(\hat{\mathcal{P}}_j\right)_{\text{Interval}} \subsetneq \left(\hat{\mathcal{P}}_j\right)_{\text{Circle}}$. As $\hat{\mathcal{P}}_j$ is symmetric we can conclude $\hat{\mathcal{P}}_j \subseteq \hat{\mathcal{P}}_j^*$ and $\left(\hat{\mathcal{P}}_j^*\right)_{\text{Circle}} \subsetneq \left(\hat{\mathcal{P}}_j^*\right)_{\text{Interval}}$. Using these two facts we can write the following

$$(\mathcal{D}_{\mathcal{P}^*})_{\text{Circle}} \subseteq (\mathcal{D}_{\mathcal{P}^*})_{\text{Interval}} = \mathscr{H}^1(I) \qquad \text{(IV.21)}$$

Hence, we already know that $\mathcal{D}_{\mathcal{P}^*}$ lies in the $\mathscr{H}$ space. We proceed like we did in the previous example.

Let $\psi \in \mathcal{D}_{\mathcal{P}^*} \Rightarrow \forall \varphi \in \mathcal{D}_{\mathcal{P}} : \left\langle \psi | \hat{\mathcal{P}}_j \varphi \right\rangle = \left\langle \hat{\mathcal{P}}_j^* \psi | \varphi \right\rangle$. We already know that $\left(\hat{\mathcal{P}}_j^*\right)_{\text{Interval}}$ is an extension of the $\left(\hat{\mathcal{P}}_j^*\right)_{\text{Circle}}$ operator. Hence, we can replace $\hat{\mathcal{P}}_j^*\psi$ by $\left(\hat{\mathcal{P}}_j^*\right)_{\text{Interval}} \psi$ as we already know the properties of $\left(\hat{\mathcal{P}}_j^*\right)_{\text{Interval}}$.

$$\begin{aligned} \int_0^{2\pi} dx\, \overline{\psi(x)}\,(-i)\,\varphi'(x) &= \int dx\, \overline{(-i)\,\psi'(x)}\varphi(x) \\ &\vdots \\ 0 &= i\left[\overline{\psi(x)}\varphi(x)\right]_0^{2\pi} \end{aligned}$$

We do not know anything about the boundaries for $\varphi(x)$ or $\psi(x)$. Let us expand the above equation and see if we can reach somewhere

$$\begin{aligned} i\,\varphi(0)\left[\psi(2\pi) - \psi(0)\right] &= 0 \\ \Rightarrow\ \psi(2\pi) &= \psi(0) \end{aligned}$$

Which gives is the domain,

$$\mathcal{D}_{\mathcal{P}^*} = \left\{\psi \in \mathscr{H}^1(I) | \psi(2\pi) = \psi(0)\right\} \qquad \text{(IV.22)}$$

So now we see that the $\mathcal{D}_{\mathcal{P}^*}$ for $\hat{\mathcal{P}}_j^*$ on a circle is not just $\mathscr{H}^1$ but $\mathscr{H}^1$ with some boundary condition. As we see, every case is unique enough to work out this everytime. So our intermediate result for the operator is

$$\begin{aligned} \hat{\mathcal{P}}_j^* &: \left\{\mathscr{H}^1(I) | \psi(2\pi) = \psi(0) \to L^2(I)\right\} \\ &\quad \psi \mapsto (-i)\,\psi' \end{aligned}$$

3. Step III : Is $\hat{\mathcal{P}}_j$ self adjoint?

Let us recall the following things :

1. $\mathcal{C}^1 \subsetneq \mathscr{H}^1$
2. These two equations

$$\begin{aligned} \mathcal{D}_{\mathcal{P}^*} &= \left\{\psi \in \mathscr{H}^1(I) | \psi(2\pi) = \psi(0)\right\} \\ \mathcal{D}_{\mathcal{P}} &= \left\{\psi \in \mathcal{C}^1 | \psi(2\pi) = \psi(0)\right\} \end{aligned}$$

Using these two facts we can effectively conclude, $\hat{\mathcal{P}}_j \subseteq \hat{\mathcal{P}}_j^* \Rightarrow \hat{\mathcal{P}}_j$ is **not** self-adjoint! Is it *essentially self adjoint?*

4. Step IV : Is $\hat{\mathcal{P}}_j$ essentially self adjoint?

We need to check $\hat{\mathcal{P}}_j^{**} = \hat{\mathcal{P}}_j^{***}$. To check that, we need to calculate the *closure.*

We know that $\hat{\mathcal{P}}_j$ is symmetric which gives us $\hat{\mathcal{P}}_j \subseteq \hat{\mathcal{P}}_j^{**} \subseteq \hat{\mathcal{P}}_j^*$. In this relation we know that $\mathcal{P} \in \mathcal{C}^1_{\text{Circle}}$ and $\mathcal{P} \in \mathscr{H}^1_{\text{Circle}}$.

Let $\psi \in \mathcal{D}_{\mathcal{P}^{**}}$, then $\forall \varphi \in \mathcal{D}_{\mathcal{P}^*}$: $\left\langle \psi | \hat{\mathcal{P}}_j^* \varphi \right\rangle = \left\langle \hat{\mathcal{P}}_j^{**} \psi | \varphi \right\rangle$. From the previous line we can say $\hat{\mathcal{P}}_j^{**}\psi = \hat{\mathcal{P}}_j^* \psi$ as $\hat{\mathcal{P}}_j^{**} \subseteq \hat{\mathcal{P}}_j^*$. So now we have

$$\left\langle \psi | \hat{\mathcal{P}}_j^* \varphi \right\rangle = \left\langle \hat{\mathcal{P}}_j^* \psi | \varphi \right\rangle$$
$$\vdots$$
$$0 = i[\overline{\psi(x)}\varphi(x)]_0^{2\pi}$$

We know $\varphi(2\pi) = \varphi(0)$ because $\varphi \in \mathcal{D}_{\mathcal{P}^*}$. So we get

$$0 = i\varphi(0)\left[\overline{\psi(2\pi)} - \overline{\psi(0)}\right]$$

This means $\psi(2\pi) = \psi(0)$. This conclusively means $\mathcal{D}_{\mathcal{P}^{**}} = \mathscr{H}^1 = \mathcal{D}_{\mathcal{P}^*} \Rightarrow \hat{\mathcal{P}}_j^{**} = \hat{\mathcal{P}}_j^*$. Hence, we have shown that it is essentially self-adjoint.

5. *Step V : Replace by the closure.*

We succeeded in constructing the unique momentum operator on a circle by taking the closure $\hat{\mathcal{P}}_j^{**}$ of our initial guess $\hat{\mathcal{P}}_j : \mathscr{H}^1(I) \to L^2(I)$ where $\forall \psi \in \mathscr{H}^1 : \psi \mapsto (-i)\psi'$.

V. CONCLUSION

The goal of this review paper was to show that defining operators in quantum mechanics mathematically precisely is not a trivial task. One needs to define the domain, check if it is self-adjoint, if it is not then check if it is essentially-self adjoint at least. We still did not discuss why we take the momentum operator as $\hat{\mathcal{P}}_j\psi \mapsto -i\psi'$. This is the goal of something known as the Stone-von Neumann theorem. After understand this review paper, a starting point would be to understand the Stone von-Neumann theorem which helps us construct observables like the momentum operator by taking analogues from Classical mechanics. Analogues like the Poisson bracket which in Quantum mechanics are *replaced* by commutator brackets, this is known as the quantization prescription.

[Schuller] *Lectures on Quantum theory, Fredric Schuller, University of Erlangen-Nuremberg*
Lecture 6 to 9 : https://www.youtube.com/playlist?list=PLPH7f_7ZlzxQVx5jRjbfRGEzWY_upS5K6

[Hall] *Quantum theory for Mathematicians, Brian C.Hall, Springer 2013*
Various topics from Chapter 7 to 10.
II.1

[R&S] *Methods of modern mathematical physics: Volume 1 - Functional Analysis, Michael Reed and Barry Simon, Academic Press 1980*
Various topics from chapter VI to VIII.

[QM Leipzig] Notes taken during the course 12-PHY-BIPTP4: Theoretical Physics IV - Quantum Mechanics at University of Leipzig, 2017. (Unpublished)

[Szekeres] *A course in Modern Mathematical Physics : Groups, Hilbert Space and Differential Geometry, Peter Szekeres, Cambridge University Press 2004.* (Chapter 13,14) (Recommended background reading).
I, II.1

[Background read] Link to transcript of a 10 page talk that might be sufficient as a quick background read. (Password : 806x)
http://rohankulkarni.me/sdm_downloads/functional-analysis0-for-qm/