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The non-self-adjointness of the radial momentum operator in n dimensions

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Abstract

The non-self-adjointness of the radial momentum operator has been noted before by several authors, but the various proofs are incorrect. We give a rigorous proof that the *n*-dimensional radial momentum operator is not selfadjoint and has no self-adjoint extensions. The main idea of the proof is to show that this operator is unitarily equivalent to the momentum operator on $L^2[(0, \infty), dr]$ which is not self-adjoint and has no self-adjoint extensions.

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1. Introduction

The radial momentum operator has been the subject of long discussions since the early days of quantum mechanics. Its exact form and relation to the Hamiltonian were considered by many authors [1–4]. Unlike the classical radial momentum, the connection between the radial momentum operator and the Hamiltonian of a free particle is not trivial [5, 6]. In fact, the connection between the radial momentum and the Hamiltonian in *n* dimensions is [6]

$$\hat{H} = \frac{\hat{P}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} + \frac{\hbar^2}{2m} \frac{(n-1)(n-3)}{4r^2}.$$

(At least formally, in principle one has to define the self-adjoint extension of \hat{P}_r^2 [7,8], which is not self-adjoint.)

Another important question that was raised is whether the radial momentum operator is an observable. Although Dirac claimed in *The Principles of Quantum Mechanics* that the radial momentum operator is 'real' [2], many authors realized that the radial momentum operator is not self-adjoint [4,9–11]. Unfortunately none of these proofs is correct.

In order to be an observable the radial momentum operator should be self-adjoint. Simply checking that the eigenvalues are real (as [4,9] do) is not sufficient (or necessary); one has to pay attention to the domain on which the operator is defined. Perhaps the most appealing (but incorrect) argument appears in [10, 11] (we use units where $\hbar = 1$):

'Since $[\hat{r}, \hat{P}_r] = i$ the unitary transformation $e^{-ia\hat{P}_r}$ shifts the operator \hat{r} by *a* (because $e^{ia\hat{P}_r}\hat{r}e^{-ia\hat{P}_r} = \hat{r} + a$) while leaving its spectrum invariant (being a unitary transformation). Therefore the spectrum of \hat{r} must be $(-\infty, \infty)$. Since the spectrum of \hat{r} is $(0, \infty)$ the operator \hat{P}_r cannot be self-adjoint'.

This statement, had it been true, would have prevented any operator which has canonical commutation relation with \hat{r} from being self-adjoint. Unfortunately, this statement cannot be true as we can see from the following counter-example. Consider the space $L^2[(0, 1), dx]$; the momentum operator $\hat{P} = -id/dx$ with a suitable domain is self-adjoint in this space [7]. The position operator \hat{X} is a bounded self-adjoint operator. Its spectrum is of course (0, 1) and we have for a suitable subspace of $L^2[(0, 1), dx]$ (say, the infinitely differentiable functions whose compact support is in (0, 1)) $[\hat{X}, \hat{P}] = i$. Following the logic of the above statement we would have concluded that \hat{P} is not self-adjoint. Therefore, from this simple example, we see that the above statement cannot be correct.

Nevertheless the operator $e^{-ia\hat{P}_r}$ should correspond to the translation operator on $L^2[(0, \infty), r^{n-1}dr]$. This operator is at least an isometry so it should be of the form

$$e^{-ia\hat{P}_r}\psi(r) = \begin{cases} \psi(r-a) & \text{if } a \leqslant r\\ 0 & \text{if } 0 < r < a. \end{cases}$$
(1)

Such an operator would not be unitary: if $\psi(r) \neq 0$ for r < a then the action of $e^{i\hat{P}_r a}$ on $\psi(r)$ is not defined. Stated differently, 'we can move everything to the right but not to the left'. Since the translation operator is not unitary we have every reason to suspect that \hat{P}_r is not self-adjoint. Therefore, it seems that a correct proof of the non-self-adjointness of the radial momentum operator is highly in order.

There seems to be almost a consensus in the literature that the operator which correspond to the radial momentum in *n* dimensions is the operator $-i(\partial/\partial r + (n-1)/2r)$ [3,5]. We shall now show that this operator is not self-adjoint and has no self-adjoint extensions.

2. The proof

It is well known that the momentum operator in $L^2[(0, \infty), dr]$ is not self-adjoint and has no self-adjoint extensions [12]. When we say the 'momentum operator' we mean the operator $\hat{P} = -id/dr$ with the domain

$$\{\psi | \psi \in L^2, \psi' \in L^2, \psi \text{ is absolutely continuous on } (0, \infty), \psi(0) = 0\}.$$

These conditions are needed to assure that \hat{P} would be symmetric (notice that since ψ is absolutely continuous $\lim_{r\to\infty} \psi = 0$ [12]). We are going to use this fact to prove our assertion.

First, define a transformation:

$$U : L^{2}[(0, \infty), dr] \to L^{2}[(0, \infty), r^{n-1}dr]$$

(U\psi)(r) := $\frac{\psi}{r^{(n-1)/2}}$. (2)

We have

$$\|\psi\|^{2} = \int_{0}^{\infty} |\psi|^{2} \mathrm{d}r = \int_{0}^{\infty} \left|\frac{\psi}{r^{(n-1)/2}}\right|^{2} r^{n-1} \mathrm{d}r = \|U\psi\|^{2},$$
(3)

so U is an isometry. U is a unitary operator since every $\varphi \in L^2[(0, \infty), r^{n-1}dr]$ has an inverse image $r^{(n-1)/2}\varphi \in L^2[(0, \infty), dr]$. This transformation (with n = 3) is well known

from elementary textbooks on quantum mechanics, where it is used to solve the Schrödinger equation for the hydrogen atom [13].

 U^{-1} is defined by

$$U^{-1} : L^{2}[(0,\infty), r^{n-1}dr] \to L^{2}[(0,\infty), dr]$$

(U⁻¹\varphi)(r) := r^{(n-1)/2}\varphi. (4)

The operator \hat{P} on $L^2[(0, \infty), dr]$ is unitarily equivalent to

$$\hat{P}_r \stackrel{def}{=} U \hat{P} U^{-1} = r^{(1-n)/2} \left(-i \frac{d}{dr} \right) r^{(n-1)/2} = -i \left(\frac{d}{dr} + \frac{n-1}{2r} \right), \tag{5}$$

which is, formally, the *n*-dimensional radial momentum operator.

If $\varphi \in D(\hat{P}_r)$ then $U^{-1}\varphi \in D(\hat{P})$. Therefore if $\varphi \in D(\hat{P}_r)$ then

- (a) $(r^{(n-1)/2}\varphi)' \in L^2[(0,\infty), dr]$
- (b) $r^{(n-1)/2}\varphi$ is absolutely continuous in $(0, \infty)$
- (c) $(r^{(n-1)/2}\varphi)(0) = 0.$

The obvious question arises: is this the 'natural' domain for \hat{P}_r ?

First of all, $\hat{P}_r \varphi \in L^2[(0, \infty), r^{n-1} dr]$, that is

$$\int_{0}^{\infty} |\hat{P}_{r}\varphi|^{2} r^{n-1} \mathrm{d}r = \int_{0}^{\infty} \left| \frac{\mathrm{d}}{\mathrm{d}r} r^{(n-1)/2} \varphi \right|^{2} (r^{(1-n)/2})^{2} r^{n-1} \mathrm{d}r \Rightarrow (r^{(n-1)/2}\varphi)' \in L^{2}[(0,\infty),\mathrm{d}r(f_{0})]$$

and we have (a).

 \hat{P}_r is (at least) symmetric, that is if $\varphi, \chi \in D(\hat{P}_r)$ then the following equality should hold:

$$\int_0^\infty \overline{\chi}(\hat{P}_r\varphi)r^{n-1}\,\mathrm{d}r = \int_0^\infty \overline{(\hat{P}_r\chi)}\varphi r^{n-1}\,\mathrm{d}r.$$
(7)

However,

$$\int_{0}^{\infty} \overline{\chi}(\hat{P}_{r}\varphi)r^{n-1} dr = (-i) \int_{0}^{\infty} \overline{\chi}r^{(1-n)/2} \frac{d}{dr} (r^{(n-1)/2}\varphi)r^{n-1} dr$$

$$= (-i) \int_{0}^{\infty} \overline{(r^{(n-1)/2}\chi)} \frac{d}{dr} (r^{(n-1)/2}\varphi) dr$$

$$= (-i) \overline{(r^{(n-1)/2}\chi)}r^{(n-1)/2}\varphi \mid_{0}^{\infty} + i \int_{0}^{\infty} \overline{\frac{d}{dr}(r^{(n-1)/2}\chi)}r^{(n-1)/2}\varphi dr$$

$$= (-i) \overline{(r^{(n-1)/2}\chi)}r^{(n-1)/2}\varphi \mid_{0}^{\infty} + \int_{0}^{\infty} \overline{(\hat{P}_{r}\chi)}\varphi r^{n-1} dr, \qquad (8)$$

where we were forced to assume (b) in order to use integration by parts. (b) also ensures that the boundary term in (8) is zero at infinity. In order that (7) will hold, we have to assume that the boundary term also vanishes at the origin, i.e. assume (c).

Thus we have defined \hat{P}_r with its proper domain and we see that it is symmetric. Furthermore it is also closed since it is unitarily equivalent to \hat{P} , which is closed [12]. As we have said earlier this operator is the radial momentum operator.

In order to find out whether this operator is self-adjoint or at least has self-adjoint extensions we have to check the dimensionality of the two subspaces: $\mathcal{K}_{-} = \ker (i + \hat{P}_{r}^{*})$ and $\mathcal{K}_{+} = \ker (i - \hat{P}_{r}^{*})$. If they do not have the same dimensionality the operator is not self-adjoint and has no self-adjoint extensions [7].

 \hat{P}_r^* is easy to find since [12] $\hat{P}_r^* = U\hat{P}^*U^{-1}$ and we have

$$\varphi \in \ker (\mathbf{i} \pm \hat{P}_r^*) \Rightarrow (\mathbf{i} \pm \hat{P}_r^*)\varphi = 0 \Rightarrow (\mathbf{i} \pm U\hat{P}^*U^{-1})\varphi = 0 \Rightarrow U(\mathbf{i} \pm \hat{P}^*)U^{-1}\varphi = 0$$
$$\Rightarrow (\mathbf{i} \pm \hat{P}^*)U^{-1}\varphi = 0 \Rightarrow U^{-1}\varphi \in \ker (\mathbf{i} \pm \hat{P}^*).$$
(9)

In a similar way we can show that

 $\psi \in \ker (i \pm \hat{P}^*) \Rightarrow U\psi \in \ker (i \pm \hat{P}^*_r)$ (10)

and we conclude that

$$\dim \ker (\mathbf{i} \pm \hat{P}_r^*) = \dim \ker (\mathbf{i} \pm \hat{P}^*). \tag{11}$$

 \hat{P}^* has the following property [12]:

dim ker (i +
$$\hat{P}^*$$
) = 0
dim ker (i - \hat{P}^*) = 1, (12)

because

$$\ker (\mathbf{i} + P^*) = \{ ce^r | c \in \mathbf{C} \} \not\subseteq L^2[(0, \infty), dr] \ker (\mathbf{i} - \hat{P}^*) = \{ ce^{-r} | c \in \mathbf{C} \} \subseteq L^2[(0, \infty), dr].$$
(13)

Therefore

 $\dim \ker (\mathbf{i} + \hat{P}_r^*) \neq \dim \ker (\mathbf{i} - \hat{P}_r^*)$ (14)

and \hat{P}_r is not self-adjoint and does not have self-adjoint extensions.

Using this equivalence we can understand the non-self-adjoint nature of the radial momentum operator on a more intuitive level, by transferring the problem into a one-dimensional problem.

In one dimension we can, in general, consider three types of interval: infinite interval, finite interval ('particle in a box') and semi-infinite interval. In the first case the momentum operator is self-adjoint because we can translate a wavepacket to both sides. In the case of a 'particle in a box' we can translate a wavepacket and whatever 'comes out' at one end we can enter at the other end (possibly with a different phase which corresponds to a specific self-adjoint extension [7]). Therefore the momentum operator, which is not self-adjoint, has self-adjoint extensions. In the case of a semi-infinite interval, we can move a wavepacket to the right but if we try to move it to the left what 'comes out' at the origin cannot be entered at the other end since the 'other end' is infinity. Therefore the translation operator is not unitary and the momentum operator is not self-adjoint and has no self-adjoint extensions.

To summarize, we have seen that the radial momentum operator is unitarily equivalent to the momentum operator on the half-line $(0, \infty)$. Since this operator is not self-adjoint (and has no self-adjoint extensions), the radial momentum operator is not self-adjoint (and has no self-adjoint extensions).

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