On the Dirac Quantisation rules and the trace anomaly

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Abstract

In this article I shall clarify three aspects of the Dirac quantisation rules of 1931, namely (i) the choice of antisymmetric Poisson brackets, (ii) the first (Poisson bracket) quantisation rule and finally (iii) the second Dirac quantisation rule, also known by him as the quantum condition, which is the best known of the canonical quantisation rules of quantum mechanics. I shall further show that (i) and (ii) do not lead to a trace anomaly for bounded operators, unlike (iii). It is at the final proposed rule (iii) that the trace anomaly emerges. Several issues that are both pedagogical and foundational arising from this study show that quantum mechanics is still not a finished product. I shall discuss options to complete its development.
I. INTRODUCTION

A recent column in this journal concerning the quantum trace anomaly Mahajan prompted me to pen this article which addresses several issues that are perhaps not widely known or even discussed in textbooks as far as I know. This relates to the origin of quantum trace anomaly, first brought to attention by Born and Jordan in 1925. In this paper all quantities with top hats are quantum operators, those without are classical variables. For the benefit of the reader, the trace anomaly arises from taking the trace of the Dirac Quantum Condition or the Born and Jordan quantum rule:

\[ [\hat{q}, \hat{p}] = i\hbar \mathbb{1}, \tag{1} \]

where the left hand side of this equation is the commutator of the two canonical quantum operators \( \hat{q} \) and \( \hat{p} \) for coordinate and momentum and the right hand side is the unit operator. Born and Jordan in their seminal paper stated that “clearly the trace anomaly implies that the quantum operators must be unbounded”, the argument adopted by Mahajan. To be clear, since bounded operators imply that the trace on the LHS of eqn(1) is zero while the RHS is finite, then Born and Jordan’s statement is that bounded operators are forbidden in quantum theory. Neither they nor subsequent writers ever go into depth as to how this anomaly is resolved by considering infinite dimensional Hilbert spaces of unbounded operators. Dirac unfortunately was very silent about the subject. We might perhaps speculate as to why at the end of this article. However, mathematicians following the axiomatic foundations of Von Neumann (1927) and algebraic generalisations see this difficulty as best overcome by treating only systems with an infinite degree of freedom, abandoning Fock Space and adopting a more sophisticated C* algebra formalism based on the type (iii) canonical quantisation, commuting (CCR) or anticommuting (ACR) rules; see for example Emch(1972). These do not however offer further insight on how their approach resolves the trace anomaly and obtains an infinite (positive) result in the limit, other than to explicitly construct exotic algebraic systems that have infinite traces. Furthermore, in solid state physics, nowadays better known as condensed matter physics, we are always dealing with bounded operators as in Born von-Karman boundary conditions, so unbounded operators do not seem to provide the resolution of the trace anomaly as purported by the earlier authors. Others such as Costella (1995) suggested that the trace anomaly could be resolved by discretization to a lattice which in the Schrodinger representation implies that the RHS
is actually off diagonal. Unfortunately such a scheme violates the essential theorem that in the energy representation the canonical commutator eqn(1) is a dynamical invariant and must be strictly diagonal, Born and Jordan 1925. In this paper I shall first show that Dirac made a specific choice in his definition of the quantum Poisson brackets. This choice must be corrected by antisymmetrisation but does reveal that several different definitions of quantum Poisson brackets are possible. For ease of notation I shall consider the one-dimensional system of length $L$, generalisation to higher dimensions is trivial by adding subscript indices for Cartesian components.

As is well known Dirac then showed using his Poisson brackets and a simple manipulation of the bracket algebra, nowadays associated as a Lie algebra, by which he arrived at his first famous quantisation rule, which we shall refer to as Dirac’s rule One:

$$[\hat{u}, \hat{v}] = i\alpha \{\hat{u}, \hat{v}\}_{P_1} ,$$

(2)

where the LHS is a commutator bracket of two quantities which are functions of canonically conjugate dynamic variables and the RHS is the quantum Poisson bracket of the same quantities, with $\alpha$ some function of $\hbar$ the Planck’s constant. Dirac chose to define this operator as the quantum operator:

$$\{\hat{u}, \hat{v}\}_{P_1} = \left( \frac{\partial \hat{u}}{\partial \hat{q}} \frac{\partial \hat{v}}{\partial \hat{p}} - \frac{\partial \hat{u}}{\partial \hat{p}} \frac{\partial \hat{v}}{\partial \hat{q}} \right) ,$$

(3)

which in operator form, eqn(2) and eqn(3) have a contradiction, although the classic 1931 text of Dirac (cf eqn(2)) referred only to the classical Poission brackets so that the definition eqn(3) is antisymmetric in (u,v). However, in the quantum operator form, this is not the case. Eqn(3) is neither symmetric or antisymmetric. This raises two issues. (i) Can we use other (explicitly antisymmetric) choices for the quantum Poisson brackets, see for example Lanczos such as:

$$\{\hat{u}, \hat{v}\}_{P_2} = \left( \frac{\partial \hat{u}}{\partial \hat{q}} \frac{\partial \hat{v}}{\partial \hat{p}} - \frac{\partial \hat{v}}{\partial \hat{q}} \frac{\partial \hat{u}}{\partial \hat{p}} \right) ,$$

(4)

and:

$$\{\hat{u}, \hat{v}\}_{P_3} = \left( \frac{\partial \hat{u}}{\partial \hat{p}} \frac{\partial \hat{v}}{\partial \hat{q}} - \frac{\partial \hat{v}}{\partial \hat{p}} \frac{\partial \hat{u}}{\partial \hat{q}} \right) ,$$

(5)

which a priori do not have to be equivalent, see for example Shewell. The second issue is should we retain Dirac’s definition and antisymmetrise it so that Dirac’s rule One, eqn(2) is no longer contradictory? In the next section, I shall discuss the answer to these two issues.
Note that any Lie algebraic or C* Algebraic quantisation approach that generates Quantum Mechanics from algebraic groups must a priori adopt one of the above P1 (antisymmetrised) see below, P2 or P3 definitions since the correspondence principle requires that as $\hbar \to 0$ the classical brackets must be antisymmetric.

II. ANTISYMMETRISED POISSON BRACKET

As I have emphasized, Dirac’s definition of the quantum Poisson bracket eqn(2), in fact has no particular symmetry or antisymmetry. As Dirac was well known to be a very particular and pedantic person, and given that he has chosen to define his Poisson brackets specifically in many places consistently there must be good reasons for this. Unfortunately I could find no sources in which he explicitly spelled out the reason for his choice, so we are left to speculate. It is very likely that he must have obtained it from the following argument. For any phase space function operator $\hat{f}$, this should be obtained from:

$$\frac{d\hat{f}}{dt} = \frac{\partial \hat{f}}{\partial t} + \frac{\partial \hat{f}}{\partial \hat{q}} \dot{\hat{q}} + \frac{\partial \hat{f}}{\partial \hat{p}} \dot{\hat{p}},$$  \hbox{(6)}

maintaining operator orderings.

Hence from Hamilton’s equations:

$$\dot{\hat{q}} = \frac{\partial \hat{H}}{\partial \hat{p}}, \quad \dot{\hat{p}} = -\frac{\partial \hat{H}}{\partial \hat{q}},$$  \hbox{(7)}

this gives:

$$\frac{d\hat{f}}{dt} = \frac{\partial \hat{f}}{\partial t} + \{\hat{f}, \hat{H}\} \text{P}_1,$$  \hbox{(8)}

and therefore:

$$\{\hat{f}, \hat{H}\} \text{P}_1 = \left(\frac{\partial \hat{f}}{\partial \hat{q}} \frac{\partial \hat{H}}{\partial \hat{p}} - \frac{\partial \hat{f}}{\partial \hat{p}} \frac{\partial \hat{H}}{\partial \hat{q}}\right),$$  \hbox{(9)}

which as the reader can see has no particular symmetry properties, being neither symmetric nor antisymmetric in $\hat{f}, \hat{H}$. From this Dirac must have generalized to the generic Poisson bracket P1, i.e. eqn(3). However it is logical that one should antisymmetrise this operator for quantisation so that Dirac’s first quantisation rule should now read:

$$[\hat{u}, \hat{v}] = i\hbar \{\hat{u}, \hat{v}\} \text{P}_1 \text{Antisymm},$$  \hbox{(10)}
The reader can confirm by straightforward manipulations that this antisymmetrised operator is now in fact given by:

\[
\{\hat{u}, \hat{v}\}_{P_1, \text{Antisymm}} = \frac{1}{2} \left[ \{\hat{u}, \hat{v}\}_{P_2} + \{\hat{v}, \hat{u}\}_{P_3} \right],
\]

Eqn(10) and eqn(11) constitute the corrected first Dirac quantisation rule.

III. SECOND DIRAC QUANTISATION RULE OR THE QUANTUM CONDITION.

The problem now reduces to one of evaluating the quantum Poisson brackets defined in the last section. Here Dirac made the simplest assumption that the canonical coordinate and momentum quantum Poisson brackets are just identical in value to the classical ones. This is not quite correct. In fact in the one dimensional case here he basically assumed that:

\[
\{\hat{q}, \hat{p}\}_{P_1} = \{q, p\}_{P_1} = \hat{1}
\]

where the large hat indicates an operator. That is, first evaluate the classical Poisson bracket then turn the result into an operator, in this case the unit operator. As can be seen, eqn(10) and eqn(12) lead to the trace anomaly. For the rest of this section I shall show that for bounded operators, eqn(11) does not lead to a trace anomaly.

A. No trace anomaly for bounded operators for the first Dirac quantisation rule

The proof of my statement follows from the use of the following theorem first published in this journal by Snygg (1980)\textsuperscript{13}. His proof however uses the Moyal-Wigner representation. The theorem can be proved otherwise which I shall show in the appendix.

Theorem:

\[
Tr \left( \hat{a}(\hat{p}, \hat{q}) \right) = \frac{1}{\hbar} \int dp \, dq \, a(p, q),
\]

where the operator \( \hat{a} \) is an arbitrary function of phase space operators \( \hat{p} \) and \( \hat{q} \), and the integral on the RHS is a classical phase space integral. Thus taking the trace of eqn(11) we have for the first term:

\[
Tr \left( \frac{\partial \hat{u}}{\partial \hat{q}} \frac{\partial \hat{v}}{\partial \hat{p}} \right) = \frac{1}{\hbar} \int dp \, dq \, \left( \frac{\partial u}{\partial q} \frac{\partial v}{\partial p} \right).\]
Now integrating by parts wrt to $q$ we now have:

$$
Tr \left( \frac{\partial \hat{u}}{\partial \hat{q}} \frac{\partial \hat{v}}{\partial \hat{p}} \right) = -\frac{1}{\hbar} \int dp \, dq \, u \left( \frac{\partial^2 v}{\partial q \partial p} \right),
$$

where we have dropped boundary terms for bounded operators or alternatively imposed periodic boundary conditions. Integrating by parts once more now wrt to $p$, we now have:

$$
Tr \left( \frac{\partial \hat{u}}{\partial \hat{q}} \frac{\partial \hat{v}}{\partial \hat{p}} \right) = \frac{1}{\hbar} \int dp \, dq \, \left( \frac{\partial v}{\partial q} \frac{\partial u}{\partial p} \right),
$$

where again we dropped boundary terms for bounded operators. The reader can now see that this term cancels the trace of the second term in eqn(4). From these results, it then follows that in fact all the quantum Poisson brackets defined here are traceless for bounded operators. In view of the neglect of boundary terms, it also follows that for unbounded operators, these terms can lead to divergences. This completes my proof.

IV. CONCLUSION

Given the results of this study, there are two ways I could see as a resolution of the trace anomaly. Strategy (A) is to adopt eqn(2) as the foundational quantisation rule and adopt an entirely new algebra that covers both bounded and unbounded operators. In this algebra the second Dirac rule eqn(10) can only be seen as an approximation, and more subtle features could emerge from such an algebra, such as in the quantisation of the harmonic oscillator that could be empirically verifiable. A second strategy (B) is to accept that Dirac’s second rule should not be read as an equation, but a (one way) algorithm. We may all inadvertently have done this for generations by instruction to students: whenever you see a quantum Poisson Bracket between $\hat{q}$ and $\hat{p}$ replace it by $i\hbar$ times a unit operator. This is fine for all practical purposes (FAPP), in the words of John Bell. Perhaps Dirac was searching for strategy (A) all his life. As he was evidently not successful initially so he proposed strategy (B) as the interim and kept silent about the matter, in the hope that he can find a better theory. Bell’s charge that Dirac was “perhaps the most distinguished of the ‘why bother?’s” would then be an overstatement.

I am indebted to Geoffrey Sewell of Queen Mary University London, for bringing the highly technical book of Emch (1972) to my attention.
V. APPENDIX

The proof of the theorem in the text begins with:

\[ \text{Tr} \, \hat{a}(\hat{p}, \hat{q}) = \frac{1}{L} \int dq \, dq' < q' | \hat{a}(\hat{p}, \hat{q}) | q > \delta(q - q') . \]  \hspace{1cm} (17)

In eqn(17) I have absorbed dimensions of $1/\sqrt{L}$ into the definition of the states while the \( \delta \) function is dimensionless. Now the action of the operator \( \hat{a} \) on the state \( |q> \) will give \( \hat{a}(\hat{p}, \hat{q}) |q> = \hat{a}(\hat{p}, q) |q> \) since the states \( |q> \) are eigenvectors of \( \hat{q} \). Thus we have:

\[ \text{Tr} \, \hat{a}(\hat{p}, \hat{q}) = \frac{1}{L} \int dq \, dq' < q' | \hat{a}(\hat{p}, q) | q > \delta(q - q') . \]  \hspace{1cm} (18)

I now introduce a complete set of momentum states \( |p> \) where \( < p|q> = \frac{1}{\sqrt{L}} e^{i\frac{pq}{\hbar}} \) and insert the identity operator: \( \frac{1}{\hbar} \int dp |p><p| \) into eqn(18) so that:

\[ \text{Tr} \, \hat{a} = \int dq \, dq' \frac{dp}{\hbar} < q' | \hat{a}(\hat{p}, q) | p > < p|q> \delta(q - q') \]  \hspace{1cm} (19)

\[ = \frac{1}{\sqrt{L}} \int dq \, dq' \frac{dp}{\hbar} < q' | a(p, q) | p > e^{i\frac{pq}{\hbar}} \delta(q - q') \]  \hspace{1cm} (20)

\[ = \frac{1}{L} \int dq \, dq' \frac{dp}{\hbar} a(p, q) e^{i\frac{(p-q')}{\hbar}} \delta(q - q'). \]  \hspace{1cm} (21)

Integration over \( q' \) is now trivial and we finally have:

\[ \text{Tr} \, \hat{a}(\hat{p}, \hat{q}) = \frac{1}{\hbar} \int dp \, dq \, a(p, q) . \]  \hspace{1cm} (22)

This completes my proof of the theorem in the text.

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