Quantum Chaos & Quantum Classical Correspondence

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Abstract- The implications of quantum chaos on Bohr’s quantum classical correspondence principle are investigated by associating operators in Hilbert space with points in phase space through Weyl's calculus. It is shown that the correspondence principle does indeed break down in the cases of motion characterized by positive Lyapunov exponents.

Keywords- Quantum Chaos, Weyl Calculus, Quantum Classical Correspondence.

I. INTRODUCTION

ONE of the cardinal principles of quantum mechanics is Bohr's correspondence principle, which provides, in substratum, that classical physics should emerge as the limit of quantum physics. However, the discovery of chaotic phenomena in microscopic quantum systems has led to considerable rethinking on the issue. Some physicists have gone to the extent of questioning its very existence [1]-[2], although the less radically minded have retained their faith in the principle and attempted to explain away the anomalies arising out of chaotic phenomena on the basis of limitations of measurement theory in quantum mechanics emanating from the Heisenberg Uncertainty Principle.

The idea of providing a common framework for quantum properties (associated with projection operators in Hilbert space) and classical properties (giving the position and momentum co-ordinates of a classical system in phase space) goes back to Wigner [3], and was, thereafter, developed by Weyl [4]. Since then, this ‘Weyl calculus’, [4]-[5], has become an important part of mathematics included in microlocal analysis and the theory of pseudo differential operators [6]-[13]. Considerable work has been done in adapting the theory of pseudo differential operators for applications to the Schrodinger equation and the Heisenberg Uncertainty Principle [14]-[15]. Another approach in the same direction has come from the interpretation of quantum mechanics in consistent histories framework advocated by Robert Griffiths and Roland Omnès [16]-[21]. Building on the work done on the time evolution of coherent states [22]-[27], explicit results were obtained for Gaussian states.

In this paper, following the approach adopted by Roland Omnès, [18]-[21], using the Weyl calculus (for associating operators in Hilbert space with symbols in phase space) and established results in microlocal analysis with pseudodifferential operators, we investigate the implications of this quantum-classical correspondence principle.

II. PSEUDODIFFERENTIAL OPERATORS

For the sake of completeness, in this section, we reproduce some of the well-established results in the theory of pseudodifferential operators that will find application in the sequel. Conventionally, we define a pseudodifferential operator $A$ by its action on a function $u(x) \in C^\infty_c$, a closed linear subspace of $C^\infty$ as

$$Au(x) = \frac{1}{(2\pi)^d} \int e^{ip\cdot x} \hat{a}(p) \hat{u}(p) dp$$

where $\hat{u}(p)$ is the Fourier transform of $u(x)$. An equivalent expression for $A$ follows from Fourier inversion of $\hat{u}(p)$ i.e.

$$Au(x) = \frac{1}{(2\pi)^d} \int e^{i(x-y)\cdot p} a(x, p) u(y) dy dp$$

with the Schwarz kernel

$$A(x) = \frac{1}{(2\pi)^d} \int e^{i(x-y)\cdot p} a(x, p) dp$$

In (1) to (3) $a(x, p)$ is construed as the symbol associated with the operator $A$. Additionally, a symbol $a(x, p)$ is of order $m \in \mathbb{R}$ if it is infinitely differentiable i.e. $a(x, p) \in C^\infty$ and to every pair of n-tuples $\alpha, \beta$ there is a constant $C_{\alpha\beta} > 0$ such that:

$$|\partial_\alpha^\beta a(x, p)| \leq C_{\alpha\beta} |(1+|p|)^{m-|\alpha|}|$$

The linear space $S^m$ of all symbols of order $m$ is a Frechet space with the seminorm:

$$\sup \left| \partial_\alpha^\beta a(x, p) \right| \left( 1+|p| \right)^{m-|\alpha|}$$

Considering $u(x) \in C^\infty_c$ as an arbitrary test function, we define the composition of two operators $A$ and $B$ and their associated symbols $a(x, p) \in S^m$ and $b(y, q) \in S^n$ as follows:-
\[ A(Bu)(x) = \frac{1}{(2\pi\hbar)^\frac{N}{2}} \int \int e^{i(x-y)\cdot p - i(y-x)\cdot a(x,y)} b(y,q) u(z) dydz dp dq \] (6)

Eq. (6) yields an expression for the symbol corresponding to composition of the two operators \( A \) and \( B \) as:

\[ c(x,p) = \frac{1}{(2\pi)^\frac{N}{2}} \int e^{i(x-y)\cdot p - i(y-x)\cdot a(x,y)} b(y,q) dy dp \] (7)

The fact that \( c(x,p) \in S^{m+n} \) may be established by differentiating (7) under the sign of integration. Using Leibnitz formula, we have:

\[ \partial_x^\alpha \partial_p^\beta c(x,p) = \frac{1}{(2\pi)^\frac{N}{2}} \sum_{\alpha \in \omega} \alpha! \int \int e^{i(x-y)\cdot p - i(y-x)\cdot a(x,y)} \partial_x^\alpha \partial_p^\beta b(y,q) dy dp \] (8)

where the last step follows from a recursive integration by parts with respect to \( y \) and \( q \). From (8), we see that \( \partial_x^\alpha \partial_p^\beta c(x,p) \) is a linear combination of terms of the kind

\[ \int e^{i(x-y)\cdot p - i(y-x)\cdot a(x,y)} \partial_x^\alpha \partial_p^\beta b(y,q) dy dp \] (9)

Noting that \( a \in S^m \) and \( b \in S^n \), we immediately have

\[ \left| \partial_x^\alpha \partial_y^\beta c(x,p) \right| \leq k \sum_{\alpha \in \omega} \left( \int_{\omega} \right)^{m+n-|\alpha|} \left( \int_{\omega} \right)^{n+1 - |\alpha|} dq \] (10)

where \( k \) is some constant.

Applying Peetre’s inequality to (10) and interchanging \( q \) and \( p-q \), we finally have

\[ \left| \partial_x^\alpha \partial_p^\beta c(x,y) \right| \leq k \left| \partial_x^\alpha \partial_y^\beta \right| \] (11)

Since \( M \) is arbitrary, we conclude that \( c(x,y) \in S^{m+n} \).

Another important result that we shall be using from the theory of pseudo differential operators concerns the asymptotic expansions of symbols and is obtained by writing the finite Taylor’s expansion of \( a(x,y,p) \) with respect to \( y \) in the neighbourhood of \( x \) as follows:-

\[ a(x,y,p) = \sum_{|\alpha| \leq N} \frac{1}{\alpha!} (y-x)^\alpha \partial_x^\alpha a(x,y,p) + R_N(x,y,p) \] (12)

Consider, now, the expression:-

\[ \int e^{i(x-y)\cdot p - i(y-x)\cdot a(x,y)} \partial_x^\alpha a(u(y)) dy dp \]

\[ \int e^{i(x-y)\cdot p} (\partial_x^\alpha a u(y)) dy dp \] (14)

\[ \int e^{i(x-y)\cdot p} (-i \partial_x^\alpha a u(y)) dy dp \]

Using the above result in (12) & (13), it follows that if \( a \in S^m \) is a symbol corresponding to the operator \( A \), there exists another for symbol \( A \) given by:-

\[ \sum_{|\alpha| \leq N} \frac{1}{\alpha!} (- \partial_x^\alpha a + R_N) \] (15)

where

\[ R_N^* = (N+1) \sum_{|\alpha| \leq N+1} \frac{1}{\alpha!} \int_0^1 (1-t)^N (-i \partial_x^\alpha a \partial_y^\beta) \] (16)

III. WEYL CALCULUS & ASSOCIATING OPERATORS IN HILBERT SPACE WITH CELLS IN PHASE SPACE [18]-[21]

In the Weyl Calculus [6], which is more compatible to the objective of this paper, we modify (2) to the symmetric compromise:-

\[ Au(x) = \frac{1}{(2\pi\hbar)^\frac{N}{2}} \int \left[ \frac{1}{2} (x+y), p \right] e^{i(x-y)\cdot p} u(y) dy dp \] (17)

This modified version of symbolic calculus has several advantages when adapted to the description of physical systems. Firstly, such symbols enjoy a fundamental invariance under a linear symplectic co-ordinate transformation \( \theta : R^{2N} \rightarrow R^{2N} \) such that \( \theta^* \omega = \omega \) where \( \omega = \sum d p_i \wedge d x_j \) is the symplectic form in \( R^{2N} \). There exists a unitary transformation \( U \in L^2 (R^n) \) uniquely determined to a constant factor, corresponding to every \( \theta \), such that:-

\[ U^{-1} a(x,p) U = (a \circ \theta)(x,p) \] (18)

There is a natural appearance of real symbols corresponding to self-adjoint operators and also much closer agreement between operator products and symbol products [5].

We consider a physical system described by the co-ordinates \( x = (x_1, \ldots, x_n) \) in the configuration space \( R^n \) with the momentum co-ordinates denoted by \( p = (p_1, \ldots, p_n) \). The Hilbert space for this system is \( H = L^2 (R^n) \).
In line with our objective of associating self-adjoint operators in Hilbert space, corresponding to quantum mechanical observables, with symbols in classical phase space, we define a cell $C$ in phase space as a connected, simply connected bounded set. We also introduce $L$ and $P$ as the characteristic scales of length and momentum which are such that $(\hbar/LP)^2$ represents the dimensionless volume of a semiclassical state in the metric

$$g(x, p) = \frac{dx^2}{L^2} + \frac{dp^2}{P^2}.$$  

Ideally, the symbol $a$ associated with an operator $A$ is the characteristic function of the cell $C$, equal to unity in $C$ and zero outside it. However, this function being discontinuous leads to unwanted singularities in the operator. We, therefore, treat $a$ as an infinitely differentiable function that is smoothed and goes gradually from unity to zero in the cell margin. For the purpose, we define the margin, in non-dimensional coordinates, as a region inside $C$ of width $\partial C$ from the cell boundary such that $\partial C \leq \left( \frac{\hbar}{LP} \right)^2$.

To facilitate the association of a projection operator in Hilbert space with cells in phase space, cell dimensions should be large enough for quantum uncertainties to be insignificant and sufficient number of semi classical states to be accommodated. Additionally, certain regularity must exist of the cell boundary, failing which, it may be impracticable to associate with it well defined projectors. This may be quantitatively expressed by requiring that the two surfaces enclosing the cell margin are such that derivatives at all points normal to the surfaces are quite larger than the derivatives parallel to the surface and the partial derivatives being of order unity in the dimensionless variables $x = \frac{Lp}{\hbar}, P$. A minimum limit may also be set for the side to side distance among opposite points of the boundary i.e. $x < \left( \frac{LP}{\hbar} \right)^{\frac{1}{2}}$.

In line with our choice of a symmetric metric, we also adopt the symmetric seminorm

$$C_{\alpha\beta} = \sup_{x, p} |P|^{\alpha} \left| \left| \partial_x^{\alpha} \partial_p^{\beta} a(x, p) \right| \right|_{m - |\alpha| - |\beta|} \left( 1 + \frac{x^2}{L^2} + \frac{p^2}{P^2} \right)^{\frac{1}{2}}$$  \hspace{1cm} (19)

Following Weyl, we associate a function $\omega(x, p)$, defined in phase space $\mathbb{R}^{2n}$ with the operator $\Omega$. The explicit representation of $\omega(x, p)$ is given by the partial Fourier transform

$$\omega(x, p) = \int \Omega \left( x + \frac{y}{2}, x - \frac{y}{2} \right) e^{-i\frac{p\cdot y}{\hbar}} \, dy,$$  \hspace{1cm} (20)

where we define $p, x = p_x x_i + \ldots + p_n x_n$.

In view of the representation (20), the adjoint operator $\Omega^\dagger$ corresponds to the conjugate function $\omega^*(x, p)$ and therefore, a real function corresponds to a self-adjoint operator. The trace, when it exists, is given by

$$Tr \, \Omega = \frac{1}{(2\pi\hbar)^n} \int \omega(x, p) \, dx \, dp.$$  \hspace{1cm} (21)

We now consider two Weyl operators $A$ and $B$ with respective symbols $a(x, p) \in S^m$ and $b(x, p) \in S^n$. Then we have,

$$ABu(x) = \frac{1}{(2\pi\hbar)^n} \int \int \int \int \int a \frac{x + z}{2} , r \frac{z + y}{2} , s, x, y, z, r, s \frac{d^4zdrdsdy}{e^{i[(x+z)/2+(y+z)/2]s, x, y, z, r, s}}$$

with the Schwartz kernel

$$K(x, y) = \frac{1}{(2\pi\hbar)^n} \int \int \int \int a \frac{x + z}{2} , r \frac{z + y}{2} , s, x, y, z, r, s \frac{d^4zdrdsdy}{e^{i[(x+z)/2+(y+z)/2]s, x, y, z, r, s}}$$  \hspace{1cm} (23)

so that

$$\begin{aligned}
K \left( \frac{x}{2}, x - \frac{t}{2} \right) & = \frac{1}{(2\pi\hbar)^n} \times \\
\int \int \int \int a \frac{x + z + t/2}{2} , r \frac{x + z - t/2}{2} , s, x, y, z, r, s \frac{d^4zdrdsdy}{e^{i[(x+z)/2+(y+z)/2]s, x, y, z, r, s}}
\end{aligned}$$  \hspace{1cm} (24)

We recover the symbol $c(x, p)$ representing the composition operator of $A$ and $B$ through a Fourier transform of (24) with respect to $t$ to get:-

$$c(x, p) = \frac{1}{(2\pi\hbar)^n} \int \int \int \int a \frac{x + z + t/2}{2} , r \frac{x + z - t/2}{2} , s, x, y, z, r, s \frac{d^4zdrdsdy}{e^{i[(x+z)/2+(y+z)/2]s, x, y, z, r, s}}$$

Eq. (25) may be written more compactly by making the following transformations:-

$$(r - p) \equiv r, \frac{-x + z + t/2}{2} \equiv z, \frac{-x + z - t/2}{2} \equiv t.$$  \hspace{1cm} (26)
The Jacobian is $2^{2n}$ and (25) becomes:
\[
c(x, p) = \frac{1}{(\pi \hbar)^{2n}} \int \int \int a(x + z, p + r) b(x + z, p + r) \times e^{i(x+y-x-r)/\hbar} \text{d}z \text{d}r \text{d}s \text{d}t
\]

In terms of Fourier transform, we can write (27) as
\[
c(x, p) = \frac{1}{(2\pi \hbar)^n} \int e^{i (p-y-q)/\hbar} \text{d}y \text{d}q \times \int \int \int \hat{a}(r, z) \hat{b}(s, t) \delta(p + s - q) \times \int \int \int \delta(z + t - y) \exp \left( \frac{i(r-x-z)h}{\hbar} \right) \text{d}z \text{d}r \text{d}t \text{d}s
\]

Expanding the exponential $e^{i(r-x-z)/\hbar}$ and noting, for example, that:
\[
\frac{\partial}{\partial x} \left[ \frac{1}{(2\pi \hbar)^n} \int a(q, y) e^{-i(p-y-q)/\hbar} \text{d}y \text{d}q \right] = \frac{1}{(2\pi \hbar)^n} \int a(q, y) \hat{a}(q, y) \text{d}y \text{d}q
\]

and similarly identifying the multiplication of the Fourier transforms of the symbols by $r$ or $z$ as a derivation acting on the corresponding symbol, we may write (28) in terms of an exponential of the Poisson Brackets i.e.
\[
e^{\chi} = \sum_{r=0}^{\infty} \frac{1}{r!} \chi^r
\]

as
\[
c(x, p) = a e^{-\frac{i\hbar}{\hbar}} b
\]

The series (31) is an asymptotic series and may be written explicitly for a finite number of terms with a remainder as in (10) to (16) i.e.
\[
c(x, p) = ab - \frac{i\hbar}{2} [a b] + \ldots + \left( \frac{1}{N!} \right) \left( -\frac{i \hbar}{2} \right)^N a \left\{ b \right\}^N + r_N
\]

where $r_n \in S^{m+n-(N+1)}$ which with the symmetric seminorm (19) implies that $r_N$ is subject to the following bounds:
\[
r_N(x, p) \leq K \left( \frac{\hbar}{LP} \right)^{N+1} \left( l + \frac{x^2}{L^2} + \frac{p^2}{P^2} \right)^{-(N+1)} \frac{m+n}{2}
\]

with similar bounds for its derivatives,[18]-[21].

IV. ESTIMATES OF OPERATORS

Quantum averages are often obtained by taking traces of operators over the bath variables. We now attempt to establish bounds for the trace norms of a given operator from the knowledge of its symbol. For the purpose, we consider a positive real symbol $a(x, p)$ and assume $A$ to be the associated operator. Let
\[
b(x, p) = [a(x, p)]^{1/2}
\]

with the associated operator being $B$. Then, by using the results of (31) and (32), we obtain the symbol associated with $B^2$ as:
\[
c(x, p) = b e^{\frac{-i\hbar}{2}} b = b^2 (x, p) - \frac{\hbar^2}{8} b \left\{ b \right\}^2 b +.
\]

Since, $b^2 (x, p) = a(x, p)$, with $A$ being the associated operator, a relation of the type $B^2 = A - A'$ follows, with $A'$ being an operator proportional to $\hbar^2$ to leading terms. Also,\[
Tr[A] = Tr \left| A A' \right|^{1/2} = Tr \left| B^2 + A' \left( b^2 + A' \right) \right|^{1/2} \geq Tr \left| B^2 \right| + Tr \left| A' \right|
\]

Bounds for the operator $A$ can be computed by applying the sharp Garding inequality, [6], to the operator $A'$ and we get
\[
Tr[A] \geq -N' \frac{\hbar}{LP} . \quad \text{Substituting } I - A \quad \text{for } A \quad \text{in the above analysis, we further conclude that}
\]

\[
Tr[A] \leq I \left( I + N' \left( \frac{\hbar}{LP} \right) \right)
\]

V. QUANTUM CLASSICAL CORRESPONDENCE

We consider a dynamical system evolving under the Hamiltonian $H(x, p)$ with the Weyl symbol $\hat{h}(x, p)$. Let $C$ be an initial regular cell with which we associate the symbol $a(x, p)$ and the corresponding operator $A$.

Let the dynamical evolution of the system as described by $H(x, p)$ result in the creation of a new cell $C'$ which is also assumed regular and has the symbol $\hat{a}'(x, p)$ and operator $A'$ associated with it respectively. Then, the transformation $A \rightarrow A'$ is the classical version of the evolution of our system.

The above evolution can be described quantum mechanically as
\[
A(t) = U^{-1}(t) A U(t)
\]
where $U(t) = e^{i \frac{t}{\hbar} H(x,p)t}$ is the unitary quantum mechanical evolution operator.

Hence, our study of the quantum classical correspondence gets confined to the determination of the bounds of the errors between the quantities $A'$ and $A(t)$.

From the Heisenberg equation of motion, we get
\[
\frac{\partial}{\partial t} F(t) = \frac{i}{\hbar} [H, F(t)].
\] (38)

Using (31) & (32) we get the following equation as equivalent to (38) in terms of the symbol $a(t)$ corresponding to the operator $A(t)$:
\[
\frac{\partial}{\partial t} a(x, p', t') + \{h, a(t')\} = -\left(\frac{\hbar^2}{24}\right) h f_{j} |^{3} a(t')
\] (39)

where we have neglected higher order terms.

We now use the mathematical framework developed earlier for estimating the bounds of operators and get an expression for the error (represented by the trace of the difference) between the classical and quantum evolution operators (in orders of magnitude) as:
\[
Tr \left| A' - A(t) \right| = \left[ C \right] (K).
\] (40)

where $[C]$ is the number of semiclassical states and $K$ is of the order of:
\[
\sup_{0 \leq t \leq \tau} \epsilon', \epsilon \sup \left( \frac{\partial x}{\partial x'}, \frac{\partial p}{\partial x'}, \frac{\partial x}{\partial p'}, \frac{\partial p}{\partial p'} \right)
\]
\[
\sup_{0 \leq t \leq \tau} \left( \frac{\partial^{3} h(x', p')}{\partial x(t')^{3}} \right) B.
\] (41)

Here, $B$ is the bound on the all combinations of third order derivatives of $(x, p)$ with respect to $(x', p')$. Eq. (41) provides a route to the identification of various scenarios where the quantum classical correspondence breaks down. In the context, an obvious situation where such distortion would occur is when $\epsilon$ or $\epsilon'$ assume significant values, both identifying chaotic motion, or when the bounds on first or third order become large enough, which again would arise in positive Lyapunov cases characterising chaos.

The above analysis gives us an insight into the possibility of breakdown of the correspondence principle in scenarios involving chaotic motion. We have examined this using an approach pioneered by Roland Omnes for associating operators in Hilbert space with points in phase space through the Wigner and Weyl formalism. Application of microlocal analysis shows, indeed, that the correspondence principle breaks down in regions of positive Lyapunov exponents.

REFERENCES