Self Adjoint Extensions of Phase and Time Operators

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Abstract

It is shown that any real and even function of the phase (time) operator has a self-adjoint extension and its relation to the general phase operator problem is analyzed.

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Problems in the definition of the quantum phase were first addressed by Fritz London [1] in 1926. One year latter Dirac [2] introduced an operator solution which was proved to be incomplete by Susskind and Glogower [3] (for history and measurements see Nieto [4]). Since then a series of workers have made many attempts to resolve the problem (for reviews see [5]).

In the present paper, the quantum phase and time problems are considered in the context of projective measurements (i.e. not in the formalism of the so-called POM or POVM observables [6]). It is shown that any real and even function of the phase (time) operator, has a self adjoint extension. There are two subspaces in which these operators are self adjoint: the subspace consisting of all the even square-integrable functions of the phase and the subspace consisting all the odd ones. That is, the non-existence of self adjoint phase and time operators does not, necessarily, preclude self adjoint extensions of their absolute value.

The quantum phase problem may be traced to two sources:

(i) The spectrum of the phase is restricted to a finite interval which is chosen in this paper, somewhat arbitrarily, to be $[-\pi, \pi]$.

(ii) The number operator (or equivalently the Hamiltonian of a simple harmonic oscillator) is bounded from below.

It can be seen very easily why condition (i) leads to a problem. The matrix elements of $[N, \Phi]$ ($N$ and $\Phi$ are the number and phase operators respectively) in the number state basis $|n\rangle$,

$$\langle n||N, \Phi||n'\rangle = (n-n')\langle n|\phi|n'\rangle$$

(1)

vanish for $n = n'$ because $|\langle n|\phi|n\rangle| \leq \pi$. That is, $[N, \Phi] \neq i$. However, as we will see in the following, this problem can be resolved. Therefore, we emphasize that it is condition (ii) which makes it impossible to define self adjoint phase or time operators.

Consider the Hilbert space, $\mathcal{H}$, consisting of square integrable functions on the segment $-\pi \leq \theta \leq \pi$, with scalar product given by

$$\langle u, v \rangle = \int_{-\pi}^{\pi} \bar{u}(\theta)v(\theta)d\theta .$$

(2)

The operator $J_z \equiv -i\frac{d}{d\theta}$ is defined over all the differentiable functions $v(\theta)$; it represents the angular momentum observable of a plane rotator. Since the spectrum of $J_z$ is not bounded from below, the analog to condition (ii) in this case is not satisfied.

The operator $J_z$ is not a self adjoint operator (see for example p.87 in [7]). Denoting the adjoint of $J_z$ by $J_z^*$ and the complex conjugate of $u(\theta)$ by $\bar{u}(\theta)$, we have

$$\langle u, J_z v \rangle - \langle J_z^* u, v \rangle = -i[\bar{u}(\pi)v(\pi) - \bar{u}(-\pi)v(-\pi)].$$

(3)

Since $v(\pi)$ and $v(-\pi)$ are arbitrary, the above expression will vanish if, and only if, $\bar{u}(\pi) = \bar{u}(-\pi) = 0$. That is, the domain of $J_z^*$ is smaller than that of $J_z$.

The family of operators, $J_{z\alpha}^a \equiv -i\frac{d}{d\theta}$ with $0 \leq \alpha \leq 1$, whose domains of definition, $\mathcal{H}_\alpha$,

$$u(\theta) \in \mathcal{H}_\alpha \iff u(\pi) = e^{2\pi i\alpha}u(-\pi),$$

(4)

are all self-adjoint operators (cf. p.88 in [7]); they are the self-adjoint extensions of $J_z$. 

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The angle operator,

\[ \Theta : \quad \Theta u(\theta) = \theta u(\theta), \]  

(5)
does not “belong” to \( \mathcal{H}_\alpha \). This is the problem that stems from condition (i) above. It is the fact that \(-\pi \leq \theta \leq \pi\) which makes it impossible to find a common domain for \( J^\alpha_z \) and \( \Theta \).

In order to resolve this problem let us define a series of differentiable functions, \( f_{\varepsilon}(\theta) \in \mathcal{H}_{\alpha=0} \), such that \( f_{\varepsilon}(\theta) = \theta \) for \(-\pi \leq \theta < \pi - \varepsilon\), and for \( \theta \geq \pi - \varepsilon \) the function smoothly goes to the value of \( f_{\varepsilon}(-\pi) \), in the limit \( \varepsilon \to 0 \). Therefore, \( f_{\varepsilon}(-\pi) = f_{\varepsilon}(\pi) \) with \( \lim_{\varepsilon \to 0} f_{\varepsilon}(\theta) \to \theta \).

Now, the family of operators \( \Theta_{\varepsilon} \equiv f_{\varepsilon}(\Theta) \) are all “belong” to \( \mathcal{H}_\alpha \); they are a good approximation of the angle operator, \( \Theta \), in the limit of small \( \varepsilon \).

The canonical commutation relations

\[ [J^\alpha_z, \Theta_{\varepsilon=0}] = -i f_{\varepsilon}'(\Theta), \]  

(6)
can not be taken at \( \varepsilon = 0 \) due to the discontinuity of the function \( f_{\varepsilon=0}(\theta) \) at the point \( \theta = \pi \). Nevertheless, sometimes it is convenient (but not rigorous) to write the canonical commutation relation of the plane rotator observables in the following form:

\[ [J^\alpha_z, \Theta_{\varepsilon=0}] = -i (1 - 2\pi \delta(\Theta - \pi)), \]  

(7)
where \( \Theta_{\varepsilon=0} \neq \Theta \) only at the point \( \theta = \pi \). Denoting the eigenstates of \( J^\alpha_z \) by \( |m\rangle \) and taking the matrix elements of both sides of the equation above give the identity

\[ (m-m')\langle m|\Theta_{\varepsilon=0}|m'\rangle = -i \delta_{m,m'} \exp[i(m'-m)\pi]. \]  

(8)

Note that for \( m = m' \) both sides of the equation are zero (cf. Eq. (1)). In this way, the problems that follow from condition (i) are (partly) resolved; although the angle operator does not belong to \( \mathcal{H}_\alpha \), any periodic function of it is a self-adjoint operator in \( \mathcal{H}_\alpha \). Therefore, we are left with the problems that arise from condition (ii).

Consider the Hilbert space, \( \mathcal{H}_r \), consisting of square integrable functions, \( u(r) \), with \( 0 \leq r < \infty \), \( u(r = \infty) = 0 \) and inner product

\[ \langle u, v \rangle = \int_0^\infty \bar{u}(r)v(r)dr \]  

(9)
The radial momentum \( p_r = -id/dr \), which is defined over all the differentiable functions \( v(r) \), is not a self-adjoint operator. It satisfies:

\[ \langle u, p_r v \rangle - \langle p_r^* u, v \rangle = i\bar{u}(0)v(0). \]  

(10)
Hence, if \( v(0) \) is arbitrary, the domain of \( p_r^* \) must be restricted by the boundary condition \( u(0) = 0 \). But, if \( u(r) \) belongs to the domain of \( p_r^* \) (i.e. \( u(0) = 0 \)) then also \( p_r^* u(r) = -iu'(r) \) belongs to the domain of \( p_r^* \). That is, also \( u'(r = 0) = 0 \), and, by induction, the \( n \)-th derivative of \( u(r) \) must be zero at \( r = 0 \) \( (u^{(n)}(r = 0) = 0) \).

Thus, it is possible to define a self-adjoint radial momentum (or time) operator only on the subspace \( \mathcal{A} \) of the Hilbert space \( \mathcal{H}_r \), where \( u(r) \in \mathcal{A} \) if, and only if, all the derivatives of \( u(r) \) vanish at \( r = 0 \). For example, the square integrable function \( u(r) = \exp\left(-\frac{1}{r}\right)/r^2 \) belongs to \( \mathcal{A} \).
From a physical point of view, the domain $\mathcal{A}$ of the self-adjoint time operator, $T \equiv -i d/dr$, is too small. Most of the physical wave functions do not belong to $\mathcal{A}$. Therefore, we would like to augment the domain of the radial momentum (time) operator. The price that we have to pay is that we have to work now only with even functions of $p_r$.

Let us define two subspaces $\mathcal{H}^+_r$ and $\mathcal{H}^-_r$ of the Hilbert space $\mathcal{H}_r$ as follows:

$$u(r) \in \mathcal{H}^+_r \iff u^{(2m+1)}(r = 0) = 0 \text{ for all } m = 0, 1, 2, ... \quad (11)$$

and, similarly,

$$u(r) \in \mathcal{H}^-_r \iff u^{(2m)}(r = 0) = 0 \text{ for all } m = 0, 1, 2, ... \quad (12)$$

Note that all the even functions belong to $\mathcal{H}^+_r$ and all the odd functions belong to $\mathcal{H}^-_r$. However, there are also non-even functions that belong to $\mathcal{H}^+_r$ and non-odd functions that belong to $\mathcal{H}^-_r$. For example, $\mathcal{A} = \mathcal{H}^+_r \cap \mathcal{H}^-_r$.

**Theorem:** Let $f(r)$ be a function that can be expressed as a Taylor series around the point $r = 0$. Then, the operator $F \equiv f(p_r)$ has two self-adjoint extensions, with domains $\mathcal{H}^+_r$ and $\mathcal{H}^-_r$, if, and only if, $f(r)$ is a real and even function.

**Proof:** First, let us take $F = p_r^2 = -d^2/dr^2$. Then we have,

$$\langle u, Fv \rangle - \langle F^*u, v \rangle = \bar{u}(0) \frac{dv}{dr}(0) - \frac{d\bar{u}}{dr}(0)v(0). \quad (13)$$

Hence, if we want $F$ to be a self-adjoint operator, we must require $\bar{u}(0) = v(0) = 0$ or $\frac{dv}{dr}(0) = \frac{d\bar{u}}{dr}(0) = 0$. But, if, the domain of $F$ and $F^*$ is restricted by the boundary condition $\bar{u}(0) = v(0) = 0$ (or $\frac{dv}{dr}(0) = \frac{d\bar{u}}{dr}(0) = 0$), then also the functions $u(r) = -u''(r)$ must satisfy the same boundary condition, i.e. $u''(r = 0) = 0$ (or $u''(r = 0) = 0$). Therefore, $p_r^2$ is a self-adjoint operator if its domain is $\mathcal{H}^+_r$ or $\mathcal{H}^-_r$. It is easy to see that any real function of $p_r^2$ also has the same self-adjoint extensions and any odd function of $p_r$ does not have a self-adjoint extension $\Box$

We are now equipped with the tools to define self-adjoint operators that represent even and real functions of the quantum phase. In order to do so we have to include condition $(i)$ to the analysis above. This can be done by replacing the continuous variable $r$ with the integer variable $n$ ($n = 0, 1, 2, ...$). After this transformation $p_r^2 \rightarrow \Phi^2$, where $\Phi$ denotes the phase operator.

Any even function $u(r) \in \mathcal{H}^+_r$ and odd function $v(r) \in \mathcal{H}^-_r$ can be written as

$$u(r) = \int_{-\infty}^{\infty} d\chi U_\chi \cos(\chi r) \text{ and } v(r) = \int_{-\infty}^{\infty} d\chi V_\chi \sin(\chi r), \quad (14)$$

where $U_\chi$ and $V_\chi$ are the Fourier components. After the transformation $r \rightarrow n$, the analogs of $u(r)$ and $v(r)$ are given by

$$u(n) = \int_{-\pi}^{\pi} d\phi U_\phi \cos(\phi n) \text{ and } v(n) = \int_{-\pi}^{\pi} d\phi V_\phi \sin(\phi n) \quad (15)$$

where $u(n) \in \mathcal{H}^+_N$ and $v(n) \in \mathcal{H}^-_N$. The subspaces $\mathcal{H}^+_N$ and $\mathcal{H}^-_N$ are the analogs of $\mathcal{H}^+_r$ and $\mathcal{H}^-_r$. Note that the inner product of $u(n)$ and $v(n)$ is given by
\[ \langle u|v \rangle = \sum_{n=0}^{\infty} \bar{u}(n)v(n). \] (16)

Consider the subspace \( \mathcal{H}_N^+ \). Since all the vectors \( u(n) \) in \( \mathcal{H}_N^+ \) can be written as in Eq. (15), the basis
\[ e_\phi^+(n > 0) \equiv \sqrt{\frac{2}{\pi}} \cos(\phi n), \quad e_\phi^+(n = 0) \equiv \frac{1}{\sqrt{\pi}} \] (17)
spans \( \mathcal{H}_N^+ \). It is normalized as follows:
\[ \int_{0}^{\pi} d\phi \ e_{\phi}^+(n)e_{\phi}(n') = \delta_{n,n'} \] and \[ \sum_{n=0}^{\infty} e_{\phi}^+(n)e_{\phi}(n) = \delta(\phi - \phi'). \] (18)
Thus, in Dirac notation we have
\[ |\phi \rangle = \frac{1}{\sqrt{\pi}} |n = 0 \rangle + \sqrt{\frac{2}{\pi}} \sum_{n=1}^{\infty} \cos(n\phi)|n \rangle \] (19)
where \( |\phi \rangle \) is an eigenstate of any real and even function of the phase operator. It is the analog of \( 1/\sqrt{2} (|\theta \rangle + | - \theta \rangle) \).

In \( \mathcal{H}_N^+ \) any real and even function of the phase \( \Phi \) is a self-adjoint operator. In particular, the absolute value of the quantum phase operator is given by
\[ |\Phi| = \int_{0}^{\pi} \phi \ |\phi \rangle \langle \phi | d\phi, \] (20)
where \( |\phi \rangle \) has been defined in Eq. (19). It is interesting to calculate the expectation values of \( |\Phi| \) in a coherent state
\[ |\gamma \rangle \equiv \exp\left(-\frac{1}{2}|\gamma|^2\right) \sum_{n=0}^{\infty} \frac{\gamma^n}{\sqrt{n!}}|n \rangle, \] (21)
where \( \gamma = \sqrt{N} e^{i\theta} \) is the eigenvalue of the annihilation operator \( a \). It can be shown [8] that in the classical limit \( N = |\gamma|^2 \to \infty \),
\[ \langle \gamma |\Phi| \gamma \rangle \to \frac{\pi}{2} - \frac{4}{\pi} \sum_{s=1,3,5,\ldots} \frac{\cos(\theta s)}{s^2} = |\theta| . \] (22)
This result proves useful for establishing that \( |\Phi| \) has the correct large-field correspondence limit.

Carruthers and Nieto [9], have defined the “phase cosine” \( C \equiv \frac{1}{2}(E + E^\dagger) \) and “phase sine” \( S \equiv \frac{1}{2i}(E - E^\dagger) \) operators, where
\[ E \equiv \sum_{n=0}^{\infty} |n \rangle \langle n + 1 |, \] (23)
represents the phase exponent. It can be seen very easily that \( C \) and \( S \) do not commute. Therefore, \( C \) and \( S \) cannot represent the sine and cosine of the phase. As we have shown here, only the cosine of the phase is a self-adjoint operator in \( \mathcal{H}_N^+ \); it is given by
\[ \cos \Phi \equiv \int_0^\pi \cos \phi \, |\phi\rangle \langle \phi| \, d\phi = C + \frac{1}{2}(\sqrt{2} - 1)(|0\rangle \langle 1| + |1\rangle \langle 0|), \]  

where the projectors involving number eigenstates |0\rangle and |1\rangle can be neglected for states with \( \langle N \rangle \gg 1 \).

The subspace \( \mathcal{H}_N^- \) is spanned by the basis

\[ e^+_\phi(n) \equiv \sqrt{2} \frac{\sin(\phi n)}{\pi}. \]  

We have shown that any even and real function of the phase is a self-adjoint operator in \( \mathcal{H}_N^- \). In Dirac notation,

\[ |\phi\rangle = \sqrt{2} \frac{\sum_{n=1}^{\infty} \sin(n\phi) |n\rangle}{\pi}, \]  

where \( |\phi\rangle \) is an eigenstate of the absolute value of the phase operator. It is the analog of \( 1/\sqrt{2}(|\theta\rangle - | - \theta\rangle) \). The quantum absolute phase observable is given by

\[ |\Phi| = \int_0^\pi \phi \, |\phi\rangle \langle \phi| \, d\phi, \]  

and the cosine of the phase is given by

\[ \cos |\Phi| = C - (|0\rangle \langle 1| + |1\rangle \langle 0|)/2. \]  

In order to understand the connection between the absolute quantum phase defined in \( \mathcal{H}_N^+ \) (see Eq. (20)) and the one defined in \( \mathcal{H}_N^- \) (see Eq. (27)) let us discuss briefly the absolute quantum angle of a plane rotator. As we have shown in the beginning, any periodic function of the angle operator \( \Theta \) has a self-adjoint extension. In particular, the absolute value of the angle operator can be written in the form:

\[ |\Theta| = \int_{-\pi}^{\pi} d\theta \, |\theta\rangle \langle \theta| = \int_0^\pi d\theta \, \theta \left( |\mathcal{E}\rangle \langle \mathcal{E}| + |\mathcal{O}\rangle \langle \mathcal{O}| \right), \]  

where \( |\mathcal{E}\rangle = (|\theta\rangle + | - \theta\rangle)/\sqrt{2} \) and \( |\mathcal{O}\rangle = (|\theta\rangle - | - \theta\rangle)/\sqrt{2} \).

Let us define the subspaces \( \mathcal{H}_e \) and \( \mathcal{H}_o \) consisting of all the even and odd functions of \( \theta \), respectively. These Hilbert spaces are the analogs of \( \mathcal{H}_N^+ \) and \( \mathcal{H}_N^- \). Therefore, the first term on the RHS of Eq. (29) is the analog of the absolute quantum phase defined in \( \mathcal{H}_N^+ \) (see Eq. (20)) and the second term is the analog of the absolute quantum phase defined in \( \mathcal{H}_N^- \) (see Eq. (27)). On the other hand, the subspaces \( \mathcal{H}_e \) and \( \mathcal{H}_o \) are orthogonal because \( \langle \mathcal{O}|\mathcal{E}\rangle = 0 \), whereas \( \mathcal{H}_N^+ \) and \( \mathcal{H}_N^- \) are not orthogonal. This is the source of the quantum phase problem, and is also the reason why we were able to define self-adjoint operators in \( \mathcal{H}_N^+ \) and \( \mathcal{H}_N^- \), but not in \( \mathcal{H}_N = \mathcal{H}_N^+ \cup \mathcal{H}_N^- \).

To summarize, in the case of a plane rotator, the z-component of the angular momentum \( \mathbf{J}_z \) has a self-adjoint extension \( \mathbf{J}_z^\alpha \) with a domain \( \mathcal{H}_\alpha \). Therefore, the condition for a bounded coordinate (condition (i) in the text) implies that only periodic functions of the angle operator, \( \Theta \), are self-adjoint operators in \( \mathcal{H}_\alpha \). In a similar manner, the lower bound for the energy or the particle number (condition (ii) in the text) imposes that only real and even functions of the time or phase operator have self adjoint extensions.
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