Superpositions of unitary operators in quantum mechanics

Hollis Williams
School of Engineering, University of Warwick, Coventry CV4 7AL, United Kingdom
E-mail: Hollis.Williams@warwick.ac.uk
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Abstract
We discuss the significance of superpositions of unitary operators in the formalism of quantum mechanics. We show that with this viewpoint, it can be demonstrated that one can observe a measurement with zero Ozawa uncertainty in a physically realisable feedback set-up which uses polarised photons coupled to spin. We derive a set of conditions under which a linear combination of unitary matrices is also a unitary matrix and confirm that the conditions are met by a realistic quantum gate.

1. Introduction
The concept of a superposition of states in quantum mechanics is by now a familiar one (it is perhaps the main defining feature of quantum mechanics which sets it apart from classical mechanics). This concept has caused a certain amount of controversy, especially because it is not possible to reconcile superpositions of states with intermediate measurements. The essential issue is that coherent superpositions of states replace continuity of realities between initial conditions and final outcomes of the quantum measurement process. There have been many attempts to reconcile quantum superpositions and classical reality by studying the causality relations between the initial condition and the measurement outcome [1, 2]. These focus on a third physical property which is measured during an intermediate measurement between a pair of observables which are measured in the initial and final measurements, respectively. The measurement of this property interrupts the causality of via the dynamics generated by . In general, quantum mechanics would seem to require that the quantum reality of be conditioned upon a change in the laws of motion which take the system from measurement of at the initial time to measurement of at the final time and so it would be desirable if the physics of this change could be included in the usual formalism within those same laws of motion [3].

The role of unitary transformations is also established in the standard theory, but it is perhaps less well-known that coherent superpositions of unitary operators themselves might be useful in understanding the process of quantum measurement. We will make a slight distinction between a superposition of unitary operators (where the coherences between the operators might have some physical significance much as they do for superpositions of states) and linear combinations of unitary matrices in linear algebra. In terms of the usual operator expansions, a superposition of unitary operators as an expansion will be defined in the right-hand side of equation (7) (alternatively, one could think of it as the usual decomposition of an operator via the generators of the Hilbert space). Any non-unitary operator can be decomposed via unitary operators and this will be key to representing the measurement operator as a superposition of unitaries. The measurement problem itself goes back to the first studies of the foundations of quantum mechanics, and there have since been many theories of measurement [4]. In the interaction model of [5], it is observed that if the eigenstates of an interaction between a system and a meter are product eigenstates, then the action of on can be expressed as a controlled unitary operator

\[ \hat{U}_{SM} = \sum_a U_{SM}(a) \otimes |a\rangle_S \langle a|_S, \]  

where \( |a\rangle \) are eigenstates of the target observable \( \hat{A} \) in the system and \( \hat{U}_M(a) \) are conditional unitaries which act on the initial eigenstate of the meter or probe to produce conditional meter states. If the parameter \( a \) is uncertain
in the sense of quantum mechanics, then it is shown in [5] that the interaction must necessarily cause entanglement between the two systems \( S \) and \( M \). A measurement of the observable \( \hat{A} \) can distinguish between the possible conditional unitaries \( U_M(a) \) such that the statistics of \( \hat{A} \) just resembles a classical mixture of unitaries with no bias towards one particular unitary operator. However, the key subtlety is that one needs to read off a measurement outcome \( m \) at the readout stage of the process. This readout stage can be represented by a measurement basis \( |m\rangle_M \) in the Hilbert space of the meter or probe. A different measurement \( |m\rangle \langle m| \) will break this classical randomness and choose a particular coherent superposition of the possible conditional unitaries. Any information on a conditional unitary \( U_M(a) \) obtained via the outcome \( m \) is represented by this superposition. This in turn implies that the measurement operators \( \hat{M}(m) \) which we use to obtain information on an intermediate state \( |m\rangle \) can be represented by superpositions of unitary operators. In this note, we will also argue that there is a plausible general link between superpositions of unitary operators and decoherence in a realistic feedback compensation scenario described in [6].

To speak briefly on this approach to the measurement problem, in [5] it is shown that the probability update associated with a measurement outcome \( r \) is responsible for the decoherence caused by interaction with the environment. It follows that a measurement is represented by conditional probabilities \( P(r|x_m) \), where \( x_m \) is the property considered in the intermediate measurement with eigenstates \( |m\rangle \). The minimal decoherence is represented by a non-unitary self-adjoint measurement operator \( \hat{M}(r) \) such that

\[
\langle b|\hat{M}(r)|a\rangle = \sum_m \langle b|m\rangle \langle m|a\rangle \sqrt{P(r|x_m)}.
\]

(2)

The measurement operator \( \hat{M}(r) \) causes a disturbance which alters the causality relation between the initial condition \( a \) and the final outcome \( b \). To write \( \hat{M}(m) \) explicitly for a measurement outcome \( m \), one would have

\[
\hat{M}(m) = \sum_a \sqrt{P(m|a)} |a\rangle \langle a|.
\]

(3)

In general, any self-adjoint operator \( \hat{A} \) can be decomposed in terms of the infinitesimal generators of the Hilbert space [7]

\[
\hat{A} = \frac{1}{n} A_0 1 + \frac{1}{2} \sum_{j=1}^{l} A_j \lambda_j,
\]

(4)

where the operators \( A_0 \) and \( A_j \) are defined as

\[
A_0 = \text{Tr}[A], \quad A_j = \text{Tr}[A \lambda_j]
\]

(5)

for generators \( \lambda_j \). Any non-unitary operator can be decomposed in this way into unitary operators \( U_j \) and the identity operator is a well-defined element in such an expansion. Taking the trace of equation (4), we obtain

\[
A_0 = \sum_a \sqrt{P(m|a)}
\]

which implies that the coefficient of the identity operator in the expansion for \( \hat{M}(m) \) is

\[
\sum_a \frac{1}{n} \sqrt{P(m|a)}
\]

(6)

where \( P(m|a) \) is a conditional probability distribution. This is confirmed when we re-write equation (4)”alt="Equation 31”> in terms of unitary operators \( U_i \):

\[
\hat{M} = \sum_i \frac{1}{n} U_i \text{Tr}(U_i^\dagger \hat{M}),
\]

(7)

The right-hand side of (7) is the general definition of a superposition of unitary operators (note also that the superposition itself is non-unitary, which it must be in order to represent a non-trivial measurement operator). Using facts of operator algebra [8] and normalising the unitary operators in the superposition by multiplying by \( 1/\sqrt{n} \), this coefficient becomes

\[
\sum_a \frac{1}{n} \sqrt{P(a|m)}.
\]

(8)

This is the Bhatacharyya coefficient (essentially a real analytic analogue of the inner product in Hilbert space) taken for all possible \( a \), which implies that the contribution of the identity operator to the decomposition (7) of the measurement operator into unitary operators cannot exceed the Hellinger distance between conditional probabilities (see [3] for further discussion). This fact might have wider significance for the measurement problem, as it implies that coherent superpositions of unitary operators could play a non-trivial role in evaluation of measurement information.
2. Connection with Ozawa Uncertainty

In a recently proposed experimental set-up, it was shown that Ozawa uncertainties can be observed empirically by compensating for the decoherence of a probe qubit $P$ induced by a weak interaction with a system $S$ between state preparation and measurement [6]. In this set-up, a probe qubit $P$ is prepared in an eigenstate of the observable $\hat{X}$ and then interacts weakly with the target observable $\hat{A}$ of the system which is being measured. The probe qubit is sensitive to phase shifts generated by an operator $\hat{Z}$. This weak interaction is described by a conditional unitary operator

$$\hat{U}_{SP} = \exp \left(-i\frac{\epsilon}{\hbar} \hat{A} \otimes \hat{Z} \right),$$

(9)

where $\epsilon$ is the parameter giving the strength of the interaction. The outcome $m$ of a measurement described by a measurement operator $\hat{M}(m)$ gives information on the value of $\hat{A}$ prior to the measurement. In particular, if $A(m)$ is the estimate of $\hat{A}$, one has another unitary operator for the feedback signal which compensates for the effect on the probe qubit

$$\hat{U}_Z(m) = \exp \left(-i\frac{\epsilon}{\hbar}(-A(m))\hat{Z} \right).$$

(10)

For a sufficiently weak interaction, the expression for the decoherence which remains in the probe qubit after feedback compensation is then

$$1 - \langle \hat{X} \rangle (\text{out}) \approx \frac{2\epsilon^2}{\hbar^2} \sum_m \text{Tr}(\hat{M}(m)(\hat{A} - A(m))\hat{\rho}_S(\hat{A} - A(m))),$$

(11)

where $\hat{\rho}_S$ is the input state and $\langle \hat{X} \rangle (\text{out})$ is the uncompensated decoherence.

This set-up can be made slightly more specific, in which case one has a simple practical method for observing zero Ozawa uncertainty. The decoherence induced in the probe qubit with no feedback compensation is

$$\langle \hat{X} \rangle (\text{out}) = \sum_a \langle a | \hat{\rho}_S | a \rangle \cos \left(\frac{2\epsilon^2}{\hbar^2} A_a \right),$$

(12)

where $|a\rangle$ is an eigenstate of $\hat{A}$ and $A_a$ is a random eigenvalue of $\hat{A}$. As stated earlier, the value of $a$ is quantum mechanically uncertain, hence the interaction entangles the probe $P$ and the system $S$ [5]. In the case where the probe qubit is a photon polarisation and $\hat{A}$ is taken to be spin angular momentum, the possible eigenstates of $\hat{A}$ are only $|R\rangle$ and $|L\rangle$ (right-handed and left-handed states, respectively) and the corresponding random eigenvalues are $A_R = +1$ and $A_L = -1$. If we substitute these values back into (12) and sum over both of the possibilities, we obtain that without feedback the decoherence is

$$\langle \hat{X} \rangle (\text{out}) = 0.$$

(13)

However, in [6] it was proved that equation (11) implies that the uncompensated decoherence induced in the qubit in such a compensation scenario is exactly equal to the Ozawa uncertainty $\eta_s$ of the measurement, so the set-up which we have outlined above provides a practical example of a measurement with vanishing Ozawa uncertainty when there is no feedback [9]. Ozawa uncertainty of zero has previously been shown to correspond to the usual projective measurements when all the weak values only have real parts

$$\eta_a = 0 \quad \text{when} \quad A(m) = \frac{\langle m | \hat{A} | \psi \rangle}{\langle m | | \psi \rangle}$$

(14)

for a pure state input $|\psi\rangle$.

The interesting point is that projections on $|a\rangle \langle a|$ are superpositions of conditional unitary operators $\hat{U}_P(a)$. As stated earlier, in the case of a weak interaction, the action of the probe $P$ on the system $S$ can be expressed via a controlled unitary operator

$$\hat{U}_{SP} = \sum_a |a\rangle_S \langle a| \otimes \hat{U}_P(a).$$

(15)

For the scenario we have described, there are only two conditional unitaries $\hat{U}_P(R)$ and $\hat{U}_P(L)$ which rotate the photon polarisation in the paths $+1$ and $-1$, respectively. However, the superposition of $\hat{U}_P(R)$ and $\hat{U}_P(L)$ is itself unitary, because a sum of two unitaries which gives an arbitrary rotation of a photon polarisation is also a unitary operator. As an example in terms of linear combinations of unitary matrices, consider the Hadamard gate:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$  

(16)


Applying the Hadamard gate to an initial eigenstate of the probe qubit we have
\[ H(0) = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle), \]
\[ H(1) = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle), \]
(17a) (17b)
hence this gate produces an equal superposition of the qubit. On the other hand, this gate can be written as a linear combination of two unitary matrices:
\[ H = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \]
(18)

It is possible that this is a more general theoretical criterion and that the Ozawa uncertainty is zero in any feedback compensation scenario as described above when all the possible superpositions of the conditional unitary operators \( U_j(a) \) are themselves unitary, and that it is non-zero otherwise.

3. Conditions for unitarity of a linear combination of unitary matrices

We mention that we have found a set of conditions under which a linear combination of unitary matrices is itself a unitary matrix. This result is an abstract mathematical statement but we do not discount the possibility that it might have a physical interpretation. To be clear, the \( c_j \)'s in this theorem are arbitrary coefficients in the linear combination whose moduli squared all add up to unity and are not the same coefficients used in expression (7).

For this reason, we are not sure if the result could describe any realistic physical scenario, although it might be useful as the starting point for something else which turns out to have physical significance. The increased number of conditions is not surprising, since it is to be expected that unit normalisation is not sufficient by itself if we deal with a unital algebra over a field as opposed to the usual normed space.

Proposition: A linear combination of \( n \) unitary matrices is unitary given a number of conditions which is equal to the \((n - 1)\)-th central polygonal number. These conditions are unit normalisation, plus the fact that each of the terms in each of the following sums is antihermitian:
\[ \sum_{i=2}^{n} c_i U_i^* U_i + \sum_{i=3}^{n} c_i c_{i-1} U_i^* U_{i-1} + \ldots + c_n - c_1 U_n^* U_1. \]
(19)

**Proof.** The proof is a simple induction argument. For the base case, take \( n = 2 \). We could also consider one unitary matrix to be a linear combination of one matrix where the coefficient is 1. The coefficients are complex numbers and for unitarity it is sufficient to check that \( U^* U = 1 \), since \( U U^* = U^* U \) in this case. For \( n = 2 \) we obtain:
\[ (a U_1 + \alpha U_2)^* (a U_1 + \alpha U_2) = (|a|^2 + |\alpha|^2) 1 + \bar{a} \alpha U_1^* U_2 + \alpha \bar{a} U_2^* U_1. \]
(20)
The linear combination of the two matrices is unitary if \( |a|^2 + |\alpha|^2 = 1 \) and if \( \bar{a} \alpha U_1^* U_2 \) is antihermitian. The number of conditions required when \( n = 2 \) is 2, which is the first central polygonal number. We now consider the case where \( n = j \) and multiply out the brackets.
\[ \begin{align*}
(a U_1 + \alpha U_2 + \ldots + c_j U_j)^* (a U_1 + \alpha U_2 + \ldots + c_j U_j) &= (\sum_{i=1}^j |c_i|^2) 1 + \bar{c}_1 \alpha U_1^* U_2 + \ldots + \bar{c}_j \alpha U_1^* U_j + c_1 \bar{\alpha} U_2^* U_1 + \ldots + c_j \bar{\alpha} U_2^* U_j \\
&\quad + \ldots \quad + c_j \bar{\alpha} U_2^* U_j + \bar{c}_1 \alpha U_j + \ldots + \bar{c}_j \alpha U_j + c_1 \bar{\alpha} U_j + \ldots + c_j \bar{\alpha} U_j \\
&\quad + c_1 \bar{c}_2 U_1^* U_2 + \ldots + c_j \bar{c}_{j-1} U_1^* U_{j-1} + c_1 \bar{c}_2 U_j^* U_1 + \ldots + c_j \bar{c}_{j-1} U_j^* U_1 \\
&\quad + \ldots \quad + c_j \bar{c}_{j-1} U_j^* U_j + \bar{c}_1 \alpha U_{j-1} + \ldots + \bar{c}_j \alpha U_{j-1} + c_1 \bar{\alpha} U_{j-1} + \ldots + c_j \bar{\alpha} U_{j-1}. \\
\end{align*} \]
(21)

If we discard the \( \bar{c}_1 \alpha U_1^* U_1 \) term which contributes to the normalisation condition, the number of remaining terms containing \( c_j \) will be \( 2j - 2 \). Pair these terms as with the base case to get \( j - 1 \) conditions: these are that every term in the sum \( \sum_{i=2}^{n} c_i U_i^* U_i \) is antihermitian.

We continue with the remaining terms which contain \( c_2 \). Discard the \( \bar{c}_2 \alpha U_2^* U_2 \) term and neglect the \( c_2 \) terms which were already multiplied with \( c_1 \); there were 2 of these so we must have \( 2j - 4 \) terms containing \( c_2 \). Pair these to get a further set of \( j - 2 \) conditions: namely, each term in the sum \( \sum_{i=3}^{n} c_i c_{i-1} U_i^* U_{i-1} \) is antihermitian. Continue in this way until we reach the remaining terms which contain \( c_{j-1} \). Discard the \( \bar{c}_{j-1} \alpha U_{j-1}^* U_{j-1} \) term and neglect the \( c_{j-1} \) terms which were multiplied with \( c_1, \ldots, c_{j-2} \); there were \( 2j - 2 \) of these, so we have \( 2j - (2j - 2) = 2 \) remaining terms containing \( c_{j-1} \). Pair these to get one final condition: \( c_{j-1} \bar{c}_j U_j^* U_{j-1} \) is antihermitian. We end up with a descending sequence of sums:
\[ \sum_{i=2}^{n} c_i U_i^* U_i + \sum_{i=3}^{n} c_i c_{i-1} U_i^* U_{i-1} + \ldots + c_n - c_1 U_n^* U_1. \]
(22)
One can see from the previous argument that the number of terms in this sequence is $\frac{(n-1)n}{2}$. Add 1 for the normalisation condition to get $\frac{(n-1)n}{2} + 1$: this is the $(n - 1)$-th central polygonal number. The fact that the argument holds for $n = j$ implies that it holds for $n = j + 1$, since adding another operator $U_{j+1}$ to the linear combination simply means there are now another two terms containing $c_1$, another two terms containing $c_2$ and so on, up to a new remaining condition that $c_n + 1 U^*_n U_{n+1}$ is antihermitian. Every term in the new sequence of sums

$$\Sigma_{j=1}^{n+1} c_1 c_j U^*_j U_j + \Sigma_{j=3}^{n+1} c_2 c_j U^*_j U_j + \ldots + c_n + 1 U^*_n U_{n+1},$$

is antihermitian. The number of terms in this sequence is again $\frac{(n-1)n}{2}$, and so we have the $(n - 1)$-th central polygonal number once more after adding the normalization condition. This completes the proof.

As a check, note that the linear combination of two unitary matrices which gives the Hadamard gate

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

does meet both the relevant conditions, since the sum of the squares of the coefficients is obviously unity, and

$$c_1 c_2 U^*_1 U_2 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

which is antihermitian.

4. Conclusion

As has been observed elsewhere, quantum measurements always require entangling interactions and the information which is transferred in the process is necessarily caused by the decoherence induced by these interactions. Registering this measurement by turning a pointer in a meter in response to the measurement leads to an irreversible change to the system which is being observed. Although this is all qualitatively clear, it is not obvious what the correct formalism would be to capture this physics and various theories of the measurement process have been proposed [5]. We have discussed the possibility of using superpositions of unitary operators and emphasised that their main importance is that they can be used to represent measurement operators [3]. However, the complete significance of this fact for quantum measurement is a complicated problem which is far from resolution. In support of our claims that the concept of a decomposition into unitary operators may be useful, we have observed that there is a specific feedback compensation scenario derived from [6] for which it would be relatively easy to demonstrate a measurement with zero Ozawa uncertainty using this particular viewpoint.

This result gives further confirmation that the Ozawa uncertainty (and weak values in general) are physically valid quantities which can be observed empirically, even though the original concept of the Ozawa uncertainty was based mostly on mathematical assumptions [9]. Given that all the superpositions of the conditional unitary operators in this simple scenario are themselves unitary, we argue that this is likely true in general and that the Ozawa uncertainty is zero in any feedback compensation scenario of the type we have described when all the possible superpositions of unitary operators are also unitary. We have also derived a set of conditions under which a linear combination of unitary matrices is a unitary matrix and checked that the Hadamard gate (a realistic quantum gate which can be used to rotate a photon polarisation) meets the required conditions when it is decomposed into a linear combination of two unitary matrices.

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Data availability statement

No new data were created or analysed in this study.

ORCID iDs

Hollis Williams https://orcid.org/0000-0003-3292-602X
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