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Measurement theory for closed quantum systems

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Abstract. We introduce the concept of a "classical observable" as an operator with vanishingly small quantum fluctuations on a set of density matrices. Their study provides a natural starting point to analyse the quantum measurement problem. In particular, it allows to identify Schrödinger cats and the associated projection operators intrinsically, without the need to invoke an environment. We discuss how our new approach relates to the open system analysis of quantum measurements and to thermalization studies in closed quantum systems.

1. Introduction

"How does Hilbert space relate to our classical reality?" The consensus answer to this fundamental question is based on decoherence [1, 2, 3, 4]. Its starting point is a separation of the universe into system and environment. The decoherence induced by the environment kills quantum effects and provides the sought-for transition from the quantum to the classical world. While the separation of large systems into different parts clearly has its merits, the ambiguity in the division between system and environment remains awkward for a fundamental theory [6, 5]. Currently, there is a thriving research activity on closed quantum systems [7]. In particular, much progress has been made in understanding their thermalisation [8, 9, 10, 11], a phenomenon where environments traditionally play a central role. In this Letter, we will address the theory of quantum measurement for closed systems.

In order to define the relation between the quantum and classical worlds, we have to specify how the observable information relates to a quantum state. A crucial experimental fact is that all we know about the world are quantities with negligible quantum fluctuations. One may think here of an image on your computer screen, even though one does not have to go that far in the macroscopic world in practice. To make the connection between a quantum mechanical system and our knowledge about it, we therefore define the concept of a classical observable as an operator with vanishingly small quantum fluctuations. An experiment then corresponds to 'reading' its expectation value. This procedure corresponds in all cases to experimental practice, where there is always a link between the quantum system and our 'knowing it', that is described in terms of an expectation value and not in terms of a projection operator (think of the light emitted by the computer screen).

2. Classicality and signal to noise ratio

We quantify the classicality of an operator with respect to a density matrix $\rho$ as

$$C(A) = \frac{\left[ \text{tr}(A\rho) \right]^2}{\text{tr}(A^2\rho)}.$$  \hspace{1cm} (1)
It satisfies \( C \leq 1 \) because of the Cauchy-Schwarz inequality. For a classical observable, the upper limit is closely approached \( (C \to 1) \), where for an observable that is subject to large quantum fluctuations, \( C \) is substantially smaller. The unit operator clearly satisfies \( C(1) = 1 \), expressing that the norm of the wave function does not fluctuate. For the density matrix of a pure state \( \rho = |\psi\rangle \langle \psi| \), also the projection operator \( P = |\psi\rangle \langle \psi| \) is classical. However, when the wave function is evolved in time, its classicality will in general quickly decrease.

\[
\text{Figure 1.} \quad \text{a) Illustration of the dynamics of observables for a wave function that evolves in Hilbert space } \mathcal{H} \text{ under Hamiltonian evolution. Shaded areas indicate the magnitude of quantum fluctuations. Most observables have most of the time a small signal to noise ratio and do not qualify as classical observables.}
\]

In order to find operators that do remain classical under time evolution, we maximize

\[
\overline{C}(A) = \frac{\int_0^T dt \{ \text{tr}[A\rho(t)] \}^2}{\int_0^T dt \text{tr}[A^2\rho(t)]}.
\] (2)

The denominator can here be seen as a natural measure for the magnitude of the operator. In order to maximize \( \overline{C} \), we expand the operator \( A \) in a basis \( B_i \) of the linear Hermitian operators acting on the Hilbert space: \( A = \sum_i a_i B_i \). Substituting this expansion in Eq. (2), one sees that for the eigenvectors of the generalized eigenvalue problem

\[
\sum_j R_{ij} a_j^{(n)} = \overline{C}_n \sum_j M_{ij} a_j^{(n)},
\] (3)

the classicality corresponds to the generalized eigenvalue \( \overline{C}_n \). In Eq. (3) The matrices \( R_{ij} \) and \( M_{ij} \) are symmetric and defined as

\[
R_{ij} = \frac{1}{T} \int_0^T dt \text{ tr}[B_i\rho(t)] \text{ tr}[B_j\rho(t)],
\] (4)

\[
M_{ij} = \frac{1}{2} \text{ tr}[(B_i B_j + B_j B_i) \overline{\rho}].
\] (5)

Two operator eigenvectors \( A_n = \sum_i a_i^{(n)} B_i \) of Eq. (3) that belong to different eigenvalues are orthogonal in the following sense:

\[
\frac{1}{2} \text{ tr}[(A_m A_n + A_n A_m) \overline{\rho}] = 0.
\] (6)

Because the unit operator is a generalized eigenvector, the other operators have all zero time averaged expectation value: \( \text{tr}(A_m \overline{\rho}) = 0 \).
For an operator with zero expectation value, the square of its expectation value is a good measure of the signal. This motivates us to define the signal to noise ratio as

$$\text{SNR}(A) = \frac{\int_0^T dt \{\text{tr}[A\rho(t)]\}^2}{\int_0^T dt \text{tr}[A^2\rho(t)] - \{\text{tr}[A\rho(t)]\}^2}. \quad (7)$$

With the definition of the classicality (1), we can write it as

$$\text{SNR}(A) = \frac{1}{1 - \mathcal{C}(A)} \quad (8)$$

This relation tells us that classical observables, with $\mathcal{C} \to 1$, show temporal variations that are much larger than their fluctuations, while the time dependence of the other operators is drowned in noise (see Fig. 1).

To complete the specification of the measurement problem, we have to choose an initial condition. If we only use the total Hamiltonian as an input for our analysis, we are restricted to formulate it in the energy eigenbasis $|n\rangle$. As an incoherent mixture of energy eigenstates precludes any dynamics, it is most natural to consider a pure state. We will assume that a finite number of $N$ energy eigenstates, in an energy window $[E, E + \Delta E]$ is populated. Because there is no dynamics in the populations of the eigenstates, we should not lose physics by making the simplifying assumption that the initial state has equal overlap with all the energy eigenstates within the energy window $[8, 9]$. We do not loose generality by taking the overlap $\langle n|\psi(t = 0)\rangle$ real for our specific initial condition, because the absolute phase of the energy eigenstates is arbitrary. We then have for the density matrix

$$\rho(t) = \frac{1}{N} \sum_{k,l=1}^N e^{-i(\omega_k - \omega_l t)} |k\rangle \langle l|. \quad (9)$$

As a basis for the Hermitian operators on the Hilbert space, we choose

$$x_{m,n} = |m\rangle \langle n| + |n\rangle \langle m| \quad (10)$$

$$p_{m,n} = -i(|m\rangle \langle n| - |n\rangle \langle m|), \quad (11)$$

with the $m \neq n$ restricted to the energy levels that are populated according to the initial condition. We then have the following expectation values

$$\text{tr}[x_{m,n}\rho(t)] = 2 \cos[(\omega_m - \omega_n)t] \quad (12)$$

$$\text{tr}[p_{m,n}\rho(t)] = 2 \sin[(\omega_m - \omega_n)t] \quad (13)$$

For sufficiently long times $T \gg 2\pi \max(|\omega_m - \omega_n|^{-1})$, the matrix elements $R_{ij}$, where $i$ is of the $x$-type and $j$ is of the $p$ type operator vanish. We can therefore restrict our search to operators of the $x$-type, and will automatically find a corresponding $p$-type operator. For long times and in the absence of degeneracies, we find that the matrix $M$ in (5) is proportional to the unit matrix: $M = (2/N)\mathbb{1}$.

The elements of the matrix $R$, restricted to the $x$-operator space can be then written more explicitly as $R_{nm,n'm'}$. Equations (4) and (12) then show that off-diagonal elements of $R$ vanish when the transition frequencies differ much more than the Heisenberg energy uncertainty, i.e.

if $|\omega_n - \omega_m| - |\omega_{n'} - \omega_{m'}| \gg 2\pi/T$. The matrix $R$ is thus approximately block-diagonal, with each block corresponding to some transition frequency. Within a block of size $N_b$, all the matrix elements are equal to $2/N^2$. The eigenvalue problem (3) has a single nonzero eigenvalue per block in $R$, with corresponding eigenvector in the block $V = (1,1,\ldots,1)^T$ (all transitions act in phase). Because $RV = 2N_b/N^2V$ and $MV = (2/N)V$, we obtain $\mathcal{C} = N_b/N$. 


3. Detection of Schrödinger cats

For a harmonic ladder of $N$ equally spaced energy levels, we have $N_b = N - 1$, so that

$$\mathcal{C}(X) = \mathcal{C}(P) = 1 - \frac{1}{N}. \quad (14)$$

As expected, the operators $X$ and $P$ are (approximately) the harmonic oscillator position and momentum operators:

$$X = \sum_{n=1}^{N-1} (|n\rangle\langle n+1| + |n+1\rangle\langle n|), \quad (15)$$

$$P = -i \sum_{n=1}^{N-1} (|n\rangle\langle n+1| - |n+1\rangle\langle n|). \quad (16)$$

They can be made arbitrarily classical by increasing the number of levels. For a two-level system, $N = 2$, we simply recover the Pauli matrices and find that $\mathcal{C}(\sigma_x) = \mathcal{C}(\sigma_y) = 1/2$. The only nonzero elements of the commutator between position and momentum operators are $([X,P])_{1,1} = -(|X,P\rangle\langle X,P|)_{N,N} = 2i$. In the limit of a large number of levels $N \gg 1$, the commutator is thus negligible with respect to $X$ and $P$. For large $N$, also powers of $X$ and $P$ have classicality close to one. Ordinary calculus can then be used for sufficiently smooth functions of $X$ and $P$.

The fact that we do not precisely recover the usual harmonic oscillator position and momentum operators [a factor $\sqrt{n+1}$ is missing in Eq. (15)] can be attributed to the fact that the energy distribution is not Poissonian, but uniform in the interval $[E, E + \Delta E]$. Note that in the limit of a small energy window $\Delta E \ll E$ at high energy $E \gg \omega$, the variation of $\sqrt{n+1}$ becomes negligible and $X$ approaches the usual harmonic oscillator position operator.

The analysis becomes more interesting when we consider a direct sum of two incommensurate harmonic oscillator ladders. The total Hilbert space is then $\mathcal{H} = \mathcal{H}_1 \bigoplus \mathcal{H}_2$, each with $N/2$ levels, but with different energies: $\omega_n = n\omega_1$ for the first ladder and $\omega_n = n\omega_2$ for the second one (see Fig 2 c). It represents a qubit coupled to a harmonic oscillator, whose cavity-QED implementation has become a fruitful testing ground for quantum physics [12, 13, 14]. For short evolution times, $T \ll 2\pi/|\omega_1 - \omega_2|$, the two harmonic oscillator ladders are indistinguishable within the Heisenberg limited energy resolution (see Fig. 2 d) and we find that $X = X_1 \bigoplus X_2$ is still a classical observable, with $\mathcal{C}(X) = 1 - 2/N$. The operators $X_1$ and $X_2$ are analogous to (15), but with the levels restricted to $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively. For evolution times much longer than the Heisenberg uncertainty time $T \gg 2\pi/|\omega_1 - \omega_2|$ on the other hand (panel d), a classical observable can no longer be found. The most classical ones are $X_1$ and $X_2$, with $\mathcal{C}(X_1) = \mathcal{C}(X_2) = 1/2 - 1/N$.

In general, the highest classicality is obtained for operators that consist of all resonant transitions $|n\rangle\langle n|$. High classicality up to time $T$ is obtained when all occupied states form part of a harmonic oscillator ladder with common transition $\omega_n$, within the Heisenberg energy uncertainty $2\pi/T$ (see Fig. 2 c). The corresponding classical observable is then fully collective: all states participate in it as in the $X$ and $P$ operators in Eqs. (15) and(16). The stringent requirements of harmonicity and collectivity provide an elementary explanation of the fact that classical phase space is so much smaller than Hilbert space.

The lack of a classical observable up to late times on the full Hilbert space $\mathcal{H}$, reflects the fact that the system turns into a Schrödinger cat. Note that we have identified the cat state without separating the universe in system and environment. Our analysis thus provides a solution to the ‘preferred-basis problem’ [2, 15, 16] in Everett’s relative-state approach [17]. Observing the expectation value of the $X$ at times $T > 2\pi/|\omega_1 - \omega_2|$ will result in the collapse of the wave function. The density matrix is then projected to a single subspace $\mathcal{H}_1$ or $\mathcal{H}_2$, with a probability
Figure 2. a) Illustration of the qubit coupled to a harmonic oscillator potential. At early times (a), the positions in the two potentials (disks) are the same. It corresponds to the poor energy energy resolution, indicated thick energy levels in panel c). At later times (panels b,d), when the two groups of transitions are dephased with respect to each other, Hilbert space ‘breaks up’. Only on the red and blue harmonic subspaces, classical observables exist. Panel (e) shows the instantaneous classicality of the $X$-operator, $C(X)$ (thick filled curve), and $(C(X) + C(P))/2$ (dashed thick). The thin lines show the same for the density matrix restricted to the subspace $H_1$. Because of the limited number of frequencies in our toy model, the classicalities show a revival at later times and are periodically repeated.

proportional to their respective dimensions. This projection is precisely what is needed to restore the classicality of the observable $X$, as illustrated in Fig. 2. Where the classicality of the $X$-operator on the total Hilbert space (filled curve) decays as a function of time, its amplitude remains constant on the projected Hilbert space (thin line).

For more complex systems, the breakup of Hilbert space will occur for different subspaces on different time scales, as schematically illustrated in Fig. 3. At every branching point, a projection takes place. A possible scenario for surviving components is shown by the dark (red) regions. Because the different branches are eigenstates of the full Hamiltonian, elimination is definitive. A ‘consistent history’ [18, 19, 20] then appears naturally.

4. Discussion
The connection with the open system decoherence approach, where the environment consists of harmonic oscillators [2, 21], is straightforward. In case the system itself has a classical observable, this remains a classical observable under linear coupling to the environment. The most familiar example is a single harmonic oscillator coupled harmonic to a harmonic bath [21, 22, 23]. On the other hand, if the system does not have a classical observable, the coupling with the environment is essential to have classicality at all. Classical observables can then be constructed for the system combined with the environment after projection. The required projection operators correspond to the usual systems pointer states [24]. Our Schrödinger cat example in Fig. 2 is the simplest illustration of this mechanism. For the qubit alone $C(\sigma_x,\sigma_y) = 1/2$, there is no classical observable. When it is coupled to a harmonic oscillator, the combined system does have classical observables after projection of the system on a pointer state. This mechanism can be generalized straightforwardly to multiple harmonic oscillators, as is the case in practice [25, 26], where the revival time (see caption of Fig. 2) tends to infinity.
It is also worth discussing the connection to studies on thermalization in closed many-body quantum systems [8, 7, 9, 10]. For generic many-body systems, it is expected that no harmonic oscillator ladders exist, i.e. that from $\omega_n - \omega_m = \omega_{n'} - \omega_{m'}$ it follows that either $n = m$ and $n' = m'$ or $n = n'$ and $m = m'$ [9, 27, 28]. We then find that at late times, all classical dynamics with large SNR decay. Our investigation is thus complementary to the thermalization studies: where they are concerned with proving that most of the time for all observables the SNR is vanishingly small [9, 10], we focus on finding the observables that do show interesting dynamics in a given time window. Our analysis also sheds light on the thermalization time. Even though generic observables thermalize very quickly on the time scale of the Boltzmann time $\tau = h/(k_B T)$ [29, 30], our construction allows to find atypical (i.e. classical) observables that do show much slower thermalization, set by the anharmonicity of the spectrum. Remember that the phase of the energy eigenstates was chosen such that the overlap $\langle n|\psi(t = 0) \rangle$ was real. This can be done for any initial state, so that in every time window $[t, t + \tau_R]$, a similar set of classical observables can be constructed: if $A$ is a classical observable in the interval $[0, \tau_R)$, then the Heisenberg backward evolved operator $A' = e^{-iHt} A e^{iHt}$ is indeed trivially classical on the interval $[t, t + \tau_R]$. The relation between a specific set of classical observables and a certain time window could mean that our classical experiences are in this way related to the history of the universe. A more detailed analysis of this relation is presented in Ref. [31].

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