Quantum typicality and initial conditions

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Abstract

If the state of a quantum system is sampled out of a suitable ensemble, the measurement of some observables will yield (almost) always the same result. This leads us to the notion of quantum typicality: for some quantities the initial conditions are immaterial. We discuss this problem in the framework of Bose–Einstein condensates.

Keywords: typicality, Bose–Einstein condensates, quantum

A Birthday Dedication

Margarita and Volodya Man’ko are a remarkable example of a life-long passion for physics. Their involvement in fundamental physics, from quantum optics to quantum mechanics, conveys the enthusiasm of two teenagers. We are therefore delighted to dedicate this article to their joint 150th anniversary. Many happy returns!

1. Introduction and motivations

When we endeavour to describe the motion of a classical system, such as a point particle, we write Newton’s equation and a given set of initial conditions. Mathematically, we try and solve a Cauchy problem for a differential equation. This is the inheritance of Pierre Simon (Marquis de) Laplace, a world that is governed by deterministic laws.

A given state of Laplace’s deterministic universe is unmistakably the cause of its future (and the effect of its past). A ‘demon’ who at a certain moment knows all forces, positions and velocities of all particles, would be able to describe their motion with arbitrary accuracy and a single equation. The future would be certain to him and he would be able to calculate it from the laws of classical mechanics. In his work, Laplace never used the word ‘demon’, which came only later, possibly to convey a feeling of awkwardness. He rather wrote of ‘une intelligence’, and for such an intellect ‘nothing would be uncertain and the future just like the past would be present before its eyes\(^3\).’ Laplace was very keen of his deterministic framework. When Napoleon asked him why he had not mentioned God in his book on astronomy, he allegedly replied that he ‘had no need of that hypothesis\(^4\).’

Later studies, in particular by Henri Poincaré, showed that Laplace’s idea of determinism requires attention and a very careful scrutiny. The motion of some systems is extremely ‘sensitive to the initial conditions’ and this has come to be called dynamical instability. Physicists like the concept of stability, that makes it meaningful to speak of state preparation, and guarantees that if one is careful in preparing the state of the (classical) system, any experiment will yield the same result. This is known as repeatability and is a milestone of Galileo’s modern scientific method [1–3]. Nowadays, to most physicists, dynamical instability is the same in meaning as chaos [4].

Quantum mechanics brought uncertainty (and with it mystery) back to the stage. Even if one sets the initial conditions of the Schrödinger equation with accurate (infinite) precision, the behaviour of the (quantum) particle is far from being deterministic, and is in fact subject to indeterminacy. Quantum indeterminacy is ontological and not epistemic like in classical statistical mechanics: it cannot be avoided even by

\(^3\) Rien ne serait incertain pour elle, et l’avenir comme le passé seraient présent à ses yeux.’ Many of Laplace books are freely available online, thanks also to an Internet Archive with funding from the University of Ottawa, www.uottawa.ca/articles/uottawa-library-s-french-language-collection-going-digital

\(^4\) ‘Je n’avais pas besoin de cette hypothèse-là.’
the most accurate definition of the initial conditions (state preparation).

But is this the whole story? Can one prepare the very same quantum state over and over? This is a very difficult question, that has mind-boggling aspects. On one hand, it is almost meaningless to state that, say, two electrons emitted by an electron gun and illuminating a double slit have the ‘same’ wave function. On the other hand, the experimental verification of this statement, as e.g. through quantum state tomography [5, 6], requires measurements over a huge number of (‘identically prepared’) electrons. A more cautious question would then be the following one: which measurements would yield the same result for a quantum state that is sampled out of a suitable ensemble? This question catapults us into the topic of this article and the notion of quantum typicality.

It should be clear from the previous discussion that in order to test the notion of quantum typicality (namely the independence of the measurement outcome on state preparation), one needs essentially two ingredients. First, some control is required on the system state: namely, one must be able to assert, with reasonable confidence, that the wave function belongs to a suitable ensemble, e.g. a given subspace of the total Hilbert space of the system, and thus the quantum state is described by a certain density matrix. This relaxes the very notion of state preparation: it is not necessary to require (and believe) that a given wave function is identically re-prepared at each experimental run. It is enough that the wave functions in different runs are drawn from a suitable statistical ensemble. Second, and equally important, one cannot expect that measurements yield (almost) the same result for any observable of the system. Some observable will be typical, other will (and can) not. This is the essence of quantum mechanics. If one were able to suppress all fluctuations (including quantum fluctuations) of all observables, the system would be classical.

It emerges that cold gases and Bose–Einstein condensates (BECs) are an ideal testbed for these ideas. Indeed, a BEC of is characterized by a macroscopic occupation of the same single-particle state, or few orthogonal states (fragmented BEC) [7, 8], and one can reasonably assume that when an experiment is repeated, almost the same wave function is re-prepared.

These ideas can be tested in double-slit experiments with BECs, where interference is observed in single experimental runs, even though the two interfering modes are independently prepared (and therefore there is no phase coherence) [9]. The presence of an interference pattern is an interesting example of a property that weakly depends on the choice of the system state: second-order (unlike first-order) interference is similar for number and phase states [7, 8] and this explains why interference patterns emerge in single experimental runs [10–19].

This article is organized as follows. In section 2 we introduce the statistical ensemble of quantum states and define the typicality of a quantum observable. In section 3 we look at a simple case-study, a two-mode system of \( N \) Bose particles. Section 4 is devoted to conclusions and perspectives.

### 2. Quantum typicality of observables

Let a quantum system live in an \( N \)-dimensional Hilbert space \( \mathcal{H}_N \) and assume that state preparation consists in randomly picking a given pure state \( |\Phi_N\rangle \) out of an \( n \)-dimensional subspace \( \mathcal{H}_n \subset \mathcal{H} \). Given a basis \( \{|\ell\rangle\} \) of \( \mathcal{H}_n \), one can write

\[
|\Phi_N\rangle = \sum_{\ell} z_\ell |\ell\rangle.
\]

The complex coefficients \( \{z_\ell\} \) are assumed to be uniformly sampled on the surface of the unit sphere \( \sum_{\ell} |z_\ell|^2 = 1 \).

Clearly

\[
\overline{z_\ell z_\ell'} = \frac{1}{n} \delta_{\ell\ell'}, \quad \overline{z_\ell} = 0,
\]

where the bar denotes the statistical average over the distribution of the coefficients. Notice the dependence on the inverse of the subspace dimension \( n \) and observe how the average of all phase-dependent quantities (including the coefficients) vanish.

Consider an observable \( \hat{A} \). The random features of state (1) will induce fluctuations on a number of quantities related to \( \hat{A} \). We now scrutinize the different origins of these fluctuations.

The expectation value of observable \( \hat{A} \) over state (1) reads

\[
\bar{A} = \langle \Phi_N | \hat{A} | \Phi_N \rangle
\]

and is itself a random variable. A relevant quantity is the statistical average of the quantum expectation (3) over the statistical distribution (2) of the coefficients

\[
\overline{\bar{A}} = \langle \Phi_N | \hat{A} | \Phi_N \rangle = \text{tr} [\rho_{\Phi_N} \hat{A}].
\]

Interestingly, this coincides with the quantum average over the (totally mixed) ‘micro canonical’ density matrix \( \rho_{\Phi_N} \), which is proportional to the projector \( \hat{P}_n \) onto the subspace \( \mathcal{H}_n \):

\[
\rho_{\Phi_N} = \langle \Phi_N | \Phi_N \rangle = \sum_{\ell_1, \ell_2} z_{\ell_1} z_{\ell_2}^* |\ell_1\rangle \langle \ell_2| = \frac{1}{n} \hat{P}_n.
\]

Another interesting quantity is the statistical variance of the quantum expectation (3)

\[
\delta_A^2 = \overline{\bar{A}^2} - \overline{\bar{A}}^2 = \langle \Phi_N | \hat{A}^2 | \Phi_N \rangle - \langle \Phi_N | \hat{A} | \Phi_N \rangle^2.
\]

This is the simplifying assumption of uniform sampling. Our results are qualitatively unchanged for a wide class of probability distributions on \( \mathcal{H}_n \).
If $A$ were deterministic, i.e. $\delta_A \approx 0$, the overwhelming majority of states in the statistical ensemble would have the same expectation value, and this would coincide with the average $\langle A \rangle$: this condition defines the typicality of the expectation value. Observe that the latter term in (6) involves a quadratic (easy-to-evaluate) average, while the former term is quartic: since the theory is not Gaussian its evaluation requires some care [20]. However, as we shall see, its evaluation is not necessary for our purposes.

A third relevant quantity is the following
\[
\Delta A^2 := \langle \Phi_N | \hat{A}^2 | \Phi_N \rangle - \langle \Phi_N | \hat{A} | \Phi_N \rangle^2,
\]
which identically vanishes if $|\Phi_N\rangle$ is an eigenstate of $\hat{A}$. This quantity describes the quantum fluctuations of observable $\hat{A}$ on state $|\Phi_N\rangle$. Since state $|\Phi_N\rangle$ is a random variable, also $\Delta A^2$ will fluctuate. Its average over the distribution of the coefficient reads
\[
\delta_A^2 := \langle \Phi_N | \hat{A}^2 | \Phi_N \rangle - \langle \Phi_N | \hat{A} | \Phi_N \rangle^2
\]
and involves the same quartic average that appears in (6). Being related to the average of $\Delta A^2$ in equation (7), $\delta_A$ vanishes identically if the ensemble is made up of eigenstates of $\hat{A}$. On the other hand, it may also vanish asymptotically (for suitable values of $n$) as $N$ increases. If this happens, the outcome of a measurement of observable $\hat{A}$ on the majority of states $|\Phi_N\rangle$ in the ensemble is within good approximation fixed by its expectation value $\langle A \rangle$.

The key quantity is
\[
\delta A^2 := \delta_A^2 + \delta_q A^2
\]
\[
= \langle \Phi_N | \hat{A}^2 | \Phi_N \rangle - \langle \Phi_N | \hat{A} | \Phi_N \rangle^2
\]
\[
= \text{tr} \left( \delta \hat{A}^2 \right) - \left[ \text{tr} \left( \delta \hat{A} \right) \right]^2.
\]
A few comments are now in order. First of all, notice the cancellation of the quartic terms and observe that this quantity depends only on quadratic averages and is expressed in terms of the density matrix (5) (as it should). As a matter of fact, $\delta A^2$, namely the quantum variance of the observable $\hat{A}$ on the microcanonical density matrix $\rho_N$, could have been introduced without reference to $\delta_A$ and $\delta_q A$. The previous ‘derivation’ aims only at elucidating the multiple aspects of the fluctuations that affect a quantum system in the framework we introduced. Since $\delta A^2$ controls both the statistical variance $\delta_A^2$ of the expectation value and the average quantum variance $\delta_q A^2$ of the observable, the condition
\[
\frac{\delta A}{A} \rightarrow 0, \quad \text{as } N \rightarrow \infty
\]
ensures that, for the overwhelming majority of wave functions in $H_n$, an experimental measurement of the observable $\hat{A}$ will fluctuate within a very narrow range around the average expectation value $\langle A \rangle$. It is clear that the limiting procedure (10) depends on the choice of the sampled subspace $H_n$, namely of the statistical ensemble (5), and on how $n$ scales with $N$.

3. Two-mode case study

Scrutiny of a simple case-study will hopefully elucidate the main ideas and be the testbed of the general framework described in the preceding section. Consider a two-mode system made up of $N$ structureless bosons. The second-quantized field operators satisfy the canonical equal-time commutation relations (in this section we remove the hats on the operators)
\[
[\Psi (r), \Psi^\dagger (r')] = 0, \quad [\Psi (r), \Psi (r')] = \delta (r - r').
\]
The $N$ bosonic particles are distributed among the ground $|\phi_0\rangle$ and the first excited state $|\phi_1\rangle$ of a harmonic oscillator, whose mode wave functions read (in suitable units)
\[
\phi_0(x) = \frac{1}{\sqrt{\pi}^{1/4}} e^{-x^2/2}, \quad \phi_1(x) = \frac{\sqrt{2}}{\sqrt{\pi}^{1/4}} xe^{-x^2/2},
\]
and whose Hamiltonian is
\[
H = \frac{1}{2} \left( p^2 + x^2 \right).
\]
One easily computes the expectation values of the even powers of the position operator in the two modes
\[
\langle \phi_0 | x^{2\nu} | \phi_0 \rangle = \frac{\Gamma(\nu+1/2)}{\Gamma(\nu)},
\]
\[
\langle \phi_1 | x^{2\nu} | \phi_1 \rangle = \frac{\Gamma(\nu+2)}{\Gamma(\nu+1)},
\]
while the expectation values of the odd powers vanish. Define the collective single-particle observable
\[
X_{2\nu} = \int dx \ x^{2\nu} \Psi^\dagger (x) \Psi (x).
\]
Let us consider the microcanonical ensemble represented by the density matrix (see equation (5))

$$\rho_{\ell} = \frac{1}{n} \sum_{\ell_1,\ell_2} |\ell\rangle \langle \ell|,$$

(17)

where in the states $|\ell\rangle := |(N/2 + \ell)\rangle$, $(N/2 - \ell)\rangle$ the occupation numbers of the two modes are well-defined, with $2\ell$ representing the particle imbalance between the modes. One can easily show that, due to the symmetry of the modes, this quantity is typical whenever the maximal imbalance satisfies $n = o(N)$. The proof is simple. The expectation value

$$X_{2\ell} = \text{Tr}(\rho_{\ell} X_{2\ell}) = \frac{N}{2} \left( \langle \phi_0 | x^{2\ell} | \phi_0 \rangle + \langle \phi_1 | x^{2\ell} | \phi_1 \rangle \right)$$

$$= N \left( \frac{(2\ell)!}{\nu!} + \frac{2(2\nu + 2)!}{(\nu + 1)!} \right),$$

(18)

splits, as one expects, into the average of expectation values of $x^{2\ell}$ in the two modes. Its variance on $\rho_{\ell}$ (9) can be expanded as a quadratic polynomial in the total number of particles $N$ and the maximal imbalance $n$, yielding [21]

$$\delta X_{2\ell}^2 = \text{Tr}(\rho_{\ell} X_{2\ell}^2) - \left[ \text{Tr}(\rho_{\ell} X_{2\ell}) \right]^2$$

$$= D_{\ell,0}^2 \frac{N^2}{4} + D_{\ell,2}^2 n^2 + O(N).$$

(19)

A straightforward computation shows that

$$D_{\ell,2}^2 = 2 \left( \langle \phi_1 | x^{2\ell} | \phi_0 \rangle \right)^2 = 0,$$

(20)

due to the opposite symmetry of the mode wave functions. By contrast, the factor multiplying $n^2$ does not vanish and reads

$$D_{\ell,2}^2 = \frac{1}{12} \left( \langle \phi_1 | x^{2\ell} | \phi_1 \rangle - \langle \phi_0 | x^{2\ell} | \phi_0 \rangle \right)^2$$

$$= \frac{1}{3} \left( \frac{2(2\nu + 2)!}{(\nu + 1)!} - \frac{2(2\nu)!}{\nu!} \right)^2.$$

(21)

These results show that, unless $n = O(N)$,

$$\frac{\delta X_{2\ell}}{X_{2\ell}} \rightarrow 0 \quad \text{as} \quad N \rightarrow \infty,$$

(22)

thus ensuring the typicality of the observable $X_{2\ell}$ for $n = o(N)$. In practice, no matters how one prepares the initial state, distributing the particles between the two modes, as far as the maximum imbalance between the two modes scales less fast than the total number of particles $N$, a measurement of the collective observable $X_{2\ell}$ will yield essentially the same result. In particular from (19), when $n = O(N^{1/2})$, the relative fluctuations around the typical value are normal, i.e. $O(N^{-1/2})$.

It is worth observing that the main result (22), being related to condition (20), can be generalized to all pairs of modes with opposite symmetry. Moreover, it can be extended to all single-particle observables that are polynomial in $x^2$. This implies that if the particles are distributed among modes with opposite symmetry, with $n = o(N)$, and confined by a symmetric potential, the potential energy of the system is always a typical observable.

4. Conclusions and outlook

We have discussed the notion of quantum typicality, defining the typicality of an observable and focusing on a two-mode Bose system. An observable is typical if its single-run measurement, performed on a system state belonging to a suitable subspace, yields the same result with very large probability.

Typical observables are therefore properties shared by the vast majority of states. By contrast, non-typical observables are characterized by wide fluctuations. Interestingly, this distinction is crucial in determining ‘good’ observables in classical and quantum statistical mechanics [22]. As measurements on typical observables yield (almost) the same result, the knowledge of the initial state with arbitrary precision becomes immaterial. This brings us back to the concepts discussed in the Introduction and the main idea of this article.

One can revisit and relax the notions of state preparation and initial conditions. As we emphasised, BESCs are an ideal testbed for these concepts in quantum statistical physics [7, 8, 14, 16, 23].

Typicality is related to the beautiful mathematical phenomenon of measure concentration [24]. This is a fecund idea that has been applied to elucidate the structure of entanglement in large quantum systems [25, 26], as well as some basic concepts in statistical mechanics [27–30]. It would interesting to apply this notion to the characterization of entanglement in BESCs and to study dynamical effects, such as phase randomization in condensates [31, 32].

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