Completely top–down hierarchical structure in quantum mechanics

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Can a large system be fully characterized using its subsystems via inductive reasoning? Is it possible to completely reduce the behavior of a complex system to the behavior of its simplest “atoms”? In this paper we answer these questions in the negative for a specific class of systems and measurements. After a general introduction of the topic, we present the main idea with a simple two-particle example, where strong correlations arise between two apparently empty boxes. This leads to surprising effects within atomic and electromagnetic systems. A general construction based on pre- and postselected ensembles is then suggested, wherein the N-body correlation can be genuinely perceived as a global property, as long as one is limited to performing measurements which we term “strictly local.” We conclude that under certain boundary conditions, higher-order correlations within quantum mechanical systems can determine lower-order ones, but not vice versa. Surprisingly, the lower-order correlations provide no information whatsoever regarding the higher-order correlations. This supports a top–down structure in many-body quantum mechanics.

emergence | reductionism | top-down | weak values | quantum mechanics

A n old dispute between reductionism and emergence questions whether the behavior of a large, complex system can be reduced to the behavior of its individual parts (1–6). We introduce a category of physical effects which fundamentally impact this issue.

While there are many definitions of emergence, we are reluctant to opine on such interpretational–philosophical issues, and, indeed, such discussions are not necessary to prove the existence of the type of physical effects proposed here. Nevertheless, the connection between our results and the existing literature is more than just semantic; we believe it may help to guide intuitions in this area of research and thereby potentially lead to further multidisciplinary discourse (7).

It is, however, useful to distinguish between weak and strong emergence (5). In a nutshell, weak emergence implies that while one may not be able to determine the behavior of the whole from the behavior of the parts, one does not challenge the basic assumption that emergent phenomena are at least in principle reducible to the more fundamental microphysics. Weakly emergent properties are said to be composed of (or supervenient upon) the lower-level properties.

In contrast, theories of strong emergence assert that there are new emergent properties which cannot in principle be reduced to or derived from any of the lower-level constituents and, in particular, cannot be reduced to the fundamental microphysical properties. Some theories of strong emergence propose the existence of downward or top–down causation, i.e., that the strongly emergent properties, which exist only at a higher level of complexity (i.e., the whole), have causal efficacy over the lower level of complexity (i.e., the parts).

However, this speculative introduction of fundamentally new arrows of causation creates overdetermined situations, as well as causal efficacies arising from different levels of complexity which may conflict with each other. For example (Fig. 1), the usual bottom–up causal efficacy of physics (part-to-whole) might tell a conglomerate of particles (at an intermediate level of complexity) to move right while the top–down (whole-to-part) causal efficacy radiating down from a higher level of complexity might tell the same conglomerate of particles to move in the opposite direction, to the left. Such arguments are often referred to as the “causal closure of the physical” or as the exclusion argument (8). These arguments apparently ruled out all claims of top–down causation up to that point in time (ref. 9, p. 11):

All of the evidence today suggests that strong emergence is scientifically irrelevant... There is no evidence that strong emergence plays any role in contemporary science... Strong emergence starts where scientific explanation ends.

Fusion Emergence

Subsequently, the attempt to get around this overdetermination inherent to strong emergence was proposed by Humphreys (10) and is known as “fusion emergence.” The idea is that properties which exist at a lower level can fuse together and create new, “emergent” properties at a higher level of complexity. During fusion, the lower-level properties (i.e., the parts which fuse together) cease to exist. Fusion thus has a number of consequences: (i) The whole can no longer be reduced to the parts (since the parts no longer exist after fusion); (ii) the overdetermination argument is eliminated, i.e., the new top–down causal efficacy of the “whole” can no longer be in conflict with the causal efficacy of the original lower-level properties which radiate their causal efficacy in the usual bottom–up fashion; and finally (iii) the new emergent properties can now have causal efficacy over the parts. A number of problems with fusion emergence were identified (ref. 11, p. 361): (i) Fusion emergence denies “the copresence

Significance

We provide quantitative evidence for the strong emergence of correlations within pre- and postselected quantum systems. These correlations are robust and can be verified by either weak or strong (projective) measurements. They give rise to intriguing effects within many-body quantum systems. Our analysis supports a top-down structure in quantum mechanics according to which higher-order correlations can always determine lower-order ones, but not vice versa.

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of their lower-level correlates, which is empirically implausible and (ii) even if it could be made plausible, a “basal loss” occurs during the fusion process (since the parts cease to exist) and this interferes with the structural integrity of the whole system.

Humphreys replied that one could apportion the parts in a delicate balance so that some fuse and some retain their identity as individual parts to maintain the structural integrity of the whole. Manafu (ref. 12, pp. 225 and 226) replied that Humphreys’ “division of labor between properties may be an ad hoc response to the problem of basal loss if we do not have independent justification for why the dichotomy between properties that can undergo fusion and those that cannot should overlap with the dichotomy between the properties that are not essential in the functioning of the system and those that are.”

Humphreys responded (ref. 13, pp. 7, 82) that a “core example of fusion emergence” is the covalent bond: When a water molecule is created by “fusing” two hydrogen atoms and one oxygen atom, electrons are shared between the atoms and hybrid (i.e., covalent) bonds are created. Humphreys argued that as a result of the formation of the covalent bond, the molecule could not be reduced to a collection of individual atoms. Kronz and Tietjen (ref. 14, p. 345) previously argued that the best-known example of fusion emergence is when the two electrons participating in a covalent bond become entangled: The new whole which emerges has “contemporaneous parts” that “cannot be characterized independently from their respective wholes.”

Manafu (12) identified several problems with Humphreys’ covalent bond example. The atoms exist at a particular level of complexity (call it level “i − 1”). Even though one might argue that they disappear when the atoms fuse together into a higher level, i.e., a molecule (call this level “i”), Manafu argued that there was still evidence of the composition of parts at level “i − 2” in terms of the electrons and nuclei.

In addition, we emphasize another limitation for any analysis of wholes described by ensembles of entangled systems: All properties of such wholes can always be fully analyzed by per-forming separate local measurements on each part along with the correlations between the parts.

We now proceed to address all of the above issues with the introduction of our family of physical phenomena.

**New Effects: Pre- and Postselection, Weak Values**

In the following, we provide simple yet fundamental arguments in favor of top–down logic and top–down causal efficacy by introducing families of pre- and postselected ensembles. Consider a conceptual example with three particles and three boxes. With appropriate preselection, postselection, and measurement during the time after the preselection and before the postselection (below), we observe the following properties: No individual particle is found in any individual box, no two particles are found in any two of the boxes, and no correlations are found between any two of the boxes. However, when we measure the correlation between all three boxes, we nevertheless find surprising, strong correlations. We could not use the one-particle or two-particle information to deduce the properties of the three-particle correlation. However, with the information of the three-particle correlation, we can now, in a top–down fashion, deduce the one- and two-particle properties and correlations.

These phenomena are completely general. We introduce states of N particles exhibiting such phenomena. We show that we obtain null results for measurements of local properties for any subpart of the full N-particle system. In addition, we show that we obtain null results for any lower-order correlations (i.e., [N − 1], [N − 2]-particle correlations, etc.). However, when we discuss the system as a whole (that is, properties involving all N particles together), strong nonlocal correlations nevertheless emerge. In other words, the higher-order (i.e., N-particle) correlations are required to construct any of the lower-order correlations, but we cannot go the other way around; i.e., we cannot deduce the N-particle correlations from any of the lower-order correlations. Because the properties of the part are determined by the whole, we argue that such systems require a top–down view of quantum mechanics and introduce the term “whole-to-part” to identify these families of states. This category of whole-to-part phenomena and the questions they raise for the reductionism–emergence debate can be fully analyzed using standard quantum mechanics. We do not need to make any modification of standard quantum mechanics to analyze these whole-to-part effects. As a consequence, it is very likely that future experiments will verify the predictions we introduce here [some of the predictions regarding the two-particle whole-to-part effects have already been verified experimentally (15, 16)]. However, the analysis of whole-to-part effects from the perspective of the standard formulation of quantum mechanics is somewhat cumbersome. By using instead a simple reformulation of standard quantum mechanics (which again provides identical predictions to those of standard quantum mechanics), the technical complications dwindle, and the results and further implications introduced in this article can be understood intuitively. The reformulation involves setting boundary conditions at two different times instead of the usual practice of setting boundary condition at a single, initial time during the earlier preparation phase (known as preselection). The second boundary condition is set at a later time, after performing the measurements which verify the strange properties of the whole-to-part state. This later boundary condition is known as postselection. This time-symmetric reformulation of standard quantum mechanics is known as the two-state vector formalism (TSVF) (17–20). Within the TSVF, quantum systems are described by the usual (preselected) state-vector |Ψ⟩ which evolves forward in time, as well as a second state-vector ⟨Φ| which evolves backward in time. The resulting two-state (|Φ⟩, |Ψ⟩) gives rise to the weak value of any operator $A$.

![Fig. 1. Overdetermination. Part-to-whole forces from low level to midlevel push particles to the right while hypothetical whole-to-part forces from top level to midlevel push the same particles in the opposite direction, to the left.](image-url)
\[ \langle A \rangle = \frac{\langle \Phi | A | \Psi \rangle}{\langle \Phi | \Psi \rangle}, \]  

which is measured weakly (21, 22) in the time between pre- and postselection. When the measured operator is dichotomic, i.e., having only two eigenvalues, and the weak value happens to be equal to one of these two eigenvalues, then we can conclude with certainty that, had we measured it strongly (projectively), we would have found the same outcome (23). That is, in this special case which is discussed throughout this paper, the weak and the “strong” values coincide. Therefore, although we discuss weak values throughout this paper, the results are quite general and can be experimentally verified by either strong (i.e., projective) measurements or weak measurements.

One question of interest regarding the two state is whether it can be inferred by using local tomography based on projective measurements. As shown in ref. 24, this task is possible when discussing preselected ensembles, but not when discussing pre- and postselected ensembles. In the latter case, a larger set of Kraus operators is needed. These results were derived for single particles, but can be easily generalized to multipartite scenarios. Therefore, broadly speaking, local projective operators are not sensitive to subtle multipartite correlations within pre- and postselected ensembles.

We are interested in a smaller set of operators, namely, those allowing “strictly local” projective measurements. By this we mean that the measurement is applied not only to a single particle but also to a single position of this particle. For instance, if the system is composed of two particles, each superposed within two different boxes, then a strictly local measurement would project on a single-particle observable localized within one of the boxes. In light of ref. 24, we know that full tomography of the two state is impossible using this set of measurements. But our aim here is different. We want to find out to what extent can higher-order multipartite correlations be inferred when using both strictly local measurements and the lower-order correlations between them. This gives rise to the phenomena explored below.

In the following, we first analyze a simple case of deductive reasoning within two-particle systems. Thereafter, we further demonstrate this whole-to-part reasoning with the aid of more effects. We then generalize this top–down structure to the N-particle case when correlations seem to emerge only when calculated at the level of the system as a whole.

### Two-Particle Systems

We begin with a simple illustration of a truly emergent correlation (Fig. 2). Consider a two-particle system, where each of the particles can be located in one of two boxes, corresponding to the states \(| L_i \rangle \) (left) and \(| R_i \rangle \) (right), where \(i = 1, 2\) corresponds to the presence of the \(i\)th particle in the left/right box in the \(i\)th pair of boxes. These two particles are prepared (i.e., preselected) at time \(t_i\) in the state

\[ | \Psi \rangle = \frac{1}{2} (| L_1 \rangle + | R_1 \rangle) (| L_2 \rangle + | R_2 \rangle). \]  

Later at \(t_f\), we postselect the system in the state
\[ \langle \Phi \rangle = \frac{1}{\sqrt{3}} \{ \langle L_1 \rangle \langle L_2 \rangle - \langle L_1 \rangle \langle R_2 \rangle - \langle R_1 \rangle \langle L_2 \rangle \}. \]  

Note that in this example, we have a total of four boxes: two boxes for particle 1 (\( L_1 \) and \( R_1 \)) and two boxes for particle 2 (\( L_2 \) and \( R_2 \)).

During intermediate times \( t \) (where “intermediate” means after the preselection and before the postselection, \( t_i < t < t_f \)), we want to know whether the particles were in their respective left-hand boxes. This can easily be checked by calculating the weak value for the projections \( \Pi^{(i)} \equiv \langle L_i \rangle \langle L_i \rangle \) for each particle \( i = 1, 2 \). According to Eq. 1, these are

\[ \langle \Pi^{(i)}_L \rangle_w = 0. \]

That is, if we weakly measure the presence of each particle in its respective left-hand box, one after the other (e.g., by weakly probing the external fields emerging from these boxes or by performing a weak scattering experiment), then we will find that both of them are empty (Fig. 2 a and b), and hence we deduce that particle 1 was in the right-hand box of the first pair of boxes and that particle 2 was in the right-hand box of the second pair of boxes. In addition to the external electromagnetic fields, the same is true for any other local property of the particles that we can measure within both of these two left-hand boxes (e.g., the gravitational field, etc.). Moreover, since projection operators are dichotomic, the null results of the existence of the particles in the left-hand boxes can also be verified with certainty by using a “strong” (i.e., projective) measurement. The particles will be found with certainty in the right-hand boxes:

\[ \langle \Pi^{(i)}_R \rangle_w = 1. \]

The above predictions seem very reasonable, but intriguingly, when calculating the correlation between the projections on the left-hand boxes we find that (Fig. 2c)

\[ \langle \Pi^{(1)}_L \Pi^{(2)}_L \rangle_w = -1. \]

When we look for the two individual particles in the left-hand boxes, we never find either individual particle in the left-hand boxes (Eq. 4). Nevertheless, we will always find a surprising correlation between the two “empty” left-hand boxes (Eq. 6). While this construction resembles Hardy’s thought experiment (15, 25, 26), we plan to use it here for a very different purpose (27). In particular, we generalize this scenario to the many-body case and from the impossibility of going the other way, i.e., constructing correlations from the single-particle weak values (in this case and in general).

Electromagnetic Field Interference Pattern

Another result stemming from the above construction can be observed by assuming that the two particles have a charge. One can then measure weakly (from a large distance) the total electromagnetic energy density of the two left-hand boxes without disturbing the particles’ states (to accentuate the effect, suppose now that both left-hand boxes are spatially separated from the right-hand boxes). The energy density will be proportional to

\[ \langle \hat{E}^2_{\text{tot}} \rangle_w = \langle \hat{E}^2_{1} \rangle_w + \langle \hat{E}^2_{2} \rangle_w + 2 \langle \hat{E}_1 \cdot \hat{E}_2 \rangle_w, \]

The reason a bottom–up approach will not work is because all of the strictly local information available through the single-particle weak values (i.e., Eqs. 4 and 5) is not sufficient to determine the two-particle correlations (i.e., Eq. 6). Pursuant to our previous discussions, this violates the compositional principle of reductionism and is in conflict with the usual bottom–up approach.

This suggests a true top–down logical structure in quantum mechanics, in cases where the experimenters are allowed only to perform strictly local projective measurements. We stress, however, that had we enlarged the set of possible operations, i.e., had we allowed each party to probe its two boxes simultaneously (which again can be a manifestly nonlocal measurement), they could have constructed the two state and could have revealed the subtle correlations between the boxes (24).

Surprising Manifestations of Top–Down Structure

Let us imagine a hydrogen atom located either in box A or in box B. We further assume that its electron can occupy the ground state \( \langle \mid gr \rangle_e \) or the first excited state \( \langle \mid ex \rangle_e \). We preselect the atom at time \( t_i \) (separated for convenience into proton, \( p \), and electron, \( e \)) as

\[ \langle \Psi \rangle = \frac{1}{\sqrt{3}} \{ \langle A \rangle_p \langle gr \rangle_e + \langle B \rangle_p \langle gr \rangle_e + \langle B \rangle_p \langle ex \rangle_e \}. \]

and later at time \( t_f \), we postselect on

\[ \langle \Psi \rangle = \frac{1}{\sqrt{3}} \{ \langle A \rangle_p \langle gr \rangle_e - \langle B \rangle_p \langle gr \rangle_e - \langle B \rangle_p \langle ex \rangle_e \}. \]

Was there a proton in box B during intermediate time \( t (t_i < t < t_f) \)? Apparently not, as

\[ \langle \Pi^p_B \rangle_w = 0, \]

i.e., the weak value of projection operator \( \Pi^p_B = \langle B \rangle_{pp} \langle B \rangle \) is zero. However, if we look for the pair proton–electron in the ground state within box B, we would find it there with certainty:

\[ \langle \Pi^{p,e}_{B} \rangle_w = 1. \]

If we use only the single-particle weak values, then Eqs. 14 and 15 would have suggested that the electron in box B is encircling nothing. To understand why the electron is in a bound state, we must take into account the observable which is the product of electron and proton. Hence we see the fundamental importance of correlations in determining the system’s behavior which goes far beyond the single-particle properties. This is also suggested by the derivation of single-particle weak values (Eqs. 4 and 5) as a sum of two correlations,

\[ \langle \Pi^p_B \rangle_w = \langle \Pi^p_B \Pi^{e,gr}_{B} \rangle_w + \langle \Pi^e_{B} \Pi^{e,ex}_{B} \rangle_w = 1 - 1 = 0, \]

and from the impossibility of going the other way, i.e., constructing correlations from the single-particle weak values (in this case and in general).
where $\vec{E}_i$ is the electric field created by the $i$th particle. However, once again, we note that since the left-hand boxes are empty, the first two contributions in Eq. 17 will be zero, and all of the energy will originate from the interference term $\langle \vec{E}_2^2 \rangle_w + 2\langle \vec{E}_1 \cdot \vec{E}_2 \rangle_w$ which depends on the correlation between the two left-hand boxes (Eq. 6).

The $N$-Body Scenario

The above example is, in fact, a special case selected from a broad family of pre- and postselected ensembles all giving rise to a completely top–down logical structure. In all these $N$-body systems, we will see that the 1-point function, the 2-point function, and all of the way up to the $(N-1)$-point function are all strictly zero, while the $N$-point function is nonzero. That is, none of the lower-order correlations reveal anything about the whole, i.e., the $N$th-order correlations.

Without loss of generality, consider one specific construction for these families of states: Let $N$ spin-1/2 particles be prepared at time $t = t_i$ in the state

$$|\Psi\rangle = \prod_{i=1}^{N} |\psi_i \rangle,$$  

where $|\psi_i \rangle = \{ (|\uparrow_1 \rangle + |\downarrow_1 \rangle) / \sqrt{2} \}$ is an eigenstate of the Pauli-X matrix characterizing particle $i$. If we interpret the operator $\sigma_x$ as a binary position operator (30), then the state given in Eq. 18 describes $N$ particles, each of which is superposed in two “boxes” (where $|\uparrow_i \rangle$, $|\downarrow_i \rangle$ are spin up in the left-hand box and spin down in the right-hand box). At $t = t_j$, the particles are postselected in the state

$$|\Phi\rangle = 2^{N/2} \prod_{i=1}^{N} |\downarrow_i \rangle + C \prod_{i=1}^{N} |\uparrow_i \rangle,$$  

where $C \neq 0$ is some complex number (the normalization of the pre- and postselected states does not influence the results of our weak value calculations).

During intermediate times $t (t_i < t < t_j)$, we use weak measurements to find specific correlations between the particles’ positions denoted by projections on the left-hand boxes, e.g., $(1 + \sigma_x^{(1)})/2$, being a projection on the left-hand box of the $i$th particle (subsequently we discuss how these weak measurements correspond to strong measurements).

It turns out that weak measurements of correlations having the form $\prod_{i=1}^{N} [(1 + \sigma_x^{(i)})/2]$, where $b_i \in \{0, 1\}$ not all 1, provide null outcomes, while the outcome of weakly measuring $\prod_{i=1}^{N} [(1 + \sigma_x^{(i)})/2]$ is nonzero. This means we would never find a particle in any of the left-hand boxes, nor would we find lower-order correlations between the particles (when limited to strictly local, projective measurements). Only the $N$th-order correlation is nonvanishing. Summarizing, we have

$$\langle \prod_{i=1}^{N} \left[1 + \sigma_x^{(i)} / 2\right] \rangle_w = 0 \quad \exists i, b_i \neq 0$$

$$1/C \quad \forall i, b_i = 1.$$  

As noted in previous sections, due to the “dichotomic operator theorem,” the absence of lower-order correlations can be verified using (counterfactual) strong measurements. When $C = 1$, we can also verify in this way the $N$th-order correlations as the $+1$ eigenvalue of a dichotomic (projection) operator.

Another interesting case is $|C| \ll 1$, where we can observe, using weak measurements only, a very large, robust $N$th-order correlation, even in the absence of all low-order correlations. The limiting case $C = 0$ is forbidden of course because then the pre- and postselected states become orthogonal.

Using a different terminology, these results also suggest that one cannot perform a full tomography of the two state using only strictly local projective measurements (and, in fact, not even by using correlations between strictly local measurements involving $N-1$ particles or fewer). However, when viewing the Hilbert space of the $N$ particles as a one-particle Hilbert space of dimension $2N$, then the task is possible in a nonlocal way using the set of $4 \cdot (2N)^2$ Kraus operators described in ref. 24.

In the following sense, this top–down structure is very stable. First, modifying the relative phase between the terms in Eq. 19, as well as the value of $|C|$, will not qualitatively change the predictions of Eq. 20 (i.e., the emergence of high-order correlations). Therefore, even in the presence of noise or unsharp final projective measurement (and also if we insert modifications of the above kind in the postselected state), we would still expect a similar effect. Furthermore, if $m$ particles are discarded during the course of the experiment (and thus are not included in the calculation of the various weak values), the top–down logical structure would still persist, and correlations will emerge at the $N - m$ level of the hierarchy.

Manifestations of Emergent Correlations

Let $N$ photons be prepared in the state

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \left( \prod_{i=1}^{N} |H\rangle_i + |0\rangle \right),$$  

where $|H\rangle$ denotes horizontal polarization and $|0\rangle$ is the vacuum state. Suppose these photons are postselected:

$$|\Phi\rangle = \frac{1}{\sqrt{2}} \left( \prod_{i=1}^{N} |V\rangle_i + |0\rangle \right).$$  

We see that the states are not orthogonal as a result of the vacuum contributions. Suppose we wish to know the values of circular polarization during intermediate times. Each projection on the clockwise or anticklockwise circular polarization will rotate the state of the corresponding preselected photon toward the postselection, but only the product of $N$ such rotations will be nonzero. Hence, we see again a situation where all of the products of $0 \leq m < N$ projections are zero, until $m = N$, which is nonzero, suggesting the emergence of the circular polarization in this pre- and postselected ensemble.

Many additional thought experiments can be designed with Fock states: For instance, if we preselect

$$|\Phi\rangle = \frac{1}{\sqrt{2}} (|1, 1, \ldots, 1\rangle + |0, 0, \ldots, 0\rangle),$$  

then the weak values of the annihilation operators $a_k$ would be null for all $l$. Any product of at most $n - 1$ different annihilation operators would also yield null weak values. In contrast, the $n$-fold product $\prod_{i=1}^{n} a_k$ has a nonzero weak value, namely 1. This leads to many other experiments.

Discussion

We have seen that in a specific category of pre- and postselected ensembles composed of $N$ particles, we obtain null results for measurements of local properties of any subpart of the full $N$-particle ensemble (i.e., properties of any subset containing
$N-1$ particles, $N-2$ particles, etc., as well as any lower-order correlations (i.e., $[N-1]$-, $[N-2]$-particle correlations, etc.). However, when we discuss the system as a whole (referring to properties involving all $N$ particles), strong nonlocal correlations ensue. Furthermore, the higher-order (i.e., $N$-particle) correlations are required to construct any of the lower-order correlations, but not vice versa. This was first shown for the case of two-level systems, and was then substantially generalized. This top–down construction is always possible due to the linearity of weak values, while, as indicated above, the bottom–up approach may fail. These predictions of the TSVF can also be verified through projective (i.e., strong) measurements and were further shown to be robust under noise and particle loss.

We emphasize that the cases discussed above are very different from those that could be achieved with classical random variables. With a set of $N$ such random variables $\{X_1, \ldots, X_N\}$ it can be arranged that the expected values $E[X_1], \ldots, E[X_N]$ and the low-order correlations are all zero, and yet $E[X_1 \cdots X_N] \neq 0$. However, in the quantum scenarios discussed above, all of the outcomes of strictly local measurements are identically zero, rather than just the averages, and hence locally one cannot have any indication concerning the existence of particles there, not to mention the possibility of correlation.

The families of states introduced here thus strengthen a top-down deductive reasoning in many-body quantum mechanics. In addition, it may shed light on some other open problems regarding the foundations of quantum physics, known as the Oxford Questions (31), such as, “Does the classical world emerge from the quantum?”

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