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Contextual Emergence of Physical Properties

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Abstract
Contextual emergence was originally proposed as an inter-level relation between different levels of description to describe an epistemic notion of emergence in physics. Here, we discuss the ontic extension of this relation to different domains or levels of physical reality using the properties of temperature and molecular shape (chirality) as detailed case studies. We emphasize the concepts of stability conditions and multiple realizability as key features of contextual emergence. Some broader implications contextual emergence has for the foundations of physics and cognitive and neural sciences are given in the concluding discussion. Relevant facts about algebras of observables are found in the appendices along with an abstract definition of Kubo-Martin-Schwinger states.

Keywords Contextual emergence · Reductionism · Stability conditions · Equivalence classes · Temperature · Chemical potential · Molecular structure

1 Introduction

Physical properties and processes are intricately interrelated in complex systems in a manner where contexts are important. A key feature characterizing contextual relations are stability conditions and contexts that can be defined precisely through contextual topologies (Sect. 2). The emphasis in contextual emergence is on making explicit the role contexts play in scientific phenomena and explanation, a role that is often left implicit. Contextual emergence was originally proposed as an inter-level

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relation for physical descriptions [19] and has been further developed into an inter-level/inter-domain relation among physical properties, processes and laws (e.g., [14, 16]).[1]

The motivation for contextual emergence is in nonlinear dynamics and the states/observables distinction found in algebraic approaches in quantum mechanics and statistical mechanics. The algebraic framework provides well-defined concepts for the latter distinction which are useful for clarifying issues and relations. Moreover, the algebraic framework offers helpful tools for categorizing algebras of observables. Nevertheless, contextual emergence is not dependent on these algebraic approaches. The contextual emergence framework is more general while putting these distinctions to use. This is important because while scientists sometimes can give similar mathematical descriptions of biological and neural phenomena in terms of states and observables, more often than not the biologist and geologist must work with more systemic and qualitative descriptions.

The formal apparatus of contextual emergence is described in Sect. 2, emphasizing multiple realizability and stability conditions (Sects. 2.2 and 2.4) and contextual topologies (Sect. 2.3). Section 3 lays out the basics of the ontic/epistemic distinction and algebras of observables (Sect. 3.2), and develops it as regards the quantum/classical distinction and emergence of classical mechanics from quantum mechanics (Sects. 3.2.1, 3.2.2). The dynamics/observables relation is discussed in Sect. 3.3. This is followed by the examples of temperature (Sect. 4) and chiral structure of molecules (Sect. 5) as contextually emergent properties. Concluding discussion is given in Sect. 6. Some facts about algebras of observables are described in three Appendices.

2 Contextual Emergence

Reduction and emergence are used in a variety of senses in the literature [12, 42, 48, 50]. These schemes are typically organized in a hierarchical manner, where levels of description or levels of reality are related to each other. For instance, one might speak of "reducing" higher-level features to lower-level features, or the emergence of higher-level features, where some of their aspects are irreducible to lower-level features.

Such levels-talk needs to be treated with some care, however. There is a tendency for reduction or emergence schemes to treat levels as reified or pre-given in some universal, timeless sense. That is an oversimplification, to be sure. Nevertheless, there are the cases of artificial systems, such as computers, where there are pre-given levels because they are constructed to be so both logically and physically [26, chap. 2]. In natural systems, by contrast, whatever levels exist arise over time. In some instances, levels are easily identifiable (e.g., elementary particles, molecules, simple crystals, or cells, organs, bodies), whereas in other cases levels can only be

[1] So-called quantum contextuality—where measurement outcomes are dependent on the measurement context—can be considered a special case of the contexts central to contextual emergence.

identified, if at all, by the length and time scales of the dynamics and dynamical structures (e.g., convection), while in some cases in quantum mechanics there is an erasure of levels (e.g., composite nonseparable quantum systems, where the joint system possesses a state, while the components lack definite states given there are many possible entanglements for the system components). Moreover, there are cases where one may explore the relationship between two domains that are not strictly hierarchically ordered [43]. In general, non-hierarchical frameworks including other notions, such as those of domains of description or domains of reality, might be more appropriate in specific cases. Finally, when we speak of a "more fundamental domain" or "lower level" of reality, we do not mean that these are somehow " more real" than "less fundamental" or "higher levels" of reality. As we will see below the idea of fundamentality is not as straightforward as often assumed in the hierarchical picture.

Contextual emergence was proposed as an inter-level/inter-domain relation that takes emergence seriously as a scientific phenomenon rather than beginning with a metaphysical assumption about what emergence must be like [14, 19]. This approach contrasts with the usual philosophical approaches to reduction or emergence which start with logical or metaphysical foundations [12].

Contexts are the heart of contextual emergence. The notion of context is multifaceted, including a family of features (many of which are inter-related or co-dependent). Among other things, contextual factors encompass

- the system/environment distinction,
- stability conditions that ensure robustness of states and observables,
- different kinds of constraints delimiting system behaviors.

An example would be constraints at larger length and time scales leading to new structures and properties, such as Rayleigh-Bénard convection [17, 23]. Contextual features can be made very precise in terms of the stability conditions leading to new states and observables (see Sects. 4 and 5).

While some necessary conditions for emergent properties may exist at smaller length and time scales, the sufficient conditions represented by contexts are found at longer length and time scales. Ontological contextual emergence focuses on the "ontological furniture" of the physical states and observables, the necessary and sufficient conditions for their existence and persistence, and the transitions that must take place from one level or domain of reality with one set of states/observables to another level or domain with new states/observables. Epistemological contextual emergence focuses on the necessary and sufficient conditions for relations among multiple levels of description.

2.1 A Framework of Conditions

A framework of necessary and sufficient conditions can be used to classify ontological relations among levels or domains of reality:

(1) *Reduction* Properties and behaviors in a lower level or domain (including its laws) offer by themselves *both necessary and sufficient* conditions for properties and behaviors at a higher level.
(2) *Contextual emergence* Properties and behaviors in a lower level or domain (including its laws) offer *some necessary but no sufficient* conditions for properties and behaviors at a higher level. Higher levels provide the needed extra conditions.
(3) *Multiple realizability* Properties and behaviors in a lower level or domain (including its laws) offer only *sufficient* conditions for the associated properties and behaviors at a higher level. Many lower-level constituents and conditions can give the same higher level results.
(4) *Radical emergence* Properties and behaviors in a lower level or domain (including its laws) offer *neither necessary nor sufficient* conditions for properties and behaviors at a higher level.

Among these relations, reductions correspond to class (1), where the entities of the fundamental level or domain are either identical to or imply everything else at a reduced level or domain (e.g., the properties of a physical system in special relativity reduce to their Newtonian mechanics counterparts in the limit $v^2/c^2 \rightarrow 0$, where v is the system velocity and c the speed of light in vacuum[2]). There are few genuine cases of class (1) reductions in the sciences outside of trivial cases.

Class (2) represents contextual emergence, where the constituents belonging to the "fundamental" level or underlying domain of reality contribute some necessary but not sufficient conditions for entities and properties in the target domain, or higher level. For instance, the domain of elementary particles contributes some of the necessary conditions for the existence of the properties and behaviors of water flowing through a faucet: no elementary particles and forces, no flowing water. On the other hand, the existence of elementary particles and their forces do not guarantee that flowing fluids will exist. The total set of necessary and sufficient conditions for flowing fluids is, itself, contingent rather than necessary, and involves more conditions than are found in the domain of elementary particles and forces. The existence of necessary conditions at the lower or underlying level means that higher-level features imply those of the lower level; however, the converse (lower-level features also imply the higher-level features) does not hold in contextual emergence.

Cases of contextual emergence arise when *contingent conditions from the target domain or higher level are added to the necessary conditions in the underlying level or domain* to create a complete set of necessary and sufficient conditions for the phenomena in the higher level or domain. The examples of temperature and molecular chirality will be given below (Sects. 4 and 5).

Class (3) represents cases of multiple realizability. There are always numerous more entities at the lower levels than at the higher levels so any particular higher level state S_1 can be realized by an equivalence class $E(S_1)$ of lower level states that

[2] This is not to imply that the spacetime of special relativity reduces smoothly to the spacetime of Newtonian mechanics in this limit.

all give the same higher level state S_1. The equivalence classes of structures and dynamics at the lower level corresponds to the emergent variables and dynamics at the higher levels.

Classes (2) and (3) complement each other as in the example of temperature which is contextually emergent (Sect. 4) while also multiply realizable (e.g., temperature is an emergent property of all kinds of gasses and liquids). In fact multiple realizability is necessary and sufficient for contextual emergence (though not all cases of multiple realizability are cases of contextual emergence). The contingent conditions from the target domain which enable contextual emergence also determine the associated equivalence classes at the lower level.

In the discussion below we focus on the contexts that characterize contextual emergence and their associated stability conditions giving rise to the associated equivalence classes. We will have nothing to say about class (4) as it is irrelevant to the sciences.

2.2 Stability Conditions

A concrete context is a set of conditions that, when added to the necessary conditions contributed by an underlying domain or level of reality, form a set of jointly necessary and sufficient conditions leading to the existence and persistence of higher-level properties of the concrete context. Temperature and molecular shape are two such properties requiring the addition of concrete contextual conditions for their existence.

A particularly important set of contextually contingent conditions are *stability conditions* that are characteristic of concrete contexts (e.g., existence of crystals in solid state physics, or molecules in a solution). These conditions guarantee the existence and persistence of appropriate states, observables, and structures of the system in question. Contextual emergence occurs when such stability conditions are not given by lower-level conditions alone. Stability conditions are integral for the identification of systems and their states as well as the persistence of their identity under various kinds of changes. As such these conditions are a central feature of contextual emergence and highlight the role that contexts play in emergence.

In typical philosophical treatments of reduction and emergence, states and observables are taken for granted meaning that the stability conditions implied by those states and observables are also taken for granted. The crucial roles played here by contexts are often neglected: There are some environmental conditions where they do not hold (for example if nuclear reactions are taking place, daily-life conservation laws do not apply). The conservation laws that always hold at the lower levels apply in particular circumstances to equivalence classes of lower level entities that together form a higher level entity displaying the conserved existence that characterizes physical objects.

Furthermore, stability conditions are related to changes in the degrees of freedom for systems: either by restricting the degrees of freedom accessible to a system (reducing the allowable states of motion, say, through constraints, symmetry breakings, or other means), or by opening the system's access to degrees of freedom that

were formerly restricted (a particularly dramatic example of this is the change in allowable states of motion in Rayleigh-Bénard convection; see [17]).

For contextual emergence, changes to the system's degrees of freedom producing new properties or structures are due to stability conditions that are never given by nor derivable from the underlying level alone. Moreover, these stability conditions are related to equivalence classes in the following way: Equivalence classes of states are indistinguishable with respect to a specific ensemble property (e.g., the class of all arrangements of gas molecules in a container with respect to the same temperature). Stability conditions lead to the distinguishing of particular equivalence classes with respect to the relevant stabilities meaning the emergent states and observables (and perhaps even the system itself) are robust under perturbations and over time. Another way to think about this is that stability conditions given by higher-levels partition the underlying state space into particular distinguished equivalence classes that are stable with respect to the dynamics of the underlying level under the higher-level constraints represented by the stability conditions. Furthermore, the context characterized by stability conditions endows the underlying state space with a new contextual topology.

2.3 Stability Conditions, Contextual Topologies and Abstraction

Any experimental observations depend on a system/environment distinction since there is always an observed object of study surrounded by elements which are not the direct object of observation. Scientists seek to control the environment as much as possible to screen off influences from the system that would interfere with the epistemic states and observables (Sect. 2.4) under investigation. As well, theories involve states and observables that are distinguished from any background conditions. Any system/environment distinction involves making abstractions about the physical domain in question.

For law-like and other relations, specifying a topology picks out the relevant relations in the set of observables that go into appropriate descriptions by specifying which elements are adjacent to each other. On the other hand, the algebras of observables characterizing different physical theories induce different topologies, and are usually related via singular limits. When the limiting procedure is singular this means that the equations at the limit are not smooth approximations of the equations when the characteristic parameter is approaching (but has not reached) the limit. Singular limits can be characterized as those in which the final set of equations has a qualitatively distinctive character to the starting set.

As an example, the very complex relationship between quantum mechanics and classical mechanics involves singular limits with respect to the Hilbert space topology. To regularize such limits (i.e., to get convergent limits) requires introducing new states and observables leading to a new *contextual topology*: a topology of a mathematical space of elements that represents a relevant extension corresponding to a mathematical space containing an expanded algebra of observables for a system in a target level or domain. Such an expansion represents information from the target level or domain's context (e.g., the target level's symmetries, stability conditions and

observables) while abstracting away from those factors considered irrelevant. The contextual information of the target domain induces a suitably enriched topology but the contextual topology is never given by the finer topology of the lower-level description. Said another way, the underlying algebra of observables conceived as being as context-free as possible based on first principles never implies the algebra of observables of the target level or domain [19, 47]. The contextual topology defines the equivalence classes at the lower level corresponding to the entities that are the genuine actors in the higher-level or target domain dynamics.

The concept of a contextual topology can be illustrated by the simple fact that there are many different possible topologies each compatible with the same starting set. For instance, suppose $S = \{A, B, C\}$ with the trivial topology $\tau = \{\oslash, \{A, B, C\}\}$, where $\oslash$ is the empty set. This is a high level description. We can restructure S to give a lower-level description as long as we preserve every relation, inducing a new topology, for example $\tau_1 = \{\oslash, \{A\}, \{A, B, C\}\}$. This illustrates that higher-level descriptions are not implied by lower-level descriptions because contextual topologies are underdetermined by the norm topology of the lower-level description ($\tau \nRightarrow \tau_1$). Hence, by imposing a hierarchy of topologies τ_N–an abstract grouping together of elements of the set–a hierarchical structure is created within the set, ordering that set. Yet, that ordering is not fixed by the lower-level description.

Stability conditions associated with the higher levels, or target domains, induce a contextual topology by picking out particular reference states and observables. These operators, in turn, form an algebra with an associated weak topology (Appendix A.2). The higher-level, (e.g., classical mechanics) has a coarser topology characterized by an algebra containing observables not found in the finer topology of the algebra associated with the lower-level theory (e.g., quantum mechanics). Although one can formally make differences between the mathematical spaces of different states of observables precise through comparing these differences in topologies, in practice physicists focus the algebras of observables themselves and their properties (see below).

These higher-level stability conditions and states represent an *abstraction* away from lower-level or underlying details to reveal patterns and constraints. Abstractions are not the same as *idealizations* (though scientists sometimes use the two terms interchangeably). The latter involve situations where we remove assumptions and apply approximations to create tractable models. In contrast, there are are many cases where we cannot remove modelling assumptions without losing necessary definitions of quantities serving to parameterize target systems. Abstractions involve hiding information about lower-level variables (e.g., variations within an equivalence class) enabling the definition of new categories of variables as sometimes are required to capture specific modal facts about systems.

If we want to know modal facts about generalities that apply across radically different microphysical systems, then abstracting away from those details is not a convenience for pragmatic idealization purposes; it is essential to characterizing the target system. Abstractions allow scientists to identify modal information concerning the circumstances under which a variety of systems share particular features, and, therefore, answer counterfactuals about when they would not share those features. This is much more powerful for understanding physical systems than simply listing

their properties and noting that some have commonalities. Abstract models are necessary for mapping the modal landscape of those commonalities in a principled way. Furthermore, they capture larger-scale or global constraints across systems sharing common features and behaviors.

The Ising model illustrates the importance of abstraction. Ferromagnetism is modeled by treating the up/down polarisations in the atomic dipoles of a metal abstractly as a regular array of points each assigned a value + 1 or − 1. Let $S_i(a)$ represent the value of the ith site in lattice arrangement a. Then $\Sigma_i S_i(a)$ is the difference between + 1 and − 1 sites in a. The degree of order of the system, M_a, is the sum of $S_i(a)$ divided by the total number of sites. If M_a is + 1 or − 1, then the lattice is maximally ordered because all the sites are either + 1 or − 1. When $M_a = 0$, the lattice is maximally disordered since just as many sites are + 1 as − 1. For each adjacent pair of sites $< j, k >$ there is an associated interaction energy $E_{jk} := -JS_jS_k$, and the total energy H_a is the sum of E_{jk} over all adjacent sites in a. In a maximally ordered arrangement, H_a is at a minimum. If H_a is positive, as the temperature decreases the probability, P_a, of disordered arrangements falls to zero; conversely, as temperature increases disordered states become more likely. The order parameter is the weighted sum over a of all arrangements P_aM_a. By counting the number of ways the lattice could be arranged, and using statistical methods, the resultant values of bulk properties such as the magnetisation can be calculated.

The Ising model is an abstraction of a ferromagnetic system rather than an idealization because it is not the case that by adding in more details the model would get more accurate. On the contrary, the Ising model would lose all of its power if it were more accurate. If more detail were added to the model, the key new variable, the order parameter, would be undefined.

2.4 Stability Conditions and Contexts

The extension to a new set of states and observables is abstraction in the sense characterized in the previous subsection. A higher-level algebra of observables does not approximate a more accurate lower-level algebra. These contextually-defined abstractions are never given by first principles of a lower-level or more fundamental theory or its domain.

Contexts, then, are those contingent conditions and features related to new states and observables, new structures and other aspects of target systems not given by lower levels or an underlying domain. In terms of descriptions, such conditions, states and observables represent the relevant features of the description of a target system at a particular level of description. To develop any description requires abstracting from or ignoring those details of a given system (and its environment) that are irrelevant. So one should not think of the stability conditions and states along with their associated algebra of observables of the higher-level descriptions as involving approximations and idealizations that deviate from the lowest-level description.

Some features irrelevant in one context may be relevant in another. For instance, temperature is relevant in thermodynamics but irrelevant in classical mechanics.

The shape of molecules is relevant in physical chemistry, but irrelevant in quantum mechanics descriptions using Schrödinger's equation focused on energy levels. Nevertheless, it is possible to implement contexts where temperature, relevant in thermodynamics, is relevant at the level of statistical mechanics (Sect. 4), or contexts where molecular shape, relevant in physical chemistry, is relevant at the level of quantum mechanics (Sect. 5).

Consider the case of higher-level descriptions. Here, there is a target system that provides the concrete context for the added necessary and sufficient conditions. Implementing a concrete context as a new algebra of observables respecting the stability conditions often requires using an asymptotic expansion: Specify a relevant reference state in the lower-level state space representing essential features of the particular target system, and expand it in terms of a perturbation parameter. Kubo–Martin–Schwinger (KMS) states in statistical mechanics or electronic ground states of a molecule in quantum chemistry would be examples of such reference states (see below). If the expansion is singular as the relevant parameter tends to some limit in the fine topology of the lower-level description simpliciter, then it is not uniformly convergent in the fine topology.

Such discontinuous limiting behavior indicates the need for a change of description because there is a change in the relevant states and observables due to stability conditions not given by the lower level. A new contextual topology that regularizes the asymptotic expansions that are singular with respect to the finer topology is needed. These expansions converge with respect to the new contextual topology (and thereby appear to be cases of reductions of class (1) to the undiscerning eye). In many cases, such regularization is possible by introducing a hierarchy of length and time scales into the description. One can then consider the motion of the system on the fast-time scales relative to almost fixed reference states corresponding to the slow time scales (e.g., [47]). The separation of time scales often leads to a partition into equivalence classes of states.[3] Nevertheless, the new algebra of observables is contingent in that it is neither given nor implied by any other elements of the lower-level description.

Contextual emergence describes cases where constraints, properties, structures, and so forth neither given nor implied by the lower level or underlying domain are at least as important as the first principles and properties of any lowest-level or "fundamental" domain. As such, it is a framework for emergence that not only relates different levels of description, but also relates properties in different levels and domains, the "ontological furniture" of states, observables, the conditions for their existence and persistence as well as the transitions necessary from lower levels or underlying domains to higher. Contexts are necessary for the transitions that manifest new properties, such as states and observables, and also for partly sustaining those properties, or even the systems possessing those properties.

[3] The coarser contextual topology is compatible with the original, finer topology if they and their dynamics are topologically equivalent with each other (Appendix A.3).

2.5 Possibility Spaces

Contexts, determined by stability conditions, large-scale constraints, symmetry breakings and regularities, are related to *possibility space*. The most basic laws of physics define what is physically possible in the world. Yet, not all of these possibilities are actualizable through the basic laws and particles of elementary particle physics by themselves. It is the specific, concrete contexts that make particular regions of possibility space accessible.

Think of contexts as specifying accessibility conditions for particular subspaces of the physical possibility space defined by the most elementary laws. Lasers illustrate this well. According to quantum mechanics, the amplification of stimulated emission of light from atoms, the key physical principle necessary for lasers to function, is physically possible. However, that portion of the possibility space is only accessible under specific contexts–appropriately engineered conditions of isolation and stability. Another example would be fluid convection [17]. The laws of fluid mechanics and dynamics define the possible states of motion of fluid molecules. Nonetheless, in the initial quiescent state of a Rayleigh-Bénard convection system, the fluid molecules cannot access any of the states of motion associated with convection cells. Yet, after the order parameter ΔT, the temperature difference between the upper and lower plates constraining the fluid, passes the critical value, many different convective states of motion are accessible, while the states of motion associated with the initial quiescent state are inaccessible. Stability conditions associated with the concrete contexts determine which of these possibility subspaces are accessible.

Thinking of contexts and possibility space also illustrates how acausal global constraints shape accessible physical possibilities. For instance, suppose spacetime has only one spatial dimension. Then, there could be no gravitational waves (and Newtonian gravity has constant magnitude between two bodies no matter their distance), and moving electrically charged particles could not radiate energy. When spacetime has two spatial dimensions, Einstein's equation in vacuum requires spacetime to be completely flat (i.e., both the Ricci and Riemann curvature tensors are zero) and gravitational waves still are not possible, while moving charged particles can radiate energy. In three spatial dimensions, gravitational waves become possible (for Einstein's equation in a vacuum, the Riemann curvature tensor can be nonzero even if the Ricci curvature tensor is zero). For a spacetime with four spatial dimensions, no stable gravitational orbits exist and the hydrogen atom under some conditions is unstable because its spectrum is unbounded from below. For five or more spatial dimensions no stable atoms can exist because the Coulomb potential dominates the $1/r^2$ centrifugal potential for small r close to the nucleus yielding an unbounded spectrum from below. Spatial dimensionality in all these cases constrains physical possibility in acausal ways. Dimensionality establishes a context into which fundamental laws must come to particular expression determining the range of possibilities these laws can delineate.

Nothing can happen outside of the most general space of possibilities delineated by the fundamental laws and dimensionality of the universe. This clarifies what fundamentality means: *Fundamental laws* are those that, along with the dimensionality of the universe, determine the total space of physical possibility. Anything lying

outside this possibility space is physically impossible. Nevertheless, these laws do not fully determine all the actual outcomes within this space of possibilities. That is the roll of concrete contexts. Returning to the laser example, although lasers are physically possible according to fundamental laws, actual lasers exist only in a particularly highly restricted subspace, where the actualization of possibilities in this subspace involves chemical, biological, psychological and embodied human possibility.

In summary, then, contextual emergence focuses on the conditions and transitions that make particular subspaces of possibility accessible or inaccessible. Concrete stability conditions include large-scale forms of constraint, both causal and acausal, as well as dynamically emerging changes in possibility ensuring particular subspaces of possibility are actualized. The detailed examples below demonstrate the kinds of conditions that make the existence of temperature and molecular shape possible, for example.

3 The Ontic/Epistemic Distinction and Algebras of Observables

Erhard Scheibe [49] first introduced the ontic/epistemic state distinction and it has been subsequently developed by others (e.g., [6, 24, 45, 46]). An *ontic state* refers to all properties of a system "the way it is" apart from any epistemic access or ignorance. Ontic states generally refer to individual descriptions with an important special case being the descriptions of point-particle states and observables in classical mechanics. In contrast, an *epistemic state* refers to the physical system's properties accessible through observation and pattern matching routines.[4] Epistemic states generally refer to statistical descriptions with an important special case being those states and observables describable in terms of probability distributions or density operators.

3.1 Algebras of Observables

The ontic or intrinsic properties of a physical system can be well-defined in a C^*-algebra (Appendix A.1) of *ontic observables* [29, 44]. C^*-algebras are equipped with a *strong norm topology* defining convergence and closure properties (Appendix A.2). Empirically accessible properties can be well-defined in a larger W^*-algebra of *epistemic observables* (there are many ways of observing the same entity). In the context of quantum mechanics, a W^*-algebra is a C*-algebra possessing a Hilbert space as a pre-dual, so it is isomorphic to a closed algebra of observables on a Hilbert space. More generally, a W^*-algebra is an abstract C^*-algebra, which is the dual

[4] On should not confuse human states of knowledge with epistemic states. Epistemic states describe those properties of systems that can be measured. Human knowledge describes what we know after a measurement has taken place.

of some Banach space.[5] This affords the definition of quantum expectation values as scalar products $\langle\psi|A|\psi\rangle$ (with A being an element of the W^*-algebra and ψ belonging to the Hilbert space), and defines a weak topology through a scalar product in Hilbert space (Appendix A.2).

A contextual topology can be defined in the following way. Given a C^*-algebra of ontic observables, many possible W^*-algebras of epistemic observables can be constructed that are unitarily inequivalent to each other. Such a construction can be carried out by applying the Gel'fand-Naimark-Segal (GNS) theorem [29, 44] from a suitably chosen reference state taken from the dual of the C^*-algebra which is the state space of the system. This reference state defines a particular restrictive context and, through the GNS constructed-W^*-algebra, an associated contextual topology (Sect. 2.3). An example would be the Kubo-Martin-Schwinger states serving as reference states for a GNS construction of a W^*-algebra containing temperature as an observable (Sect. 4).

3.2 Quantum and Classical Algebras

Algebras of observables can be distinguished as follows. A *quantum algebra* of observables will be noncommutative. In contrast, a *classical algebra* of observables is commutative, where every observable commutes with all other observables in the algebra. Finally, there is the *mixed case*, a quantum/classical algebra of observables, which has a nontrivial center. In this context, this means there is also a set of commuting or classical observables in the algebra. In algebraic approaches, conceptually the distinction between commuting and noncommuting observables is the core of the classical/quantum observable distinction rather than classical vs. quantum physics. For a quantum system the C^*-algebra does not contain observables that commute with every other observable (except the identity); it has a trivial center only. Similarly for a quantum W^*-algebra. These algebras, therefore, describe quantum systems with a non-Boolean propositional calculus.

There are some subtleties to the commuting/noncommuting distinction. For instance, it can be shown under very general conditions that chaotic nonlinear dynamical systems have some noncommuting observables, and these observables can be found in classical statistical mechanics systems [39, 40]. On the other hand, the Hamiltonian operator in quantum mechanics often commutes with a number of quantum observables, but is not considered to be a proper observable of classical physics. Nor are quantum Hamiltonians found in the center of the respective algebra. So, a particular observable may have particular commutation properties, but not be classified as a quantum or classical observable based on its peculiarities. Nonetheless, it is always the case that quantum observables will not be found in a classical algebra of observables nor in the nontrivial center

[5] This is to say that a C^*-algebra, $\mathcal{A}$, is a W^*-algebra if there exists a Banach space $\mathcal{A}_*$ such that $(\mathcal{A}_*)^* = \mathcal{A}$, where $(\mathcal{A}_*)^*$is the dual Banach space of $\mathcal{A}_*$. The Banach space $\mathcal{A}_*$ is the predual of $\mathcal{A}$. An important example of a commutative W*-algebra is the Banach space L_∞ where the predual space is the separable Banach space L_1.

of a quantum/classical algebra. In the special case where all the properties of a system are identical to the observables in the center of an algebra, that system can be classified as classical since all its properties are identified with classical observables.

Lastly, as is well known, for any nontrivial operator A defined on a Hilbert space $\mathcal{H}$, there exists a state vector $\psi \subseteq \mathcal{H}$ such that $\langle\psi|A|\psi\rangle$ is not dispersion free (i.e., $\langle\psi|A^2|\psi\rangle \neq \langle\psi|A|\psi\rangle^2$) [54]. Quantum mechanics allows all bounded operators on $\mathcal{H}$, so contains no dispersion-free, or classical observables.

3.2.1 Classical Algebras

A classical algebra is equal to its center; hence, all observables commute and are described by a Boolean propositional calculus. Classical mechanics is an example where the algebra of observables is commutative. For a C^*-algebra $\mathcal{A}$, a dispersion-free state on $\mathcal{A}$ is a one-dimensional representation of $\mathcal{A}$, so every dispersion-free state is a pure state. Moreover, if every pure state on a W*-algebra is dispersion-free, then this algebra is commutative. The ontic states of of every classical system are dispersion-free, so every pure state on such a W*-algebra of observables is a possible ontic state of the system.

This means that there can be an interleaving of levels of description: The dispersion-free states of a W^*-algebra at one level of description can serve as the ontic states that can be related to epistemic states at a higher level of description in a relation of relative onticity [9]. It is always possible to represent any classical system by a commutative W^*-algebra of observables.

3.2.2 Quantum/Classical Algebras

A W^*-algebra may contain a center of commuting—and therefore classical—observables, and, hence, be a mixed quantum/classical algebra. Observables in the center of a quantum/classical algebra will be dispersion-free and their time evolution defines a classical dynamical system.

The existence of classical observables in an algebra $\mathcal{A}$ has an important consequence if it is a *-algebra defined on $\mathcal{H}$. The space is split into sectors separated by a superselection rule. The sectors are indexed by the possible dispersion-free values of the classical observables. The superselection rule implies that all transition probabilities $|\langle\Psi_j|A|\Psi_k\rangle|^2$ for $\Psi_j \subseteq \mathcal{H}_j$, $\Psi_k \subseteq \mathcal{H}_k$, when $\mathcal{H}_j$ and $\mathcal{H}_k$ are different sectors, vanish for all $A \subseteq \mathcal{A}$. Hence, the normalized state vector $\Psi = c_1\Psi_j + c_2\Psi_k$, c_1, $c_2 \subseteq \mathbb{C}$ is a mixture rather than a pure state. Coherent superpositions across sectors are forbidden. For example, Ψ cannot be a superposition of chiral states of a single molecule (Sect. 5). This fact implies classical observables restrict the validity of the principle of superposition for quantum state vectors.

Finally, one also can use a Hilbert space formulation of classical physics [32, 33] to pursue a unified mathematical framework for quantum and classical mechanics.

3.3 Algebras and Dynamics

For a classical W^*-algebra, the dynamics is given by a semigroup of positive, identity-preserving normal maps of the algebra of observables into itself. In the case of general W^*-algebras, the dynamics is given by completely positive maps. The homomorphisms and the one-norm projections represent important classes of completely positive maps. Every positive linear map on a commutative C^*-algebra is completely positive.

The importance of complete positivity can be seen from the following. Consider two non-interacting systems, where the algebra of observables is given by the W^*-tensor product $\mathcal{A}_1 \bar{\otimes} \mathcal{A}_2$. The tensor product of two linear maps is not guaranteed to be positive, whereas the tensor product of completely positive maps is a completely positive map. To summarize, a dynamical semigroup $\{\alpha_t | t \geqslant 0\}$ on an arbitrary W^*-algebra is a weakly continuous one-parameter completely positive, identity-preserving normal map of $\mathcal{A}$ into itself. Time evolution in the Heisenberg picture is given by dynamical semigroups $\alpha_t : \mathcal{A} \to \mathcal{A}$, while time evolution in the Schrödinger picture is given by the pre-adjoint semigroup $\alpha_{*_t} : \mathcal{A}_* \to \mathcal{A}_*$.[6] For the dynamics to be invertible, α_t is required to be a *-automorphism.

This is the algebraic machinery for dynamics. In the context of quantum mechanics, it corresponds to the usual textbook dynamics, where $\hat{U}(t_1, t_2)$ is a completely positive unitary operator defined by the evolution equation

$$i\hbar \frac{d}{dt} |\Psi_t\rangle = \hat{H} |\Psi_t\rangle. \tag{1}$$

In contrast to classical systems, (1) is insufficient to describe the complete evolution of a quantum system due to the fact that $|\Psi_t\rangle$ is a linear superposition of states. In a measurement, only a specific eigenvalue–a definite classical outcome–is observed rather than a superposition. This is the measurement problem in quantum mechanics, which we briefly comment on in Sect. 6.2.

4 Temperature as a Contextually Emergent Property

Temperature is an example of a thermodynamic property that often is discussed both in physics and philosophy literatures as a "textbook case" of reduction. Temperature is usually glossed as the mean motion of molecules in a gas or liquid. Work in algebraic statistical mechanics shows that the relationship of temperature to the motion of molecules is more complex than this.

[6] Dynamics on the dual $\mathcal{A}^*$ is also well-defined, but the time evolution of non-normal states are not guaranteed to have desirable continuity properties.

4.1 Two Transitions

Temperature actually arises as the result of two transitions, one from the domain of particle mechanics to that of statistical mechanics, and the other from the latter domain to that of thermodynamics. The first transition involves the formation of ensembles of particles, where system properties are defined in terms of ensembles. Typically this is represented as statistical moments of a many-particle distribution function. There is a transition from individual particle states to ensembles as the physically relevant states. An example would be the mean kinetic energy of a system of N particles calculated from the distribution of the momenta of all particles. Assuming the applicability of limit theorems, such as the law of large numbers, the expectation value of kinetic energy is defined through the limit of infinitely many particles. Any expectation value of a thermodynamic property whose definition is based on a statistical ensemble presupposes (infinitely) many degrees of freedom in the form of thermodynamic or other continuum limits [22]. In turn equivalence classes of the particles having the same properties are defined in the chosen limit.

Textbooks typically gloss the thermodynamic limit as a limit where the volume V of a system is allowed to increase without bounds, $V \rightarrow \infty$, while keeping constant the ratio of V/N. In addition, the condition that E/N remains constant, where E is the total energy, must be added for the microcanonical ensemble, or that the temperature remains constant for the canonical ensemble, or that the chemical potential and temperature remain constant for the grand canonical ensemble. The thermodynamic limit is equivalent to a scale transformation, where all dimensions of the system increase by some indefinite factor, and all thermodynamic properties are recovered in this limit.

As an alternative, Ludwig Boltzmann proposed "*a definite limit when the number of the particles is made ever larger and their size ever smaller. We can then assert of these properties that they belong to the continuum and this in my view is the only non-contradictory definition of a continuum endowed with certain properties*" [38]. This is a continuum limit that reverses the scale transformation: The size of the particles decrease without limit (in contrast to letting V increase without limit) while $N \rightarrow \infty$. Properties of the system as a whole, such as V, total mass Nm, total energy, total entropy, temperature and system chemical potential $N\mu$, where μ is the chemical potential of the particles, remain constant or attain an asymptotic value [22]. In this continuum limit, all microscopic and intensive quantities vanish, while all macroscopic and extensive quantities are at least asymptotically constant as one would expect for actual-world systems. Continuum limits correspond to a change of scale, where a similarity transformation acts on the particles. In contrast, thermodynamic limits re-scale system size. The important point is that thermodynamic and continuum limits share a common feature of mathematically indicating a physical transition from individual particle states and observables to ensemble states and observables with distinguished equivalence classes.

The second transition is from the statistical mechanics domain to thermodynamics. Temperature presupposes thermodynamic equilibrium, a special stable state based on the zeroth law of thermodynamics: Two systems in thermodynamic equilibrium with a third system at time t are in thermodynamic equilibrium with each

other at t. Thermodynamic properties, such as temperature and chemical potential, are uniform and unchanging throughout the system. Therefore, if two systems are in thermodynamic equilibrium, they are at the same temperature.

While thermodynamic equilibrium is central to the definition of temperature in thermodynamics, such equilibrium is neither formally nor conceptually available in the domain of statistical mechanics. In the latter there are always fluctuations, so there are no uniform, unchanging properties as in thermodynamic equilibrium. Moreover, the very concept of temperature is absent from the statistical mechanics domain simpliciter (in textbooks it is usually introduced through some form of phenomenological argument). Not only is thermodynamic equilibrium not definable for statistical mechanics simpliciter, temperature cannot be a mechanical property, contrary to the usual picture communicated in textbooks (see Sect. 4.3).

4.2 The Contextual Origin of Temperature

Temperature contextually emerges as a novel thermodynamic property. Thermodynamic equilibrium is a context providing stability conditions for the existence of temperature. Thermodynamic equilibrium as a stability condition implies a distinguished set of equivalence classes, namely all ensemble classes consistent with such stability.

For temperature, the thermodynamic stability conditions are physically implemented through the KMS condition leading to a set of equivalence classes of statistical states with very special properties, the so-called KMS states. These states are a generalization of Gibbs states that possess remarkable stability properties (Sect. A.4). Physically, the KMS condition is a stability condition guaranteeing the existence and persistence of KMS states stable against local perturbations. These states have temperature as a well-defined classical observable.

Some of the stability properties of the KMS condition are [28][7]:

(1) *Local thermodynamic stability* Fluctuations of KMS states confined to bounded regions of space cannot increase the system's free energy.
(2) *Global thermodynamic stability* KMS states that are translation invariant do not raise the spatial density of the free energy.
(3) *Local dynamical stability* Arbitrarily small local perturbations of the system dynamics admit stationary states that are arbitrarily close to KMS states.
(4) *Passivity* If a system is initially in a KMS state, no local perturbations applied over any finite time interval to the dynamics can result in energy being extracted from the system.
(5) *Reservoir stability* Any system in a KMS state can serve as a thermal reservoir when weakly coupled to a finite system.

[7] While what follows is based on results from quantum statistical mechanics, since the end result always leads to a quantum/classical algebra (Sect. 3.2.2) with temperature as a classical observable, it makes no difference to the case for contextual emergence whether one discusses classical or quantum statistical mechanics.

The KMS states originally were derived for infinite systems [30, 35, 37]. Later, Haag et al. [31] gave a rigorous derivation for finite systems based on three physically reasonable stability conditions for equilibrium states, which avoid some continuum limits:

(1) *Stationarity* Expectation values of observables do not change over time.
(2) *Stability* The dynamics such states participate in is stable against perturbations.
(3) *Asymptotic abelianness* Correlations between local quantities at different times vanish sufficiently fast as the time differences go to infinity.

Any equilibrium states will meet the first condition. The second condition reflects stability under arbitrarily small perturbations; namely, such states are always given by density matrices that are functions of the system Hamiltonian. The third condition ensures there are no fluctuations in intensive system variables and implies that temporally distinct observables eventually become compatible. These are the same conditions that will lead to thermodynamic equilibrium. Taken together, this represents a thermodynamic stability condition that picks out an equivalence class of relevant states. We regard this step from infinite to finite systems as conceptually important, as infinite systems do not exist in physical reality [27].

An important point to notice is that, as with conservation laws, the conditions underlying KMS states are neither quantum, nor classical. Rather, they are global or universal stability conditions implying that as soon as objects arise in the universe fulfilling these conditions, KMS states emerge along with temperature as an observable. So, for instance, as soon as there are quarks fulfilling these conditions–if these are the first particles–KMS states emerge with temperature as an observable.

Physically, the thermodynamic stability condition implements the contextual contingent stability conditions of thermodynamics in the statistical mechanics domain. For example, the second law of thermodynamics implements this stability condition in terms of maximization of entropy [28]. When a system is in a KMS state it is in the canonical Gibbs state, uniquely defining a parameter whose natural interpretation is (inverse) temperature. In the framework of algebraic statistical mechanics, KMS states serve as reference states for a GNS construction. Mathematically, these reference states are functionals defined on the algebra of observables of the statistical mechanics domain through a new contextual topology, which is coarser than the original topology. The stability condition gives rise to a new algebra of observables including temperature as a property of the system. Takesaki [52] demonstrated how temperature must be a classical observable, rather than an element in the underlying quantum statistical algebra of observables.

4.3 A Contextually Emergent Property

Temperature is an element of an algebra $\mathfrak{M}$ of contextual observables. Mechanical descriptions are given by type I W^*-algebras, while the contextual W^*-algebra $\mathfrak{M}$ is of type III (Appendix A.1). This means temperature cannot be an element of a mechanical description, implying the underlying statistical mechanics domain does

not reduce temperature to molecular motion in any straightforward sense. In contrast to several textbook claims, thermodynamics is not simply a coarse-grained description of statistical mechanics. Moreover, KMS states have the remarkable property that different temperatures are disjoint [52], a property also inconsistent with mechanical states underlying the ensembles of statistical mechanics. Finally, KMS states of different temperatures fall into different superselection sectors. This means that temperature is a dispersion-free, i.e., classical, observable. So supposing the quark-gluon plasma is the first object that achieves the KMS condition, it would have both quantum and classical observables at one of the earliest stages of the universe's development.

Temperature, then, is an example of a contextually emergent property neither contained in nor derivable from the laws and properties of the underlying mechanical and statistical mechanics domains simpliciter. Hence, the need for the two transitions discussed above. Distribution states determined by the thermodynamic stability condition are required for the existence of thermodynamic states and properties. The KMS states are not implied by the laws and properties of the statistical mechanics domain; rather, they result from the noncausal global stability constraints. When crucial contextual details are made explicit, thermodynamic properties can be seen acting as constraints for the mechanical properties of particles.

5 Chemical Potentials and Chirality as Contextually Emergent Properties

The case is similar for chemical potentials and molecular structure.

5.1 Chemical Potentials

Chemical potential as a contextually emergent property follows from the KMS states for specific constituents. They require a transition from an ensemble of molecules (statistical mechanics domain) to a rich context for such ensembles (chemical thermodynamics domain). Araki et al. [4] and Müller-Herold [41] have shown that this transition is nontrivial. The stability condition of thermodynamic equilibrium must be implemented through KMS states parameterized by temperature. These KMS states are disjoint for different chemical potentials meaning that states with different chemical potentials fall into different superselection sectors. Hence, chemical potential also is a dispersion-free or classical observable.

5.2 The Problem of Molecular Structure

The chemical structure of molecules is another example of contextual emergence. Although the role of contexts in quantum mechanics is familiar as the differences between single and double-slit experiments illustrate with wave-particle duality, the role of contexts in the emergence of molecular structure often goes unacknowledged.

To begin, we should always keep in mind that there is no such thing as an isolated molecule–all molecules are always coupled to the radiation field of the environment. Furthermore, chemists always deal with molecules having environmentally-determined aspects of structure, such as chirality in amino acids or drugs such as thalidomide.

Chiral molecules have structures that are not superposable as mirror images. For instance, (R)-bromochlorofluoromethane is not superposable on (S)-bromochlorofluoromethane. According to quantum mechanics, the superposition state for properly chiral molecules, $\Psi_0 = \frac{1}{\sqrt{2}}(\Psi_R + \Psi_S)$, should exist as a totally symmetric pure ground state, but is never encountered in laboratories. The reason for this absence is that when the coupling to the radiation field is taken into account, the chiral state vectors Ψ_R and Ψ_S exist in two different selection sectors, implying their structure is a classical (i.e., dispersion-free) observable. The chirality of DNA is a biologically important example of structure as a classical observable.[8]

For improperly "chiral" molecules, things are more subtle. Consider an ammonia molecule interacting with nothing other than its environment. It has two distinct pyramidal forms, Ψ_L and Ψ_R. The superpositions $\Psi_+ = \frac{1}{\sqrt{2}}(\Psi_L + \Psi_R)$ and $\Psi_- = \frac{1}{\sqrt{2}}(\Psi_L - \Psi_R)$ are the proper ground state and first excited state, respectively. Both Ψ_+ and Ψ_- are eigenstates of the molecular Hamiltonian, and are stationary states of the time-dependent Schrödinger equation. But, neither eigenstate has a nuclear frame, therefore neither has a molecular structure. On the other hand, Ψ_L and Ψ_R can be written as the superpositions $\Psi_L = \frac{1}{\sqrt{2}}(\Psi_+ + \Psi_-)$ and $\Psi_R = \frac{1}{\sqrt{2}}(\Psi_+ - \Psi_-)$. The latter two superpositions are nonstationary states of the time-dependent Schrödinger equation. The two sets of superposition states reflect a tunneling process which transforms Ψ_L into Ψ_R and vice-versa. This implies that such a non-interacting ammonia molecule has no nuclear frame.

Without a well-defined nuclear frame, there is no molecular structure since there is no fixed position for nuclei relative to electrons. A key reason for this lack of molecular shape is that according to quantum mechanics molecules are always entangled: nuclei with electrons as well as molecules being entangled with their environment (e.g., other molecules, electromagnetic and gravitational fields) unless these entanglements are suppressed or broken. There is no such thing as a single molecule as an individual system since the interaction with the electromagnetic field yields a molecule + field system (so-called dressed states). Interactions with electromagnetic and gravitational fields can never be decoupled from molecules though these interactions can be partially screened.

Even considering an isolated molecule, quantum entanglement among nuclei and electrons implies that there are no separate nuclei and electrons as individual subsystems that could take on the kinds of spatial relationships needed for molecular

[8] The knot-type of DNA is also dispersion-free, hence, is a classical observable that has actual-world consequences (e.g., [36]).

shape. Therefore, considering quantum mechanics simpliciter there are no states or observables for molecular shape apart from concrete contexts.

5.3 The Importance of Molecular Shape

On the other hand, many chemical properties depend crucially on molecular shape, and such structure plays important roles in chemistry and biology. Consider 2-butene. It is a stereoisomer, meaning its two forms have the same chemical formula, yet different spatial orientations. These orientations cannot be related by translation or rotational transformations between the isomers. The cis and trans forms have different properties (e.g., different boiling points and densities). Perhaps the most famous example is DNA which has left-handed chiral symmetry, and the most tragic example is thalidomide which originally was not known to have two complementary chiralities until it was discovered in the 1960s that one species of handedness was harmful while the other was beneficial in thalidomide-based treatments.

These are examples of what are known as chemical isomers–molecules having identical chemical formulas, but different chemical properties due to their differing structural arrangements. An oft-discussed example is C_3H_4, which is the formula for three distinct chemical compounds: allene, cyclopropene, and methyl acetylene. There is no first-principles quantum Hamiltonian for C_3H_4 capable of distinguishing these three isomers. In general, no chemical isomers can be distinguished quantum mechanically because the first-principles or context-free quantum Hamiltonian only accounts for the total number of nucleons and electrons and their Coulomb forces. There are no specific spatial arrangements in the Hamiltonian because the electrons and nuclei are in entangled states. This can be seen from the fact that there are no shape observables in the first-principles quantum algebra of observables (see below).

Even taking the inter-particle distances and using the symmetric sum over them to produce an observable that is represented by a self-adjoint operator on the Hilbert space of functions fails to define molecular structure. For instance, in the case of C_8H_8 the expectation values of these spatial observables imply that all the carbon-hydrogen inter-particle distances are the same on average, so no structural interpretation can be given. The only self-adjoint quantum observable that can be formed in first-principles quantum mechanics corresponding to classical observables associated with molecular structure yields results consistent with there being no molecular structure. Attempts involving charge density functions fare no better at yielding molecular structure [51].

Along with these problems, context-free first-principles quantum Hamiltonians also would have too many of the nuclear permutation and rotational symmetries, along with spherical and inversion symmetries, missing from actual-world molecules. There are many reasons, then, for the fact that the context-free quantum domain lacks molecular structure and, thus, provides no basis for distinguishing isomers or explaining optical activity, or other phenomena dependent on molecular shape. The algebras of observables for quantum mechanics and quantum chemistry indicate that shape observables are always classical rather than quantum observables [44]. The observables characterizing molecular structure are commutative, and the

algebra of observables of quantum chemistry turns out to be a quantum/classical algebra with a nontrivial center (Sect. 3.2.2). More than the context-free laws and properties of quantum mechanics are needed for the emergence of states and observables for molecular structure.

5.4 Ontological Emergence of Molecular Structure

Although molecular shape was proposed in the mid-nineteenth century, it first was made precise by Born and Oppenheimer through the Born-Oppenheimer "approximation" [20]. The scare quotes indicate that this is a mischaracterization of what is going on in the Born-Oppenheimer procedure. Molecular models, such as the Born-Oppenheimer procedure, often actually refer to new states and observables (recall the idealization vs. abstraction discussion in Sect. 2.3). The basic idea is to follow the physical implications of the nucleus being very much more massive than the electron mass, and treat the nucleus as if it is (almost) stationary with respect to electronic motions. This corresponds to an asymptotic series expansion in powers of the parameter $\epsilon = (m_e/m_n)^{1/4}$, where m_e and m_n are the electron and nuclear masses, respectively. As m_n becomes indefinitely large with respect to the electron mass, $\epsilon \to 0$.

Slightly more accurate results can be achieved with other adiabatic procedures, where the electrons are considered to move much faster than the heavier nuclear frame of a molecule. All of these adiabatic procedures are ways of implementing the fixed or clamped-nucleus assumption, the only assumption under which the singular limits involved can be regularized. Interestingly, the clamped nucleus assumption is the only one that leads to self-adjoint Hamiltonians for quantum chemistry [51]. This represents a context where:

(1) Nuclear and electronic motions are distinguished, so entanglements between the nucleus and electrons are broken.
(2) Nuclear permutation, rotational and translational symmetries of the underlying quantum domain are broken.
(3) Electrons in molecules are distinguishable.

These are properties actual-world molecules have that are not found in the underlying first-principles quantum domain [2, 14, 19, 44]. They correspond to P.W. Anderson's key comment that emergence of new properties is associated with broken symmetries [3].

The regularization of such limits tracks with ontological changes that occur, such as the broken entanglements among nuclei and electrons and broken symmetries, leading to distinguishable particles and, in particular, new states and observables. The clamped nuclei assumption represents the stability condition distinguishing nuclear and electronic frames that is implemented in the quantum chemistry context via a new contextual topology containing the relevant states and observables missing from the underlying quantum domain. Furthermore, this stability condition induces nuclear and atomic orbital equivalence classes [34], which play important

roles in nuclear magnetic resonance and electron spin resonance spectroscopy (e.g., [10, 11]). There are new observables corresponding to molecular shape, while states corresponding to individual atoms vanish and are replaced by states corresponding to molecules.

It is worth repeating that the clamped nuclei assumption is not merely an idealization (Sect. 2.3). Physically, it relates to a stability condition, where the electrons and nuclear motions are distinguished (breaking of entanglements and symmetries), with electronic motions taking place against the background of a relatively slow moving nuclear frame that provides physical conditions for the existence of states and classical (commuting) observables absent from the underlying quantum domain.

5.5 The Associated Algebras

This is indicated by the quantum/classical algebra of observables of quantum chemistry. In the underlying quantum domain, the position and momentum observables do not commute, and the nucleons and electrons have no definite positions or momenta. Actual-world molecules, in contrast, are coherent objects maintaining very sharp positions and momenta with semi-rigid structures. These properties are used in chemical experiments, drug research, and so forth on a daily basis. A transition has occurred in the character of the position and momentum observables in the algebra of observables that our adiabatic procedures try to capture. The algebra of observables changes from a noncommutative algebra with a trivial center to a noncommutative algebra with a nontrivial center. Corresponding to this is a transition in the dynamics of the system where a Boolean logic emerges in the center of the algebra of observables.

Consider the context-free quantum mechanical Hamiltonian for molecules and examine the equations of motion for the electrons and nuclei. This algebra of observables forms a W^*-algebra given by a tensor product of the electronic and nuclear observables, $A = A_n \otimes A_e$, where A_n and A_e are both factors of type I (technically I_∞). The position and momentum operators of the electrons are the generators of A_e, while the canonical position and momentum operators of the nuclei are the generators for A_n. Time evolution, then, is given by the equations of motion for these two sets of canonical observables. Note that for $t > 0$, the electrons are not a dynamical system autonomous from the nuclei when only considering context-free first-principles quantum mechanics.

Under the clamped nuclei assumption, the algebra A contracts to $A_e \otimes \mathfrak{N}$, where A_e is still of type I describing the degrees of freedom of the electrons, but $\mathfrak{N}$ is a commutative W^*-algebra describing the molecular structure and motions of the nuclei. The algebras of observables describing the electronic and nuclear motions is factorizeable indicating the quantum entanglement between nuclei and electrons is broken in this limit. This is reflected in the equations of motion as the electronic observables now form a distinguished system. The electronic motions are entrained by the motion of the nuclear frame.

This is the transition where the quantum entanglements between nuclei and electrons are broken, several nuclear symmetries are broken, nuclear and atomic orbital

equivalence classes are distinguished, and new, classical states and observables for nuclear motion and molecular shape arise. The algebra $A_e \otimes \mathfrak{N}$ is a mixed quantum-classical algebra (Sect. 3.2.2). A classical control variable now appears in the electronic Hamiltonian. The nuclei form a classical stochastic system with classical observables in the center of A. The nuclei behave approximately like Newtonian point particles, but there are at least two correction factors to consider. First, there is an often small stochastic feedback from the electrons. Second, there is the remaining quantum nature of the nuclei, where the classical position and momentum observables fulfil a stochastic version of Heisenberg's inequality. The fluctuations represented in these relations are much more rapid than the collective translational, vibrational and rotational motions of the nuclei. Furthermore, the mean distribution of these stochastic trajectories corresponds to the trajectories of the nuclei given by the quantum observables in A_n.

5.6 Transition of the Algebra

The important point is that the original quantum algebra of observables in the underlying, formerly context-free quantum domain has undergone a transition to now include observables corresponding to molecular shape. This is the impact of the stability condition represented in the clamped nuclei situation. Although these observables do not exist in the underlying quantum domain simpliciter–the underlying algebra contains no such observables–in relevant contexts, these classical observables emerge, and have the properties chemists study. The context-free quantum domain provides a necessary part of the total set of conditions necessary and sufficient for molecular structure. However, it is the concrete context provided by the stability condition in an environment that gives rise to the remaining necessary and sufficient conditions for the states and observables relevant for molecular shape. Molecular structure is a contextual feature of the actual world.

Of course, the environment in which molecules exist plays a key role in such coherence and localization–environmental decoherence–but care is needed in understanding precisely what this claim means. The environment involves heat baths with properties such as temperature and chemical potential, which themselves are contextually emergent properties (Sect. 4), so decoherence presupposes a richer context than just the underlying quantum domain. For instance, this environment already has the KMS stability condition in place, hence temperature is a contextually emergent dispersion-free observable with KMS states of different temperatures in different superselection sectors. The KMS condition acts like a global acausal constraint for the formation of chemical molecules. More importantly, the electromagnetic field in quantum electrodynamics has uncountably many superselection sectors (e.g., [21]), meaning that molecules are always interacting with classical states in the environment. This is the context that leads to the emergence of the classical states and observables associated with molecular shape. Decoherence itself is an example of contextual emergence when the details are considered (for more discussion, see [18], Sect. 6.2.1).

6 Discussion

Contextual emergence is a framework that makes explicit what is often left implicit in inter-level/inter-domain relations. The concrete examples of temperature and molecular structure illustrate how stability conditions relevant to concrete contexts play crucial roles in the emergence of physical phenomena, where particular equivalence classes are distinguished. Contextual topologies express the new information needed for understanding the relationship between lower-levels/underlying domains that are relatively context-free, and higher-level context-rich phenomena, where there are transitions between the relevant algebras of observables. Contextual emergence reveals that the physical world is more subtle than the reductionistic impressions based on "fundamental physics" that have been popularized [5, 18, 55].

6.1 Possibilities and Constraints

Contextual emergence clarifies how to think about fundamentality in physics. The oversimplified view is that elementary particles and forces sit at the bottom of a hierarchy as the most fundamental elements of reality "governing" everything that transpires in the sense of making everything else happen in the universe. According to this metaphor, our writing and your reading of this text are just the complex outworkings of elementary particles in response to elementary forces. In contrast, contextual emergence indicates we should not think in terms of governance but in terms of possibility and constraint. What the most elementary or underlying particles and forces contribute are the necessary conditions defining the space of physical possibility. What is required for the actualization of specific possibilities are stability conditions characterizing concrete contexts (e.g., dimensionality of space, KMS condition for temperature, clamped nuclei–separation of nuclear and electronic frames and the entrainment of the latter by the former–for molecular structure).

Contexts are as fundamental as the elementary particles and forces because even the "most fundamental" laws always have to come to expression in, and are conditioned by, concrete contexts [7, 15, 18, 26]. First principles are "fundamental" in the sense of being universal: they establish the space of physical possibility holding for all of reality, but do not determine all of what happens in reality. Concrete contexts are restrictions under various kinds of constraints that lead to actual phenomena and events, and as such are just as important for the existence and behavior of physical phenomena as the first principles.[9]

[9] This implies that any talk of a universal wavefunction as a fundamental entity is incoherent if anything more is meant than the basic fact that quantum mechanics contributes necessary conditions defining the space of physical possibility [18, Sect. 6.3]. Any wavefunctions are already coming to expression in some concrete context. What is more, as noted above, any physical environment already has classical thermal and electromagnetic states.

6.2 Extended Applications

Contextual emergence can also shed light on the measurement problem though this problem is dependent on the quantum theory in question. For example, taking von Neuman's projection postulate seriously as well as the details of quantum measurements in concrete contexts (e.g., that the environment within which any experiment takes place always contains classical states interacting with quantum systems, and the specifics of the measurement apparatus such as a Geiger counter), any theory treating the wave function as ontically real involves an irreducible classical context that is sufficient to produce the measurement outcome in interaction with the quantum system. The classical structure of the measurement device (e.g., structure of atoms, macroscopic properties, nature of the internal heat bath) acts as a stability condition for a reliable transition from the quantum system's superposition state to a particular eigenvalue and subsequent amplification of this outcome. Hence, any measurement outcome for a quantum system is the result of a top-down (classical-to-quantum) constraint [25, 18, Sects. 6.2–6.3]. The interaction between quantum system and measurement apparatus is not describable by entanglement because of the presence of ineliminable classical thermal and electromagnetic states (one of the details missing from typical decoherence accounts). Therefore, any measurement of a quantum system always involves a crucial classical contextual constraint leading to the particular eigenprojection of the wavefunction. Moreover, models for the quantum-measurement system in concrete contexts always involve quantum/classical algebras of observables.

Beyond foundations of physics, contextual emergence as a framework has also been applied to cognitive science and neuroscience [1, 8, 13]. For instance, the Hodgkin-Huxley equations describing the generation and propagation of action potentials involve the electric conductance transmembrane currents, and the kinetics of sodium and potassium ion channel openings. The lower-level ion channels are macro-molecular quantum objects that would be in an entangled state of electrons and nuclei as described in the previous section, where the molecular structure necessary for pores to be in open or closed states is contextually emergent. In turn, the fluctuations of ion channels are stochastic and the Hodgkin-Huxley equations describe a contextually-emergent stochastic dynamics [13]. At a higher level, the contextual emergence of mental states from neural states can be described in this framework [1, 8].

The breadth of applicability of contextual emergence as a framework along with the clarification of fundamentality implies there is an intricate interleaving of levels, where both "bottom-up" causes and "top-down" constraints are involved. For example, quantum mechanics provides some necessary laws and properties for the existence of properties such as molecular structure, while the clamped-nuclei stability condition provides the remaining necessary and sufficient conditions for molecular structure. In turn, the laws and properties of chemistry provide some necessary laws and properties for the existence and behavior of biomolecules and biological organisms, while stability conditions at the levels of biochemistry and biology provide the remaining necessary and sufficient conditions for the existence and behavior of biomolecules.

Put another way, quantum mechanics provides a broad physical possibility space within which chemical phenomena can emerge, but concrete chemical contexts determine the subspace of chemical possibilities and its accessibility. In turn, the subspace of these chemical possibilities provides the possibility space within which biochemical phenomena can emerge, but concrete biochemical contexts determine the subspace of biochemical possibilities and its accessibility. Similarly, the subspace of these biochemical possibilities provides the possibility space within which biological phenomena can emerge, but concrete biological contexts determine the subspace of biological possibilities and its accessibility.

So there are interleaving ontological relations among the different possibility spaces and their differing accessibility all within the basic physical space of possibilities. And this is why there are interleaving patterns of descriptions across the sciences. Interleaving of descriptions is well illustrated by fields such as biophysics and biochemistry. The ineliminable role of contexts is made explicit in contextual emergence making clear what has always been present in physics and other sciences, but has often been taken for granted or underestimated in its importance.

Useful extensions of this work could develop the relation between the topologies that characterize contextual emergence, their associated equivalence classes of states, and the accessibility relations for the different possibility subspaces defined by concrete contexts (e.g., accessibility conditions for the transition from chemistry to biochemistry). As well there is much to be explored regarding how the framework of contextual emergence can provide a unified view of the sciences while respecting the particularities of the different domains and disciplines.

Finally, we note that there are deep connections between contextual emergence and renormalization group approaches. This is being explored in other publications.

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Appendices

The Appendices cover *-Algebras (Appendix A.1), Strong/Weak Topologies (Appendix A.2), and Structural Stability and the Topological Equivalence of Dynamical Systems (Appendix A.3). The final Appendix defines KMS states (Appendix A.4).

A.1: *-Algebras

A *-algebra admits an involution $^* : \mathcal{A} \rightarrow \mathcal{A}$ with the usual properties. A *-algebra is normed, if there is a mapping $||.|| : \mathcal{A} \rightarrow \mathbf{R}_+$ with the usual properties. A complete normed *-algebra is a Banach *-algebra. A C^*-algebra is a Banach *-algebra $\mathcal{A}$ with the additional property $||x^*x|| = ||x||^2$ for all $x \in \mathcal{A}$ [53, chap. I.1]. The associated concept of a state is introduced in terms of positive normalized linear functionals defined over $\mathcal{A}$. For a fundamental theory in physics, the state space is chosen such that only the most basic assumptions are required for its definition.

Algebras can be classified by their central decompositions or factors. A factor is of type I if it contains an atom.[10] It is of type II if it is atom-free and contains some nonzero finite projection. It is of type III if it does not contain any nonzero finite projection [53, p.296]. Every factor of type I has normal pure states, though for type I_∞ not all pure states are normal. Factors of types II and III lack normal pure states. For the example of statistical mechanics/thermodynamics, mechanical observables used to develop statistical ensembles and their expectation values reside in a type I W^*-algebra, while the contextual W^*-algebra defined through the KMS condition is of type III, meaning temperature cannot be reducible to statistical mechanics in any straightforward sense (Sect. 4).

The center of an algebra contains elements that commute with the rest of the elements in the center. A center is trivial when these elements are simply multiples of the identity operator.

A.2: Strong/Weak Topologies

Algebras of observables are related to the topologies of the state spaces over which they are defined. Topologies define the convergence properties for a sequence of elements in a space, and can be characterized as strong/fine or weak/coarse. For instance, in a Banach space the $\|\cdot\|$ norm induces a topology τ, while its dual, the set of all continuous linear functions, induces a topology σ on the Banach space. The latter topology is weak while the former is strong; that is to say, $\sigma \subseteq \tau$.

The differences between strong and weak topologies can be illustrated by means of series expansions [13]. An example of convergence in a strong topology would be uniform convergence of a Taylor series of a function within its convergence radius. An example of convergence in a weak topology would be the Fourier series of a function, which converges only in quadratic norm L^2.

A.3: Structural Stability and Topological Equivalence of Dynamical Systems

A fundamental notion of stability for a dynamical system is the stability of a point $x^* \in \mathfrak{X}$ under the flow $\Phi^t : x^* = \Phi(x^*)$. This means x^* is a fixed-point attractor for the flow. The technique of Poincaré sections can be used to relate limit cycles or higher-order tori as attractors to fixed points. More generally, attractors are invariant sets $A \subset \mathfrak{X}$, such that $\Phi(A) = A$ and $\Phi^{-1}(A) \subseteq A$. This invariance property of A extends to probability measures μ, where $\mu(\Phi^{-1}(A) = \mu(A)$, which are called stationary or invariant measures. Similarly, a statistical state ρ_μ over the algebra of continuous functions assigned to the measure μ has the invariance property. The invariance of thermal equilibrium states is the first condition for KMS states given in Haag et al. [31].

[10] An atom is a minimal nonzero element of a lattice, which is to say that it cannot be decomposed into two proper subsets: For $\alpha \subseteq \mathcal{A}$, α is an atom iff for every β, either $\beta \wedge \alpha = \alpha$ or $\beta \wedge \alpha = 0$.

Structural stability refers to perturbations in the function space of the flow map Φ. A system $(\mathfrak{X}, \Phi)$ is structurally stable if there is a neighborhood $\mathcal{N}$ of Φ such that all $\Psi \in \mathcal{N}$ are topologically equivalent to Φ. Two maps Φ and Ψ are *topologically equivalent*, or conjugated, if there is a homeomorphism h such that $h \circ \Phi = \Psi \circ h$. As Haag et al. [31] pointed out, structural stability is closely related to ergodicity: An invariant probability measure μ is said to be ergodic under the flow Φ if an invariant set A, has either measure zero or one, $\mu(A) \in \{0, 1\}$. If μ is non-ergodic, there is an invariant set A with $0 < \mu(A) < 1$ corresponding to an accidental degeneracy. Such degeneracies are not stable under small perturbations. Therefore, non-ergodic systems are in general not structurally stable [31].

A.4: Defining KMS States

Consider a C^*-dynamical system with an associated algebra of observables. Suppose $\mathcal{A}$ be a C^*-algebra and $t \to \tau_t$ a strongly continuous group of automorphisms of $\mathcal{A}$. An element $A \subseteq \mathcal{A}$, is analytic if there exists a strip $I_\eta = \{z \in \mathbb{C} : | \mathfrak{G}(z) | < \eta\}$ and a function $f : I_\eta \to \mathcal{A}$ such that

(1) $f(t) = \tau_t(A)$ for all $t \in \mathbb{R}$
(2) $z \to f(z)$ is analytic for $z \in I_\eta$

For the C^*-dynamical system $(\mathcal{A}, \tau, \mathbb{R})$, a state ϕ defined over $\mathcal{A}$ is a τ-KMS state with value $\beta \in \mathbb{R}$ if $\phi(A_\beta(B)) = \phi(BA)$ for all A, B in a norm-dense, τ-invariant *-subalgebra of $\mathcal{A}_\tau$, where β is inverse temperature.

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