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Unification of Energy Concepts in Generalized Phase Space Theories

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We consider how to describe Hamiltonian mechanics in generalized probabilistic theories with the states represented as quasiprobability distributions. We give general operational definitions of energy-related concepts. We define generalized energy eigenstates as the purest stationary states. Planck's constant plays two different roles in the framework: the phase space volume taken up by a pure state and a dynamical factor. The Hamiltonian is a linear combination of generalized energy eigenstates. This allows for a generalized Liouville time-evolution equation that applies to quantum and classical Hamiltonian mechanics and more. The approach enables a unification of quantum and classical energy concepts and a route to discussing energy in a wider set of theories.

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Introduction.—Generalized probabilistic theories (GPTs) constitute a metatheoretical framework developed within the foundations of quantum mechanics. Two key goals of GPTs are to understand the structure of quantum theory, particularly which elements necessarily arise from its probabilistic nature, and to elucidate the relations between classical and quantum mechanics [1–4]. Classical and quantum theories, as well as classical-quantum hybrid models, appear as special cases [3–5]. The states in GPTs are viewed as compressed lists of probabilities of possible measurement outcomes, with specifications contingent on the system preparation and subsequent dynamical transformations. While the initial emphasis was on the underlying probabilistic structure of GPTs, there is now a growing focus on a unified treatment of energy concepts within GPTs and the exploration of natural generalizations of classical and quantum dynamics [6–11].

In Refs. [6–9], the quantum theory Hamiltonian was extended in various ways to GPTs. In Ref. [7] it was shown that the phase space formalism can represent continuous-variable generalized probabilistic theory models. Thus one may use the phase space formalism for a dynamical description of hypothetical post-quantum theories of mechanics [7,9]. Using the phase space approach, Ref. [10] recently presented postquantum toy models of real systems including hydrogen atoms, by hypothesizing a generalized phase-space time evolution that is based on a generalization of a quantum-mechanical Moyal bracket [11].

These promising results create hope that we can develop self-consistent postquantum theories of Hamiltonian mechanics as well as gain a deeper understanding of quantum and

classical mechanics and their interrelations. There are certain hurdles lying ahead. For example, the formal classical limit of quantum theory where the Planck constant is taken to zero is singular [12], creating a further potential block towards a unified framework: how does one generalize this constant? There is also the fact that well-defined energy states in classical mechanics have descriptions (for example, Liouville density written in terms of positions and momenta), that evolve explicitly, whereas quantum energy eigenstates are stationary and thus akin to functions of action and angle variables. Thus it may appear as though at least some classical energy concepts are incompatible with quantum energy concepts.

We tackle these questions via a generalized phase space approach. By introducing postulates that reduce to the standard assumptions of the quantum and classical theories in the appropriate limits, we are able to describe dynamics in terms of a generalized Hamiltonian $H(q, p)$. The generalized evolution equations are obtained with the help of a theory-specific integration kernel $\mathcal{K}(k)$. In the particular case of $\mathcal{K}(k) \rightarrow (2/k)\delta(k - \hbar)$, the quantum evolution is recovered. When $\mathcal{K}(k) \rightarrow (2/k)\delta(k)$, the classical evolution is obtained. General functions $\mathcal{K}(k)$ model post-quantum theories.

The Hamiltonian of a closed system is an observable with a time-invariant expectation value $\langle E \rangle = \int H(q, p)f(q, p)dqdp$, where f is a GPT state. We construct the Hamiltonian as $H = \sum_i E_i V_{g_i}$, where E_i are the generalized energy eigenvalues and g_i are their generalized eigenstates that are ascribed a phase space volume V_{g_i} . This volume acts as a generalization of the

Bohr-Sommerfeld elementary volume, reducing to $V_{g_i} = (2\pi\hbar)^n$ for a quantum system with n degrees of freedom. The generalized energy eigenstates g_i are defined as the purest stationary states. In other words, they are time-invariant states that are not mixtures of other time-invariant states [13]. They coincide with the standard energy eigenstates if the GPT is a quantum theory and are uniform distributions over phase space orbits in the case of classical mechanics.

These results provide a unified framework within which one can derive statements relating to energy in such a manner that they apply directly to both quantum and classical mechanics as well as to a wider set of theories.

We proceed as follows. First, we briefly summarize the key rules of the quantum and classical phase space description. We then generalize (i) the Born rule and Planck's constant therein, (ii) the energy eigenstates, (iii) the equation of motion, and (iv) the Hamiltonian. Detailed derivations and additional results are given in an accompanying paper [14].

Phase space representation.—Consider first classical mechanics of a nonconstrained system with a finite number of degrees of freedom. Its states and (the algebra of) observables are smooth functions on the phase space \mathfrak{P} [12,15]. Mathematically, it is a symplectic manifold that is a cotangent bundle of the configuration space with local coordinates q . The local coordinates on \mathfrak{P} are $z = (q, p)$, where p are the generalized momenta.

The Poisson bracket of two phase space functions $\{f, g\}$ is defined as

$$\sum_j \left(\frac{\partial f}{\partial q_j} \frac{\partial g}{\partial p_j} - \frac{\partial f}{\partial p_j} \frac{\partial g}{\partial q_j} \right) \equiv f(\overleftarrow{\partial}_q \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_q) g \equiv -f \Lambda g, \quad (1)$$

where j runs through all the degrees of freedom (we will focus on one-dimensional systems hereafter), and arrows indicate the direction of action of the differential operators. The Poisson bracket governs the dynamics of observables via the canonical equations of motion $\dot{q} = \{q, H\}$ and $\dot{p} = \{p, H\}$, that are generated by the system's Hamiltonian H .

Our knowledge about a system is encapsulated in a probability (Liouville) density $\rho(z)$. Its evolution is given by the Liouville equation,

$$\frac{\partial \rho(q, p)}{\partial t} = \{H, \rho\} = -H \Lambda \rho. \quad (2)$$

The most common *quantum* phase space representation [11,16,17] is the Wigner function $W(q, p)$, a real function which may be negative for regions of q, p , and is therefore termed a quasiprobability density [11,12,16,18–20]. The Wigner function corresponding to a Hermitian operator \hat{A} is the Fourier transform of the off-diagonals of \hat{A} (the Wigner transform of \hat{A}):

$$\begin{aligned} A(q, p) &:= \text{Wigner}_k \{ \hat{A} \} (q, p) \\ &= \int dx e^{ipx/k} \left\langle q - \frac{1}{2}x | \hat{A} | q + \frac{1}{2}x \right\rangle. \end{aligned} \quad (3)$$

The Weyl transform [11,16]

$$\hat{A} = \frac{1}{4\pi^2 k^2} \int \text{Wigner}_k \{ \hat{A} \} (q, p) e^{i \frac{a(q-\hat{q})+b(p-\hat{p})}{k}} dq dp dadb, \quad (4)$$

effects the inverse transformation, with obvious generalization to n degrees of freedom. In quantum mechanics $k = \hbar$. Both transforms do not affect the dimension. Since $\hat{\rho}$ is dimensionless, the Wigner function as a quasiprobability distribution on \mathfrak{P} is defined as $W_{\hat{\rho}} := \text{Wigner}_{\hbar} \{ \hat{\rho} / (2\pi\hbar) \}$ [16].

The Born rule is reproduced by the following inner product,

$$P(i|\hat{\rho}_j) = \text{Tr}(\hat{E}_i \hat{\rho}_j) = h \int W_i W_j dq dp, \quad (5)$$

where $h = 2\pi\hbar$, and W_i and W_j are Wigner functions corresponding to \hat{E}_i (the effect) and $\hat{\rho}_j$ (the state), respectively.

The (noncommutative) product of operators is represented as $\text{Wigner}_{\hbar} \{ \hat{A} \hat{B} \} = \text{Wigner}_{\hbar} \{ \hat{A} \} \star \text{Wigner}_{\hbar} \{ \hat{B} \}$, where $\star = \exp(-\frac{1}{2}i\hbar\Lambda)$ is the Moyal star product. Finally, the time evolution of the density operator $\hat{\rho}$ under the (Weyl-ordered) Hamiltonian \hat{H} is equivalently represented as the evolution of the Wigner function W_{ρ} ,

$$\begin{aligned} \frac{\partial W_{\rho}}{\partial t} &= \frac{1}{i\hbar} (H \star W_{\rho} - W_{\rho} \star H) \\ &= -\frac{2}{\hbar} H(q, p) \sin\left(\frac{\hbar}{2}\Lambda\right) W_{\rho}(q, p). \end{aligned} \quad (6)$$

When $\hbar \rightarrow 0$, Eq. (6) becomes the classical evolution Eq. (2).

Generalized Born rule and inner product from symmetries.—A key ingredient of any generalized probabilistic theory (GPT) is the assignment of probabilities of the outcomes i of tests on preparations f , $P(i|f) = e_i(f)$ [1–3,21–23]. In the terminology of quantum foundations research, the functional e_i on the state space is called an effect [24,25]. In GPTs the states are represented as real vectors, which here correspond to continuous real distributions $f(z)$ [7].

It is standard to assume linearity of the effects in a GPT, such that the probability of a discrete outcome can always be represented via

$$P(i|f) = e_i(f) = c_i \int f(z) g_i(z) dz, \quad (7)$$

where g_i is a real-valued normalized function and c_i is a positive constant. g_i does not necessarily represent a valid

state. For the effects to form a complete measurement the identity $\sum_i e_i(f) = 1$ should hold for any allowed state f . Thus $\sum_i c_i g_i = 1$, which is known as the *completeness condition* for a measurement.

Similar expressions give the probability of continuous effects labeled by a continuous variable μ . The probability of falling into an interval $(\mu, \mu + d\mu)$ is $dP(\mu; d\mu|f) = \rho(\mu|f)d\mu$, where $\rho(\mu|f)$ is the probability density for the outcome μ given the state f . We can represent the density by the general expression $\rho(\mu|f) = c_\mu \int f(z)g_\mu(z)dz$. For example, classical (sharp) phase space localization has $\mu = z_0 \in \mathfrak{P}$, and the state is given by the Liouville density: $f = \rho(z)$. The probability of being within the volume dz_0 around z_0 in \mathfrak{P} is $dP = \rho(z_0)dz_0$. Comparison with the general expression identifies $g_{z_0}(z) = \delta(z - z_0)$ and $c_{z_0} = 1$.

While the g_i of effects in Eq. (7) are in general not associated with specific states, it is possible that g_i is a function representing a state such that Eq. (7) can be interpreted as the probability being proportional to the inner product between two states, with

$$\langle f, g \rangle = \int f(q, p)g(q, p)dqdp \quad (8)$$

being a possible form of the inner product. We find that Eq. (8) is, up to a multiplier, the unique inner product under three symmetries. The symmetries read as follows: 1. Translation: $(q, p, t) \mapsto (q + a, p + b, t + c)$, for any $a, b, c \in \mathbb{R}$, 2. Switch: $(q, p, t) \mapsto (Cp, q/C, -t)$, where C is an arbitrary constant fixing unit, 3. Time reversal: $(q, p, t) \mapsto (q, -p, -t)$. (See the Supplemental Material [26] for details).

Equation (8) allows us to interpret the inner product with a state g_i as a possibly allowed effect $e_i(f) \propto \langle g_i, f \rangle \propto \int fg_i dqdp$. The proportionality constant is fixed if $e_i(g_i) = 1$:

$$1 = e_i(g_i) = c_i \int g_i g_i dqdp := c_i \|g_i\|^2, \quad (9)$$

resulting in $c_i = \|g_i\|^{-2}$. We call complete sets of such effects *state-dual measurements*. Projective measurements in quantum theory are an example. State-dual measurements are guaranteed to exist in so-called self-dual theories [2,3].

Equation (9) associates a property of state g_i with the corresponding state-dual measurement. This relationship ascribes a quantity with the units of $[qp]$ to the effect g_i . We will show this c_i can be given the meaning of volume that is occupied by the corresponding state in \mathfrak{P} .

Generalized Planck constant of uncertainty: State volume.—Consider a set of state-dual measurements on the system whose states are confined within the region $\mathfrak{D} \subset \mathfrak{P}$. The functions $\{g_i\}$ that represent the effects have joint support in the same domain. Completeness of the

measurement inside \mathfrak{D} implies $\sum_{i=1}^N c_i g_i = 1_{\mathfrak{D}}$, where $1_{\mathfrak{D}}$ takes value 1 inside the domain \mathfrak{D} and 0 outside it. As the support of any g_i is in \mathfrak{D} , the phase space volume $V_{\mathfrak{D}}$ satisfies

$$V_{\mathfrak{D}} = \int 1_{\mathfrak{D}} dz = \sum_i c_i \int_{\mathfrak{D}} g_i dz = \sum_i c_i, \quad (10)$$

enabling the interpretation of the coefficients c_i as the effective phase space volume of the states g_i . We will accordingly use the terminology of the *state volume* V_{f_i} of a function f_i in \mathfrak{P} as

$$V_{f_i} := \left(\int f_i^2 dqdp \right)^{-1} = \frac{1}{\|f_i\|^2}. \quad (11)$$

The generalized Born rule for state-dual measurements can now be written as

$$P(i|f) = V_{g_i} \int g_i(q, p)f(q, p)dqdp. \quad (12)$$

For example, in quantum theory the purity of a state $\hat{\rho}$ is bounded via Eq. (5) as $\text{Tr}(\hat{\rho}^2) = h \int W_i^2 \leq 1$. Thus the state volume of any pure quantum state is given by the Planck constant, $V_\rho = \|W_\rho\|^{-2} = h$, while mixed states have larger state volumes.

Classical pure states are associated with points in \mathfrak{P} and Dirac-delta distributions centred on those points [12]. For concreteness, consider a mixed state $f_{\delta\varepsilon}$ that is given by a uniform distribution in the volume $\Delta q \Delta p$, where we set $\Delta q = \delta$, $\Delta p = \varepsilon$ and take the limit of zero uncertainty by $\varepsilon\delta \rightarrow 0$. A normalized rectangular function is $1/(\varepsilon\delta)$ on this domain and zero elsewhere. Equation (11) then implies that in the limit $\varepsilon\delta \rightarrow 0$ the volume $V_{f_{\delta\varepsilon}}$ approaches zero. In an epistemically restricted classical theory simulating quantum mechanics [27] $V_f \geq h$.

If we demand that similarly to classical and quantum theories all pure states in a GPT have the same 2-norm (this does not hold in the example of the probabilistic theory known as box world [28]) we can define a state-independent generalization of h as $\|g_p\|^{-2} = V_p$, where g_p is an arbitrary pure state. The number N of distinguishable states (associated with the state-dual measurements in \mathfrak{D}) can be interpreted as the amount of information (as measured in the number of states) one can store in the system, and then obeys $N \leq (V_{\mathfrak{D}}/V_p)$ in line with Eq. (10).

Generalized energy eigenstates.—We generalize the energy eigenstates of quantum mechanics as the set of purest stationary states of a GPT. For stationary states the probabilities of all time-independent effects are time independent, and thus they are given by time-independent functions on \mathfrak{P} .

Probabilistic mixtures of stationary states are, by inspection, also stationary, so there is a convex set of stationary

states. *Pure stationary states* are the extreme points of the set of stationary states. Pure stationary states are not necessarily pure states of the corresponding GPT, i.e., the extreme points [12,25] of the convex set of all states.

Wigner functions that represent the energy eigenstates of quantum mechanics are stationary by construction. On the other hand, if the action-angle $I-\theta$ variables can be introduced [15,29,30], then the invariance of the action variables is an explicit manifestation of stationarity. The classical energy eigenstates are then $\delta(I-I_0)/(2\pi)$, for all the possible I_0 , corresponding to uniform distributions over phase-space orbits. Thus pure stationary states of classical mechanics are not classical pure states. These correspond to the phase space points and in the Schrödinger picture are explicitly given as $f_{z_0}(t) = \delta(z - z_0(t))$, where $z_0(t) \in \mathfrak{P}$ is the phase space trajectory. The pure stationary states moreover coincide with the eigenfunctions of the Liouvillian operator in the Koopman–von Neumann quantumlike formulation of classical mechanics [14]. However, the dual role of the Hamiltonians as the generator of dynamics and as an observable, which we incorporate in the GPT framework, is not respected in the Koopman–von Neumann formulation, which has important consequences for the hybrid quantum-classical mechanics [31].

We will show in subsequent sections that pure stationary states further satisfy two natural desiderata for generalized energy eigenstates: (i) pure stationary states can be assigned sharp energy values, always giving the same value in an energy measurement, and (ii) they determine the time evolution of the system.

Generalized equation of motion.—A class of generalized equations of motion for the states $f(z, t)$ is obtained if their generator \mathcal{G} is assumed to be a bilinear functional of the state f and the generalized energy eigenstates $\mathcal{G}(f, \sum e_i g_i) = \sum e_i \mathcal{G}(f, g_i)$. Imposing the additional assumptions of (i) the symmetries of canonical coordinates; (ii) preservation of the inner product; (iii) $\mathcal{G}(g_i, g_j) = 0$ for all i, j results in (see Supplemental Material [26] for details):

$$\begin{aligned} \frac{\partial f}{\partial t} &= \sum_i \varepsilon_i \int \mathcal{K}(k) f \sin\left(\frac{k}{2}\Lambda\right) g_i dk \\ &= \sum_i \varepsilon_i \int \frac{i}{2} \mathcal{K}(k) \text{Wigner}_k\{\{\hat{f}_k, (\hat{g}_i)_k\}\} dk, \end{aligned} \quad (13)$$

where ε_i are constant coefficients and $\mathcal{K}(k)$ is a theory-specific distribution. $\text{Wigner}_k\{\}$ represents the Wigner transform of Eq. (3), and $\hat{f}_k, (\hat{g}_i)_k$ are the Weyl transforms [Eq. (4)] of f and g_i (their units are different from density matrices). To include the continuous spectrum (unbounded quantum states, classical mechanics), the sum over should be replaced by integration. This generalized evolution provides a restricted version of the generalized Moyal bracket in Ref. [10], here derived from physical principles.

We recover the quantum dynamics [Eq. (6)] if we identify $\mathcal{K}(k) = 2\delta(k - \hbar)/k$ [and $H(q, p) \equiv \sum_i \varepsilon_i g_i$]. To obtain the classical theory [Eq. (2)] we have to take a (singular) limit $\hbar \rightarrow 0$. Thus $\mathcal{K}(k)$ can be viewed as generalizing the *dynamically* important Planck constant.

As a simple example of a self-consistent theory where the dynamical and state Planck constants differ, consider d -dimensional quantum systems with a restriction on the information about the preparation such that the allowed pure states of the restricted theory are the states of the form $\frac{1}{2}|\psi\rangle^{(a)}\langle\psi|^{(a)} + \frac{1}{2}|\psi\rangle^{(b)}\langle\psi|^{(b)}$, where $|\psi\rangle^{(x)} = \sum_{i=1}^d c_i^{(x)}|i\rangle$ and $\langle\psi|^{(a)}|\psi\rangle^{(b)} = 0$. Then the generalized Planck constant for states is $V = 2h$, whereas the dynamical Planck constant remains h (see Ref. [14] for details).

For a general $\mathcal{K}(k)$ the evolution is given by the integral of commutators with different commutation relations. A nonassociative algebra replaces the associative Moyal bracket or the operator product. Therefore, the transformation is no longer described by a Lie group, but a quasigroup, or what may be termed a *loop* [32]. We have not found any principle that rejects this possibility.

Generalized energy and Hamiltonian.—We now complete the discussion by providing an explicit expression for the Hamiltonian as an observable and writing the generalized time evolution equation in terms of that Hamiltonian.

The set of energy eigenstates provides a set of state-dual measurement effects in quantum mechanics. Generalizing this idea, we postulate that there exists a state-dual measurement corresponding to the pure stationary states $\{g_i\}$ ($\{g_\mu\}$ in the case of a continuum labeled by μ).

A restriction on how to define generalized energy values is that the identification $H = \sum_i \varepsilon_i g_i$ in Eq. (13) in the quantum cases indicates that the energy eigenvalues (scalars with the dimension of energy) are $E_i = \varepsilon_i/(2\pi\hbar) = \varepsilon_i/V_i$, where we used Eq. (12) and that $V_i = 2\pi\hbar$ for all pure states in quantum mechanics.

Extending the definition of the Hamiltonian as the generator of time evolution, we demand

$$\frac{\partial f}{\partial t} = \int dk \mathcal{K}(k) f \sin\left(\frac{\Lambda k}{2}\right) H, \quad (14)$$

i.e., the dynamics of a GPT is determined by the set (g_i, ε_i) and the kernel $\mathcal{K}(k)$. Thus the Hamiltonian can be written as

$$H(q, p) = \sum_i E_i g_i V_{g_i} + \int E_\mu g_\mu dV_\mu, \quad (15)$$

an expression that also defines the generalized energy eigenvalues (both the discrete and continuous parts of the spectrum). In Ref. [14], we give a detailed discussion about how the generalized energy is a conserved and additive quantity.

We have seen that the above definition reduces to the standard expression for the energy in quantum theory. In

TABLE I. Comparison between quantum, classical, and our generalized framework.

Quantum	Classical	Generalization
Wigner function	Non-negative phase space distribution	Arbitrary distribution in the phase space
Energy eigenstates	Delta functions of action	Pure stationary states
Uncertainty \hbar	0	State volume
Dynamical \hbar	$\{q, p\} = 1$	Nonlocalized dynamics factor $\mathcal{K}(k)$ in Eq. (13)
Equation (6)	Liouville equation Eq. (2)	Time evolution Eq. (14)

classical mechanics we have $g_{I_0}(I) = (1/2\pi)\delta(I - I_0)$, where I stands for the action in the action-angle coordinate [15], such that

$$H = \int E_{I_0} \frac{1}{2\pi} \delta(I - I_0) 2\pi dI_0, \quad (16)$$

where E_{I_0} is the classical energy that corresponds to the I_0 , $(1/2\pi)\delta(I - I_0)$ is a normalized state, and $2\pi dI_0$ gives dV_{I_0} . It trivially satisfies Eq. (15).

Consider the expectation value of energy. By the generalized Born rule of Eq. (12), $P(i|f) = \int V_{g_i} g_i f dq dp$. Combining that with the definition of the Hamiltonian [Eq. (15)], we have that the expectation value of energy for state f is given by

$$\langle E \rangle = \int H f dq dp, \quad (17)$$

which for the generalized energy eigenstate g_i is just its value E_i .

Summary and outlook.—We built a generalized phase-space framework centered around generalizations of the quantum energy concepts, like Hamiltonian and energy eigenstates (as listed in Table I). We define the generalized energy eigenstates operationally: the most pure stationary states. Based on these pure stationary states, we derive a generalized equation of motion in phase space that encompasses the quantum and classical Liouville equations of motion. This includes generalizing Planck’s constant. In our framework, Planck’s constant provides the volume occupied by pure states and also appears in the commutation relation in the equation of motion. The two generalizations of Planck’s constant can have different values in general theories. The axioms used are listed together in the Supplemental Material [26]. A specific theory is obtained by specifying the set of pure states of the theory, the dynamical kernel $\mathcal{K}(k)$, and a general postmeasurement state update rule, as can be seen, e.g., from comparison with summaries of classical and quantum axioms [12,25,33]. An accompanying extended article contains a derivation of the generalized Born rule from symmetries and examples of theories other than quantum and classical, among other things [14].

This framework can be employed and developed in several directions: (i) The link between the generalized evolution, state or effect negativity, “jumping in phase space,” and contextuality deserve investigation [14]. (ii) Other forms of mechanics can be built, that are neither classical nor quantum, e.g., by letting Planck’s constant in the equation of motion differ from Planck’s constant for uncertainty or choosing a nontrivial $\mathcal{K}(k)$. (iii) The framework enables clear analogies and comparisons between quantum and classical dynamics and could, for example, help clarify the apparent speed-up of Hamiltonian-based quantum walks over classical walks [34]. (iv) It may be possible to reduce or alter the set of postulates (see the Supplemental Material [26] for a list), and (v) it is natural to employ the framework to create a theory of thermodynamics that is independent of the underlying choice of mechanics.

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