Causal evolution of wave packets

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Drawing from the optimal transport theory adapted to the relativistic setting we formulate the principle of a causal flow of probability and apply it in the wave-packet formalism. We demonstrate that whereas the Dirac Hamiltonian impels a causal evolution of probabilities, even in the presence of interactions, the relativistic-Schrödinger model is acausal. We quantify the causality breakdown in the latter model and argue that, in contrast to the popular viewpoint, it is not related to the localization properties of the states.

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I. INTRODUCTION

Causality, understood as the impossibility of superluminal transfer of information, is considered one of the fundamental principles, which ought to be satisfied in any physical theory. Whereas it is readily implemented in classical theories based on Lorentzian geometry, the status of causality in quantum theory was controversial from its dawn. As expressed in the famous Einstein-Podolsky-Rosen (EPR) paper [1], the main stumbling block is the inherent nonlocality of quantum states. However, quantum nonlocality on its own cannot be utilized for superluminal transfer of information; neither can quantum correlations be communicated between spacelike separated regions of spacetime [2]. In fact, the principle of causality can be invoked to discriminate theories that predict stronger than quantum correlations [3].

Since the EPR controversy, a multitude of different approaches to causality in quantum theory have been proposed. The challenge is to provide a sensible notion of causality, which accurately disentangles the nonlocality of quantum states from the causality violation effects as, for instance, interference fringes can travel with superluminal speed, but cannot be utilized to transfer information [4].

One of the lines of study in this field focused on the "causal propagation of observables" [5–8]. This perspective is closely related to the "no-signalling" or "microcausality" axiom in quantum field theory [9,10]. The latter is often presented as the only sensible framework to study causality in quantum theory (see for instance [11–13]). Moreover, some researchers conclude that causality—seemingly broken in one-particle relativistic quantum mechanics—is magically restored at the QFT level [14–16]. On the other hand, the recent results of [17] suggest that if a relativistic quantum system is acausal before the second quantization, then this drawback cannot be cured by the introduction of antiparticles.

A second approach to causality focuses on the dynamics of quantum states and relates to the problem of localization [18]. The results usually invoked in this context are those of Hegerfeldt [19] (see also [20–22] and references therein), which show that an initially localized [23] quantum state with positive energy immediately develops infinite tails. Hegerfeldt's approach, however, faced criticism [12] based on the impossibility of preparing a "localized" state [24] (compare [25] though). It is usually concluded that Hegerfeldt's theorems, which are mathematically correct, provide an alternative argument against the localization of quantum relativistic states [12,14,26] rather than a "proof of acausality."

The two mentioned viewpoints on causality in quantum theory share the common intuition that probabilities should not propagate faster than light, as this would allow for a superluminal communication. From the viewpoint of quantum field theory, the wave-packet formalism gives a phenomenological rather than fundamental description of Nature. Nevertheless, it serves as a handy low-energy approximation commonly used in atomic, condensed matter [27–29], or neutrino physics [30]. Regardless of the adopted simplifications, its statistical predictions confronted with the experiments cannot be at odds with the principle of causality.

In this paper we rigorously formalize the intuition of a causal probability flow within the wave-packet formalism, suitable to study phenomena in which the creation of particles can be neglected. To this end we employ the notion of causality for Borel probability measures developed in our recent articles [31,32]. The adopted formalism allows us also to quantify the breakdown of causality, which may prove handy in discriminating different models of a given quantum system.

To demonstrate the adequacy of the employed notion of causality we investigate the evolution of probability densities in two "basic" relativistic quantum models, described respectively by the Dirac and relativistic-Schrödinger equations. We demonstrate that in the Dirac model, the evolution of *any* initial wave packet is causal, even in the presence of interactions. On the other hand, the propagation governed by the relativistic-Schrödinger Hamiltonian turns out to be at odds with the principle of causality, regardless of the localization properties of the initial state.

The study of the Dirac equation is motivated by its usefulness in modeling the electron transport in graphene [33] and

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its pertinence for the study of topological insulators [28,34]. Moreover, Dirac fermions have recently been simulated with cold atoms [35], trapped ions [36], and photonic systems [37], which opens the door to an experimental study of their causality and localization properties.

The relativistic-Schrödinger model seems less interesting from the empirical point of view, but it is of great importance for theoretical analysis. It allows us to confirm and clarify the conclusions of Hegerfeldt concerning the acausal behavior of exponentially localized states with positive energy. In addition, we provide explicit examples of quantum states with heavy tails, that do not fulfill Hegerfeldt's localization assumption, but do break the principle of causality. The relativistic-Schrödinger model provides us also a simple illustration of the causality breakdown quantification and facilitates the comparison with the results of [17]. In particular, we confirm the transient character of causality violation in this model, detected in [17] for compactly supported initial states. On the other hand, we obtain a significantly larger value of the amount of causality violation in the limit of a perfectly localized initial state, as compared to [17].

For the Dirac model we were able to provide an analytic proof of causality, whereas in the relativistic-Schrödinger case the numerical analysis was relatively straightforward. Let us stress, however, that the formalism developed in this paper is much more general and can be applied to any, possibly nonlinear, dynamics of probabilities, for instance governed by the Gross-Pitaevskii equation. We shall expand on this point at the beginning of Sec. III and in the Outlook.

The paper is organized as follows: In Sec. II we present the basic definition of causality for probability measures from [31] along with the physical intuition behind it. Therein, we also coin the notion of a *causal evolution* and discuss its Lorentz invariance. Then, in Sec. III, we apply the developed theory in the wave-packet formalism. After some general considerations concerning the quantification of causality breakdown, we turn to the n-dimensional Dirac equation and show that it impels a causal evolution of probability measures, regardless of the choice of the initial spinor. This result holds also when an, possibly non-Abelian, external gauge field is minimally coupled to the system. Then, we take a closer look at the relativistic-Schrödinger equation in two dimensions. We confirm the breakdown of causality in the course of evolution of a initial Gaussian state, derived in [20] and checked also in [17]. Next, we turn to states with exponentially bounded tails and show, via explicit examples, that Hegerfeldt's bound is superficial. Finally, we demonstrate the violation of causality for wave packets of powerlike decay. A summary of our work, together with further comparison with Hegerfeldt's theorem, comprises Sec. IV. Therein, we also make an outlook into the potential applications of our formalism in discriminating theoretical models of various quantum systems. Last, we discuss a possible extension of the adopted notion of causality to the study of dynamics of POVM's.

II. CAUSALITY FOR PROBABILITY MEASURES

A. Causal relation

We start with a brief summary of the main concepts contained in [31]. This requires some notions from Lorentzian geometry, topology, and measure theory, which we invoke without introducing the complete mathematical structure behind. For a detailed exposition on these topics the reader is referred to standard textbooks on general relativity [38] and optimal transport theory [39] or, simply, to the "Preliminaries" section in [31].

Let $\mathcal{M}$ be a spacetime. For any $p,q \in \mathcal{M}$ we say that p *causally precedes* q (denoted $p \preceq q$) iff there exists a future-directed piecewise smooth causal curve $\gamma : [0,1] \to \mathcal{M}$, such that $\gamma(0) = p$ and $\gamma(1) = q$. It is customary to denote the set of causally related pairs of events by J^+, i.e., $J^+ := \{(p,q) \in \mathcal{M}^2 \mid p \preceq q\}$. For any $p \in \mathcal{M}$ one defines the *causal future (past)* of p as

$$J^+(p) := \{q \in \mathcal{M} \mid p \preceq q\}$$
$$(J^-(p) := \{r \in \mathcal{M} \mid r \preceq p\}).$$

Similarly, for any set $\mathcal{X} \subseteq \mathcal{M}$ one denotes $J^\pm(\mathcal{X}) := \bigcup_{p\in\mathcal{X}} J^\pm(p)$.

Let us now consider $\mathscr{P}(\mathcal{M})$—the set of all Borel probability measures on $\mathcal{M}$ (which we shall simply call "measures" from now on), i.e., measures defined on the σ-algebra $\mathscr{B}(\mathcal{M})$ of all Borel subsets of $\mathcal{M}$, and normalized to 1. In particular, $\mathscr{P}(\mathcal{M})$ contains all measures of the form $\rho \cdot \lambda_{\mathcal{M}}$, where ρ is a probability density on $\mathcal{M}$ and $\lambda_{\mathcal{M}}$ is the measure associated to the canonical volume form on $\mathcal{M}$. Also, one can regard $\mathcal{M}$ as naturally embedded in $\mathscr{P}(\mathcal{M})$, the embedding being the map $p \mapsto \delta_p$, where the latter denotes the Dirac measure concentrated at the event p.

In [31] we demonstrated that the causal relation $\preceq$ extends in a natural way from the spacetime $\mathcal{M}$ onto $\mathscr{P}(\mathcal{M})$ [31, Definition 2]. Concretely, we have the following:

Definition 1. [31] Let $\mathcal{M}$ be a spacetime. For any $\mu,\nu \in \mathscr{P}(\mathcal{M})$ we say that μ *causally precedes* ν (symbolically $\mu \preceq \nu$) iff there exists $\omega \in \mathscr{P}(\mathcal{M}^2)$ such that (i) $\omega(A \times \mathcal{M}) = \mu(A)$ and $\omega(\mathcal{M} \times A) = \nu(A)$ for any $A \in \mathscr{B}(\mathcal{M})$, and (ii) $\omega(J^+) = 1$. Such an ω is called a *causal coupling* of μ and ν.

The above definition mathematically encodes the following physical intuition: The existence of a joint probability measure ω provides a (nonunique) probability flow from μ to ν and the condition $\omega(J^+) = 1$ says that the flow is conducted exclusively along future-directed causal curves. We shall denote the set of all couplings between $\mu,\nu \in \mathscr{P}(\mathcal{M})$ (i.e., joint probability measures satisfying (i)) by $\Pi(\mu,\nu)$ and the set of causal ones by $\Pi_c(\mu,\nu)$.

In spacetimes equipped with a sufficiently robust causal structure one has the following characterization of the causal precedence relation:

Theorem 1. Let $\mathcal{M}$ be a causally simple spacetime [40] and let $\mu,\nu \in \mathscr{P}(\mathcal{M})$. Then, $\mu \preceq \nu$ if and only if for all compact $\mathcal{K} \subseteq \operatorname{supp} \mu$

$$\mu(\mathcal{K}) \leqslant \nu(J^+(\mathcal{K})). \tag{1}$$

Proof. On the strength of [31, Theorem 8], μ causally precedes ν iff for all compact $C \subseteq \mathcal{M}$

$$\mu(J^+(C)) \leqslant \nu(J^+(C)),$$

which trivially implies (1). In order to show the converse implication, let $C \subseteq \mathcal{M}$ be any compact set. Recall that every measure on $\mathcal{M}$, including μ, is *tight*, i.e., the μ-measure of any Borel subset of $\mathcal{M}$ can be approximated from below by

μ-measures of its compact subsets. In particular, for any $\varepsilon > 0$ there exists a compact set $\mathcal{K}_\varepsilon \subseteq J^+(C) \cap \operatorname{supp} \mu$ such that $\mu(J^+(C) \cap \operatorname{supp} \mu) \leqslant \mu(\mathcal{K}_\varepsilon) + \varepsilon$. Using (1), one thus can write that

$$\begin{aligned}\mu(J^+(C)) &= \mu(J^+(C) \cap \operatorname{supp} \mu) \leqslant \mu(\mathcal{K}_\varepsilon) + \varepsilon \\ &\leqslant \nu(J^+(\mathcal{K}_\varepsilon)) + \varepsilon \leqslant \nu(J^+(J^+(C) \cap \operatorname{supp} \mu)) + \varepsilon \\ &\leqslant \nu(J^+(J^+(C))) + \varepsilon = \nu(J^+(C)) + \varepsilon,\end{aligned}$$

which yields (ii) as soon as one takes $\varepsilon \to 0^+$. ■

Condition (1) provides a link with the "no-signalling" intuition behind the principle of causality. Indeed, imagine that there exists a physical process, which impels a probability flow $\mu \rightsquigarrow \nu$—i.e., there exists $\omega \in \Pi(\mu,\nu)$—which is superluminal, i.e., $\omega(J^+) < 1$. Then, Theorem 1 says that there exists a compact region of spacetime $\mathcal{K}$, such that the probability leaks out of its future cone. In this case, an observer localized in $\mathcal{K}$ could encode some information in the probability measure μ, for instance by collapsing a nonlocal quantum state of a larger system, and transfer it to a recipient beyond $J^+(\mathcal{K})$—the causal future of $\mathcal{K}$. Such a method of signaling would be rather inefficient, due to its statistical nature, but would be a priori possible (compare similar arguments given in [22] or [20]).

Let us also note that Theorem 1 harmonizes with the definition of causal propagation of observables adopted in [6, (3.2a) and (3.2b)] and [8, (3.1) and (3.2)] (see also [7]). The main difference is that the works [6–8] focused on the evolution of quantities localized on time slices in the Minkowski spacetime. This situation is encompassed by Definition 1, as explained in Sec. II B, but our formalism, together with Theorem 1, provides a rigorous definition of causality in a much wider—generally covariant—setting. Further comments on the relationship of our approach to the works [6–8] are included in Secs. II C and II D.

If $\mathcal{M}$ is causally simple, then the condition $\omega(J^+) = 1$ can be equivalently expressed as $\operatorname{supp} \omega \subseteq J^+$ [31, Remark 5]. This, in particular, implies the following necessary condition for the causal precedence of two measures [31, Proposition 5].

Proposition 2. [31] Let $\mathcal{M}$ be a causally simple spacetime and let $\mu,\nu \in \mathscr{P}(\mathcal{M})$, with μ compactly supported. If $\mu \preceq \nu$, then $\operatorname{supp} \nu \subseteq J^+(\operatorname{supp} \mu)$.

In other words, if the measure μ is compactly supported, then the support of any ν causally preceded by μ should lie within the future of $\operatorname{supp} \mu$. Whereas this condition is necessary, it is not sufficient, even in the case of both μ and ν compactly supported. This is readily illustrated by the counterexample presented in Fig. 1.

B. Causal dynamics of measures

The formalism developed in [31] and summarized above establishes the kinematical structure of $\mathscr{P}(\mathcal{M})$. We shall now formalize the requirement that any evolution of measures should respect the inherent causal structure. This task has been accomplished in [32] in full generality of curved space times. Since the main objective of this paper is the application in wave-packet formalism, we will focus exclusively on the $(1+n)$-dimensional Minkowski spacetime $\mathcal{M} := \mathbb{R}^{1,n}$ and assume the measures to be localized in time, i.e., concentrated on parallel time slices.

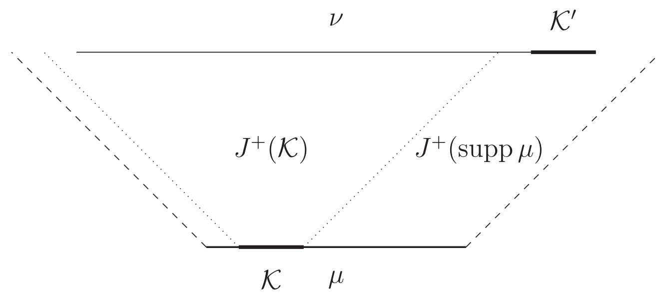

FIG. 1. Although $\operatorname{supp} \nu$ lies in the future of $\operatorname{supp} \mu$, the excessive weight condensed in the region $\mathcal{K}$ cannot flow causally to $\mathcal{K}'$. Hence, $\operatorname{supp} \nu \subset J^+(\operatorname{supp} \mu)$, but $\mu \not\preceq \nu$.

Let us fix an interval $I \subseteq \mathbb{R}$ and consider a measure-valued map

$$\mathcal{E} : I \to \mathscr{P}(\mathbb{R}^n), \quad t \mapsto \mathcal{E}(t) =: \mu_t,$$

which describes a time-dependent probability measure on $\mathbb{R}^n$. This map can be equivalently regarded as a family of measures $\{\boldsymbol{\mu}_t\}_{t\in I} \subseteq \mathscr{P}(\mathcal{M})$, where $\boldsymbol{\mu}_t := \delta_t \times \mu_t$. One can think of the map $t \mapsto \mu_t$ as a *curve in* $\mathscr{P}(\mathbb{R}^n)$ parametrized by $t \in I$. If $\mu_t = \delta_{x(t)}$, then one recovers a curve $t \mapsto x(t)$ in $\mathbb{R}^n$, whereas $\boldsymbol{\mu}_t = \delta_{(t,x(t))}$ becomes the corresponding world line in $\mathcal{M}$ of a classical point particle. We shall refer to the map $\mathcal{E}$, or equivalently to the corresponding family $\{\boldsymbol{\mu}_t\}$, as the *dynamics of measures* or *evolution of measures*.

The compatibility of the dynamics of measures with the causal structure of $\mathscr{P}(\mathcal{M})$ is formalized in the following definition:

Definition 3. We say that an evolution of measures is *causal* iff

$$\forall\, s,t \in I \quad \text{with } s \leqslant t \quad \boldsymbol{\mu}_s \preceq \boldsymbol{\mu}_t,$$

in the sense of Definition 1.

One may be concerned about the apparent frame dependence of thus defined (causal) evolution of measures. Indeed, the measures $\boldsymbol{\mu}_t$ live on t-slices, and so this way of describing the dynamics of a nonlocal phenomenon manifestly depends on the slicing of the spacetime associated with the chosen time parameter. To put it differently, consider two observers O and O', one Lorentz-boosted with respect to the other, who want to describe the dynamics of the same nonlocal phenomenon. Their evolutions of measures $\mathcal{E}$ and $\mathcal{E}'$, respectively, employ two different time parameters t and t', hence, consequently, two different collections of time slices. In particular, it is a priori not clear whether O and O' would always agree on the causality of their respective evolution of measures.

This matter has been thoroughly analyzed in [32, Sec. 2], in a much broader class of spacetimes. It turns out that, in spite of the apparent frame dependence of Definition 3, the property of the evolution of measures being causal is independent of the choice of the time parameter. Interested readers can find all the details in [32].

$\mathscr{P}(\mathbb{R}^n)$-valued maps can be utilized to model various physical entities evolving according to some dynamics. The most natural examples concern classical spread objects, such as charge or energy densities (see Sec. II D). We shall argue that the same concept can be successfully applied to probability measures obtained from wave functions in the position representation.

As pointed out in the Introduction, the wave-packet formalism has a phenomenological character from the viewpoint of relativistic quantum theory. The latter is believed to be causal par excellence, on the strength of the microcausality axiom of quantum field theory [9,10]. Therefore, it seems more adequate to speak of causality of the *model* rather than the system itself.

Definition 4. We say that the *model of a physical system is causal* iff any evolution of measures on $\mathbb{R}^n$ governed by its dynamics is causal in the sense of Definition 3.

By a model of a dynamical phenomenon we shall understand a family of measures $\{\boldsymbol{\mu}_t\}$, as explained at the beginning of this section. This concept will be illustrated with some examples from classical physics in Sec. II D. Then, in Sec. III we will explain the role of the model in the description of quantum systems within the wave-packet formalism.

Equipped with the rigorous definition of a causal evolution we can express the demand of causality of the statistical predictions of any physical model.

Principle 1. Any model of a physical system, which involves an evolution of probability measures on $\mathbb{R}^n$ ought to be causal in the sense of Definition 4.

C. Continuity equation

In physics one often encounters the *continuity equation*, which describes the transport (or the *flow*) of a certain conserved quantity, described by a density function $\rho : [0,T] \times \mathbb{R}^n \to \mathbb{R}$. Typically, the equation has the form

$$\frac{\partial}{\partial t}\rho + \nabla_x \cdot \mathbf{j} = 0, \tag{2}$$

for (sufficiently regular) ρ and a time-dependent vector field $\mathbf{j} : [0,T] \times \mathbb{R}^n \to \mathbb{R}^n$ called the *flux* of ρ. If there is a *velocity field* $\mathbf{v}$, according to which the flow runs (as it happens for instance in fluid mechanics), then $\mathbf{j} = \rho\mathbf{v}$.

The intuition that the continuity equation of some physical quantity should imply its causal flow was expressed in [7,8]. The aim of this section is to show that this viewpoint is also captured in Definition 4. A slight conceptual difference is that in [6–8] the evolution of observables is considered, whereas we concentrate on the corresponding probability distributions. Also, we do not take into account particle creation processes, which were considered in [8, pp. 279–280]. On the other hand, the measure-theoretic framework allows for a more rigorous formulation, which relies on the assumption that the velocity field $\mathbf{v}$ is subluminal.

We begin with the definition of the continuity equation in the space of measures, as given, e.g., in [41, Definition 1.4.1].

Definition 5. [41] Let $I = [0,T]$, for some $T > 0$. We say that an evolution of measures $\mathcal{E} : t \mapsto \mu_t$ satisfies the continuity equation with a given time-dependent Borel velocity field $\mathbf{v} : [0,T] \times \mathbb{R}^n \to \mathbb{R}^n$, $(t,x) \mapsto \mathbf{v}_t(x)$ iff

$$\frac{\partial}{\partial t}\mu_t + \nabla_x \cdot (\mathbf{v}_t \mu_t) = 0 \tag{3}$$

holds in the distributional sense, i.e., for all $\Phi \in C_c^\infty((0,T) \times \mathbb{R}^n)$,

$$\int_0^T \int_{\mathbb{R}^n} \left[\frac{\partial \Phi}{\partial t} + \mathbf{v}_t \cdot \nabla_x \Phi\right] d\mu_t dt = 0. \tag{4}$$

The continuity equation allows one to regard the time-dependent measure μ_t as some sort of a fluid. Its density flows, but overall constitutes a conserved quantity. Its "particles" (fluid parcels) move according to the velocity field $\mathbf{v}$ in a continuous manner. One would intuitively expect that if the flow of measures is to behave reasonably, the magnitude of $\mathbf{v}$ should be bounded. This expectation is attested by the following theorem [42, Theorem 3] (see also [43, Theorem 3.2] or [41, Theorem 6.2.2] for other formulations):

Theorem 2. [42] Let $T > 0$ and denote $\Gamma_T := C([0,T],\mathbb{R}^n)$. Let $\mathcal{E}$ satisfy the continuity equation with velocity field $\mathbf{v}$ such that

$$\exists\, V > 0\ \forall t \in [0,T]\ \forall x \in \mathbb{R}^n \quad \|\mathbf{v}_t(x)\| \leqslant V. \tag{5}$$

Then, there exists a measure $\sigma \in \mathscr{P}(\Gamma_T)$ such that

(i) σ is concentrated on absolutely continuous curves $\gamma \in \Gamma_T$ satisfying

$$\dot\gamma(t) = \mathbf{v}_t(\gamma(t)) \quad \text{for } t \in (0,T) \text{ a.e.}; \tag{6}$$

(ii) $(\mathrm{ev}_t)_*\sigma = \mu_t$ for every $t \in [0,T]$, where $\mathrm{ev}_t : \Gamma_T \to \mathbb{R}^n$ denotes the evaluation map $\mathrm{ev}_t(\gamma) = \gamma(t)$.

One can say that the measure σ prescribes a family of curves along which the infinitesimal "parcels" flow during the evolution. Since we put very few requirements on $\mathbf{v}$ (namely, that it is Borel and bounded), curves satisfying (6) might cross each other and the measure σ itself is in general not unique.

One would intuitively expect that the probability flow is causal if the norm of the velocity field governing its dynamics is bounded by the speed of light c at every point of $\mathcal{M}$. The following theorem shows that this is indeed the case:

Theorem 3. Let $T > 0$ and let the evolution of measures $\mathcal{E}$ satisfy the continuity equation with a velocity field $\mathbf{v}$ such that

$$\forall t \in [0,T]\ \forall x \in \mathbb{R}^n \quad \|\mathbf{v}_t(x)\| \leqslant c. \tag{7}$$

Then, $\mathcal{E}$ is causal in the sense of Definition 3.

Proof. By inequality (7), there exists a measure $\sigma \in \mathscr{P}(\Gamma_T)$ with the properties listed in Theorem 2.

We claim the following: For every absolutely continuous curve $\gamma \in \Gamma_T$ satisfying (6), we have

$$(s,\gamma(s)) \preceq (t,\gamma(t)), \quad 0 \leqslant s \leqslant t \leqslant T. \tag{8}$$

Note that the curve $t \mapsto (t,\gamma(t))$, being absolutely continuous, has tangent vectors $(1,\gamma'(t))$ for almost all $t \in (0,T)$. Moreover, these tangent vectors are causal by (7). However, this curve need not be piecewise smooth, so (8) does not follow (that) trivially.

On the other hand, in the Minkowski spacetime (8) is equivalent to the inequality

$$\|\gamma(t) - \gamma(s)\| \leqslant c(t - s), \quad 0 \leqslant s \leqslant t \leqslant T \tag{9}$$

and this can be easily proven by means of the fundamental theorem of calculus, which is valid precisely for absolutely continuous functions. Namely, we can write

$$\forall s,t \in [0,T] \quad \gamma(t) = \gamma(s) + \int_s^t \gamma'(\tau)d\tau.$$

Therefore, if $s \leqslant t$, then

$$\|\gamma(t) - \gamma(s)\| = \left\| \int_s^t \gamma'(\tau)d\tau \right\| \leqslant \int_s^t \|\gamma'(\tau)\| d\tau$$
$$= \int_s^t \|\mathbf{v}_\tau(\gamma(\tau))\| d\tau \leqslant c(t-s),$$

where in the last inequality we employed (7), thus proving (9) and, consequently, (8).

Now, for any $s,t \in [0,T]$, $s \leqslant t$ define the map $\mathrm{Ev}_{(s,t)} : \Gamma_T \to \mathcal{M}^2$ by $\mathrm{Ev}_{(s,t)}(\gamma) := ((s,\gamma(s)),(t,\gamma(t)))$. We claim that $\omega := (\mathrm{Ev}_{(s,t)})_* \sigma$ is a causal coupling of $\boldsymbol{\mu}_s$ and $\boldsymbol{\mu}_t$.

Indeed, for any $A \in \mathscr{B}(\mathcal{M})$, using its characteristic function χ_A, one can write

$$\omega(A \times \mathcal{M}) = \int_{\mathcal{M}^2} \chi_A(p)d\omega(p,q) = \int_{\Gamma_T} \chi_A(s,\gamma(s))d\sigma(\gamma)$$
$$= \int_{\mathbb{R}^n} \chi_A(s,y)d\mu_s(y) = \boldsymbol{\mu}_s(A).$$

One similarly shows that $\omega(\mathcal{M} \times A) = \boldsymbol{\mu}_t(A)$.

To demonstrate $\omega(J^+) = 1$, notice that we have

$$\omega(J^+) = \int_{\mathcal{M}^2} \chi_{J^+} d\omega = \int_{\Gamma_T} \underbrace{\chi_{J^+}((s,\gamma(s)),(t,\gamma(t)))}_{=1} d\sigma(\gamma)$$
$$= \int_{\Gamma_T} d\sigma = 1,$$

where we made use of (8). This concludes the proof of ω being a causal coupling and, by the arbitrariness of s,t, we have thus shown that the evolution $\mathcal{E} : t \mapsto \mu_t$ is causal. ∎

As a corollary of Theorem 3, we unravel the following relation between the continuity equation for probability densities (2) and the causality of the four-current (compare also [8, (3.5) and (3.9)]).

Corollary 6. Let $T > 0$ and let $\rho, \mathbf{j}$ satisfy Eq. (2). Suppose, additionally, that $\rho \geqslant 0$ and that $\int_{\mathbb{R}^n} \rho(0,x)dx =: Q \in (0,+\infty)$. Then, if $J := (c\rho,\mathbf{j})$ is a causal vector field on the Minkowski spacetime $\mathbb{R}^{1,n}$, then the evolution $\mathcal{E} : t \mapsto \mu_t$ with $d\mu_t(x) := \frac{\rho(t,x)}{Q} d^n x$ is causal.

Proof. Note that (2) guarantees that $\int_{\mathbb{R}^n} \rho(t,x)dx = Q$ for any $t \in [0,T]$ and the definition of μ_t is sound.

Now, observe that $\mathcal{E}$ satisfies the continuity equation (3) with the velocity field $\mathbf{v} = (v^k)_{k=1,\ldots,n}$ defined, for all $(t,x) \in [0,T] \times \mathbb{R}^n$, as

$$v_t^k(x) := \begin{cases} \frac{j^k(t,x)}{\rho(t,x)}, & \text{for } (t,x) \text{ such that } \rho(t,x) \neq 0 \\ 0, & \text{for } (t,x) \text{ such that } \rho(t,x) = 0 \end{cases}.$$

Indeed, for any $\Phi \in C_c^\infty((0,T) \times \mathbb{R}^n)$ one has (we employ Einstein's summation convention),

$$\int_0^T \int_{\mathbb{R}^n} \left[\frac{\partial \Phi}{\partial t} + \mathbf{v}_t \cdot \nabla_x \Phi \right] d\mu_t dt$$
$$= \frac{1}{Q} \int_0^T \int_{\mathbb{R}^n} \frac{\partial \Phi}{\partial t} \rho \, d^n x dt + \frac{1}{Q} \int_0^T \int_{\mathbb{R}^n} \rho \, v_t^k \frac{\partial \Phi}{\partial x^k} d^n x dt$$
$$= -\frac{1}{Q} \int_0^T \int_{\mathbb{R}^n} \Phi \frac{\partial \rho}{\partial t} d^n x dt - \frac{1}{Q} \int_0^T \int_{\mathbb{R}^n} \Phi \frac{\partial j^k}{\partial x^k} d^n x dt$$
$$= -\frac{1}{Q} \int_0^T \int_{\mathbb{R}^n} \Phi \underbrace{\left[\frac{\partial \rho}{\partial t} + \frac{\partial j^k}{\partial x^k} \right]}_{=0 \text{ by } (2)} d^n x dt = 0$$

and so condition (4) is satisfied.

In remains now to check that condition (7) holds, which amounts to proving that for all $(t,x) \in [0,T] \times \mathbb{R}^n$,

$$\|\mathbf{j}(t,x)\| \leqslant c|\rho(t,x)|.$$

But the latter is precisely the condition for the vector field $J := (c\rho,\mathbf{j})$ to be causal, which is true by assumption. ∎

D. Examples from classical physics

Corollary 6 shows that Definition 3 correctly encodes the common intuitions concerning the causal flow, at least in the domain of classical physics. Before we move to the quantum realm, let us provide further evidence in favor of Principle 1 by invoking concrete examples.

Example 7. By Maxwell's equations, if ρ and $\mathbf{j}$ denote, respectively, the *charge density* and the *current density* (on $\mathbb{R}^3$), then they satisfy the continuity equation (2). It is well known that $J := (c\rho,\mathbf{j})$ is a causal four-vector field [44, Sec. 28]. Suppose that $\rho \geqslant 0$ or $\rho \leqslant 0$ and that the total charge Q is finite. Then, Corollary 6 assures that the evolution of ρ is causal.

Example 8. Consider a time- and space-dependent electromagnetic field $\mathbf{E}$, $\mathbf{B}$. In the absence of external charges and currents, the electromagnetic energy density $u := \frac{1}{2}(\varepsilon_0 \|\mathbf{E}\|^2 + \frac{1}{\mu_0}\|\mathbf{B}\|^2)$ satisfies the continuity equation

$$\frac{\partial}{\partial t} u + \nabla_x \cdot \mathbf{S} = 0,$$

where $\mathbf{S} := \frac{1}{\mu_0} \mathbf{E} \times \mathbf{B}$ is the Poynting vector.

As is well known, the quadruple $(cu,\mathbf{S})$ is a causal four-vector field, which is actually equal to $cT^{\mu 0}$, where $T^{\mu\nu}$ constitutes the stress-energy tensor of the electromagnetic field [44, Secs. 32–33]. If we now assume that the total energy $\int_{\mathbb{R}^3} u(0,x)dx$ is finite, Corollary 6 guarantees that u evolves causally, in full accordance with [7, Sec. 5.3].

Example 9. Generalizing the previous example, consider a stress-energy tensor $T^{\mu\nu}$ such that $T^{\mu 0}$ is a causal vector field (cf. [8, Eq. (3.5)]). The energy conservation principle takes the form (in the Minkowski spacetime) of the continuity equation $\partial_\mu T^{\mu 0} = 0$. This fact, on the strength of Corollary 6, implies that the energy density $\rho := T^{00}$ evolves causally, provided that the total energy $\int_{\mathbb{R}^n} \rho(0,x)dx$ is finite. In this way the results of Gromes [8] are incorporated in the presented formalism.

III. WAVE-PACKET FORMALISM

We have illustrated the techniques from the optimal transport theory on classical examples. Now, we will argue that the same concept proves useful in quantum theory described via the wave-packet formalism. The first hint in favor of this claim is provided by Example 8: It was observed by

Białynicki-Birula [45] that the energy density of the electromagnetic field admits a probabilistic interpretation and can be written as the modulus square of the photon wave function. Example 8, on the strength of Corollary 6, immediately implies that the description of the one-particle quantum electromagnetism via photon wave function impels a causal probability flow and thus harmonizes with Principle 1. Let us stress that this result, although clearly based on the Lorentz invariance of Maxwell's equations, is not trivial. The wave function, being a complex object, induces interference effects in the probability density, which could in principle spoil the causal flow of probability. The fact that this is not the case shows that Definition 3 correctly disentangles causality violation from quantum superposition effects.

Since the concept of a photon wave function is in close analogy with the Dirac formalism, it is natural to expect that the latter also satisfies Principle 1. This is indeed the case, as we will shortly show (see Sec. III C). Before doing so, let us establish the general framework for the study of causality in wave-packet formalism on the $(1+n)$-dimensional Minkowski spacetime.

We assume that the quantum system at hand is modelled by a normalized wave function $\psi \in L^2(\mathbb{R}^{1+n},\mathbb{C}^k)$ for some $k \in \mathbb{N}$. Its time evolution $t \mapsto \psi(t,\cdot)$ is governed by some, possibly nonlinear and time-dependent, dynamical equation. As the wave function ψ is normalized to 1 at any instant of time, it defines a probability density $\|\psi(t,\cdot)\|^2$ on $\mathbb{R}^n$ for every $t \in \mathbb{R}$. By fixing a time interval $[0,T]$ we obtain an evolution of measures $\mathcal{E} : t \mapsto \mu_t$, with $d\mu_t(x) = \|\psi(t,x)\|^2 d^n x$. Equipped with Definition 3 we can thus rigorously study the issue of causality of the evolution. Let us note that $\mathcal{E}$ is *not*, in general, uniquely determined by the initial measure μ_0, as initial wave functions differing by a (nonconstant) phase factor will yield the same initial probability distribution μ_0, but different evolutions.

Below, we shall focus on two models of relativistic quantum systems, described by the Dirac and relativistic-Schrödinger equations respectively. These models can be seen as the most basic ones from a theoretical point of view [46] and they will serve us to justify that the proposed notion of causality is sound.

In realistic quantum systems accessible experimentally the true dynamics of probabilities is typically much more complicated as it involves many body interactions, nonzero temperature effects, etc. To describe the dynamics of the wave function of a given quantum system one is always condemned to adopt approximations. For instance, in the Bose-Einstein condensate one often assumes the Hartree mean-field approximation, which leads to the Gross-Pitayevskii equation [29]. Moreover, one needs to account for the atom-atom interactions by choosing a suitable effective potential [47]. Similarly, in condensed matter physics, one starts with the Dirac equation to model topological insulators [28]. However, to obtain a more adequate description one can, for instance, introduce a quadratic correction [34]. Finally, in modeling the experimental amplitudes one should take into account the characteristic of the detector, which can influence the effectively observed dynamics [48].

The above considerations justify the standpoint that the notion of a causal evolution of wave packets should refer to the model rather than the system itself. One could, in principle, have two competing models of a given quantum phenomenon—one of them being causal and the other not. It is also evident that one cannot hope to have Principle 1 exactly satisfied in an effective description of some complicated quantum dynamics. It is thus desirable to have some measure of causality breakdown in a given model, to check how far the adopted simplifications haven taken us from the true quantum relativistic description.

A. Quantifying the breakdown of causality

A suitable measure of causality breakdown should take into account, in addition to the free parameters of the model at hand, the initial state and the time scale of the effect. As for the former, it might turn out that the states, for which causality violation occurs, are not physically realizable—for instance if they have compact spatial support (cf. [10,24]). It is also desirable to study the duration of the superluminal flow of measures, as the effect might turn out evanescent and irrelevant from the perspective of the characteristic time scale of a given model. For instance, the results of [17] show that the causality breakdown in the relativistic-Schrödinger model is a transient effect and it becomes marginal rather quickly.

In our formalism, the most natural quantification of causality violation is the following:

$$\begin{aligned}\widetilde{N}(t,\psi_0) &:= \inf\{\omega(\mathcal{M}^2 \setminus J^+) \,|\, \omega \in \Pi(\boldsymbol{\mu}_0,\boldsymbol{\mu}_t)\} \\ &= 1 - \sup\{\omega(J^+) \,|\, \omega \in \Pi(\boldsymbol{\mu}_0,\boldsymbol{\mu}_t)\}. \qquad (10)\end{aligned}$$

With Definitions 1 and 3 we have $\widetilde{N}(t,\psi_0) = 0$ if and only if $\boldsymbol{\mu}_0 \preceq \boldsymbol{\mu}_t$.

However, Eq. (10) is not very convenient for concrete computations as one needs to explore the whole space $\Pi(\boldsymbol{\mu}_0,\boldsymbol{\mu}_t)$, which is vast. Also, its relationship with the actual possibility of superluminal information transfer is not visible.

Drawing from Theorem 1 we can define another measure of causality violation:

$$M(t,\psi_0) := \sup\{M(t,\psi_0,\mathcal{K}) \,|\, \mathcal{K} \text{ compact}, \mathcal{K} \subseteq \text{supp } \boldsymbol{\mu}_0\},$$

where

$$M(t,\psi_0,\mathcal{K}) := \max\{0, \boldsymbol{\mu}_0(\mathcal{K}) - \boldsymbol{\mu}_t(J^+(\mathcal{K}))\}.$$

The number $M(t,\psi_0,\mathcal{K}) \in [0,1]$ can be thought of as the "capacity of the superluminal communication channel"—discussed in Sec. II A. In this context, it is desirable to keep track of the dependence of $M(t,\psi_0,\mathcal{K})$ on $\mathcal{K}$ to see whether the latter is not unreasonably large (or small) for the information transfer to be possible—even in principle.

The quantity $M(t,\psi_0,\mathcal{K})$ mimics, to some extent, the "outside probability" defined in [17], which, in our notation, can be written as

$$\begin{aligned}N(t,\mu_0) &= \boldsymbol{\mu}_t(\mathcal{M} \setminus J^+(\text{supp } \boldsymbol{\mu}_0)) \\ &= 1 - \boldsymbol{\mu}_t(J^+(\text{supp } \boldsymbol{\mu}_0)) \\ &= (\boldsymbol{\mu}_0 - \boldsymbol{\mu}_t)(J^+(\text{supp } \boldsymbol{\mu}_0)).\end{aligned}$$

Clearly, this quantity makes sense only for strictly localized initial states, as if supp $\mu_0 = \mathbb{R}^n$ and thus supp $\boldsymbol{\mu}_0 = \{0\} \times \mathbb{R}^n$, then $N(t,\mu_0) = 0$ for all $t \geqslant 0$. Also, one should write

$N(t,\psi_0)$, with $\mu_0 = |\psi_0|^2$, rather than $N(t,\mu_0)$ to take into account for mean momentum of the initial packet, which does influence its evolution.

Note that the difference $\boldsymbol{\mu}_0(\mathcal{K}) - \boldsymbol{\mu}_t(J^+(\mathcal{K}))$ cannot, in general, be understood as the "outside probability" [17], i.e., the pure "leak out" of the probability. The latter holds only if $\mathcal{K} = \operatorname{supp} \boldsymbol{\mu}_0$. In general, $J^+(\mathcal{K})$ depends causally on the region $J^-(J^+(\mathcal{K})) \supseteq \mathcal{K}$, so the flow of probability into $J^+(\mathcal{K})$ from outside of $\mathcal{K}$ can diminish, or even completely compensate, the visible acausal effect. In fact, the superluminal flow can conspire in such a way that it might be hard in practice to find a compact region $\mathcal{K} \subseteq \{0\} \times \mathbb{R}^n$, for which $M(t,\psi_0,\mathcal{K}) > 0$ for given t and ψ_0. Nevertheless, we shall demonstrate on the example of the relativistic-Schrödinger model that the quantity $M(t,\psi_0)$ helps to understand the acausal behavior.

The introduced causality breakdown measures are dimensionless, but the parameters on which they depend are dimensionful. We shall adopt the natural units by setting $\hbar = c = m_e = 1$. These determine the natural scales of length $\hbar/(m_e c) = \alpha$ a.u. $\approx 7.3 \times 10^{-3}$ a.u. and time $\hbar/(m_e c^2) = \alpha^2$ a.u. $\approx 5.3 \times 10^{-5}$ a.u.

B. A nonrelativistic model

To demonstrate the use of Definition 3 in practice let us first consider a nonrelativistic quantum model, from which one would expect an acausal behavior. Indeed, for instance the well-known spreading of the Gaussian wave packet of a free massive quantum particle is acausal in the sense of Definition 3. Let us illustrate this fact by considering an initial wave function $\psi_0(x) = (\pi d)^{-1/4} e^{-x^2/(2d)}$, with $d > 0$, on the two-dimensional Minkowski spacetime $\mathbb{R}^{1,1}$ evolving under the Hamiltonian $\frac{1}{2m}\partial_x^2$. The resulting evolution of probability measures reads

$$d\mu_t(x) = \sqrt{\frac{dm^2}{\pi(d^2m^2 + t^2)}} \exp\left(-\frac{dm^2x^2}{d^2m^2 + t^2}\right) dx.$$

To show that the evolution $\mathcal{E} : t \mapsto \mu_t$ is acausal we exploit Theorem 1. If we take $K = [-a,a]$ for some $a > 0$, then

$$\boldsymbol{\mu}_t(J^+(\{0\} \times K)) = \mu_t([-a-t,a+t]) = \int_{-a-t}^{a+t} d\mu_t$$
$$= \operatorname{Erf}\left(\frac{\sqrt{d}m(a+t)}{\sqrt{d^2m^2 + t^2}}\right),$$

where Erf is the error function. Since the latter increases monotonically, we conclude that for $a > \frac{md}{t}(\sqrt{m^2d^2 + t^2} + md)$ we have $\int_{-a-t}^{a+t} d\mu_t < \int_{-a}^{a} d\mu_0$ for every $t,d,m > 0$. Hence, for any $t,d,m > 0$ there exists a compact set $\mathcal{K}_a = \{0\} \times [-a,a] \subset \mathbb{R}^{1,1}$, such that the inequality $\boldsymbol{\mu}_t(J^+(\mathcal{K})) < \boldsymbol{\mu}_0(\mathcal{K})$ holds and so $\boldsymbol{\mu}_0 \not\preceq \boldsymbol{\mu}_t$.

For the sake of comparison with the relativistic-Schrödinger model it is instructive to plot the quantity $M(t,\psi_0,\mathcal{K}_a)$ showing the amount of causality violation in the nonrelativistic model (see Fig. 2).

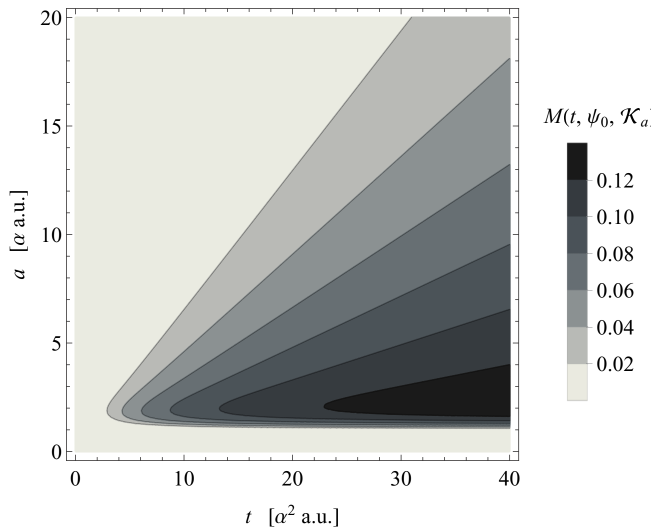

FIG. 2. Quantification of causality breakdown in the nonrelativistic model with mass $m = 1 = m_e$ and an initial Gaussian state of width $\sqrt{d} = 1 = \alpha$ a.u.

C. Dirac model

Let us now turn to the Dirac model, which is generally believed to conform to the principle of causality [17,22,26]. Below, we confirm this statement in the rigorous sense of Definition 4.

Proposition 10. Let $\psi \in L^2(\mathbb{R}^{1+n}) \otimes \mathbb{C}^{2^{\lfloor (n+1)/2 \rfloor}}$ be a solution to the $(1+n)$-dimensional Dirac equation [49]

$$i\gamma^\mu \partial_\mu \psi - m\psi = 0$$

and let $\psi^\dagger(t,\cdot)\psi(t,\cdot)$ be the corresponding time-dependent probability density. Then, the Dirac model is causal in the sense of Definition 4.

Proof. The proof is a straightforward application of Corollary 6. The associated continuity equation is satisfied with $\rho := \psi^\dagger\psi$ and $\mathbf{j} := (\psi^\dagger\gamma^0\gamma^k\psi)_{k=1,\ldots,n}$. In this case, ρ is a probability density function (and so $Q = 1$) and the quantity $J := (\rho,\mathbf{j})$ can be simply written as

$$J^\mu := \psi^\dagger\gamma^0\gamma^\mu\psi.$$

J is well known to possess the transformation properties of a vector field on the $(1+n)$-dimensional Minkowski space time.

Moreover, this vector field is causal everywhere. Indeed, assume that J is spacelike at some event p. Then, we can find an inertial frame in which $J'^0(p) = 0$, that is $\psi'^\dagger(p)\psi'(p) = 0$ and therefore $\psi'(p) = 0$. But this would mean that also $\psi(p) = 0$, because $\psi(p)$ and $\psi'(p)$ are related through a unitary transformation. On the other hand, $\psi(p) = 0$ would imply $J(p) = 0$—a contradiction with the assumption that J was spacelike at p. ■

Let us emphasize the fact that in the Dirac model causality is satisfied during the evolution of *any* initial spinor. In particular, we impose no restrictions on its energy or localization. This fact does not contradict Hegerfeldt's results (see [22]), as it is well known [16,26] that positive-energy Dirac wave packets cannot have the localization properties required by Hegerfeldt's theorem [20].

We conclude this section with an extension of Proposition 10 to interacting Dirac model.

Remark 11. The proof of causality of the Dirac model relies on the basic continuity equation

$$\partial_\mu J^\mu = 0 \tag{11}$$

enjoyed by the probability current J^μ. The latter, as a fundamental law of probability conservation, holds also in presence of external electromagnetic or Yang-Mills potentials, in which case the wave function ψ acquires additional degrees of freedom. In general, the Dirac model with *any* interaction which does not spoil the continuity Eq. (11) is causal in the sense of Definition 4.

D. Relativistic-Schrödinger model

We now turn to the relativistic-Schrödinger model, i.e., we consider wave packets evolving under the Hamiltonian $\hat{H} = \sqrt{\hat{p}^2 + m^2}$, with $\hat{p} = -i\partial_x$ and $m \geqslant 0$. For the sake of simplicity, we restrict ourselves to the case of spin 0 representation and one spatial dimension.

Since in the relativistic-Schrödinger model $\hat{H} \geqslant 0$, Hegerfeldt's theorem applies and we expect the evolution of a localized initial state to be acausal. This has been checked (and quantified) in [17] for a family of compactly supported initial wave packets $\psi_0(x) = \frac{1}{\sqrt{2d}}\chi_{[-d,d]}(x)$, with χ being the characteristic function. Because of Proposition 2, this result implies that the evolution of measures in this case is acausal. We consequently conclude that the relativistic-Schrödinger model is not causal and thus does not meet Principle 1. However, compactly supported states are unphysical idealizations (cf. for instance the Reeh-Schlieder theorem [24]). Moreover, in the relativistic-Schrödinger model the property of compact spatial support is lost whenever the wave packet is boosted to any other frame [17]. It is therefore instructive to study the evolution of other classes of initial wave packets to gain better understanding of the nature of causality violation in this system.

Given any initial state $\psi_0 \in L^2(\mathbb{R})$, the evolution under $\hat{H}$ yields for any $t \geqslant 0$,

$$\psi(t,x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widehat{\psi}_0(p)\, e^{-i\sqrt{p^2+m^2}t + ipx}\, dp, \tag{12}$$

where $\widehat{\psi}_0$ is the Fourier transform of ψ_0.

To check whether the evolution of measures $\mathcal{E} : t \mapsto \mu_t$ with $d\mu_t = |\psi(t,x)|^2 dx$ breaks causality in the sense of Definition 3 we exploit Theorem 1, similarly as we did for the nonrelativistic Hamiltonian. In the relativistic case, an explicit formula for the Fourier integral (12) is not available, therefore we had to resort to numerical integration. The complete analysis performed with the help of Wolfram *Mathematica* 10.0.4 is available online [50]; below we summarize its essential points.

The analysis presented below concerns the behavior of the quantity $M(t,\psi_0,\mathcal{K}_a)$ for $\mathcal{K}_a = \{0\} \times [-a,a]$, with $a > 0$ and initial wave packets with zero average momentum. This simplifies the analysis and is sufficient to understand qualitatively the causality violation effects. On the other hand, the quantitative picture is limited by the choice of working with symmetric intervals only. In particular, we obviously have

$$\widetilde{M}(t,\psi_0) := \sup_{a\in\mathbb{R}} M(t,\psi_0,\mathcal{K}_a) \leqslant M(t,\psi_0). \tag{13}$$

Note also that the supremum in $M(t,\psi_0)$ can involve disconnected subsets of $\operatorname{supp}\mu_0$. Nevertheless, the estimate $\widetilde{M}(t,\psi_0)$, being only a lower bound of $M(t,\psi_0)$, already gives significantly larger values than $N(t,\mu_0)$ of [17] in the limit of a perfectly localized initial state.

In [50] we analyzed the impact of a nonzero average momentum of the wave packet ψ_0 on $M(t,\psi_0,\mathcal{K}_a)$ and found that it does not change the qualitative picture presented below. Note also that a state with a nonzero average momentum can always be boosted to a frame where $\langle\hat{p}\rangle = 0$, which, in view of the discussion following Definition 3, will not change the conclusions about the (a)causal behavior, though it will affect the quantitative picture. In [50] we have also studied the asymmetric case—with $\mathcal{K} = \{0\} \times [a,b]$. It turns out, not surprisingly, that for symmetric initial wave functions with vanishing average momentum the maximum of $M(t,\psi_0,\{0\} \times [a,b])$ is actually attained for some symmetric interval $[-a,a]$. This is no longer true if the initial wave packet has a nonvanishing expectation value of $\hat{p}$. In the case of $\langle\hat{p}\rangle > 0$, the maximal causality violation is observed by picking the interval $[a,b]$ with $a < 0 < b$ and $|b| < |a|$. This confirms the supposition that causality breakdown is best visible when the spreading effects are more important than the average motion of the packet.

We shall first focus on the massive case $m > 0$ and then briefly comment on the massless one. If $m > 0$, we can set $m = 1$ without loss of generality. Indeed, note that (12) implies

$$\psi(t,x,\psi_0;m) = \psi(mt,mx,\psi_0(\cdot/m);1),$$

hence

$$\begin{aligned} &M(t,\psi_0,\{0\} \times [a,b];m) \\ &\quad = M(mt,\psi_0(\cdot/m),\{0\} \times [a/m,b/m];1), \\ &M(t,\psi_0;m) = M(mt,\psi_0(\cdot/m);1). \end{aligned} \tag{14}$$

The first class of initial states in the relativistic-Schrödinger model that we have analyzed in detail are the Gaussian wave packets

$$\psi_0^G(x;d) = (\pi d)^{-1/4} \exp\left(\frac{-x^2}{2d}\right),$$

with the width $\sqrt{d} > 0$.

Figure 3 illustrates the behavior of the quantity $M(t,\psi_0^G,\mathcal{K}_a)$, with $\mathcal{K}_a = \{0\} \times [-a,a]$ and $d = 1$.

At first, the quantity $M(t,\psi_0,\mathcal{K}_a)$ is zero suggesting a causal evolution. Then, for some $t = t_0$, it starts increasing, manifesting the breakdown of causality. For later times ($t > t_1$), the probability flow "slows down" and the quantity $M(t,\psi_0,\mathcal{K}_a)$ can even decrease to 0 for $t > t_2$ and a suitably chosen compact set $\mathcal{K}_a$.

In [50] we studied the dependence of the values of time instants t_0, t_1, and t_2 on the choice of the "size" of the compact set $\mathcal{K}_a = \{0\} \times [-a,a]$, as parametrized by a. It leads to the following conclusions:

(i) For a small enough, the quantity $M(t,\psi_0,\mathcal{K}_a)$ is zero for all times and the breakdown of causality is not visible. On

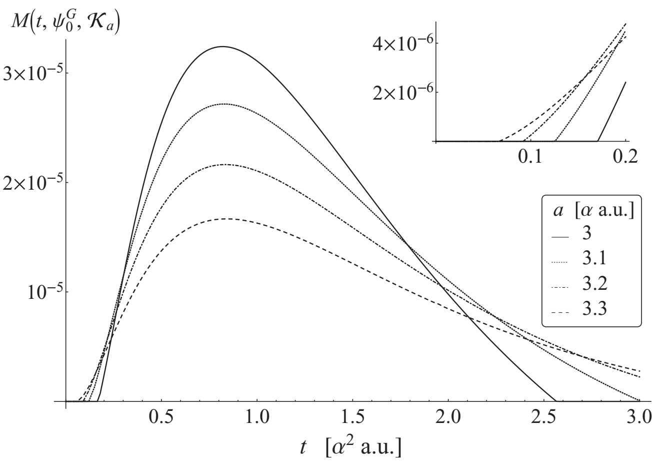

FIG. 3. Quantification of the acausal evolution of a Gaussian probability density in the relativistic-Schrödinger model. The inset pictures the closeup of the plot for short times.

the contrary, the values of a larger than $a_0 \approx 2.65$ lead to the acausal behavior as illustrated in Fig. 3.

(ii) The first time scale t_0 decreases with larger values of a. It suggests that, as in the nonrelativistic case, for any $t > 0$ there exists a compact set $\mathcal{K} \subset \{0\} \times \mathbb{R}$, such that the inequality $\boldsymbol{\mu}_t(J^+(\mathcal{K})) < \boldsymbol{\mu}_0(\mathcal{K})$ holds and thus causality is actually broken immediately once the evolution starts.

(iii) On the other hand, the scale of causality breakdown, quantified by (13), becomes smaller for larger regions $\mathcal{K}_a$. It attains a maximum $\widetilde{M}(t,\psi_0^G) = 3.55 \times 10^{-5}$ for $t_1 = 0.81$ and $a_M = 2.89$—see Fig. 4.

(iv) The causality breakdown has a transient character quantified by the time scale $t_1(\mathcal{K}_a) = \arg\max_{t\geqslant 0} M(t,\psi_0,\mathcal{K}_a)$. The quantity $t_1(\mathcal{K}_a) \approx 0.8$ does not depend significantly on the choice of a, provided $a > a_0$.

(v) The third time scale t_2, capturing the restoration of causality, can be made arbitrarily large by choosing a large enough.

TABLE I. Amount of causality violation in the relativistic-Schrödinger model with $m = 1$ for Gaussian initial states of width $\sqrt{d}$. The units of t_1 and a_M are as in Fig. 4.

d	1	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}
$\widetilde{M}(t_1)$	0.000035	0.0066	0.039	0.079	0.106	0.121
t_1	0.81	0.68	0.64	0.58	0.53	0.48
a_M	2.89	0.63	0.165	0.048	0.015	0.0047

With the narrowing of the initial Gaussian width d, the quantity $\widetilde{M}(t,\psi_0^G;d)$ grows, whereas the time scale t_1 decreases slightly, as illustrated by Table I.

In the limit $d \to 0$, the quantity $\widetilde{M}(t,\psi_0^G)$ tends to the maximum of approximately 0.13. This value is by 60% larger than the maximal outside probability computed in [17]. It shows that to quantify the amount of the causality breakdown for arbitrary wave packets it is not sufficient to look at one specific region of space from which the probability "leaks out too fast."

In the massless limit, the causality breakdown in the model driven by the Hamiltonian $\hat{H} = \sqrt{\hat{p}^2}$ has a persistent rather than transient character: The quantity $\widetilde{M}(t,\psi_0^G)$ is greater than 0 for any $t > 0$ and increases monotonically—see Fig. 5. It approaches asymptotically the value 0.13, in consistency with the above results and formula (14).

Let us now return to the massive case ($m = 1$) and analyze a second class of initial states with exponentially bounded tails,

$$\psi_0^e(x) = \sqrt{\frac{\beta}{2}}\,\mathrm{sech}(\beta x), \tag{15}$$

for $\beta > 0$. Thanks to the fact that sech is its own Fourier transform, the states (15) have exponential tails also in the momentum representation, which makes them convenient for numerical integration.

According to Hegerfeldt's result, one expects an acausal evolution for $\beta > m = 1$. Table II illustrates the amount of

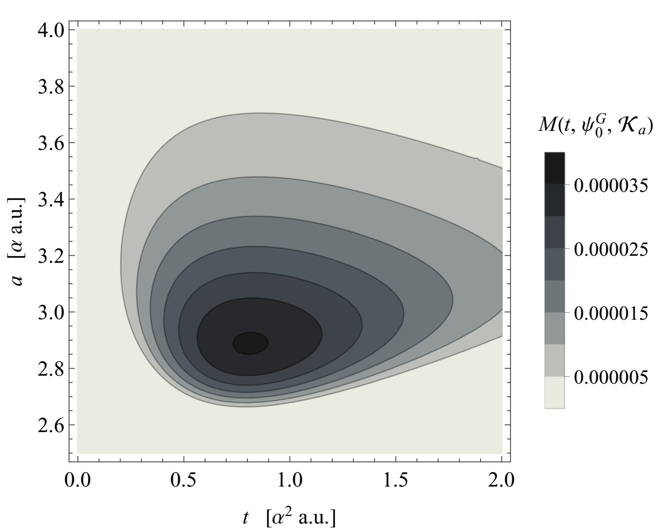

FIG. 4. Estimation of the time scale t_1 [α^2 a.u.] and length scale a_M [α a.u.] of causality violation in the relativistic-Schrödinger model.

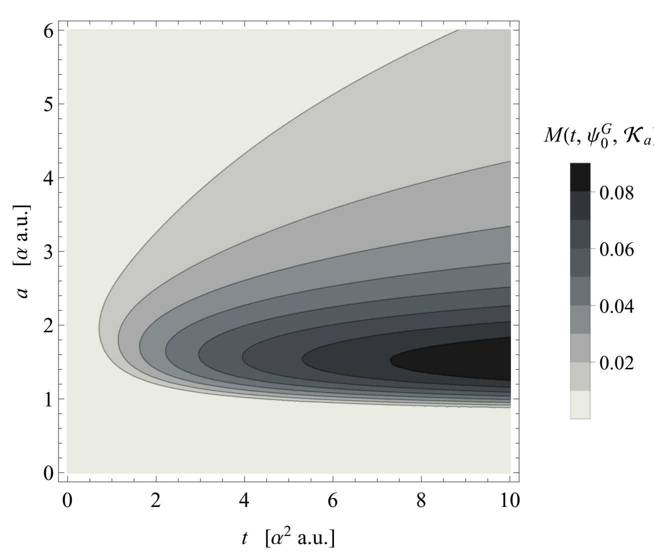

FIG. 5. In the massless limit of the relativistic-Schrödinger model the causality violation has a persistent character.

TABLE II. Quantification of causality violation in the relativistic-Schrödinger model for initial states in the class (15). The units of t_1 and a_M are as in Fig. 4.

β	3	2	5/3	3/2
$\widetilde{M}(t_1)$	3×10^{-4}	2×10^{-6}	1.4×10^{-8}	10^{-10}
t_1	0.79	0.83	0.84	0.85
a_M	1.4	3.2	5.2	7.4

causality violation quantified by formula (13) as β approaches the Hegerfeldt's bound.

As β tends to infinity one obtains a maximal amount of causality violation around 13%. This is consistent with the result we obtained above for the δ-like limit of the initial Gaussian states.

On the other hand, the amount of causality violation decreases fast as β approaches $m=1$. It suggests that the evolution of measures triggered by the initial state (15) with $\beta=m=1$ is causal. Indeed, in [50] we found no evidence of causality violation during the evolution of such an initial wave packet.

This observation is, however, only an artefact of the chosen class of states. The next example shows that the Hegerfeldt's bound is in fact artificial.

We now investigate the evolution of initial states

$$\psi_0^{SE}(x) = \mathcal{N}\,\frac{\sin x}{x}\,\mathrm{sech}(\beta x), \tag{16}$$

for $\beta > 0$, with the normalization constant $\mathcal{N}$. States in this class still have exponentially bounded tails both in position and momentum representation.

By computing the quantity $\widetilde{M}(t,\psi_0^{SE})$ we found in [50] a clear evidence of causality violation for all values of $\beta \in [0,4]$, as shown on Fig. 6.

We see that initial states decaying as $e^{-m\|x\|}$ play no special role in the causality violation effects in the relativistic-Schrödinger model. Although there seems to be local minimum for $\beta \approx 1.5$, which may well be an artefact of the fact

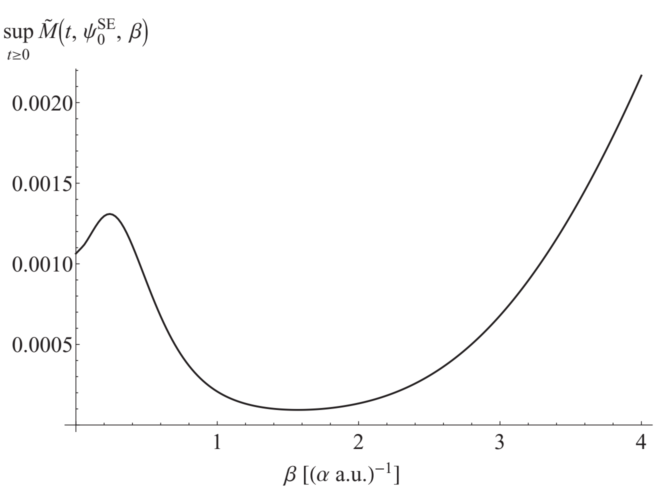

FIG. 6. The maximal amount of causality violation during the evolution of initial states in class (16).

that $\widetilde{M}(t,\psi_0^{SE})$ is only a lower bound of $M(t,\psi_0^{SE})$, the quantity $\widetilde{M}$ is manifestly positive for all β.

In particular, note that causality of the evolution is spoiled for initial states in the class (16) with $\beta = 0$, which decay only as $\mathcal{O}(x^{-1})$. In fact, our numerical analysis suggests that the breakdown of causality is generic also in a wider class of states with heavy tails:

$$\psi_0^{S}(x) = \mathcal{N}\left(\frac{\sin p_m x}{p_m x}\right)^n,$$

with $n \in \mathbb{N}$ and $p_m > 0$. In [50] we checked it explicitly for $n \in \{1,2,3\}$ and $\frac{1}{10} \leqslant p_m \leqslant 10$.

Let us now summarize our analysis, draw conclusions, and compare them with the upshot of Hegerfeldt.

IV. DISCUSSION

A. The claim of Hegerfeldt

To facilitate the comparison let us first briefly summarize Hegerfeldt's results on causality presented in [20] and his other works [19,21,22,51]. We find it important to clarify the field, as the outcomes of [20] are sometimes misinterpreted or overinterpreted (see below).

Hegerfeldt's conclusion concerning the acausal behavior of the wave packets relies on three assumptions [20]:

(1) For any region of space $V \subseteq \mathbb{R}^3$, there exists a positive operator $N(V) \leqslant 1$, such that $\langle\psi|N(V)|\psi\rangle$ yields the probability of finding in V a particle in the state ψ.

(2) The time evolution of states is driven by the Schrödinger equation with a positive (possibly time-dependent [52]) Hamiltonian operator $\hat{H}$.

(3) There exists a state ψ_0 with exponentially bounded tails, i.e.,

$$\langle\psi_0|N(\mathbb{R}^3 \setminus B_r)|\psi_0\rangle \leqslant K_1 \exp(-K_2 r^k), \tag{17}$$

for sufficiently large r, with B_r—a closed ball of radius r centered at the origin.

The constants K_1, K_2 depend on ψ_0 and the exponent k depends on the chosen Hamiltonian. More concretely, one has [20] $k=1$, $K_2 > m$ for the free relativistic-Schrödinger Hamiltonian $\hat{H} = \sqrt{\hat{p}^2 + m^2}$ and $k=2$, K_2 arbitrarily small for more general systems with interactions.

Under the above assumptions, Hegerfeldt obtained the following result:

Theorem 4 (Hegerfeldt's theorem [20]). In the quantum system fulfilling the assumptions (1) and (2) let ψ_0 be a state satisfying (17). Then,

$$\forall t > 0\ \exists\, \mathbf{a} \in \mathbb{R}^3\ \exists r > 0$$
$$\langle\psi_t|N(B_{\mathbf{a},r})|\psi_t\rangle > \langle\psi_0|N(\mathbb{R}^3 \setminus B_{\|\mathbf{a}\|-r-t})|\psi_0\rangle, \tag{18}$$

where $B_{\mathbf{a},r}$ denotes a closed ball of radius r centered at $\mathbf{a}$.

Let us stress that, although condition (18) is never mentioned explicitly in Hegerfeldt's works, it is this condition which is actually proven in [20].

In the original formulation, Hegerfeldt demonstrated the above result under the assumption of arbitrary finite propagation speed c'. However, since the strict inequality (18) holds for any $t > 0$, we can set $c' = 1$ without loss of generality.

Since it is obviously true that $\mathbb{R}^3 \setminus B_{\|\mathbf{a}\|-r-t} \supseteq B_{\mathbf{a},r+t}$, therefore (18) implies that

$$\forall t > 0 \ \exists \mathbf{a} \in \mathbb{R}^3 \ \exists r > 0$$
$$\langle \psi_t | N(B_{\mathbf{a},r}) | \psi_t \rangle > \langle \psi_0 | N(B_{\mathbf{a},r+t}) | \psi_0 \rangle. \tag{19}$$

This result, albeit somewhat weaker than (18), has a clearer interpretation. Namely, it shows that for any $t > 0$ *there exists a ball* in $\mathbb{R}^3$, into which the probability "has been leaking too fast" by the time t has elapsed.

We emphasize the "there exists a ball" phrase in the above results. This makes them considerably weaker statements than the one alleged by Hegerfeldt in [51], where the author announces the superluminal flow of probability from *any* ball centered at the origin. The latter claim is in fact false in the relativistic-Schrödinger model, as we have seen in the previous section. Additionally, notice that (19) speaks about the inflow of probability into a ball rather than the outflow.

B. Summary of the obtained results

In our approach to causality in quantum theory we have adopted a geometrical viewpoint. We have shown that the inherent causal structure of the underlying spacetime $\mathcal{M}$ induces a rigorous notion of the causal relation in the space $\mathscr{P}(\mathcal{M})$ of probability measures over $\mathcal{M}$. Our Definition 3 encodes the demand that the dynamics of measures should respect the natural geometry of $\mathscr{P}(\mathcal{M})$—in complete analogy to classical physics. Instead of focusing on a particular dynamics of probabilities induced, for instance, by a Schrödinger equation—as in the works of Hegerfeldt [19,20] or a continuity equation—as advocated in [7,8], we established the general kinematical structure. Nevertheless, our Definition 3 accurately encodes the common viewpoint on causality in quantum mechanics [4,8,51] in that it should be about the *flow of probability*.

The developed formalism allowed us for an analytical proof of causality of the evolution of measures modelled by the Dirac equation. To this end we have invoked the continuity equation (3), which provides a connection between our formalism and the works [6–8]. Surprisingly enough, we did not need to assume the positivity of energy of the wave packet. It shows that bizarre phenomena resulting from the interference of positive and negative frequency parts of the packet [53], such as Zitterbewegung [54], do not spoil the causal evolution of probabilities.

By a close inspection of the relativistic-Schrödinger equation, we were able to check the pertinence of the assumptions of Hegerfeldt's theorem. We have shown that the causality violation in this model is not restricted to localized initial states. In particular, Hegerfeldt's assumption (18) seems to be merely an artefact of his technique of proving Theorem 4. On the other hand, with the help of tools developed in Sec. III A we have quantified the causality breakdown in the relativistic-Schrödinger model and have confirmed its transient character detected in [17] for compactly supported initial states. The time scale of maximal violation of causality is 1 in natural units, i.e.,$\hbar/(mc^2)$, and the distances, where the effect is relevant, are of the order of the Compton wavelength $\hbar/(mc)$. This result, especially when contrasted with the nonrelativistic model (see Fig. 2), shows that the acausality of the relativistic-Schrödinger model is in fact irrelevant for all practical purposes.

C. Outlook

The potential usage of the proposed notion of causality is not limited to the two "basic" models studied in the present paper. As stressed at the beginning of Sec. III, within our formalism one can rigorously study the issue of causality in any, possibly nonlinear, dynamics of probability measures. With the help of the tools tailored to quantify the breakdown of causality, one can analyze different models of a given quantum phenomenon and promote the one that is the "closest" to satisfy Principle 1.

For instance, one could inspect from this point various models of atom-atom interactions in Bose-Einstein condensate [47], which lead to an effective evolution of the atomic cloud density governed by a modified Gross-Pitaevskii equation. With the help of our formalism, one may also study the sudden change in the character of the atom-atom interaction—from contact δ-type to long range—provoked by the Rydberg dressing of atoms in the condensate [55].

In the same vein, one could investigate the domain of applicability of modified Dirac dynamics of topological insulators [28,34] or address the fidelity of quantum simulators [56].

Let us observe that, somewhat in the same spirit, the principle of causality was invoked in [57] to demonstrate the advantage of the Unruh-deWitt model of detection in quantum field theory over the popular Glauber scheme. Curiously, the Unruh-deWitt detector was deemed more accurate in [57] despite the fact that it responds also to the negative field frequencies. This harmonizes with our results suggesting that to respect causality in the wave-packet formalism one should allow for negative energy components—as in the Dirac model—rather than forcing the positive frequencies—as in the relativistic-Schrödinger case.

We also emphasize that the usage of the "nonrelativistic" (cf. [16]) position operator $(\hat{x}\psi)(x) = x\psi(x)$ is not an essential feature of our formalism. As stressed in the Introduction, wave functions should not be considered as physical objects—they are just a way to compute probabilities [2]. In fact, we regard the probability measures on a given spacetime $\mathcal{M}$ as mixed states on the *commutative* C^*-algebra of observables $C_0(\mathcal{M})$. They can thus be seen as *potential outcomes of the measurement*—a channel transforming quantum information into the classical one [58]. One could choose to work with the "relativistic" position operator $\hat{x}_{\mathrm{NW}}$ of Newton and Wigner [18], as one can reexpress the probability measure obtained with $\hat{x}_{\mathrm{NW}}$ in terms of the standard "modulus square principle" via the Foldy-Wouthuysen transformation [16]. The corresponding transformed wave packets can never have compact spatial supports, but the question of causality can still be rigorously approached.

Let us conclude with an outlook into the potential extensions of the developed formalism. Since the framework of [31] is generally covariant, it seems natural to envisage an extension of the outcomes of Sec. III to curved spacetimes. The wave-packet formalism in the external gravitational field (see for instance [14]) is particularly useful in the study of neutrino oscillations [30]. Such an extension, which would require a covariant continuity equation for measures is, however, not that straightforward. The stumbling block is the foundational Theorem 2 in the optimal transport theory, which has been formulated only on $\mathbb{R}^n$.

For the sake of completeness, it would be also desirable to study the status of Principle 1 in the Klein-Gordon model. This would require an extension of our formalism to signed measures, as the density current in the latter model does not have a definite sign. A more radical generalization would consist of extending the causal relation onto the space $\mathscr{P}(\mathcal{M},\mathcal{B}(\mathcal{H}))$ of Borel probability measures on spacetime $\mathcal{M}$ with values in a, possibly noncommutative, algebra of observables $\mathcal{B}(\mathcal{H})$. Definition 1 can be easily adapted to this case: condition (i) stays unaltered, whereas the second requirement will take the form $\omega(J^+) = \mathrm{id}_{\mathcal{H}}$. The details of such a construction, in particular an analog of Theorem 1, require more care and remain to be unravelled. In this framework, one could construct positive-operator valued measures on $\mathcal{M}$ with the spacetime events regarded as possible outcomes of a generalized observable. With a definite causal order on $\mathscr{P}(\mathcal{M},\mathcal{B}(\mathcal{H}))$ one might be able to address the pertinent problem [59] of finding a unified framework for the study of quantum correlations between spacelike and timelike separated regions of spacetimes.

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