Necessity of negative Wigner function for tunneling

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(Received 14 April 2020; accepted 23 October 2020; published 15 December 2020)

We consider in what sense quantum tunneling is associated with nonclassical probabilistic behavior. We use the Wigner function quasiprobability picture. We give a definition of tunneling that allows us to say whether in a given scenario there is tunneling or not. We prove that this can only happen if the Wigner function is negative and/or a certain measurement operator which we call the tunneling rate operator has a negative Wigner function. We also investigate tunneling in postquantum theories.

DOI: 10.1103/PhysRevA.102.062210

I. INTRODUCTION

Quantum objects can "tunnel" into and through barriers. Tunneling plays a crucial role in a range of systems, including radioactivity [1], nanodevice quantum electronics [2], as well as adiabatic quantum computing and annealing [3]. It is both inherently interesting and technologically important.

While it appears well accepted that tunneling contrasts with classical mechanics, being a wavelike behavior exhibited by particles, from a quantum information science viewpoint one may wonder whether it is also nonclassical in a probability theory sense. For example, in the context of adiabatic quantum computing and annealing it is conjectured that tunneling plays a role in achieving quantum speedup in computations [3]. For this to be the case, we expect that tunneling should involve nonclassical probabilistic behavior, so that this process is nonclassical at the level of data and probabilities. In fact there are intriguing examples connecting tunneling with *negativity* in the quasiprobability Wigner function [4] representation of the quantum state [1,5,6]. We therefore here aim to clarify the relation between negative Wigner function and tunneling.

We give a clear mathematical definition of tunneling which allows us to clarify this relation. We prove mathematically that a nonzero tunneling rate necessitates a negative Wigner function. More specifically the Wigner function of the state and/or the tunneling rate operator have to contain negative values at some phase-space points (see Fig. 1). We thus make it concrete how tunneling is associated with negative Wigner function, a prototypical nonclassical probabilistic behavior. We show how to apply the main theorem to several examples, including explaining how positive Wigner function states can tunnel due to negativities in an operator associated with the energy.

To investigate the phenomenon more deeply we also consider whether postquantum theories could have a higher tunneling rate than quantum theory. This is analogous to how the postquantum Popescu-Rohrlich (PR) boxes, a hypothetical alternative to a pair of entangled quantum bits, have more Bell violation than the standard quantum theory, violating Tsirelson's bound [7]. We pose that as an open question and contribute tools for tackling it, by showing that the Wigner function, as a real-vector representation of quantum states, fits into the generalized probabilistic framework, thus allowing for a natural extension to postquantum theories.

We proceed as follows. First we give a brief technical introduction to tunneling and Wigner functions. Then we give our definition of tunneling and our main theorem. We discuss the interpretation of the theorem. Finally we consider tunneling and Wigner functions in postquantum theories.

A. Quantum tunneling

Quantum tunneling refers to the phenomenon where a quantum state with insufficient energy penetrates and/or passes through a potential barrier, which defies the laws of classical mechanics[1] [1]. It is usually demonstrated mathematically with energy eigenstates for a rectangular potential barrier [8–10]:

[1]Note on terminology: we have included the phenomenon, sometimes known as barrier penetration, as a case of tunneling. We therefore, for example, call the ground state of a quantum simple harmonic oscillator a tunneling state.

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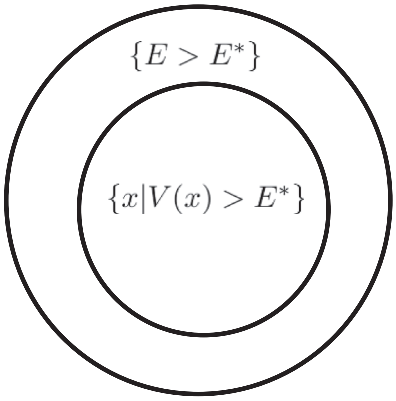

FIG. 1. Why negative quasiprobability is needed for tunneling. The phase-space points where the potential energy $V(x) > E^*$, for some given energy E^*, are a subset of the points for which the energy $E > E^*$. Thus for classical probability theory we have an inequality between the associated probabilities: $P(x|V(x) > E^*) \leqslant P(E > E^*)$. We define quantum tunneling as violation of this inequality. In the quantum phase space the Wigner function replaces the classical probability density, and the former can be negative, which makes violation of the inequality possible.

Definition 1: Standard definition of tunneling. For a system with a rectangular potential barrier with the form

$$V(x) = \begin{cases} V_0, & x \geqslant 0 \\ 0, & \text{otherwise}, \end{cases} \tag{1}$$

an energy eigenstate with definite energy E is a tunneling state if and only if $E < V_0$ and the probability of finding the state in the region $x \geqslant 0$ is nonzero.

Similar behaviors had been studied substantially in quantum systems in other potentials, such as series of rectangular barriers [11] and double wells [12], where there is a finite probability of locating an energy eigenstate in a classically forbidden region. However, it is difficult to conceive an analogous definition for quantum systems in a superposition of energy eigenstates or in a more complicated potential, because it is less clear what the corresponding classically forbidden regions are for both cases.

B. Phase-space formulation of quantum mechanics

In order to provide a more general definition of quantum tunneling and to understand this phenomenon in terms of nonclassical probabilistic behavior, we have chosen the phase-space formulation of quantum mechanics as the fundamental framework [4]. In this formulation, the state of a quantum system is described by a quasiprobability distribution, and observables are replaced by ordinary c-number functions in phase space. Mathematically, a quantum state described by a vector in the Hilbert-space formulation $|\psi\rangle = \int \psi(x)\,|x\rangle\,dx$ can be transformed to a real function *Wigner function* $W(x, p)$

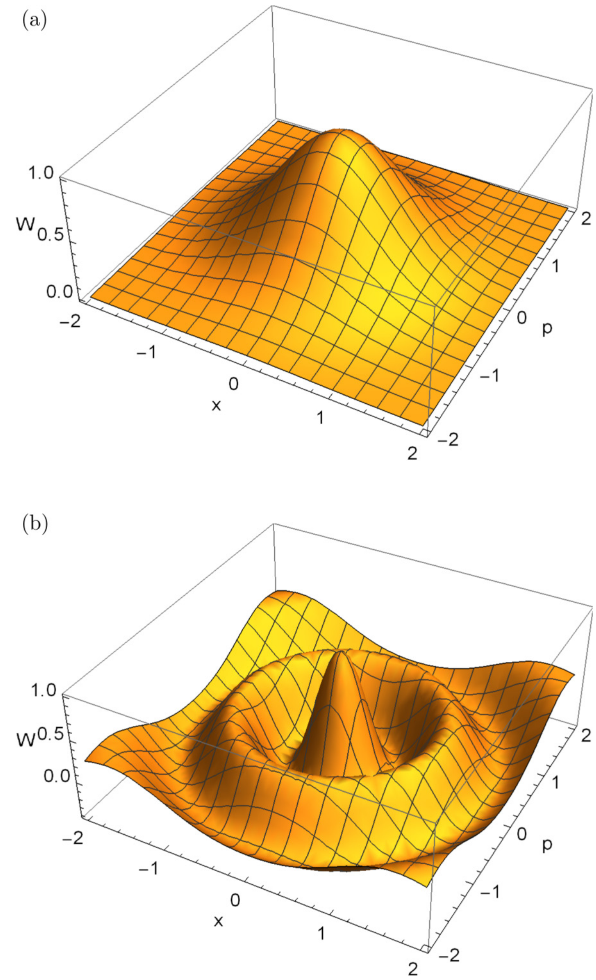

FIG. 2. Examples of Wigner functions $W(x, p)$. (a) Wigner function of the ground state of a quantum harmonic oscillator, which is positive everywhere and Gaussian. (b) Wigner function of the fourth excited state of a quantum harmonic oscillator, which has negative values in places and is non-Gaussian. x is in units of $\sqrt{\hbar/m\omega}$ and p is in units of $\sqrt{\hbar m\omega}$, where the parameters are defined in Sec. III B 2.

in the phase-space formulation as[2]

$$W(x, p) = \frac{1}{\pi\hbar}\int e^{2ipy/\hbar}\psi^*(x+y)\psi(x-y)\,dy. \tag{2}$$

Such a function satisfies the normalization condition $\int W(x, p)\,dx\,dp = 1$. However, Wigner functions cannot be considered legitimate joint probability distributions in phase space in general, as they can be negative, an example of which is shown in Fig. 2. It was demonstrated that a Wigner function of a pure continuous-variable state is positive if and only if the state is Gaussian, which is known as Hudson's theorem [13].

A more general approach to describe states and operators $\hat{\Omega}$ as phase-space functions $\mathcal{O}(x, p)$ is via the transformation,

$$\mathcal{O}(x, p) = \frac{1}{\pi\hbar}\int e^{2ipy/\hbar}\,\langle x+y|\hat{\Omega}|x-y\rangle\,dy, \tag{3}$$

[2]Note on notation: unless specified, all integral signs $\int \equiv \int_{-\infty}^{\infty}$ in this article.

and the inverse transformation, the Wigner transformation, given by the formula

$$\hat{\Omega} = \frac{1}{(2\pi)^2} \iiiint \mathcal{O}(x,p) e^{i[\alpha(\hat{X}-x)+\beta(\hat{P}-p)]}\, d\alpha\, d\beta\, dx\, dp. \tag{4}$$

It is clear, from Eqs. (2) and (3), that the Wigner function of a pure state is the Weyl transformation of a pure density operator $|\psi\rangle\langle\psi|$. With the fact that a general density operator is represented by $\hat{\rho} = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$, any mixed state in the phase-space representation is described by a convex sum of pure Wigner functions $W(x,p) = \sum_i \lambda_i W_i(x,p)$, where $W_i(x,p)$ are the pure Wigner functions and $\sum_i \lambda_i = 1$ (for normalized states).

Another point to note about the transition between Hilbert-space formulation to phase-space formulation of quantum mechanics is the preservation of the noncommutative nature of operators via the introduction of the star product, $\star$:

$$\star \equiv \exp\left[\frac{i\hbar}{2}(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x)\right]. \tag{5}$$

Here, $\overleftarrow{\partial}$ and $\overrightarrow{\partial}$ are used to denote left and right derivatives, respectively, which operates on a pair of functions as

$$\mathcal{O}_1 \overleftarrow{\partial}_x \mathcal{O}_2 = \frac{\partial \mathcal{O}_1}{\partial x}\mathcal{O}_2,$$
$$\mathcal{O}_1 \overrightarrow{\partial}_x \mathcal{O}_2 = \mathcal{O}_1 \frac{\partial \mathcal{O}_2}{\partial x},$$

and the exponential function could be understood as a shorthand notation of its standard power-series expansion $\exp(x) = \sum_{k=0}^{\infty} x^k/k!$.

Given the star product, the mapping can be written as

$$\hat{\Omega}_1\hat{\Omega}_2 \to \mathcal{O}_1(x,p) \star \mathcal{O}_2(x,p), \tag{6}$$

where $\mathcal{O}_i(x,p)$ is the Weyl transformation of the corresponding operator $\hat{\Omega}_i$.

In the phase-space formulation, the probability of a measurement outcome $P(\Omega = \omega) = \mathrm{Tr}(|\omega\rangle\langle\omega||\psi\rangle\langle\psi|)$ (where $\Omega|\omega\rangle = \omega|\omega\rangle$) for a quantum state $|\psi\rangle$ and a corresponding Wigner function $W_\psi(x,p)$ becomes

$$P(\Omega = \omega) = 2\pi\hbar \iint W_\omega(x,p) W_\psi(x,p)\, dx\, dp, \tag{7}$$

where $W_\omega(x,p)$ is the Wigner function of the state $|\omega\rangle$. In other words, this probability is simply the integral of the product of Wigner functions corresponding to the measurement outcome and the quantum state itself up to a normalization constant $2\pi\hbar$. This result is analogous to its classical counterpart described by a distribution function $f(x,p)$, where the probability of a dynamic variable $\Omega = \omega$ is given by

$$P(\Omega = \omega) = \iint \delta[\Omega(x,p) - \omega] f(x,p)\, dx\, dp, \tag{8}$$

where $\delta[\Omega(x,p) - \omega]$ is the Dirac delta function, which is zero everywhere except at $\Omega(x,p) = \omega$ and $\iint \delta[\Omega(x,p) - \omega]\, dx\, dp = 1$.

It should be clear that the probability corresponding to a measurement of a dynamic variable $\Omega = \omega$ is the inner product of the state of the system $f(x,p)$, and a function that describes the measurement of probability of a certain dynamic variable, which is known as an effect $\mathcal{E}$. For instance, in the examples above, the effects for calculating the probability $P(\Omega = \omega)$, $\mathcal{E}_{\Omega=\omega}(x,p)$ are $\delta[\Omega(x,p) - \omega]$ and $2\pi\hbar W_\omega(x,p)$ for classical and quantum cases, respectively.

C. Generalized probabilistic theories

From the brief discussions above, it is apparent that the mathematical structures of classical and quantum theories in phase space are rather similar to one another. Such similarities could have been anticipated by the fact that classical probability theories and finite-dimensional quantum theories can be described by a unified framework known as the generalized probabilistic theories (GPTs) [14].

A finite-dimensional probabilistic theory under the framework of GPTs has three major components:

a. Preparation. A state of a finite-dimensional system is represented by a real vector from a convex *state space* within a finite-dimensional vector space. The state space represents all possible states that the physical system can be in (including normalized states and subnormalized postoperation states) and is the convex hull of the set of allowed normalized states, or *pure states*, and the zero vector, or *null state*. Any state can therefore be described as a convex sum of pure states and the null state [7]. Here a state represents our knowledge about probabilities of outcomes on possible future measurements on the system.

b. Transformation. The evolution of any state vector is represented by a linear map that maps any state vector into another within the state space.

c. Measurement. The probability of a particular measurement outcome for any state is described by the inner product between the state vector and an *effect vector* corresponding to such measurement. The inner product calculated must be ranging between zero and 1 as a valid probability [15]. The set of valid effects is known as the *effect space*.

Under the GPT framework, it is possible to construct probabilistic theories other than classical and quantum theories by varying its state space, the effect space, and the set of allowed transformations, hence providing a way of generalizing existing theories into postquantum theories. It was shown via these constructed postquantum theories that certain quantum phenomena, such as nonunique decomposition of mixed states into pure states, and the no-cloning theorem [7,16], which were thought to be novel to quantum systems, were actually generic properties of generalized probabilistic theories. However, these studies are limited to finite-dimensional systems and therefore cannot be immediately applied to the study of quantum tunneling, which is normally treated as a wave-mechanical quantum phenomenon. Therefore, if it is possible to rewrite infinite-dimensional quantum mechanics in the framework of GPTs, we could determine whether tunneling is unique to quantum theories, and examine the phenomenon in postquantum theories.

II. RESULTS

A. Definition of tunneling

It is clear from the previous section that Definition 1 is too restrictive to describe the entire class of tunneling behavior. A general quantitative definition of tunneling is therefore required. It should be able to (i) recover Definition 1 as a special case, (ii) reflect the nonclassicality of the behavior, and (iii) supply quantitative criteria of tunneling for systems with general potentials and states without definite energy.

In order to construct such a definition of tunneling, we start with the law of conservation of energy for a classical particle in a potential $V(x)$. Due to the momentum p being a real number, classical kinetic energy $p^2/2m$ is positive. By conservation of energy, for a particle with energy E^*,

$$E^* - V(x) = \frac{p^2}{2m} \geqslant 0,$$
$$E^* \geqslant V(x). \tag{9}$$

This implies that a particle with energy E^* is not allowed in the region $\{x|V(x) > E^*\}$ classically, where x is a real variable representing position. Denote this region as $\mathcal{X}(E^*)$, the classically forbidden region for states with energy E^*. The inequality relationships of these energies then translates into subset relationships between their corresponding classically forbidden regions. Explicitly, consider two energies E_1^* and E_2^*, such that $E_1^* > E_2^*$. Since for all $x^* \in \mathcal{X}(E_1^*)$ implies $V(x^*) > E_1^*$ by definition, $V(x^*) > E_2$ and hence $x^* \in \mathcal{X}(E_2^*)$. Therefore, $E_1^* > E_2^*$ implies $\mathcal{X}(E_1^*) \subseteq \mathcal{X}(E_2^*)$. Classically, only a particle with energy $E > E^*$ is allowed to be in $\mathcal{X}(E^*)$, since (i) for $E = E^*$, $\mathcal{X}(E^*)$ is classically forbidden region, and (ii) for $E < E^*$, $\mathcal{X}(E^*) \subseteq \mathcal{X}(E)$ is also classically forbidden.

With the last concluding statement, and with the general principle that tunneling is a phenomenon that violates this classical constraint, we formulate the definition of tunneling to be the following.

Definition 2: General definition of tunneling. A state in a system with a potential given by $V(x)$ is tunneling if and only if there exists some energy E^*, such that the probability of locating the state in a region where $V(x) > E^*$ is greater than that of measuring the state to have energy $E > E^*$. Mathematically, a state is tunneling if, for the state,

$$\exists E^* : P(x|V(x) > E^*) > P(E > E^*).$$

Notice that this definition does not require the state in question to be quantum or classical, and therefore allows the definition to be applied as a condition of a general phenomenon on any physical systems, provided they can be described by energy and position as physical parameters. Naturally, for quantum systems, one cannot simultaneously measure the position and the energy of a state as their corresponding operators do not have simultaneous eigenstates. Yet, operationally, one can carry out this tunneling test by preparing identical copies of that state, and building up the statistics to get the probabilities. Here, some copies should be reserved for calculating the energy statistics, and others for the position statistics as the two observables do not commute. In addition to the benefits of providing an empirical recipe to determine whether a state is tunneling or not, another advantage of using such a general definition is its capacity for extension to other nonclassical behavior, such as reflection over a barrier as discussed in Appendix A.

B. Main theorem: Tunneling necessitates negative Wigner function

It has been observed in several examples that nonclassical behavior of quantum systems, such as tunneling, is associated with negativities in Wigner functions [1,5,6]. In this section, we use the general definition of tunneling to mathematically demonstrate and clarify the logical relations between the two.

Theorem 1: Necessary and sufficient phase-space condition for tunneling. A state represented by a distribution function $f(x, p)$ in phase space is tunneling if and only if there exists some E^*,

$$\iint [\mathcal{E}_{E>E^*} - \mathcal{E}_{\{x|V(x)>E^*\}}](x, p) f(x, p)\, dx\, dp < 0,$$

where $\mathcal{E}_{E>E^*}$ and $\mathcal{E}_{\{x|V(x)>E^*\}}$ are the effects associated with the probability of measuring the outcome $P(E > E^*)$ and $P(x|V(x) > E^*)$, respectively.

Proof. This statement is basically a rewritten form of the general definition. As by the definition of the effects $\mathcal{E}$ as stated in the theorem,

$$P(E > E^*) = \iint \mathcal{E}_{E>E^*}(x, p) f(x, p)\, dx\, dp,$$
$$P(x|V(x) > E^*) = \iint \mathcal{E}_{\{x|V(x)>E^*\}}(x, p) f(x, p)\, dx\, dp.$$

By Definition 2, the necessary and sufficient condition of tunneling is therefore $\exists E^*$:

$$P(E > E^*) - P(x|V(x) > E^*) < 0,$$
$$\iint [\mathcal{E}_{E>E^*} - \mathcal{E}_{\{x|V(x)>E^*\}}](x, p) f(x, p)\, dx\, dp < 0,$$

which is the theorem to be proved. ■

The theorem therefore shows that tunneling is related to the distribution function and $\mathcal{E}_{E>E^*} - \mathcal{E}_{\{x|V(x)>E^*\}}$, and the latter is denoted as $\Delta\mathcal{E}_{E^*}$, the *tunneling rate operator* at E^*. Two important consequences of Theorem 1 are as follows:

Corollary 1. A state is nontunneling if, for every energy E^*, the tunneling rate operator and the distribution function are non-negative everywhere in the phase space.

Proof. From the above, and the fact that a state is either tunneling or not, a state is nontunneling if, for all E^*, $\iint \Delta\mathcal{E}_{E^*}(x, p) f(x, p)\, dx\, dp \geqslant 0$. It is clear that if both $\Delta\mathcal{E}_{E^*}(x, p)$ and $f(x, p)$ are non-negative over all of phase space, then this condition will hold. ■

Corollary 2. If a state is tunneling, then either the tunneling rate operator at some E^* and/or the distribution function contain negativities.

Proof. By directly replacing the differences in effects with the tunneling rate operator in Theorem 1, for some energy E^*,

$$\iint [\mathcal{E}_{E>E^*} - \mathcal{E}_{\{x|V(x)>E^*\}}](x, p) f(x, p)\, dx\, dp < 0,$$
$$\iint \Delta\mathcal{E}_{E^*}(x, p) f(x, p)\, dx\, dp < 0.$$

As it is impossible for the statement above to hold if any of the two functions $\Delta\mathcal{E}_{E^*}(x, p)$ or $f(x, p)$ are positive over the entire phase space, then at least one of them must contain negativities. ■

The last statement demonstrates the main claim of this article: Under a phase-space framework, tunneling implies negativities in the distribution representing the state and/or the tunneling rate operator at some energy levels. In the case of quantum systems, tunneling implies negativities in the Wigner function of the state and/or the tunneling rate operator.

However, it is worth noting that it is still possible to have negativities in either of these two functions and a nontunneling state. An illustration of this can be found in Sec. III B 2.

III. DISCUSSION

A. Quantum versus classical case

The results of the previous section can immediately be applied to the study of generic behaviors of classical and quantum theories. One important result is that classical phase-space mechanics does not allow tunneling, because as shown in Appendix B, both the phase-space distributions representing a state and the tunneling rate operator do not contain non-negativities, and by Corollary 1, classical states cannot tunnel. However, in quantum theories, the non-negativity conditions of the functions are relaxed. This can be attributed to the following two elements of quantum phase-space theory:

a. Wigner function as quasiprobability distribution. A quantum state in phase space is represented by the Wigner function, which generally contains negative values in general.

b. Deformation of effect $\mathcal{E}_{E>E^*}$. Generally speaking, the effect $\mathcal{E}_{\{x|V(x)>E^*\}}$ is identical for the both classical and quantum cases, whereas the effect $\mathcal{E}_{E>E^*}$ is altered in the quantum case.

We show that both phenomena can be explained by the alteration in the eigenvalue equations for the phase-space position and Hamiltonian operators, respectively. Generally, for any dynamical variables $\Omega(x,p)$, for both classical and quantum systems, their eigenstate with respect to the corresponding algebra has definite value ω if one conducts a measurement of Ω on the system.

Consider first the dynamical variable x as the position. The eigenvalue equation in classical systems with eigenstate $f_0(x,p)$ and eigenvalue x_0 is

$$x f_0(x,p) = x_0 f_0(x,p), \tag{10}$$

and this equation has an obvious solution of $f_0(x,p)=\delta(x-x_0)g(p)$, where g is an arbitrary positive real function which is normalized to unity: $\int g(p)\,dp = 1$. If the state in question is of such a form, the measurement of position on the state must give $x = x_0$. Similarly, to measure the probability of a given state with a position of x for some set $\mathcal{X}$, the corresponding effect could be constructed out of these δ functions such that $\mathcal{E}_{x\in\mathcal{X}} = \int_{x_0\in\mathcal{X}} \delta(x-x_0)\,dx_0 = I_{\mathcal{X}}(x)$, where the indicator function $I_{\mathcal{X}}(x)$ is 1 when $x\in\mathcal{X}$ and zero otherwise.

In the case of quantum systems, the product of any operators is replaced by the star product of functions as a result of deformation quantization. Therefore, the eigenvalue problem is mapped to an equation with position eigenstate $W_0(x,p)$ and eigenvalue x_0:

$$x \star W_0(x,p) = x_0 W_0(x,p). \tag{11}$$

One simple way of solving the problem is to switch back to the Hilbert-space picture, where the equivalent problem is $\langle x|\hat{X}|\psi_0\rangle = x_0\langle x|\psi_0\rangle$, which has a well-known solution of $\langle x|\psi_0\rangle = \psi_0(x) = \delta(x-x_0)$. The Wigner function for such a state is given by

$$\begin{aligned}
&\frac{1}{\pi\hbar}\int e^{2ipy/\hbar}\delta(x-x_0+y)\delta(x-x_0-y)\,dy\\
&=\frac{1}{\pi\hbar}e^{2ip(x-x_0)/\hbar}\delta[x-x_0+(x-x_0)]\\
&=\frac{1}{\pi\hbar}e^{2ip(x-x_0)}\frac{1}{2}\delta(x-x_0)\\
&=\frac{1}{2\pi\hbar}\delta(x-x_0),
\end{aligned} \tag{12}$$

which is again of the form of a Dirac delta function in position space after integrating away the momentum dependence. By the duality of effects and states in quantum theory, the effect for $x\in\mathcal{X}$ is therefore $\mathcal{E}_{x\in\mathcal{X}} = 2\pi\hbar\int_{x\in\mathcal{X}} W_0(x,p)\,dx_0 = I_{\mathcal{X}}(x)$. Therefore, the effects corresponding to measurement in position space are identical, which implies $\mathcal{E}_{\{x|V(x)>E^*\}}$ is of the same form for both classical and quantum calculations.

However, this is not the case for $\mathcal{E}_{E>E^*}$. The energy eigenstate $f_E(x,p)$ with energy E for a classical system satisfies

$$H(x,p)f_E(x,p) = E f_E(x,p), \tag{13}$$

which gives $f_E(x,p)\sim\delta[H(x,p)-E]$. The quantum energy eigenvalue equation in phase space for an energy eigenstate $W_E(x,p)$ and energy E, however, is altered to be

$$H(x,p)\star W_E(x,p) = E W_E(x,p). \tag{14}$$

Here, the energy eigenstate as a Weyl map of $\hat{\rho} = |E\rangle\langle E|$ is no longer of the form $\delta[H(x,p)-E]$, as the introduction of the star product implies the functional dependence of the energy eigenstate is no longer purely on the functional form of the dynamical variable. This can be seen by the Bopp shift representation of star product (5), where the functional dependence of the energy eigenstate depends also on the position and momentum derivatives of the Hamiltonian function. Therefore, the energy eigenstate $\mathcal{E}_{E>E^*}$ is not identical to its classical counterpart.

With the energy effect $\mathcal{E}_{E>E^*}(x,p) = 2\pi\hbar\int_{E^*}^{\infty} W_{E'}(x,p)\,dE'$, and the fact that Wigner functions are generally not completely positive, $\mathcal{E}_{E>E^*}(x,p)$ generally contains negativity. Therefore, the function $\Delta\mathcal{E}_{E^*}$ generally contains negativity, given that $\mathcal{E}_{\{x|V(x)>E^*\}}$ is non-negative. This demonstrates how this operator can violate the classical case by containing negativities.

B. Tunneling in pure Gaussian states

A special class of states in quantum mechanics is pure Gaussian states, which have non-negative Wigner functions in the phase-space representation. By Corollary 1, a statement for Gaussian states could be made as follows:

Corollary 3. A pure Gaussian state can tunnel only if the function $\Delta\mathcal{E}_{E^*}$ contains negativities for some E^*.

Proof. By Corollary 1, if a state is tunneling, then either $\Delta\mathcal{E}_{E^*}(x,p)$ or $W(x,p)$ contains negativities for some energy E^*. By Hudson's theorem [13], the Wigner function representing the Gaussian state is non-negative over all of phase space. Therefore, if a pure Gaussian state is tunneling, then $\Delta\mathcal{E}_{E^*}$ must contain negativities for some energy E^*. ■

This corollary serves two purposes. First of all, since a pure Gaussian state is represented by a positive Wigner function over phase space, it is often considered to be a valid joint probability distribution and as the "least nonclassical" state [17]. This corollary serves as a reminder that, despite it being true that negativity in Wigner functions as distribution functions is a novel feature in phase-space quantum theory, a completely positive Wigner function can still exhibit nonclassical behaviors, which, in this specific case, is due to the deformation in effects as discussed in the last section. It has been demonstrated that the subtheory of Gaussian quantum mechanics can be constructed by imposing certain epistemic restrictions on classical phase-space mechanics [18], in which only Gaussian states, measurements, and operations are considered. This reinforces the conclusion that the tunneling rate operator corresponding to the measurements in question is the culprit for a pure Gaussian state to exhibit tunneling; otherwise, the state would be analogous to a classical one and cannot tunnel.

Second, the discussion of tunneling in pure Gaussian states allows for simplified examples of the application of the previous results, as the tunneling rate operator $\Delta\mathcal{E}_{E^*}$ determines the tunneling behavior of these pure Gaussian states. Consider the following two examples of pure Gaussian states.

1. Quantum tunneling of wave packets

Wave-packet states, quasilocalized superpositions of energy eigenstates, are often used in the study of quantum tunneling and quantum mechanics problems [8,19]. By studying Gaussian wave packets incident on a rectangular potential barrier, one also introduces dynamical aspects into the problem of tunneling, as the position probability distribution of a quantum system now changes over time due to the relative phase differences between the different components of its energy eigenstates.

A Gaussian wave packet that centers at position $x = x_0$ and momentum $p = p_0$, with uncertainty in position as $\Delta x = \sigma_x$, has the form

$$\psi(x) = \left(\frac{1}{2\pi\sigma_x^2}\right)^{1/4} \exp\left[-\frac{(x-x_0)^2}{4\sigma_x^2}\right] \exp\left(\frac{ip_0x}{\hbar}\right), \quad (15)$$

which has a Gaussian distribution over position space,

$$P(x) = \sqrt{\frac{1}{2\pi\sigma_x^2}} \exp\left[-\frac{(x-x_0)^2}{2\sigma_x^2}\right]. \quad (16)$$

It is possible to solve for the dynamics of the Gaussian wave packet as the superposition of time-dependent energy eigenstates of the rectangular potential barrier, or via numerical simulation of the Schrödinger equation. An example of such a simulation is shown in Fig. 3, where a wave packet, with initial Gaussian shape and average energy lower than the potential height, passes through the barrier, and the Gaussian nature of the wave packet is destroyed.

The fact that there is no definite energy for such a Gaussian wave packet creates difficulties in applying the standard definition of tunneling to this case. However, using our general

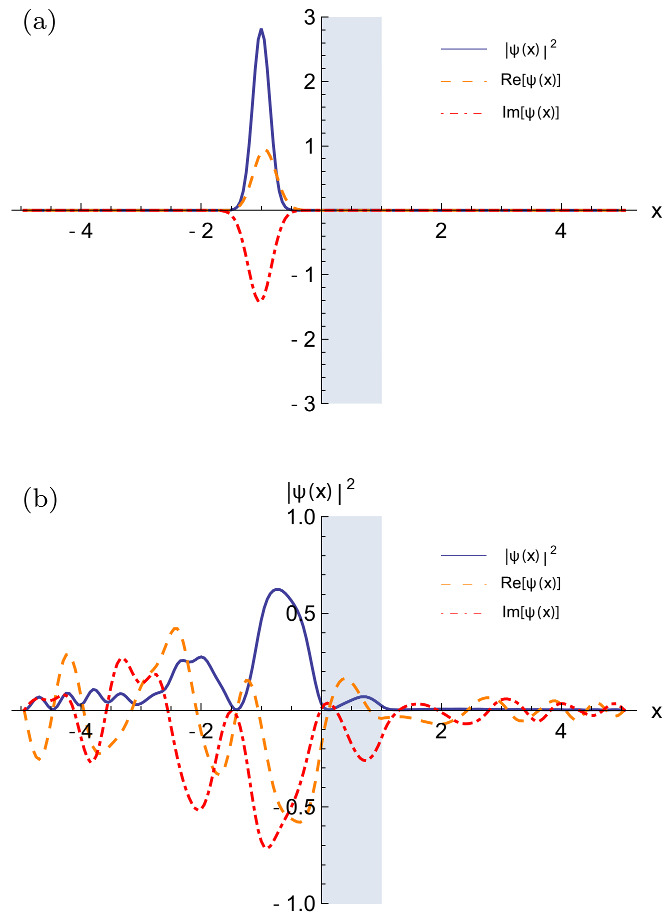

FIG. 3. The probability distribution, real and imaginary components of the wave function of a Gaussian wave packet tunneling through a barrier (a) before and (b) while "passing" the barrier. The unit for x is $\sqrt{\hbar/mV_0}$, where V_0 is as defined in Eq. (1).

definition, it could be demonstrated that such a state is indeed tunneling at certain times during the propagation of the wave packet, as $\exists E^* : P(E > E^*) > P(x|V(x) > E^*)$ as shown in Fig. 4. The detailed calculations can be found in Appendix C.

2. Simple harmonic oscillator

A simple harmonic oscillator has a potential of the form

$$V(x) = \tfrac{1}{2}m\omega^2x^2, \quad (17)$$

where m is the mass of the particle, and ω is the angular frequency of the oscillator. A simple harmonic oscillator is one of the most well-studied potentials in physics, and has many nice features that are exploited in both classical and quantum theories.

A particle as a classical simple harmonic oscillator will oscillate sinusoidally [20]:

$$x(t) = C\cos(\omega t + \phi), \quad (18)$$

where the amplitude C and the phase ϕ depend on the initial conditions of the particle. By conservation of energy, a particle with energy E is only allowed to be in

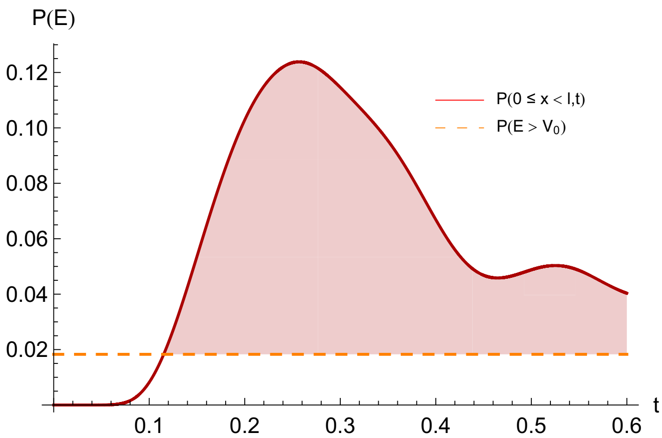

FIG. 4. Plot of probabilities $P(0 \leqslant x < l)$ (bold) and $P(E > V_0)$ (dashed) for a Gaussian wave packet tunneling through a barrier as a function of time t. At times that $P(0 \leqslant x < l, t) \geqslant P(E > V_0)$, the state is considered to be tunneling. The unit of t is $\hbar/V_0$.

the region $-\sqrt{2E/m\omega^2} \leqslant x \leqslant \sqrt{2E/m\omega^2}$, for otherwise the particle would have negative kinetic energy.

In the quantum case, the wave function of interest is the ground state of the quantum harmonic oscillator, $\psi_0(x) = \langle x|0\rangle$, which can be solved by the equation $\langle x|\hat{a}|0\rangle = 0$, where $\hat{a}$ is the annihilation operator [8–10]. Solving the equation would give the solution

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right), \tag{19}$$

which has a Gaussian waveform. Since this energy eigenstate has energy $E_0 = \hbar\omega/2$, and the Gaussian wave function has nonzero amplitudes over the entire position space, there is nonzero probability of finding the ground state in the classically forbidden region where $V(x) > \hbar\omega/2$, hence $P(x|V(x) > E_0) > P(E > E_0)$, satisfying the criteria of tunneling. This phenomenon also applies to excited states, which can be clearly seen in Fig. 5.

To mathematically develop the statement about whether the ground state is indeed tunneling from the viewpoint of the phase space, one could refer to Corollary 3 and consider the operator $\Delta\mathcal{E}_{E^*}$ at $E^* = E_0 = \hbar\omega/2$. It can be shown, in Appendix D, that such an operator for the quantum case is calculated to be

$$\Delta\mathcal{E}_{E_0}(x,p) = \begin{cases} -2\exp\left(-\frac{m\omega x^2}{\hbar}\right)\exp\left(-\frac{p^2}{m\omega\hbar}\right) & \text{for } V(x) > E_0, \\ 1 - 2\exp\left(-\frac{m\omega x^2}{\hbar}\right)\exp\left(-\frac{p^2}{m\omega\hbar}\right) & \text{otherwise,} \end{cases} \tag{20}$$

which contains negativities, indicating the ground state of a quantum harmonic oscillator can tunnel. To demonstrate such a state is indeed tunneling, one could calculate the inner product between this tunneling rate operator and the Wigner function of the ground state, which is indeed negative as shown in Appendix D. By Theorem 1, the ground state of a quantum harmonic oscillator is a tunneling state.

By modifying the ground state of a simple harmonic oscillator, it is possible to construct a scenario where there are

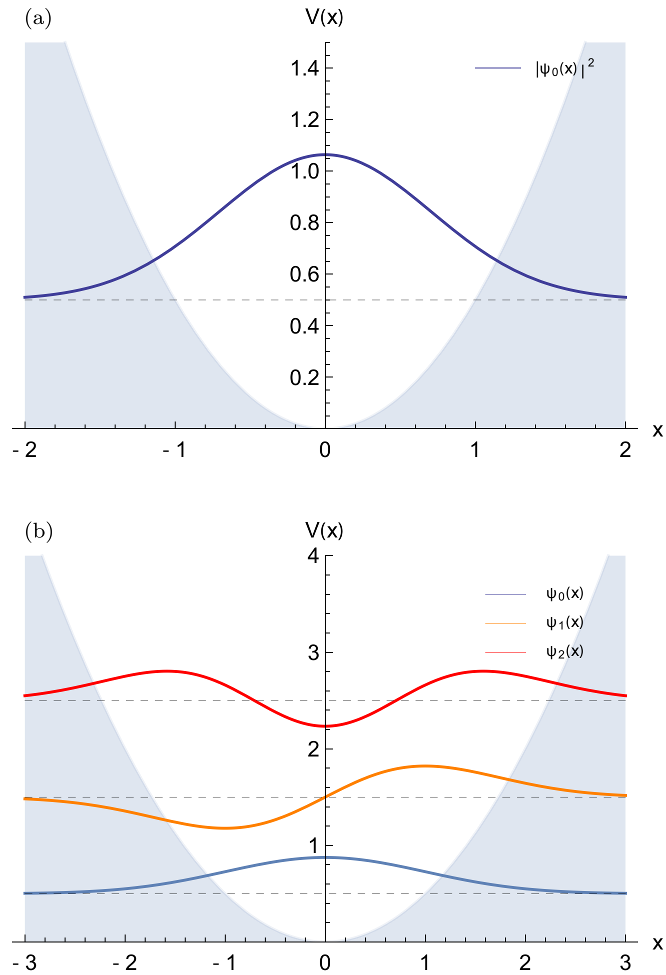

FIG. 5. (a) Probability distribution of locating the ground state of the quantum harmonic oscillator. (b) Wave functions of the first three eigenstates of the quantum harmonic oscillator (states shown in descending order, from top to bottom, of their respective energy levels). The dashed lines represent the zeros of the corresponding wave functions and probabilities, with its value being its eigenenergy level. The shaded region specifies the classically forbidden region. x is in units of $\sqrt{\hbar/m\omega}$, and $V(x)$ and the energy levels are in units of $\hbar\omega$.

negativities in both the state and the tunneling operator but the state is not classified to be tunneling. Construct a wave function:

$$\psi(x) = \begin{cases} \mathcal{N}\psi_0(x) & \text{when } V(x) > E_0 \\ 0 & \text{otherwise,} \end{cases}$$

where $\mathcal{N}$ is the normalization factor such that $\int \psi(x)\,dx = 0$. Consider first for energy levels $E^* > E_0$, $P(x|V(x) > E^*) = 0$ and therefore $P(x|V(x) > E^*) \leqslant P(E > E^*)$ necessarily. Consider next for energy levels $E^* \leqslant E_0$, given that the eigenenergies of such a system have to be higher than that of the ground-state energy, $P(E > E^*) = 1$, and therefore again $P(x|V(x) > E^*) \leqslant P(E > E^*)$. Combining both cases, this state is not a tunneling state by Definition 2. However, since the constructed state $\psi(x)$ is not Gaussian, by Hudson's theorem, the Wigner representation of such a state must contain negativity. Also, the tunneling operator at $E^* = E_0$, as an example, also contains negativity.

C. Wigner function as example of generalized probabilistic theory

In order to demonstrate that phase-space quantum theory can be structured under the generalized probabilistic theory framework, it is necessary to recover the mathematical objects corresponding to the three components of a GPT.

1. Preparation. A state of a one-spatial-dimensional quantum state can be described by a Wigner function $W(x, p)$, which is essentially the Weyl transformation of a density operator representing that quantum state in Hilbert-space formulation. However, there may be difficulties in designating such state as a real vector, which is demanded by the framework of GPT, for mathematical manipulations may not be well behaved for objects in infinite-dimensional spaces [9].

Nonetheless, real functions $f(x, p)$ in the phase space can be considered vectors in a vector space, with the vector addition as addition of functions and scalar multiplication as multiplying a scalar [21], in which the set of valid phase-space functions, or the state space, is a subset. In addition, one can define an inner product on such a vector space such that, for any two functions Ω_1 and Ω_2,

$$\langle \Omega_1, \Omega_2 \rangle = \iint \Omega_1(x, p)\Omega_2^*(x, p)\, dx\, dp, \tag{21}$$

such that a Wigner function corresponding to a pure state is square integrable,

$$\iint |W(x, p)|^2\, dx\, dp = \frac{1}{2\pi\hbar}, \tag{22}$$

which implies that the function converges and the inner product exists for these states as a sign of well-behaved theory. Moreover, for general normalized states that are represented by $\hat{\rho} = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$ with $\sum_i \lambda_i = 1$ and $0 \leqslant \lambda_i \leqslant 1$, the Wigner representation is

$$\begin{aligned} &\frac{1}{\pi\hbar}\int e^{2ipy/\hbar}\langle x - y|\sum_i \lambda_i|\psi_i\rangle\langle\psi_i|x + y\rangle\; dy \\ &\quad = \sum_i \lambda_i W_i(x, p), \end{aligned} \tag{23}$$

where $W_i(x, p)$ are Wigner functions corresponding to the pure states $|\psi_i\rangle\langle\psi_i|$. In this case, since $\sum_i \lambda_i = 1$, these Wigner functions correspond to the normalized states, and therefore any normalized state is a convex sum of the pure states W_i. Therefore, it is demonstrated that the Wigner functions corresponding to the pure states are the extremal states of the GPT, and the set of normalized states is the convex hull of such extremal states. Therefore, these normalized mixed states are square integrable as well, as

$$\begin{aligned} &\iint W^2(x, p)\, dx\, dp \\ &= \iint \left[\sum_i \lambda_i W_i(x, p)\right]^2 dx\, dp \\ &= \sum_{i,j} \lambda_i\lambda_j \iint W_i(x, p)W_j(x, p)\, dx\, dp \\ &\leqslant \sum_i \frac{\lambda_i^2}{2\pi\hbar} + \sum_{i\neq j}\frac{\lambda_i\lambda_j}{2\pi\hbar}\frac{1}{2\pi\hbar}\left(\sum_i \lambda_i\right)^2 = \frac{1}{2\pi\hbar}, \end{aligned} \tag{24}$$

which implies $1/2\pi\hbar$ is the maximum of the square integral of any Wigner function. In fact, such a result is related to the purity measure $\mu \equiv \mathrm{Tr}(\hat{\rho}^2)$. This measure can be mapped to

$$\mathrm{Tr}(\hat{\rho}^2) = 2\pi\hbar \iint W^2(x, p)\, dx\, dp = \mu, \tag{25}$$

where $0 \leqslant \mu \leqslant 1$, with $0 \leqslant 2\pi\hbar \iint W_i(x, p)W_j(x, p) \leqslant 1$. This implies the square integral, or the inner product of the state on itself, or geometrically the square of the length of the state vector, is linearly related to purity. An interesting comparison to be made here is that the length of a vector in the Bloch sphere corresponds also to the purity measure of a qubit, and that in quantum theory of qubits, such length is also related to the uncertainty of a state.

Subnormalized states can be generated by rescaling a normalized Wigner function with some non-negative constant $\nu \leqslant 1$ and therefore, in general, any state can be expressed as

$$W(x, p) = \nu \sum_i \lambda_i W_i(x, p) = \sum_i \lambda_i[\nu W_i(x, p)], \tag{26}$$

as the convex sum of extremal states and the null vector. Therefore, the states of phase-space formulation concur with the requirements of the GPT framework.

There is, however, one caveat: The conventional Wigner representation of a position eigenstate is linearly related to a Dirac delta function $\delta(x - x_0)$. This state is not well behaved in the sense that the square integral of the function diverges, causing problems in defining the inner product of such vector space as the integral of two phase-space functions. Nonetheless, it should be noted that the same problem arises in the Hilbert-space formulation of quantum theory, where the wave function of a position eigenstate is not considered to be a state in Hilbert space and therefore does not correspond to a physical state [9]. Therefore, the introduction of such states in the GPT framework does not lead to additional nonphysical features other than the ones inherent in the conventional quantum theory [9].

2. Transformation. The set of valid transformations is the set of functions with star product as the Weyl transform of transformations in the Hilbert-space formulation. An example of such transformation is the unitary evolution of state. The Weyl transformation of such an evolution is given by

$$\hat{U}\rho\hat{U}^\dagger \rightarrow U(x, p) \star W(x, p) \star U^*(x, p),$$

where $U(x, p)$ is the Weyl transform of the unitary operator $\hat{U}$. It can be demonstrated that complex conjugate transposition of an operator in the Hilbert-space formulation is mapped to a complex conjugation of the phase-space function, or $(U^\dagger)(x, p) = U^*(x, p)$.

Therefore, the unitary condition for a reversible transformation is expressed as

$$\hat{U}^\dagger \hat{U} = \mathbf{1} \to U^*(x,p) \star U(x,p) = 1.$$

It is also interesting to note that unitary transformations preserve purity by

$$\mathrm{Tr}([\hat{U}\hat{\rho}\hat{U}^\dagger]^2) = \mathrm{Tr}(\hat{U}\hat{\rho}^2\hat{U}^\dagger) = \mathrm{Tr}(\hat{U}^\dagger\hat{U}\hat{\rho}^2) = \mathrm{Tr}(\hat{\rho}^2).$$

In the phase-space formulation, this is equivalent to the case where the unitary transformations preserve the length of the state vector. In general, unitary transformations preserve the inner products between two states, and therefore in the phase-space picture such transformations resemble an orthogonal transformation, despite the dimension of the state space being infinite. This feature is analogous to the isomorphism between SU(2) and SO(3) in the Bloch sphere representation of quantum theory of qubits.

In order to demonstrate that transformations in the phase-space formulation of quantum theory concur with that of a GPT, it is necessary to demonstrate that such transformations are linear. Since it is the case in the Hilbert-space formulation that a transformation, represented by a completely positive and trace preserving (CPTP) map as $\hat{\Phi}$, must be linear, by the Weyl transformation,

$$\hat{\Phi}\left(\sum_i \lambda_i \hat{\rho}_i\right) = \sum_i \lambda_i \hat{\Phi}(\hat{\rho}_i),$$
$$\Phi(x,p) \star \sum_i \lambda_i W_i(x,p) = \sum_i \lambda_i \Phi(x,p) \star W_i(x,p),$$

where $\Phi(x,p)$ is the operator in phase-space representation, and $W_i(x,p)$ are Wigner functions corresponding to density operators $\hat{\rho}_i$. This can also be seen from the construction of star product (5), where the fact that the operators $\vec{\partial}_x$ and $\vec{\partial}_p$ are linear implies that the star product as an expansion of these operators is linear as well, and therefore is consistent with the formulation of transformation in a GPT.

It is also relatively straightforward to demonstrate that such transformations map any valid state into another by directly converting such result from the Hilbert-space formulation via the Weyl transformation. Since it is the case that each state in the Hilbert-space formulation can be mapped to a Wigner function as a valid state, and that each CPTP map is a transformation that maps one valid state into another, it must be the case that these transformations in the phase-space formulation map any state into valid states.

3. Measurement. The set of valid effects in the phase-space formulation is the set of functions as the Weyl transformation of positive operator valued measurements, or POVMs, in the Hilbert-space formulation. In particular, the set of pure effects $\mathcal{E}_i$ are the phase-space functions corresponding to projective measurement in the form $\hat{\Pi}_i = |\omega_i\rangle\langle\omega_i|$, such that

$$\mathcal{E}_i(x,p) = 2\int e^{2ipy/\hbar}\langle x-y|\hat{\Pi}_i|x+y\rangle\, dy$$
$$= 2\int e^{2ipy/\hbar}\langle x-y|\omega_i\rangle\langle\omega_i|x+y\rangle\, dy,$$

which is isomorphic to the set of pure states.

Notice that under the Weyl transformation, a probability of some event corresponding to ω_i occurring is given by the inner product of the effect $\mathcal{E}_i$ and the state W,

$$\mathrm{Tr}(\hat{\Pi}_i\hat{\rho}) \to \iint \mathcal{E}_i(x,p)W(x,p)\,dx\,dp.$$

Here, the probabilities satisfy $0 \leqslant \mathrm{Tr}(\hat{\Pi}_i\hat{\rho}) \leqslant 1$. These projectors correspond to a measurement summing to identity by the completeness equation, and the set of orthogonal eigenstates is mapped to a set of orthogonal functions in phase space as shown in Appendix E. Therefore, for some projection operators $\hat{\Pi}$ corresponding to multiple outcomes, $0 \leqslant \mathrm{Tr}(\hat{\Pi}\hat{\rho}) \leqslant \mathrm{Tr}(\mathbf{1}\hat{\rho}) \leqslant 1$. Hence, for general states and general effects, the inner product has the upper bound

$$\mathrm{Tr}\left(\sum_i \mu_i\hat{\Pi}_i \sum_j \lambda_j |\psi_j\rangle\langle\psi_j|\right)$$
$$= \sum_{i,j}\mu_i\lambda_j \mathrm{Tr}(\hat{\Pi}_i|\psi_j\rangle\langle\psi_j|)$$
$$\leqslant \sum_{i,j}\mu_i\lambda_j \leqslant \left(\sum_i \mu_i\right)^2\left(\sum_j \lambda_j\right)^2 \leqslant 1, \tag{27}$$

by the Cauchy-Schwarz inequality and the conditions $\sum_i \mu_i \leqslant 1$ and $\sum_j \lambda_j \leqslant 1$. This inner product is also non-negative, as $0 \leqslant \mu_i, \lambda_j \leqslant 1$ and the trace of pure states and pure effects must be non-negative. By mapping these results into the phase-space formulation, these effects satisfy the requirement of the GPT framework as to give valid probability values under the inner product with any states in state space.

IV. TUNNELING IN POSTQUANTUM THEORIES

To study the phenomenon of tunneling in postquantum theories, one will have to devise a method of consistently extending the existing state space in the phase-space picture to include nonphysical states. Extension of the state space is relatively easy with the Wigner function representation, as by varying the values of the Wigner function at some phase-space points, it is possible to generate a nonphysical state. The difficulty, however, lies in construction of the corresponding effect space, and the physical interpretation of these postquantum states. While a complete postquantum theory is not devised in this article, some preliminary work on Gaussian states is carried out as a precursor towards an eventual development of a postquantum phase-space theory.

A Gaussian bivariate distribution in phase space $W_G(x,p)$ has the form [18]

$$W_G(x,p) = \frac{1}{2\pi\det(\gamma)^{1/2}}\exp\left[-\frac{1}{2}(\vec{x}-\vec{\mu})^T\gamma^{-1}(\vec{x}-\vec{\mu})\right], \tag{28}$$

where $\vec{x}$ is a vector of coordinates, $\vec{\mu}$ is a vector of mean values of coordinates, and γ is the covariance matrix, where γ_{ij} is the covariance of the ith and jth coordinates. A possible way of generalizing the existing state space is to include Gaussian distributions that violate the purity condition (25), such that

$$\mu = 2\pi\hbar\iint W_G^2(x,p)\,dx\,dp > 1. \tag{29}$$

The main advantage of considering only Gaussian distributions as postquantum states is that it is a proper joint probability distribution in phase space, and therefore such an object gives proper probabilities when one conducts measurement in position or momentum space. Another advantage is that such a distribution is positive over all phase space, and therefore, by Corollary 3, any analysis of tunneling on these postquantum states is dependent only on the effects $\mathcal{E}_{E>E^*}$ and $\mathcal{E}_{\{x|V(x)>E^*\}}$, provided that the effects remain valid under such an extension of state space.

It is interesting to note the physical meaning behind extension of purity. One way of understanding such an extension is to calculate the variances in both position and momentum for $W_G(x, p)$. Since it is the property of a Gaussian bivariate distribution to yield a Gaussian distribution in one coordinate after integrating the distribution over the other coordinate, the variances in x and p are simply $\sigma_x^2 = \gamma_{xx}$ and $\sigma_p^2 = \gamma_{pp}$. For a state with given purity μ,

$$\mu = \frac{2\pi\hbar}{4\pi\sqrt{\sigma_x^2\sigma_p^2 - \gamma_{xp}^2}} \geqslant \frac{\hbar}{2\sqrt{\sigma_x^2\sigma_p^2}}, \tag{30}$$

since $\gamma_{xp}^2 \geqslant 0$. This implies that $\sigma_x\sigma_p \geqslant \hbar/(2\mu)$. The final result of the calculation closely resembles the uncertainty principle. In fact, if one substitutes $\mu = 1$ as the condition of a pure state, the uncertainty principle is recovered. Therefore, by relaxing the purity relation to states that have $\mu > 1$, the lower bound of the uncertainties $\sigma_x\sigma_p$ reaches below the lower bound allowed by quantum theory, and therefore violates the quantum uncertainty principle. This matches the intuition on an extreme case where a Dirac delta function $\delta(x - x_0)\delta(p - p_0)$, which represents a distribution with perfect information of both position and momentum, is a state with infinite purity μ since $\iint \delta^2(x - x_0)\delta^2(p - p_0)\,dx\,dp \to \infty$, which maximally violates the uncertainty principle.

It should be noted that certain studies had related purity and uncertainty before [22]; yet the results are limited to purity being in the range $0 \leqslant \mu \leqslant 1$. Nonetheless, the practical implication of this result is that one can simply change the purity condition and generate postquantum states according to Eq. (29) by altering the covariant matrix γ in Eq. (28).

Another way of interpreting the violation of the purity condition is to look at the Hilbert-space formulation of quantum mechanics. For a general state $W(x, p)$ such that it is real, it is mapped by Wigner transformation to an operator $\hat{\rho}$ such that $\hat{\rho}^\dagger = \hat{\rho}$, or the reality condition of a Wigner function is mapped to the Hermiticity of the density operator. Since it is possible to find an eigendecomposition for any Hermitian operators [10], one can write a density operator as $\hat{\rho} = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$, where λ_i are eigenvalues corresponding to $|\psi_i\rangle$ as the ith eigenvector. In this representation, by the orthogonality of eigenvectors, purity is simply $\mathrm{Tr}(\hat{\rho}^2) = \mathrm{Tr}(\sum_i \lambda_i^2 |\psi_i\rangle\langle\psi_i|) = \sum_i \lambda_i^2$. Therefore, for a general normalized postquantum state with purity $\mu > 1$ represented by a real Wigner function, it can be mapped to a density operator in its eigenbasis $\hat{\rho} = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$, such that the two conditions $\sum_i \lambda_i = 1$ and $\sum_i \lambda_i^2 > 1$ are satisfied.

Assume that all $\lambda_i \geqslant 0$. By some algebraic manipulation, $1 = (\sum_i \lambda_i)^2 = \sum_i \lambda_i^2 + \sum_{i\neq j} \lambda_i\lambda_j \geqslant \sum_i \lambda_i^2 > 1$. Therefore, it is impossible to satisfy both conditions together with the assumptions $\lambda_i \geqslant 0$. By *reductio ad absurdum*, it is necessary for the density operator corresponding to postquantum states with purity greater than unity to have negative eigenvalues. In other words, in the Hilbert-space formulation, these postquantum states violate quantum theory by introducing non-positive-definite operators as states. This serves as a warning of altering the state space without correspondingly changing the effect space, as this would introduce observable nonphysical probabilities beyond the conventional range between zero and 1.

With the procedure (29) ultimately related to introducing negativities into the density operator, there is an obvious problem with the extension towards postquantum theory: It can no longer be conceived that the set of measurements is invariant under such an alteration, for to do so is to allow negative probabilities when one conducts an inner product of an effect corresponding to the eigenstate with negative eigenvalue and the state. Therefore, the set of allowed measurements must shrink accordingly. Despite that the effect $\mathcal{E}_{\{x|V(x)>E^*\}}$ is still valid by the construction of Eq. (28), it is not so apparent that $\mathcal{E}_{E>E^*}$ remains valid. If in certain states for which the set of effects corresponding to energy measurement is invalid, then one must find another set of effects corresponding to a new energy measurement, which creates great difficulties in interpreting energy as a physical and observable quantity.

Nonetheless, a qualitative argument could be given here regarding the status of tunneling as a phenomenon in postquantum scenarios. Consider the ground state of the quantum harmonic oscillator (19): If one varies the state by shrinking σ_x and σ_p simultaneously, and therefore violating the uncertainty principle and purity condition by altering the covariance matrix γ in Eq. (28), then while the ground-state energy effect vector would shrink correspondingly, the variation is continuous and therefore the inner product that specifies the tunneling rate would still retain negativity in the close vicinity of the quantum case. Therefore, it seems that tunneling can be a generic property of postquantum theories and is not unique to quantum theory. However, to fully study the phenomenon of tunneling in postquantum theories rigorously, it is necessary to construct a systematic theory that describes the effects on the effect space by alteration of the state space.

V. CONCLUSION

We have shown that tunneling necessitates a negative Wigner function of the state and/or a tunneling rate operator at some energies as we have defined. This links tunneling with nonclassical probabilistic behavior (negative quasiprobabilities) in a concrete manner. We also argued that our approach can be used to investigate tunneling in generalized probabilistic theories, showing the Wigner function representation fits into that framework. A very intriguing question for future research is how these results relate to recent studies that suggest negative Wigner function is equivalent to contextuality [23]. Preparation contextuality, meaning that extra context beyond the density matrix ρ is needed for an ontic model to be able to accurately mimic quantum theory, is linked to random access encoding, wherein more than one bit is encoded per qubit but only one bit can be decoded according to choice of measurement [24,25]. Preparation contextuality can be revealed by communication games [26] and is necessary for achieving optimal quantum state discrimination [27]. Limiting preparation contextuality gives Tsirelson's bound on the Bell nonlocality [28]. Contextuality, and thus indirectly the negative Wigner function, has also been argued to be the "source" of the putative power of quantum computation [29], hinting at a route together with our results towards linking tunneling with computational power in a probability theory sense. We are also optimistic that our operational definition of tunneling will be useful for discriminating between classical hopping and quantum tunneling in experiments.

ACKNOWLEDGMENTS

We are grateful for discussions with Dan Browne, Jonathan Halliwell, Benjamin Yadin, Andrew Garner, Vlatko Vedral, Dominic Branford, Myungshik Kim, and Marco Genoni. O.C.O.D. is grateful for funding from the EU collaborative project TherMiQ (Grant Agreement No. 618074), Wolfson College, University of Oxford, the London Institute for Mathematical Sciences and the National Natural Science Foundation of China (NSFC).

APPENDIX A: REFLECTION OVER BARRIER

The general definition, Definition 2, could be thought of as a case of nonclassical behavior in position space. A corresponding nonclassical behavior, known as reflection over barrier, could be considered under the same framework as tunneling in momentum space. Following the same analysis, the classically forbidden region for a particle with energy E^* is $\{p||p| < \sqrt{2m(E^* - \sup_{\mathbb{R}} V)}\}$, denoted as $\mathcal{P}(E^*)$, where p is a real variable representing momentum. Such constraint also applies to states with energy $E > E^*$, or that $\mathcal{P}(E^*) \subseteq \mathcal{P}(E)$. Therefore, one can formulate the definition of reflection over barrier as follows.

Definition 3: General definition of reflection over barrier. For a state in a potential given by $V(x)$, it is reflecting over barrier if and only if there exists some energy E^*, such that the probability of locating the state in a region where $|p| < \sqrt{2m(E^* - \sup_{\mathbb{R}} V)}$ is greater than that of measuring the state to have energy $E < E^*$, or, mathematically,

$$\exists E^* : P\left(p\middle||p| < \sqrt{2m\left(E^* - \sup_{\mathbb{R}} V\right)}\right) > P(E < E^*).$$

It should be noted that the two definitions, Definition 2 and Definition 3, have similar structure, and this provides an example of constructing a mathematical formulation of various nonclassical quantum processes: starting from certain classical relations between physical quantities, such as position x and energy E in Definition 2, one could define some classically forbidden region $\mathcal{X}(E^*)$ which relates the two quantities, and any states that violate this relation are considered to be nonclassical states.

APPENDIX B: TUNNELING IN CLASSICAL PHASE-SPACE DISTRIBUTIONS

With the framework of tunneling in phase space stated in Theorem 1 and Corollary 1, it is straightforward, then, to demonstrate that it is impossible for classical systems to tunnel in the following manner:

Theorem 3: Impossibility of tunneling in classical systems. A classical system, specified with the Hamiltonian $H(x, p)$ and the distribution function $f(x, p)$, cannot allow tunneling.

Proof. For a general classical system, the effect corresponding to probability $P(x|V(x) > E^*)$ is

$$\mathcal{E}_{\{x|V(x)>E^*\}}(x, p) = \begin{cases} 1 & \text{for } V(x) > E^* \\ 0 & \text{otherwise,} \end{cases}$$

and similarly, the effect corresponding to probability $P(E > E^*)$ is

$$\mathcal{E}_{E>E^*}(x, p) = \begin{cases} 1 & \text{for } H(x, p) > E^* \\ 0 & \text{otherwise.} \end{cases}$$

However, since the set $\{(x, p)|V(x) > E^*\} \subseteq \{(x, p)|H(x, p) > E^*\}$, $V(x) > E^*$ implies $H(x, p) > E^*$ for a classical system, which suggests that the function $\Delta\mathcal{E}_{E^*}(x, p) \geqslant 0$. Also, since $f(x, p)$ in this scenario is a joint probability function, $f(x, p)$ must be non-negative over all phase space. Therefore, by Corollary 1, a classical state cannot tunnel. ■

In some sense, this proof is anticipated by the design of the general definition, as part of the original intentions of constructing such a definition. However, this exercise is still valuable, because the previous discussion in the main text is largely based on classical particles rather than phase-space ensembles. Another important point is that this proof illustrates the dual nature of tunneling in phase space, as tunneling does not only depend on condition on the state, i.e., the distribution function, but also the difference in effects, $\Delta\mathcal{E}_{E^*}$. In particular, both functions have to be non-negative for a state to not tunnel. This concurs with the discussion on Corollary 3, where a Gaussian state has a positive Wigner function representation, yet in certain scenarios such states could indeed tunnel.

APPENDIX C: QUANTUM TUNNELING OF WAVE PACKETS

While it is rather difficult to obtain the energy distribution of a wave packet due to the piecewise nature of the energy eigenstate wave functions, there are certain features of the problem that simplify the analysis in principle. First, despite the time evolution of the state, the cumulative probability distribution $P(E > E^*)$ is invariant. This is due to the fact that a general state can be considered a superposition of energy eigenstates $|\psi\rangle = \sum_i c_i |E_i\rangle$, and under the unitary operator $\exp[-i\hat{H}t/\hbar]$, the probability $P(E > E^*)$ is the sum of the norm squared amplitude corresponding to energy eigenstates with energy greater than E^*, or

$$P(E > E^*) = \sum_{E_i > E^*} |c_i|^2, \tag{C1}$$

which is independent of time. Hence, the dynamical nature of the wave packet only changes the probability $P(x|V(x) > E^*)$.

Second, given that for a rectangular potential barrier $P(x|V(x) > E^*) = P(0 \leqslant x < l)$ is a constant value in the range $0 < E^* < V_0$, it can then be demonstrated that the state is tunneling if and only if $P(E > V_0) < P(0 \leqslant x < l)$, by demonstrating that $P(E > V_0) < P(0 \leqslant x < l)$ is equivalent to the condition $\exists E^* : P(x|V(x) > E^*) > P(E > E^*)$, i.e., the condition of a tunneling state:

a. $\exists \mathbf{E}^* : \mathbf{P}(\mathbf{x}|\mathbf{V}(\mathbf{x}) > \mathbf{E}^*) > \mathbf{P}(\mathbf{E} > \mathbf{E}^*)$ *implies* $\mathbf{P}(\mathbf{E}>\mathbf{V_0}) < \mathbf{P}(\mathbf{0} \leqslant \mathbf{x} < \mathbf{l})$. Assume it is the case that $\exists E^* : P(x|V(x) > E^*) > P(E > E^*)$ and $P(E>V_0) \not< P(0\leqslant x<l)$. Construct $P(x|V(x) > E^*)$,

$$\begin{aligned} &P(x|V(x) > E^*) \\ &= \begin{cases} 1 & \text{for } E^* = 0 \\ P(0 \leqslant x < l) \leqslant P(E > E^*) & \text{for } 0 < E^* < V_0 \\ 0 & \text{for } E^* \geqslant V_0 \end{cases} \\ &\leqslant P(E > E^*), \end{aligned}$$

where in the region $0 < E^* < V_0$, $P(E > V_0) = P(E > E^*) - P(V_0 > E > E^*) \leqslant P(E > E^*)$, and in the region $E^* \geqslant V_0$, $0 \leqslant P(E > E^*)$. Therefore, for all possible E^*, $P(x|V(x) > E^*) \leqslant P(E > E^*)$, which contradicts the premise $\exists E^* : P(x|V(X) > E^*) > P(E > E^*)$. Therefore, by *reductio ad absurdum*, $\exists E^* : P(x|V(x) > E^*) > P(E > E^*) \rightarrow P(E > V_0) < P(0 \leqslant x < l)$.

b. $\mathbf{P}(\mathbf{E} > \mathbf{V_0}) < \mathbf{P}(\mathbf{0} \leqslant \mathbf{x} < \mathbf{l})$ *implies* $\exists \mathbf{E}^* : \mathbf{P}(\mathbf{x}|\mathbf{V}(\mathbf{x}) > \mathbf{E}^*) > \mathbf{P}(\mathbf{E} > \mathbf{E}^*)$. Since $P(0 \leqslant x < 1)$ is simply $P(x|V(x) > V_0)$, $P(E > V_0) > P(x|V(x) > V_0)$ implies $\exists E^* : P(x|V(x) > E^*) > P(E > E^*)$.

What the previous exercise shows is that it suffices to use two probabilities, $P(E > V_0)$ and $P(0 \leqslant x < l)$, of a state in a rectangular potential barrier to determine whether the state is tunneling or not, which could be applied to our example of Gaussian state tunneling through a rectangular barrier. Using the approximation that the energy eigenstates are roughly free momentum eigenstates, one can conduct a Fourier transform on Eq. (15) and obtain the Gaussian wave packet that has a probability distribution over momentum space as

$$P(p) = \sqrt{\frac{2}{\pi}} \frac{\sigma_x}{\hbar} \exp\left[-\frac{2\sigma_x(p - p_0)^2}{\hbar}\right], \tag{C2}$$

which is also Gaussian, as expected from the property of Fourier transform of Gaussian probability distributions. Therefore, the cumulative energy probability is given by

$$\begin{aligned} &P(E > E^*) \\ &= \int_{-\infty}^{-\sqrt{2mE^*}} P(p)\,dp + \int_{\sqrt{2mE^*}}^{\infty} P(p)\,dp \\ &= 1 - \frac{1}{2}\text{erf}\left(\frac{\sqrt{2}\sigma_x}{\hbar}(\sqrt{2mE^*} - p_0)\right) \\ &\quad + \frac{1}{2}\text{erf}\left(\frac{\sqrt{2}\sigma_x}{\hbar}(\sqrt{2mE^*} + p_0)\right). \end{aligned}$$

While it is difficult to find the close form of the probability $P(0 \leqslant x < l)$, via some numerical simulation it is possible to obtain this probability as a function of time, as shown as Fig. 4.

Regardless, this analysis demonstrates how the general definition of tunneling can be used to determine whether a general state as a superposition of energy eigenstates is tunneling or not, as well as to assign a quantitative value to how such a state violates the classicality constraints. It therefore provides evidence on how the general definition satisfies the criteria of providing quantitative criteria of tunneling for systems with states without definite energy.

APPENDIX D: QUANTUM TUNNELING OF GROUND STATE OF QUANTUM HARMONIC OSCILLATOR

For a quantum harmonic oscillator, the ground-state wave function $\psi_0(x)$ is given by Eq. (19). Such a wave function can be mapped to a Wigner function $W_0(x, p)$ by Weyl transformation to be

$$W_0(x, p) = \frac{1}{\pi\hbar} \exp\left(-\frac{m\omega x^2}{\hbar}\right) \exp\left(-\frac{p^2}{m\omega\hbar}\right). \tag{D1}$$

Notice here that such a Wigner function, as a map of a Gaussian state, is a bivariate Gaussian distribution which is positive over all phase space. This example is hence a direct verification of Hudson's theorem.

As stated in the main text, the analysis of tunneling for Gaussian states lies predominantly on the effects. First of all, consider the effect $\mathcal{E}_{\{x|V(x)>E^*\}}$. By the condition $V(x) > E^*$, the region corresponding to each E^* can be found as $|x| > \sqrt{2E^*/m\omega^2}$, which implies the function $\mathcal{E}_{\{x|V(x)>E^*\}}$ has the form

$$\begin{aligned} &\mathcal{E}_{\{x|V(x)>E^*\}} \\ &= \begin{cases} 1 & \text{for } x > \sqrt{2E^*/m\omega^2} \text{ or } x < -\sqrt{2E^*/m\omega^2} \\ 0 & \text{otherwise,} \end{cases} \end{aligned} \tag{D2}$$

which is simply its classical counterpart. Second, the effect $\mathcal{E}_{E>E^*}$ is simply $2\pi\hbar \sum_{n=n^*}^{\infty} W_n(x, p)$, where $W_n(x, p)$ is the Wigner function for the nth energy eigenstate of the quantum harmonic oscillator, and n^* is the minimum quantum number that corresponds to an energy eigenstate with energy greater than E^*, or $n^* = \lceil \frac{E^*}{\hbar\omega} - \frac{1}{2} \rceil$.

For analysis of tunneling of the ground state, the most relevant energy E^* is the ground-state energy at $E^* = \hbar\omega/2$. Therefore, consider the effects $\mathcal{E}_{\{x|V(x)>\hbar\omega/2\}}$ and $\mathcal{E}_{E>\hbar\omega/2}$, which are calculated to be Eqs. (D2) and

$$\begin{aligned} &\mathcal{E}_{E>\hbar\omega/2}(x, p) \\ &= 1 - 2\pi\hbar W_0(x, p) \\ &= 1 - 2\exp\left(-\frac{m\omega x^2}{\hbar}\right)\exp\left(-\frac{p^2}{m\omega\hbar}\right). \end{aligned} \tag{D3}$$

An interesting point to note here is that despite that the effect corresponding to the probability $E > \hbar\omega/2$ is simply the difference between identity $\mathbf{1}$ and the rescaled Wigner function of the ground state of the quantum harmonic oscillator $W_0(x, p)$, which is a positive function, the function as the difference between the two effects still contains negativities.

Despite that the two fundamental components to the effect are positive functions and can sometimes be interpreted as classical effects and distributions, ultimately the combination of the two leads to nonclassical behaviors.

Moving on with the analysis, the difference between the two effects is

$$\Delta\mathcal{E}_{\hbar\omega/2}(x,p) = \begin{cases} -2\exp\left(-\frac{m\omega x^2}{\hbar}\right)\exp\left(-\frac{p^2}{m\omega\hbar}\right) & \text{for } |x| > \sqrt{\hbar/m\omega} \\ 1-2\exp\left(-\frac{m\omega x^2}{\hbar}\right)\exp\left(-\frac{p^2}{m\omega\hbar}\right) & \text{otherwise,} \end{cases}$$

which clearly shows that such a function contains negativities. By Corollary 3, the ground state of a quantum harmonic oscillator can indeed tunnel. As a comparison and an example to the discussion in the main text regarding quantum and classical cases of tunneling, the classical and quantum versions of the tunneling rate operator are shown in Fig. 6, which clearly demonstrates that only the quantum case of the function contains negativities.

Although it is shown by Corollary 3 that the ground state can tunnel, to demonstrate that it is indeed tunneling is to consider the integral

$$\begin{aligned} &\iint \Delta\mathcal{E}_{\hbar\omega/2}(x,p)W_0(x,p)\,dx\,dp \\ &= -\iint \mathcal{E}_{\{x|V(x)>\hbar\omega/2\}}(x,p)W_0(x,p)\,dx\,dp \\ &= -\iint_{-\infty}^{-\sqrt{\hbar/m\omega}} W_0(x,p)\,dx\,dp - \iint_{\sqrt{\hbar/m\omega}}^{\infty} W_0(x,p)\,dx\,dp, \end{aligned}$$

since $\iint \mathcal{E}_{E>\hbar\omega/2}(x,p)W_0(x,p)\,dx\,dp = 0$. By Hudson's theorem, $W_0(x,p)$ is positive, and therefore the last line of the derivation is negative. By Theorem 1, the ground state of the quantum harmonic oscillator is indeed a tunneling state.

APPENDIX E: ORTHOGONALITY OF WIGNER FUNCTIONS OF EIGENSTATES

The Weyl transformation between Hermitian operator and real function in phase space provides a method of generating sets of orthogonal functions in phase space. A Hermitian density operator can generally be expressed as $\hat{\rho} = \sum_{i,j}\lambda_{i,j}|\omega_i\rangle\langle\omega_j|$, where $|\omega_i\rangle$ form a set of basis states. Consider, then, the Weyl transformation of the operator $|\omega_i\rangle\langle\omega_j|$ as $F_{i,j}$, such that for a Wigner function $W(x,p)$,

$$\hat{\rho} = \sum_{i,j}\lambda_{i,j}|\omega_i\rangle\langle\omega_j| \rightarrow W(x,p) = \sum_{i,j}\lambda_{i,j}F_{i,j}(x,p), \quad \text{(E1)}$$

where the set of functions $F_{i,j}$ are orthogonal,

$$\begin{aligned} &\mathrm{Tr}(|\omega_{i_1}\rangle\langle\omega_{j_1}|\omega_{j_2}\rangle\langle\omega_{i_2}|) \\ &= 2\pi\hbar\iint F_{i_1,j_1}(x,p)F^*_{i_2,j_2}(x,p)\,dx\,dp \\ &= \delta_{i_1,j_1}\delta_{i_2,j_2}, \end{aligned} \quad \text{(E2)}$$

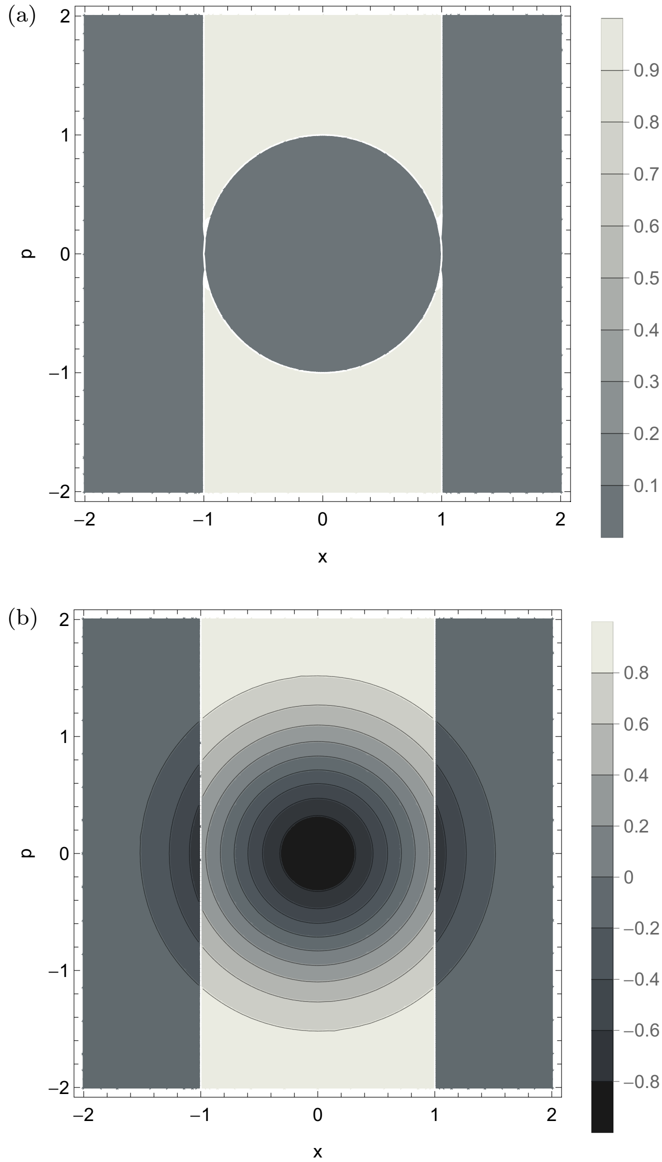

FIG. 6. Contour plots of the function $[\mathcal{E}_{E>\hbar\omega/2} - \mathcal{E}_{\{x|V(x)>\hbar\omega/2\}}](x,p)$: (a) classical case and (b) quantum case of the tunneling operator. x is in units of $\sqrt{\hbar/m\omega}$ and p is in units of $\sqrt{\hbar m\omega}$.

and completeness of the operators $|\omega_i\rangle\langle\omega_j|$ in Hermitian matrices is mapped to the completeness of the corresponding functions $F_{i,j}(x,p)$ in real functions. Therefore, the coefficients $\lambda_{i,j}$ can be calculated by

$$\lambda_{i,j} = \mathrm{Tr}(\hat{\rho}|\omega_j\rangle\langle\omega_i|) = 2\pi\hbar\iint W(x,p)F^*_{i,j}(x,p)\,dx\,dp. \quad \text{(E3)}$$

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