

Quantum phase for an arbitrary system with finite-dimensional Hilbert space

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A representation of the phase observable in terms of a positive-operator-valued measure for an arbitrary quantum system with a finite Hilbert space is consistently defined. The phase for systems with rational relations between the energy eigenvalue differences is treated explicitly and the phase in the case of the irrational relations is obtained as a well-defined limit of the rational approximations.

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I. INTRODUCTION

State vector evolution of a quantum system with a finite Hilbert space \mathcal{H}^n is either periodic or quasiperiodic, depending on the characteristic frequencies, i.e., the ratios of the energy eigenvalue differences $(E_i - E_j)/(E_k - E_l)$, with $i, j, k, l = 1, 2, \dots, n$, being rational or irrational. Classical Hamiltonian systems that support only periodic and quasiperiodic orbits are integrable and for such systems a variable called phase, which is directly related to the time parameter, is well defined and simply expressible in terms of the canonical variables [1]. Following the spirit of the correspondence principle, one would expect that for periodic and quasiperiodic quantum dynamics an observable phase of the quantum motion should be well defined in general. Such an observable for systems with finite-dimensional Hilbert space is essential in the context of quantum information theory. However, a proper definition of the quantum phase even for the simplest system, such as the harmonic oscillator, proves to be a highly nontrivial task primarily because of the well-known Pauli obstacle [2]. Many different nonequivalent answers were suggested. Some of the relevant references are Refs. [3–11] (a comprehensive list of more than 500 items containing works on the phase observable published up to 1996 is available in Ref. [12]). The major breakthrough was to realize that measurements of quantum observables can be consistently described using an appropriate positive-operator-valued measure (POVM), which provides nonorthogonal resolutions of unity and cannot be reduced to the more common projective measures (PMs) [13,14]. In the simplest cases of the harmonic oscillator, the phase is mathematically represented by the corresponding POVM denoted $\hat{M}(d\theta)$, which satisfies the covariance condition [13,14]

$$\exp[i\theta_1 \hat{H}] \hat{M}(a, b) \exp[-i\theta_1 \hat{H}] = \hat{M}(a + \theta_1, b + \theta_1) \text{mod} 2\pi, \quad (1)$$

where θ_1 is a particular phase parameter value, (a, b) and $(a + \theta_1, b + \theta_1)$ are an interval of the phase and its θ_1 shift, and \hat{H} is the Hamiltonian. The covariance condition is taken as the defining property of the phase observable. However, a definition of the phase observable for an arbitrary quantum system with a periodic or quasiperiodic state vector dynamics has not been formulated in full generality. Examples of POVM

representations of phase observables have been constructed for qubits and qutrits [15–20] using polar decomposition, analogously to the case for the harmonic oscillator. An interesting approach explores the complementarity of the putative phase and amplitude observables formalized using the concept of mutually unbiased bases [21].

It is the purpose of this Brief Report to introduce a consistent definition of the POVM for the phase observable in general for an arbitrary quantum system with a finite number of energy eigenstates and eigenvalues. We shall see that such a phase observable satisfies the covariance condition and is always given by a POVM (and not by a PM), as should be expected on quite general arguments [22]. The definition can be generalized to systems with an infinite Hilbert space.

We would like to stress that the phase introduced here is not considered a parameter to be estimated from the system's state like in Ref. [23,24]. In addition, the phase of an arbitrary N -level system is here considered a single quantity determined by the system's Hamiltonian and not as N objects conjugated to the N inversions as in, for example, Refs. [19–21]. In this sense the single phase studied here could be called the master phase of the system. The system's phase introduced here is comparable to the phase observable introduced by Holevo [13] for the equidistant spectrum of the harmonic oscillator or for the systems with rationally related energy levels discussed in Refs. [25,26]. However, our results provide a consistent definition of the phase for finite systems with arbitrary spectra and point out the relations between the spectra of systems with similar distributions of the phase values.

II. RESULTS

Without any substantial loss of generality in the presentation of the main ideas, we start the analysis with three-dimensional systems with three different energy eigenvalues $E_0 < E_1 < E_2$. All such systems can be divided into groups characterized by the three energy eigenvectors. The systems in one group have the same energy eigenvectors denoted $|0\rangle, |1\rangle$, and $|2\rangle$ and are distinguished by all possible triplets of different energy eigenvalues E_0, E_1 , and E_2 . The definition of the phase observable will be given in terms of arbitrary E_0, E_1 , and E_2 and arbitrary fixed $|0\rangle, |1\rangle$, and $|2\rangle$. A generalization, based on the same ideas, to systems with an arbitrary finite number of possibly degenerate energy eigenvalues is sketched in Sec. III.

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The characteristic frequency of the three-dimensional system is given by the ratio of the energy differences

$$\nu = \frac{E_2 - E_1}{E_1 - E_0}, \quad (2)$$

which could be a rational or an irrational number implying a periodic or quasiperiodic state vector dynamics. There is no special purpose in our presentation in using the ratio of the energy differences instead of the independent pair $E_2 - E_1$ and $E_1 - E_0$. The main point is that the two energy differences could be integer or noninteger multiples of some unit ΔE . Of course, in the first case the characteristic frequency is rational and in the second it is irrational. In the case of more than three energy eigenvalues there will be more characteristic frequencies, each corresponding to the ratio of independent energy value differences, some of which are rational and some irrational. In any case, the characteristic frequencies are fully determined by the energy spectrum. Our strategy to define the phase observable for an arbitrary ν will be to define it first for an arbitrary rational ν and then to consider the limit of such an observable for a sequence of rational frequencies converging to an irrational frequency.

A systematic way to reproduce and organize all rational and irrational numbers in the interval $[0,1]$ is provided by the Farey algorithm, which we briefly recapitulate. The result of the algorithm is an infinite sequence of rows of rational numbers called the Farey tree and is organized as follows. The first row contains only $p_1/q_1 = 0/1$ and $p_2/q_2 = 1/1$. The second row contains the numbers obtainable as $p/q = (p_1 + p_2)/(q_1 + q_2)$, which is just $1/2$. The third row adds two more rational numbers as $(0 + 1)/(1 + 2) = 1/3$ and $(1 + 1)/(2 + 1) = 2/3$. The rational numbers that appear at the next row are $1/4 = (0 + 1)/(1 + 3)$, $2/5 = (1 + 1)/(3 + 2)$, $3/5 = (1 + 2)/(2 + 3)$, and $3/4 = (2 + 1)/(3 + 1)$. Each new rational number at the k th row has the numerator and the denominator equal to the sum of numerators and denominators of the two neighboring rational numbers obtained at all the previous rows. Following the algorithm *ad infinitum* generates all rational numbers in $[0, 1]$. A sequence of successively better rational approximations with the smallest denominators of irrational numbers is obtained by following the connected decreasing paths in the Farey tree. Such a sequence for a particular irrational number can be obtained analogously by its continued fraction expansion. The dynamical role of the rational approximations of the frequencies of structures with quasiperiodic motion in classical Hamiltonian systems is well known [27].

After this brief recapitulation of the Farey tree construction we proceed to define the phase observable for the quantum system with energy ratios (2) equal to a rational $\nu = p_k/q_k$ belonging to the k th level of the Farey tree. The energy differences satisfy

$$E_{k1} - E_{k0} = p_k \Delta E_k, \quad E_{k2} - E_{k1} = q_k \Delta E_k, \quad (3)$$

where ΔE_k is the energy unit that fits exactly p_k times into the interval $E_{k1} - E_{k0}$ and q_k times into $E_{k2} - E_{k1}$. Notice that as k is increased p_k/q_k converges to an irrational number and p_k and q_k both converge to infinity, implying that $\Delta E_k \rightarrow 0$ in Eq. (3). The semispectral measure [28] of the phase observable for the system with the rational number p_k/q_k is constructed

using the following vectors indexed by a continuous index $t \in [0, 2\pi\hbar/\Delta E_k]$:

$$|t\rangle_k = \sqrt{\frac{\Delta E_k}{2\pi\hbar}} \sum_{n=0}^2 \exp(i E_{kn} t/\hbar) |n\rangle, \quad (4)$$

where $|n\rangle, n = 0, 1, 2$ are arbitrary but fixed eigenvectors of the Hamiltonians in the considered group.

The domain of the semispectral measure representing the phase observable, denoted θ , should always be $\theta \in [0, 2\pi)$, irrespective of the system considered, i.e., of the rational number p_k/q_k . Therefore we rescale the interval of the index $t \in [0, 2\pi\hbar/\Delta E_k]$ by defining $\theta = t\hbar/\Delta E_k$. The phase interval $(a, b) \subset [0, 2\pi)$ corresponds to the t interval $(t_a, t_b) \subset [0, 2\pi\hbar/\Delta E_k]$, where $t_a = a\hbar/\Delta E_k$ and $t_b = b\hbar/\Delta E_k$. The semispectral measure of the phase observable θ is now defined as

$$\begin{aligned} \hat{M}_\theta^{p_k/q_k}(a, b) &= \hat{M}_t^{p_k/q_k}(t_a, t_b) = \frac{\Delta E_k}{2\pi\hbar} \int_{t_a}^{t_b} dt |t_k\rangle \langle t_k| \\ &= \frac{\Delta E_k}{2\pi\hbar} \int_{t_a}^{t_b} dt \sum_{n,m=0}^2 \exp[i(E_{kn} - E_{km})t] |n\rangle \langle m|. \end{aligned} \quad (5)$$

The phase semispectral measure $\hat{M}_\theta^{p_k/q_k}(a, b)$ obviously satisfies the covariance condition (1). Its off-diagonal and diagonal matrix elements in the $|n\rangle$ bases are

$$\begin{aligned} [M_\theta^{p_k/q_k}(a, b)]_{m \neq n} &= \frac{\Delta E_k}{2\pi\hbar} \int_{t_a}^{t_b} dt \exp i [E_{nk} - E_{mk}] t/\hbar \\ &= \frac{1}{2\pi i} \left(\frac{\Delta E_k}{E_{nk} - E_{mk}} \right) \left[\exp i \frac{(E_{nk} - E_{mk})b}{\Delta E_k} \right. \\ &\quad \left. - \exp i \frac{(E_{nk} - E_{mk})a}{\Delta E_k} \right] \end{aligned} \quad (6)$$

and

$$[M_\theta^{p_k/q_k}(a, b)]_{m=n} = (b - a)/2\pi. \quad (7)$$

Obviously $[M_\theta^{p_k/q_k}(0, 2\pi)]_{m \neq n} = 0$ and $[M_\theta^{p_k/q_k}(0, 2\pi)]_{m=n} = 1$. The matrix element $\hat{M}_\theta^{p_k/q_k}(a, b)$ for arbitrary p_k/q_k generates a resolution of unity. The resolution is obviously nonorthogonal.

Thus the family $\hat{M}_\theta^{p_k/q_k}(a, b)$ given by Eq. (5) provides the POVM representation of the phase observable for an arbitrary system with a rational ratio (2). In Fig. 1 we illustrate the phase expectations $\langle \psi | \hat{M}_\theta^{p_k/q_k}(0, b) | \psi \rangle$, with $b \in (0, 2\pi)$, in the three states $|\psi\rangle$ forming an orthonormal basis: $|1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3}\rangle$ [Fig. 1(a)], $|1/\sqrt{2}, -1/\sqrt{2}, 0\rangle$ [Fig. 1(b)], and $|1/\sqrt{6}, 1/\sqrt{6}, -\sqrt{2}/3\rangle$ [Fig. 1(c)]. In fact, $m(b; \nu = p_k/q_k, \psi) \equiv \langle \psi | \hat{M}_\theta^{p_k/q_k}(0, b) | \psi \rangle - b/2\pi$ for the three rational numbers $p_k/q_k = 2/3, 3/5$, and $5/8$ is illustrated. One should notice that the amplitudes of the oscillations in the curves becomes smaller for the rational numbers with larger q_k . In fact, the curves converge at the x axis as $q_k \rightarrow \infty$.

The phase observable for systems with irrational ratios (2) are defined by considering the limits of phases given by Eq. (5) for systems with rational ratios. An irrational ν determines the sequence of rational approximations p_k/q_k with both $p_k, q_k \rightarrow \infty$. This is equivalent to $\Delta E_k \rightarrow 0$, which is applied in Eq. (5)

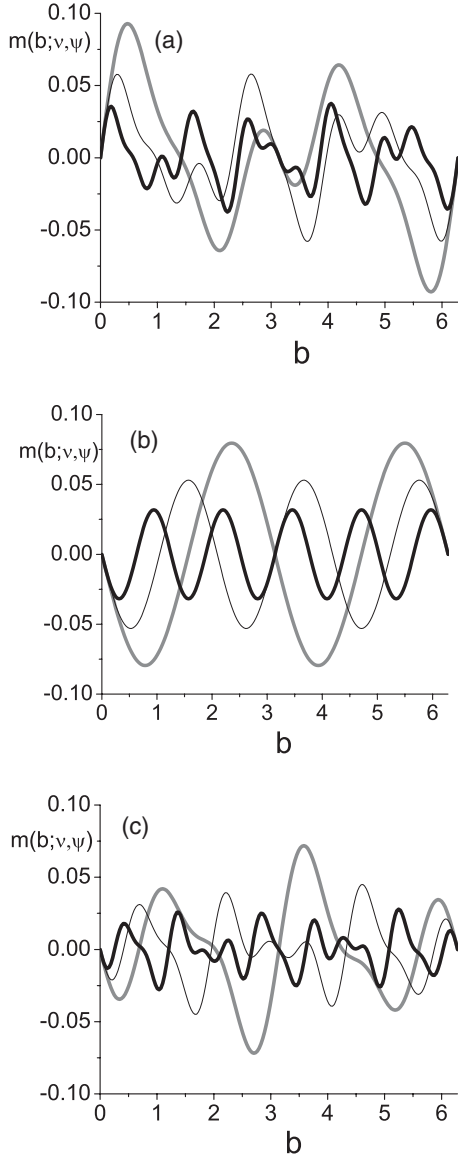


FIG. 1. Illustration of $m(b; v, \psi)$ for (a) $|\psi\rangle = |1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3}\rangle$, (b) $|\psi\rangle = |1/\sqrt{2}, -1/\sqrt{2}, 0\rangle$, and (c) $|\psi\rangle = |1/\sqrt{6}, 1/\sqrt{6}, -\sqrt{2}/3\rangle$ for $v = 2/3$ (thick gray line), $3/5$ (thin gray line), and (thick black line).

to give the POVM for the phase observable of the system with the irrational v . Due to the rescaling involved in the transition from the parameter t to the phase θ , the limiting process results with a well-defined finite POVM, which satisfies the coherence property (1). The matrix elements of this POVM are obtained from Eqs. (6) and (7) in the limit $k \rightarrow \infty$, with $\Delta E_k \rightarrow 0$, and are equal to

$$[M_\theta^v(a, b)]_{m \neq n} = 0 \tag{8}$$

and

$$[M_\theta^v(a, b)]_{m=n} = (b - a)/2\pi. \tag{9}$$

The phase observables for systems with the irrational ratio (2) are represented by the same POVM given by the matrix elements (8) and (9) independently of the irrational v .

III. DISCUSSION

The definition of the phase POVM for systems with N energy levels that are all nondegenerate and such that the ratios of the energy eigenvalue differences are all rational is a straightforward generalization of the three-level case. Vectors $|t\rangle$ are defined with formula (4) where the summation is over the nondegenerate energy eigenbases. The term ΔE_k denotes the small interval such that the independent energy eigenvalue differences are presented as integer multiples p_1, p_2, \dots, p_N of ΔE_k . The phase variable θ and the POVM $M_\theta^{p_1, p_2, \dots, p_N}$ are defined as in the three-level case, i.e., $\theta = t\hbar/\Delta E_k$ and formula (5). More discussion is needed to treat systems with degenerate energy and/or irrational ratios of the energy eigenvalue differences.

In the case that some of the energy levels are degenerate the summation over the energy eigenvectors in the definition of the vector $|t\rangle$ needs to be supplemented by the summation over a basis in each of the degenerate energy eigenspaces. The choice of the basis within each of the degenerate eigenspaces is in general arbitrary, but it is natural to respect the symmetry underlying the degeneracy and use the common eigenbases of the complete set of operators commuting with the Hamiltonian.

The phase POVM of the irrational case is obtained as the limit of POVMs over the sequence of systems with rational ratios where the rational numbers fixing the energies are chosen to be the successive continued-fraction approximants of the corresponding irrational ratios. Like in the three-level case, it is important to realize that the phases of two systems are similar only if the involved rational numbers are close to each other in the Farey tree. Otherwise a system with energy levels that are small perturbations of another system could have a quite different phase distribution in the same state. This is illustrated in Fig. 2 for an example of a four-level system. The following comparisons are made: in Fig. 2(a) the phase POVM for two systems with energy levels $E_1, E_2 = E_1 + 1\Delta E$, $E_3 = E_1 + 3\Delta E$, and $E_4 = E_1 + 5\Delta E$ (thin line) and $E_1, E_2 = E_1 + 10\Delta E$, $E_3 = E_1 + 31\Delta E$, and $E_4 = E_1 + 51\Delta E$ (thick line) and in Fig. 2(b) for two systems with energy $E_1, E_2 = E_1 + 1\Delta E$, $E_3 = E_1 + 3\Delta E$, and $E_4 = E_1 + 5\Delta E$ (thin line) and $E_1, E_2 = E_1 + 1\Delta E$, $E_3 = E_1 + 5\Delta E$, and $E_4 =$

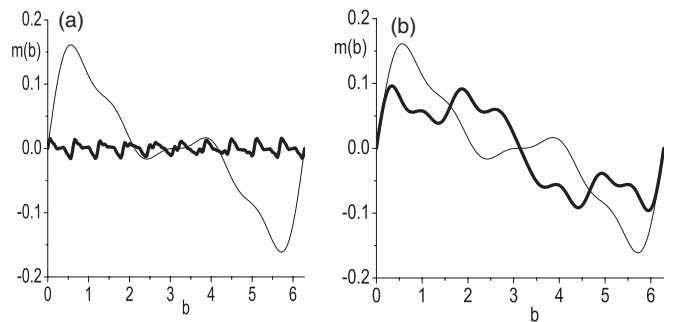


FIG. 2. Illustration of the phase distribution of (b) two systems with the characteristic frequencies nearby in the Farey tree being much more similar than for (a) two systems with the slightly different characteristic frequencies but far away in the Farey tree. The angle b is in radians and $m(b)$ is dimensionless. The details are given in the main text.

$E_1 + 8\Delta E$ (thick line). As shown in Fig. 1, $m(b) \equiv m(b; E_1, E_2, E_3, E_4, \psi) \equiv \langle \psi | \hat{M}_\theta^{E_1, E_2, E_3, E_4}(0, b) | \psi \rangle - b/2\pi$, where $|\psi\rangle = (1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4})$. The characteristic frequencies of the two systems in Fig. 2(a) are closer than those of the two systems in Fig. 2(b), but the difference in the phase distributions is much more similar for the pair of systems in Fig. 2(b) because the characteristic frequencies are closer in the Farey tree. In other words, the phase POVMs of a sequence of systems with rational ratios will converge to a well-defined limit and can be used to define the phase POVM of the system with some irrational ratios only if the rational ratios are chosen as the continued-fraction approximants of the irrational energy difference ratios. This can be considered the main point of our work. The systems with an infinite Hilbert space and an infinite number of discrete energy eigenvalues such that the energy spectrum contains accumulation points requires a careful analysis.

IV. CONCLUSION

We have shown how to define the POVM representation of the phase observable for an arbitrary quantum system with a finite-dimensional Hilbert space. The matrix elements of the phase POVM are given explicitly. The phase POVM is nonorthogonal, provides a resolution of unity, and satisfies the covariance condition required for the phase observable. In the case of rationally related characteristic frequencies the phase POVM is given by Eq. (5). The case of irrationally related characteristic frequencies is treated as a well-defined limit of the rational approximations.

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