Quantum phase for a system with an arbitrary discrete energy spectrum

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Positive operator valued measures representing phase observables for systems with arbitrary discrete, possibly degenerate, spectra are constructed. The general construction is presented and discussed using illustrative examples. The phase POVM shows intricate discontinuous dependence on the eigenfrequencies. Special discussion is devoted to the systems with degenerate energy spectrum, in which case the phase observable is nonunique. We present arguments that can be used to reduces this nonuniqueness.

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I. INTRODUCTION

Classical mechanical systems which are integrable possess only periodic and quasiperiodic motions, and have a well-defined physical quantity representing the phase of a point evolving on a periodic or a quasiperiodic orbit. A state vector of a bounded quantum system always undergoes periodic or quasiperiodic motion in the corresponding Hilbert space. This paper is devoted to a construction of a measurable quantity that represents the phase of the state vector motion on its orbit in the Hilbert space. An adequate and mathematically correct definition of the phase of quantum motion, as corresponding to the notion of phase of classical oscillatory dynamics, proves to be a highly nontrivial task, even for the simplest systems, like the harmonic oscillator. Constructions of a meaningful object representing the phase of quantum motion have been attempted in at least three conceptually different frameworks. In the first approach [1,2], the phase is considered as a parameter and the problem is then to estimate the phase shift during evolution of a state vector. In the second [3], which might be called semiclassical, one again treats the phase as a parameter of the quantum state introduced using the geometry of the quantum phase space. The third approach attempts to define the phase as an observable conjugate to the system's Hamiltonian. The main well-known problem with this approach is the Pauli's obstacle [4,5] coming from the semibounded nature of the energy spectrum. Many different nonequivalent answers were suggested. Illustrative references for this approach are Refs. [6–15]. 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 (PM) [16,17]. In the simplest case of the harmonic oscillator, the phase is mathematically represented by the corresponding (POVM) denoted $\hat{M}(d\theta)$, which satisfies the covariance condition [16,17]:

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

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. Obviously, in cases of systems with symmetries, implying Hamiltonians with degenerate spectrum, the covariance condition does not fix uniquely the phase POVM. Nevertheless, the covariance condition is taken as the defining property of the phase observable. Corresponding construction of the phase observable for an arbitrary quantum system with periodic or quasiperiodic state vector dynamics has not been formulated in full generality. The original definition of the covariant phase observable provided for the harmonic oscillator by prof. Holevo [16] has been generalized for systems with rationally related nondegenerate energy eigenvalues in Refs. [18,19]. Alternative constructions of POVM representations of phase observables have been suggested for qubits and qutrits [20–25] using polar decomposition analogously as 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 [26].

In a recent publication we have briefly sketched a definition of a covariant phase observable for an arbitrary system with finite dimensional state space and no degeneracy [27]. It is the purpose of this communication to provide a detailed and general construction of the POVM for the phase observable for an arbitrary quantum system given by a discrete possibly infinite and degenerate energy spectrum, and to compare the phase POVM of systems with different characteristic frequencies. In the elementary case of a system with an equidistant energy spectrum, the phase introduced here reduces to the known phase observable for the harmonic oscillator [16] and in the case of finite systems with rationally related nondegenerate energy levels to the one discussed in Refs. [18,19]. The physical interpretation of the phase observable for periodic systems introduced here (and in Ref. [27]) is that of the system's normalized phase (or normalized age, or angle), normalized to the system's period. This is different from the notion of an absolute phase or absolute age [9]. The notion of normalized phase has been criticized in Ref. [28]. Step by step comments on this criticism appear in Ref. [29], and shall be discussed in Sec. IV. At this point, it is enough to stress that the normalized phase, introduced here, is a direct analog of the classical phase variable, and it measures the part of the total period T undergone by the system during an interval $(0,t)$. In this way the normalized ages of two systems with different periods can be meaningfully compared.

The paper is organized as follows. In the second section we present an explicit construction of the phase POVM valid for arbitrary, possibly degenerate, energy spectrum with rationally related eigenvalues. We than discuss the case of a system whose energy spectrum has an accumulation point and systems with irrationally related energy eigenvalues. Peculiar discontinuous dependence of the phase POVM on the system's parameters is illustrated and discussed in Sec. III A using the Morse potential as an example. In Sec. III B we illustrate the nonuniqueness of the phase POVM for systems with degenerate spectrum and discuss physically the most plausible way to reduce such nonuniqueness. Section IV contains an example of a system with clear physical interpretation, that can be studied experimentally. Detailed discussion and summary are given in Secs. V and VI, respectively.

II. GENERAL CONSTRUCTION OF THE PHASE POVM

Consider a system with a discrete spectrum of possibly degenerate energy eigenvalues E_k, $k = 0,1,2\ldots$. If all the energy levels are rationally related then there exists the corresponding smallest interval ΔE such that all the eigenvalues can be written as

$$E_k = E_0 + \Delta E q_k, \tag{2}$$

where q_k, $k = 1,2\ldots$ are positive integer numbers. The spectra with irrationally related energy eigenvalues can be approximated arbitrary well by the form (2) with sufficiently small ΔE and sufficiently large integers q_k. However, it will turn out that the phase observables for systems with spectra that have nearby energy eigenvalues might be quite different so that the phase observable of an irrational cannot be approximated by a simple continuity argument.

We shall first define the phase observable for arbitrary but fixed sequence of integers q_k, and then compare the phase observables for different integer approximations of a spectra with some irrationally related eigenvalues.

The covariance condition on putative $\hat{M}(\theta)$ suggests to attempt the construction of $\hat{M}(\theta)$ as a discrete Fourie sum over the eigenbases of the Hamiltonian, as was done for the case of the equidistant spectrum of the harmonic oscillator [16]. In the case of a nondegenerate spectrum with arbitrary rational ratios of the eigenenergies, the discrete Fourie transform with an appropriate rescaling would indeed result in a POVM with the desired covariance property (1). However, the simple procedure does not work in the case of a degenerate spectrum. One difficulty is that the simple Fourier sum in the degenerate case does not give an object which represents a resolution of unity. Some of the matrix elements of the simple Fourier transform have to be eliminated in a consistent way. However, there are different possible ways that this can be done and as a result the phase POVM is not uniquely defined. This will be illustrated after we introduce the procedure that works also in the degenerate case. There is also another source of nonuniqueness of the phase POVM in the degenerate case with a more transparent physical origin. Suppose that the eigenvalue E_n is twofold degenerate with the corresponding two-dimensional (2D) eigenspace P_n. In the construction of the discrete Fourier sum one is free to chose arbitrary bases in P_n, and different choices might render different results. This nonuniqueness of the phase POVM satisfying the covariance condition, like the degeneracy of the spectrum, is a consequence of the system's symmetry. In fact, if $\hat{M}(\theta)$ satisfies (1) the equation is satisfied also by $\hat{M} + \hat{C}$ where $\hat{C}$ generates symmetry transformations. A unique choice of the phase POVM may be attempted by imposing conditions additional to the covariance Eq. (1).

In what follows we shall present a sufficiently general algorithm for the construction of phase POVMs which works in the case of arbitrary degeneracy. It will turn out that the matrix elements of the phase POVM in the chosen bases depend also on the procedure that is used in the definition to split the degenerate energy eigenspaces. In order to formulate the general procedure that defines the phase POVM we shall first introduce the notion of a legitimate partition of the energy eigenbases.

Denote by $\Pi = \{Q_i,\, i = 1,2,3\ldots\}$ a partition of the spectra and the relevant integers numbers q_k into cells Q_i, and introduce a double index (i,j) so that all integers $q_{i,j}$ are from the ith cell, and those from the ith cell are enumerated by the index j: $Q_i = \{q_{i,j},\, j = 1,2,3\ldots\}$. Furthermore, require that the partition is such that no two integers $q_{i,l}$ and $q_{i,m}$ from the same cell Q_i (and different $l \neq m$) correspond to the same energy eigenvalue. In other words, if $E_{i,j} = E_0 + \Delta E q_{i,j}$ then

$$l \neq m \rightarrow q_{i,l} \neq q_{i,m} \rightarrow E_{i,l} \neq E_{i,m}. \tag{3}$$

For convenience, we call partitions satisfying the condition (3) legitimate. Motivation for the introduction of legitimate partitions will be cleared during the construction of the phase POVM.

Which are the legitimate partitions is determined by the degeneracy of the energy spectrum. For example, consider a system with the Hilbert space C^4 of complex dimension 4, and energy eigenvectors $|1\rangle,|2\rangle,|3\rangle,|4\rangle$. Let the vectors $|2\rangle$ and $|4\rangle$ belong to the same energy eigenvalue. Then, for example, the partitions $\Pi_1 = \{\{|1\rangle,|2\rangle\},\{|3\rangle,|4\rangle\}\}$, $\Pi_2 = \{\{|1\rangle,|2\rangle,|3\rangle\},\{|4\rangle\}\}$, and $\Pi_3 = \{\{|1\rangle\},\{|2\rangle\},\{|3\rangle\},\{|4\rangle\}\}$ are legitimate, while the partitions $\Pi_4 = \{\{|1\rangle,|2\rangle,|4\rangle\},\{|3\rangle\}\}$ and the trivial one $\Pi_5 = \{\{|1\rangle,|2\rangle,|3\rangle,|4\rangle\}\}$ are not legitimate. In the case of partition Π_1 the vectors would be indexed as $|1\rangle = |1,1\rangle, |2\rangle = |1,2\rangle, |3\rangle = |2,1\rangle, |4\rangle = |2,2\rangle$. Notice that if the spectra are nondegenerate then all partitions, and in particular the trivial one with all the levels in a single cell like in Π_5, are legitimate. As another example, we might consider a one-dimensional (1D) free particle with doubly degenerate energy spectrum $p^2/2m$. Each 2D eigenspace is spanned by the generalized eigenvectors $|p\rangle,|-p\rangle$. A legitimate partition is, for example, the one with only two cells Q_+, Q_- such that Q_+ contains all $|p\rangle, p > 0$ and Q_- contains all $|p\rangle, p \leqslant 0$. Of course there are infinitely many other legitimate partitions.

We can now proceed with the definition of the phase observable corresponding to a general legitimate partition of an energy spectrum $E_{i,j}$ with rationally related eigenfrequencies. First define for each cell the vector $|\theta,i\rangle$ using the Fourier

combination of all N_i vectors from the cell Q_i:

$$|\theta,i\rangle = \frac{1}{\sqrt{2\pi}} \sum_{j=0}^{N_i} \exp(i q_{i,j}\theta)|i,j\rangle. \quad (4)$$

Then define positive operator valued density $\hat{\mathcal{M}}(\theta)$ as

$$\hat{\mathcal{M}}(\theta) = \sum_{i=1}^{N_Q} |\theta,i\rangle\langle i,\theta| = \sum_{i=1}^{N_Q} \frac{1}{2\pi} \sum_{n=0}^{N_i}\sum_{m=0}^{N_i} \exp[(i q_{i,n} - i q_{i,m})\theta]|i,n\rangle\langle m,i|, \quad (5)$$

where N_Q is the number of cells in the considered partition.

Finally construct the quantity,

$$\hat{M}(\theta_1,\theta_2) = \int_{\theta_1}^{\theta_2} \hat{\mathcal{M}}(\theta) d\theta. \quad (6)$$

Properties of the expression (6) are best studied by explicitly computing its matrix elements. For the vectors in different cells, i.e., those with necessarily different eigenenergies and different values of the coefficients satisfying (3), one has

$$i \neq j \rightarrow \langle i,n_i|\hat{M}(\theta_1,\theta_2)\rangle|j,n_j\rangle = 0. \quad (7)$$

For example, cells containing a single element contribute only the corresponding diagonal elements.

Matrix elements between different vectors from the same cell are

$$\langle i,n|\hat{M}(\theta_1,\theta_2)\rangle|i,m\rangle = \frac{1}{2\pi i} \frac{[\exp i(q_{i,n} - q_{i,m})\theta_2 - \exp i(q_{i,n} - q_{i,m})\theta_1]}{q_{i,n} - q_{i,m}}. \quad (8)$$

Finally, the diagonal elements are

$$\langle i,n|\hat{M}(\theta_1,\theta_2)\rangle|i,n\rangle = \frac{1}{2\pi}(\theta_2 - \theta_1). \quad (9)$$

With these formulas it is easily checked that with any legitimate partition the formula (6) indeed gives a POVM on the interval $[0,2\pi]$. One can now see clearly the reason for partitioning of the eigenvectors. If all vectors belong to a single cell then there are off-diagonal matrix elements in $\hat{M}$ that correspond to the eigenvectors with the same energy eigenvalues, and those do not give zero after integration over $[0,2\pi]$. Such $\hat{M}(\theta)$ does not generate a partition of unity. This is avoided by the above procedure based on the legitimate partitions.

We propose to represent the phase observable of the system with the energy spectra given by integers $q_{i,j}$ by the POVM (6) constructed using any of the legitimate partitions. Any such POVM indeed satisfies the covariance condition (1). In fact it can be shown, using the explicit formulas for the matrix elements, that the following commutation relation between the phase observable $\hat{\theta} = \int \theta \hat{M}(d\theta)$ based on the POVM (6) and the Hamiltonian $\hat{H} = \sum_{i,j} E_{i,j}|i,j\rangle\langle i,j|$,

$$[\hat{H},\hat{\theta}] = i\Delta E[\hat{\mathbf{1}} - 2\pi\hat{\mathcal{M}}(0)], \quad (10)$$

where $\hat{\mathcal{M}}(0)$ is given by formula (5) for $\theta = 0$, is satisfied.

The phase POVM given by (6) obviously depends on the arbitrary phase factor $\exp i\theta^0_{i,j}$ that might multiply each of the energy eigenvectors $|i,j\rangle$. This dependence is analogous to the dependence of the phase of an integrable classical system on the arbitrary initial phases. Furthermore, in the degenerate case the quantity $\hat{M}(\theta_1,\theta_2)$ depends on the choice of the energy eigenbasis $\{|i,j\rangle\}$ and also, for a fixed basis, on the partition into the legitimate cells. Nonuniqueness of the phase POVM due to the choice of the energy bases and the legitimate partition will be discussed in Sec. IV.2.

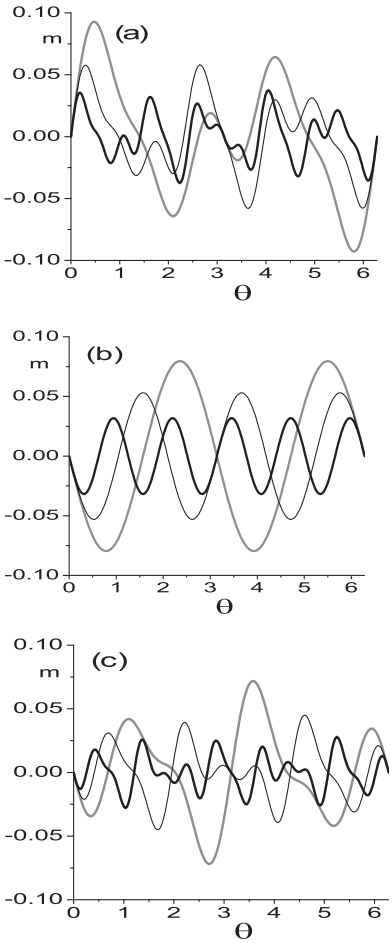

FIG. 1. $m \equiv m(\theta;q_1,q_2;\psi) \equiv \langle\psi|\hat{M}^{q_1,q_2}(0,\theta)|\psi\rangle - \theta/2\pi$ are plotted for pairs of rationals $(q_1,q_2-q_1) = (2,3)$ (gray); $(q_1,q_2-q_1) = (3,5)$ (thin line); $(q_1,q_2-q_1) = (5,8)$ (thick line) and in the states (a) $|1/\sqrt{3},1/\sqrt{3},1/\sqrt{3}\rangle$; (b) $|1/\sqrt{2},-1/\sqrt{2},0\rangle$; and (c) $|1/\sqrt{6},1/\sqrt{6},-\sqrt{2/3}\rangle$. In this, and all other figures all quantities are dimensionless.

Figures 1 and 2 illustrate some of the main properties of the phase observable in the simple case of only three nondegenerate rationally related energy eigenvalues. The system is three-dimensional, so that there are two integers (q_1,q_2) in the formula (2). In fact, the phase is determined by the ratio of the energy eigenvalue differences given by $\nu = q_1/(q_2 - q_1)$, which might be called the characteristic frequency.

Figures 1(a)–1(c) illustrate shapes of the phase expectations $\langle\psi|\hat{M}^{q_1,q_2}(0,\theta)|\psi\rangle$ over the full domain $\theta \in (0,2\pi)$, and for three different states $|\psi\rangle$. The three states are chosen such as to form an orthonormal bases: $|\psi\rangle = |1/\sqrt{3},1/\sqrt{3},1/\sqrt{3}\rangle$; $|\psi\rangle = |1/\sqrt{2},-1/\sqrt{2},0\rangle$; and

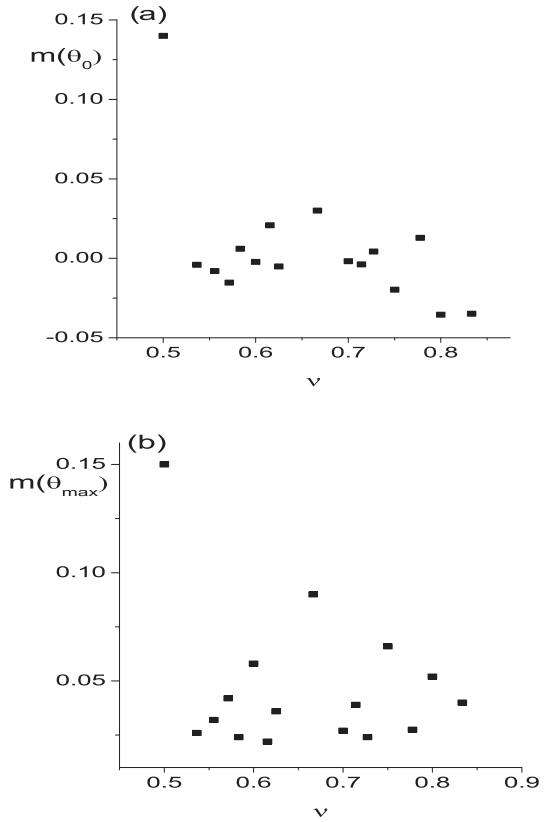

FIG. 2. Plotted are value of $m(\theta_0;q_1,q_2;\psi) \equiv \langle\psi|\hat{M}^{q_1,q_2}(0,\theta_0)|\psi\rangle - \theta_0$ for the same state as in Fig. 2(a) and for several co-prime rational $\nu \equiv q_1/(q_2 - q1)$ that appear at the first six levels of the Farey tree and are bigger then $1/2$. The fixed angle $\theta_0 = 1$. Figure 2(b) illustrates the same quantity but at different values of the angle $\theta = \theta_{\max}$ for different ν as in Fig. 2(a), such that $m(\theta;q_1,q_2;\psi)$ obtains its maximum at $\theta_{\max}$.

$|\psi\rangle = |1/\sqrt{6},1/\sqrt{6},-\sqrt{2/3}\rangle$. The shapes of the phase expectations are illustrated for their systems with the spectra (2) with integers q_1,q_2 satisfying $(q_1,q_2 - q_1) = (2,3);(3,5);(5,8)$.

Figure 2(a) illustrates the value of $m(\theta_0;q_1,q_2;\psi) \equiv \langle\psi|\hat{M}^{q_1,q_2}(0,\theta_0)|\psi\rangle - \theta_0/2\pi$ for $\psi = |1/\sqrt{3},1/\sqrt{3},1/\sqrt{3}\rangle$ and for several co-prime rational $\nu \equiv q_1/(q_2 - q_1)$ that appear at the first six levels of the Farey tree and are bigger then $1/2$. The fixed angle $\theta_0 = 1$. Figure 2(b) illustrates the same quantity for ν as in Fig. 2(a) but at different values of the angle $\theta = \theta_{\max}$ such that $m(\theta;q_1,q_2;\psi)$ obtains its maximum at $\theta_{\max}$. The dependence of the phase expectation on the characteristic frequency, at the given θ [Fig. 2(a)] or at θ corresponding to the maximum [Fig. 2(b)], is obviously discontinuous.

It is seen, from the above examples, that the phase observables for systems with spectra that have nearby energy eigenvalues might be quite different. In particular, the phase observable for a spectrum with some irrationally related eigenvalues cannot be approximated by a simple continuity argument. However, special sequences of sets of rational numbers $\{q_2/q_1,q_3/q_1 \ldots q_k/q_1 \ldots\}_j$, such that the kth entry of the jth and $j+1$st sets are the neighbors in jth and $j+1$th level of the Farey tree of rational numbers, which we call Farey close sets of q_k's, prove to be of special significance for the treatment of phase observables. In fact, the major observation is that expectations of phase observables for two systems with spectra (2) corresponding to jth and $j+1$st sets of Farey close $q_k's$ are much closer to each other then in the case the two sets are such that the kth entries of the corresponding $q_2/q_1,q_3/q_1 \ldots q_k/q_1 \ldots$ are quite close but are in the same time on quite distant Farey levels. The phase observables for systems with spectra corresponding to this special set of sequences are in fact continuously approaching the phase for irrationally related energy eigenvalues. The nontrivial dependence of the phase POVM on the characteristic frequencies was reported for the first time in Ref. [27], where slightly more details about the Farey tree construction can be found. Such dependence of physical dynamical quantities on the number-theoretic nature of characteristic frequencies is commonly encountered in classical Hamiltonian dynamics [30]. Thus, the phase POVM for a system with irrationally related energy eigenvalues is defined as the limit of the phase POVMs over the special sequence of systems with Farey close sets of q_k's. The result of such limiting procedure is a phase POVM with zero off-diagonal matrix elements and the diagonal ones given by (9) independently of the energy spectra. In this way the unique phase POVM given by uniform density is associated with any system with irrational ratios of the energy eigenvalues. This is as it should be expected since the orbits of a system with irrationally related energy levels generate a linear irrational rotation, which is an ergodic system with uniform invariant measure independent of the irrationally related rotation numbers. Differences among the invariant measures for different irrational rotations is to occur only in the case of nonlinear rotations, and these do not occur in quantum mechanics.

Previous general prescription works in the case of an arbitrary discrete spectrum without an accumulation point. Spectra with an accumulation point can be considered as a limit of a sequence of approximations as follows. Suppose that the accumulation point in the energy spectrum corresponds to the index $k \to \infty$. Then all energy eigenvalues for $k > k_0$ where k_0 is large enough are close. k_0 approximation is obtained if all levels with $E_k < E_{k_0}$ are the same as in the spectra with the accumulation point but the levels with $E_k > E_{k_0}$ are considered as equal to E_{k0}, that is, as a single infinitely degenerate eigenvalue. The phase POVM of such k_0th approximation is computed using formulas for the matrix elements (7)–(9). The first $k_0 \times k_0$ matrix elements of the k_0+1th approximation coincide with the k_0th approximation, and this is true for any k_0. In the limit $k_0 \to \infty$ we obtain the phase POVM for the original spectrum with the accumulation point. The procedure indicates that the constructed phase distribution of a system with an accumulation point in its spectrum is uniform, like for systems with irrationally related eigenenergies.

III. ILLUSTRATIVE EXAMPLES

In this section we shall first illustrate further the peculiar discontinuity of the phase POVM dependence on the parameters in a given Hamiltonian, and then illustrate and discuss the nonuniqueness of the phase POVM in the case of a degenerate spectrum.

A. Morse spectrum

The phase POVM depends discontinuously on the characteristic frequencies and on the parameters in the Hamiltonian. These discontinuous dependencies are illustrated in this subsection using the well-known Morse oscillator [31]. The potential of the Morse oscillator is given by

$$V(x) = D\{1 - \exp[-a(x - x_0)]\}^2, \tag{11}$$

where $x - x_0$ is the distance from the equilibrium x_0, and D and a are parameters that describe the depth and the width of the potential well, respectively. The discrete energy eigenvalues are nondegenerate and are given by the following formula:

$$E_k = h\nu_0(k + 1/2) - \frac{[h\nu_0(k + 1/2)]^2}{4D}, \tag{12}$$

where k is an integer valued quantum number, and ν_0 has dimension of a frequency and is related to the particle mass m and the Morse constant D via

$$\nu_0 = \frac{a}{2\pi}\sqrt{2D/m}. \tag{13}$$

The potential (11) has a finite number of the discrete eigenvalues (12) and the maximal possible k is determined as

$$k_{\max} = \left[\frac{2D - h\nu_0}{h\nu_0}\right], \tag{14}$$

where the brackets denote the integer part of the argument. For fixed values of D and a (and $h = 1$) the energy eigenvalues and $k_{\max}$ are functions of the mass m only.

The difference between the successive E_k is not constant but is such that the ratio $(E_k - E_{k-1})/(E_{k-1} - E_{k-2})$ is constant. Thus, although there could be a large number of E_k, i.e., q_k in Eq. (2), their relations can be characterized by a single characteristic frequency $\nu = (E_k - E_{k-1})/(E_{k-1} - E_{k-2})$.

The number of discrete eigenvalues, the characteristic frequency, the corresponding numbers $q_1, \ldots q_k$, and consequently the phase POVM depend on the mass m, with a and D conveniently fixed as $a = 1/\sqrt{2}$ and $D = 1/\pi$. This dependence is illustrated in Fig. 3, where the values of m are chosen such as to illustrate the discontinuous dependence of the phase on m. For example, following three values of m: $m_1 = 2.26354$; $m_2 = 2.29192$; and $m_3 = 2.19335$ all imply the same number of discrete energy eigenvalues $k_{\max} = 4$. m_1 implies $\nu_1 = 1/4 = 0.25$, m_2 implies $\nu_2 = 10/41 = 0.268293$, and m_3 implies $\nu_3 = 1/5 = 0.2$. The corresponding eigenvalues in the three considered cases are obtained, for example, with $\{q_1,q_2,q_3\}_1 = \{64,80,84\}$; $\{q_1,q_2,q_3\}_2 = \{68921,87412,92373\}$; $\{q_1,q_2,q_3\}_3 = \{125,150,155\}$ with the corresponding appropriate choice of ΔE. As was pointed out, the phase observable does not depend on ΔE but only on the triplet $\{q_1,q_2,q_3\}$, in fact on the ratio $\nu = (q_3 - q_2)/(q_2 - q_1)$.

In Figs. 3(a) and 3(b) we plot the phase expectation in the state $|\psi\rangle = (|0\rangle + |1\rangle + |2\rangle + |3\rangle)/\sqrt{4}$ for (a) $\nu_1 = 1/4$ and $\nu_2 = 11/41$ and in (b) for $\nu_1 = 1/4$ and $\nu_3 = 1/5$. The expectation of the phase for $\nu_2 = 11/41$ gives numbers of the order 10^{-5} which cannot be distinguished from zero on the scale of Fig. 3(a). Figures 3(a) and 3(b) convincingly demonstrate that although $|m_2 - m_1| < |m_3 - m_1|$ and

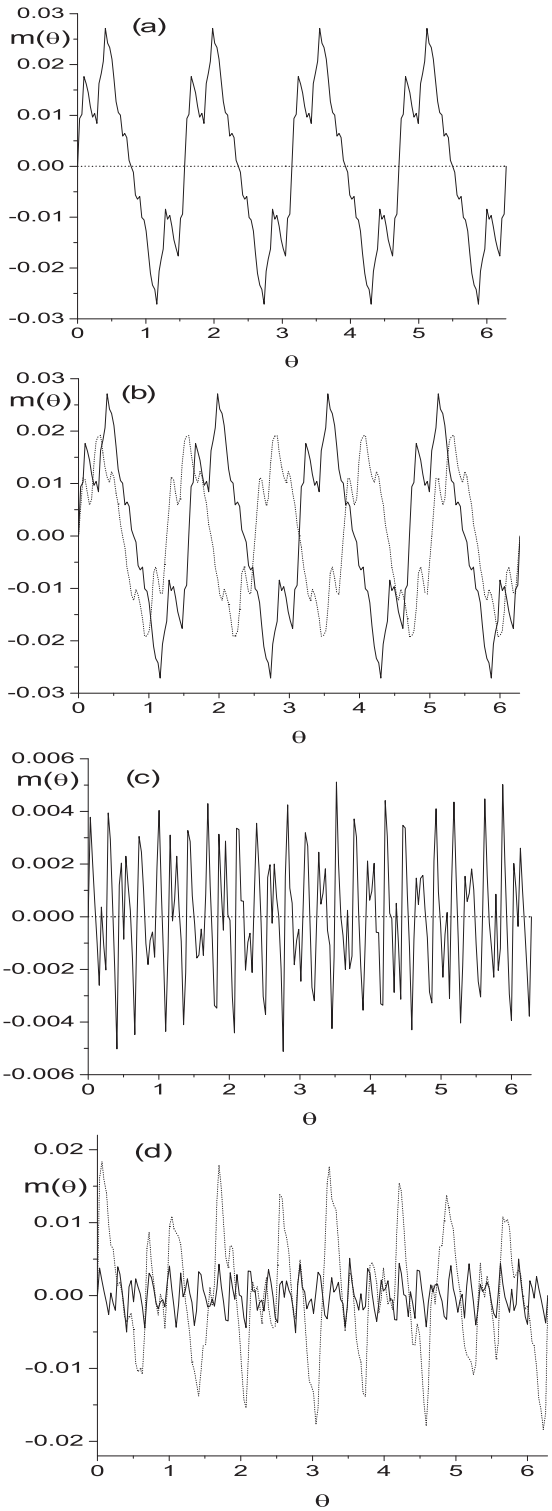

FIG. 3. Function $m(\theta) \equiv \langle\psi|\hat{M}_\theta^{q_1,q_2}(\theta)|\psi\rangle - \theta/2\pi$ for the Morse oscillator is illustrated in the state $|\psi\rangle = (|E_0\rangle + |E_1\rangle + |E_2\rangle + |E_3\rangle)$ for (a) $\nu = \nu_1 = 1/4$; $\nu = \nu_2 = 11/41$ (dotted); (b) $\nu = \nu_1 = 1/4$, $\nu = \nu_3 = 1/5$ (dotted); (c) $\nu = \nu_1 = 3/5$; $\nu = \nu_2 = 31/51$ (dotted); (d) $\nu = \nu_1 = 3/5$, $\nu = \nu_3 = 2/3$ (dotted).

$|\nu_2 - \nu_1| < |\nu_1 - \nu_3|$ the phase expectations satisfy $|\langle M_1\rangle - \langle M_3\rangle| \ll |\langle M_1\rangle - \langle M_2\rangle|$ since 1/5 and 1/4 are Farey neighbor appearing at the successive levels of the Farey tree, while 11/41 appears at the level distant from the level of 1/4.

The same conclusion is illustrated in Figs. 3(c) and 3(d) corresponding to $m_1 = 4.47623; m_2 = 4.53611; m_3 = 5.09296$ with $k_{\max} = 5$ and $\nu_1 = 3/5; \nu_2 = 31/51; \nu_3 = 2/3$. The phase expectation for $\nu_2 = 31/51$ given in Fig. 3(c) cannot be distinguished from zero on the scale of the figure.

The previous examples show that, although the parameter values m_1 and m_2, and the corresponding energy eigenvalues are relatively good approximations of each other, much better approximation of the phase observable $\hat{M}_1$ is obtained with $\hat{M}_3$ chosen such that the characteristic frequencies are close in the Farey tree.

B. Coupled spins: The case of a degenerate spectrum

In the case of a degenerate spectrum there are two qualitatively different reasons for nonuniqueness of the phase POVM.

As was pointed out, different energy eigen-bases and different legitimate partitions give different phase POVMs. We illustrate this facts using examples of two spins in a magnetic field coupled in such a way that the system is symmetric with respect to rotations around the field axes, implying degenerate spectrum.

The Hamiltonian is

$$H = \omega\left(\sigma_z^1 + \sigma_z^2\right) + \mu\sigma_z^1\sigma_z^2, \tag{15}$$

where ω and μ are parameters and $\sigma_z^{1,2}$ are Pauli σ_z matrices of the first and the second spin.

For $\omega = 2$ and $\mu = 1$ the Hamiltonian has eigenvalues $-3,-1,-1,5$. Vectors $|1,1\rangle \equiv |1\rangle \otimes |1\rangle$ and $|-1,-1\rangle \equiv |-1\rangle \otimes |-1\rangle$, where $(|1\rangle,|-1\rangle$ denote the two eigenvectors of σ_z, are the eigenvectors corresponding to the nondegenerate 5 and -3 eigenvalues, respectively. Preferred choice of two orthogonal eigenvectors in the degenerate eigenspace E_{-1} is suggested by the symmetry of (15). Minimal complete set of compatible observables (MCSCO) for the system (15) is, for example, $(\hat{H},\hat{\sigma}_z^1 \otimes 1)$ or $(\hat{H},1 \otimes \hat{\sigma}_z^2)$, and either choice of MCSCO selects the same two orthogonal vectors $|1,-1\rangle \equiv |1\rangle \otimes |-1\rangle$ and $|-1,1\rangle \equiv |-1\rangle \otimes |1\rangle$. Thus, the nonuniqueness of the phase POVM due to the arbitrary choice of the bases in the degenerate eigenspace is removed by selecting the common eigenbases of the MCSCO. It is natural to apply the same recept for the choice of the preferred bases in the general case.

Let us now turn onto the dependence of the phase POVM on the choice of a legitimate partition for the bases fixed as above. Here we propose to consider only those legitimate partitions such that the vectors belonging to the same cell correspond to the same eigenvalues of the operators in the MCSCO additional to the Hamiltonian. Vectors from different cells must correspond to different additional eigenvalues. Such restriction on the legitimate partitions is dictated by the reason of simplicity, and is suggested by the analyses of the phase POVM already obtained in simple cases like free 1D particle or 2D particle. For example, in the 1D case, each energy eigenvalue $p^2/2m$ is doubly degenerate. Construction of the standard phase POVM [16] proceeds by using the partition with only two cells $\{Q_+, Q_-\}$ such that the cell $Q_\pm$ contains only the $\hat{P}$ generalized eigenvectors with positive or negative P eigenvalues. This prescription uniquely fixes the phase POVM in the case of 1D free particle.

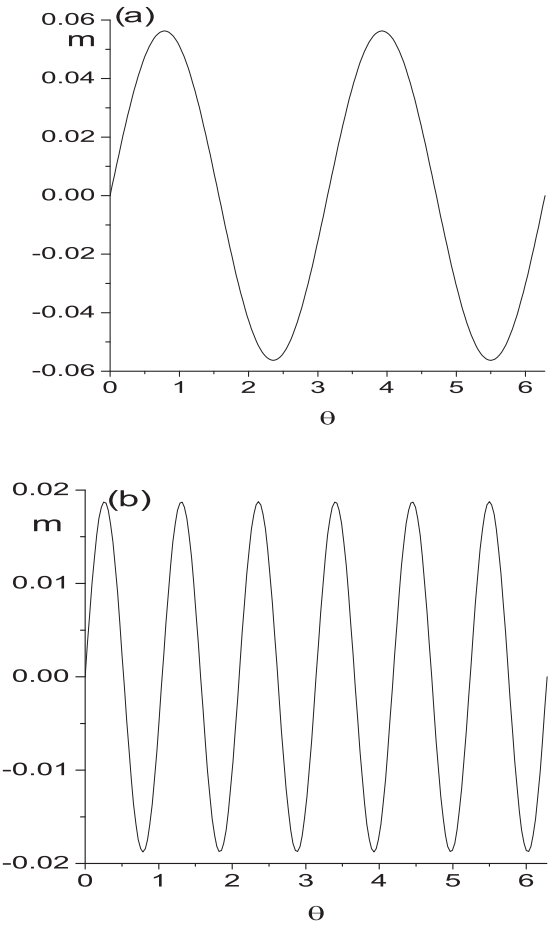

FIG. 4. Figures illustrate nonuniqueness of the phase POVM, due to the possibility of different legitimate partitions. $m(\theta)$ for the system (15) is calculated with partition Π_1 (a) and Π_2 (b) in the state $\psi = (1/2,1/\sqrt{2},0,1/2)$.

In the example (15), with already fixed bases $|1,1\rangle,|1,-1\rangle,|-1,1\rangle,|-1,-1\rangle$ there are two partitions that satisfy the above criterion. If MCSCO is chosen as $\{\hat{H},\hat{\sigma}_z^1 \otimes 1\}$ then the corresponding partitions are $\Pi_1 = \{\{|1,1\rangle,|1,-1\rangle\},\{|-1,-1\rangle,|-1,1\rangle\}\}$. On the other hand, if MCSCO is chosen as $\{\hat{H},\hat{1} \otimes \sigma_z^2\}$ then the corresponding partitions are $\Pi_2 = \{\{|-1,1\rangle,|1,1\rangle\},\{|-1,-1\rangle,|1,-1\rangle\}\}$.

In Figs. 4(a) and 4(b) we illustrate the expectation values of the phase POVM (6) for the state $\psi = (1/2,1/\sqrt{2},0,1/2)$ obtained with the bases $|1,1\rangle,|1,-1\rangle,|-1,1\rangle,|-1,-1\rangle$ and with the two partitions Π_1 [Fig. 4(a)] and Π_2 [Fig. 4(b)]. The two natural legitimate partitions generate different phase POVM. We do not see any additional physically justified criterion that can be used to single out any of these two phase POVMs as more natural.

IV. TRAPPED BEC AND PHASE MEASUREMENT

In order to measure the phase of a state vector motion one must be able to observe experimentally the evolution in time of the full state vector at least at some sufficiently representative

set of time instants. An example of physical systems where this can be done is provided by Bose-Einstein condensate (BEC) trapped in some potential. Absorption experiments performed successively at times t_i with such systems provide information abut the distribution of density of atoms at those time, or in other words provide the functions $|\psi(x,t_i)|^2$, where x are the spacial coordinates. Such measurements of $|\psi(x,t_i)|^2$ and other derived quantities for a BEC in a double well, which is relevant for the model treated in what follows, have been reported, for example, in Ref. [32]. Since the number of atoms in the BEC is constant during its evolution the state space of the system is finite dimensional, and therefore the function $|\psi(x,t)|^2$ at any fixed t uniquely determines the expansion coefficients $c_i(t)$ of the state vector $\psi(x,t)$ at those t. The coefficients $c_i(t)$ are periodic functions of t and such oscillatory motion is characterized by the corresponding phases, one for each periodic function $c_i(t)$. The corresponding master phase represents the phase of the state vector evolution. Thus, image processing of the measured $|\psi(x,t)|^2$ provides $c_i(t)$ and therefore the evolution of the phase of the state vector motion. Such experimentally measured phase of the state motion, renormalized onto the period of the particular state vector evolution, is mathematically represented by the expectation value of the phase operator $\hat{\theta}$ introduced here.

Dynamics of the density profiles in different models of BEC have been numerically treated in many references, for example, in Refs. [33–35]. Main points of the computations are here illustrated using a particularly simple model of the BEC in a double-well potential. The two-mode Bose-Hubbard (2mBH) system is given, up to c-number terms, by the following Hamiltonian (see, for example, [36] and the references therein):

$$\hat{H} = \epsilon_1 \hat{a}_1^\dagger \hat{a}_1 + \epsilon_2 \hat{a}_2^\dagger \hat{a}_2 - \delta(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) + \frac{c}{2}\left((\hat{a}_1^\dagger)^2 \hat{a}_1^2 + (\hat{a}_2^\dagger)^2 \hat{a}_2^2\right), \tag{16}$$

where the operators $\hat{a}_1^\dagger$, $\hat{a}_1$ and $\hat{a}_2^\dagger$, $\hat{a}_2$ are the bosonic creation and annihilation operators for the two degrees of freedom. The Hamiltonian (16) approximates the physical situation created experimentally by confining an atomic Bose-Einstein condensate in a double-well trap [37,38]. In this case operators $a_1^\dagger$ and $a_2^\dagger$ are interpreted as creating atoms in the condensate confined in the potential wells 1 and 2, respectively. The term proportional to δ describes the tunneling of atoms between the two wells and the term proportional to c describes the nonharmonicity of the potential wells. The operator $\hat{N} = \hat{N}_1 + \hat{N}_2 = \hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2$ commutes with the Hamiltonian (16) and represents the conserved total number of atoms in the trapped condensate.

Introducing operators,

$$\hat{J}_x = (\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1)/2, \tag{17a}$$

$$\hat{J}_y = i(\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1)/2, \tag{17b}$$

$$\hat{J}_z = (\hat{a}_2^\dagger \hat{a}_2 - \hat{a}_1^\dagger \hat{a}_1)/2, \tag{17c}$$

that satisfy the standard SU(2) commutation relations the Hamiltonian (16) becomes, up to a constant term,

$$\hat{H} = (\epsilon_2 - \epsilon_1)\hat{J}_z - 2\delta \hat{J}_x + c\hat{J}_z^2. \tag{18}$$

The quantity J_z gives the population imbalance between the two modes,

The invariant subspaces of the total Hilbert space are the spaces of irreducible SU(2) representations. The total number operator $\hat{N}$ is related to the Casimir operator of the SU(2) by the relation $\hat{J}^2 = \hat{N}/2(\hat{N}/2+1)$. Interpretation of the relevant quantities is best described using SU(2) coherent states. These are parametrized by the canonical coordinates q,p related to the SU(2) coherent state expectations of $\hat{J}_x, \hat{J}_y, \hat{J}_z$ by the formulas,

$$\langle \hat{J}_x \rangle(p,q) = \frac{q}{2}(4j - q^2 - p^2)^{1/2}, \tag{19}$$

$$\langle \hat{J}_y \rangle(p,q) = -\frac{p}{2}(4j - q^2 - p^2)^{1/2}, \tag{20}$$

$$\langle \hat{J}_z \rangle(p,q) = \frac{1}{2}(q^2 + p^2 - 2j). \tag{21}$$

The canonical coordinate q represent the relative phase $q = \phi$ between the two modes in Eq. (16) and the canonical momenta $p = \cos^2(\theta/2)$ gives the population of the second mode. Here the angles θ,ϕ provide an alternative parametrization of S^2, i.e., of the SU(2) coherent states. The polar angle coordinate of the SU(2) coherent state is the phase difference of the two modes in Eq. (16).

Consider 2mBH with a fixed total number N of atoms. N determines the representation of the SU(2). The Hamiltonian matrix (18) is diagonalized to obtain the spectrum in terms of the parameters $\delta, \epsilon = \epsilon_2 - \epsilon_1, c$ and then the integers $q_1, q_2, \ldots$ corresponding to some fixed values of the parameters are determined. Obviously the spectrum must be computed numerically for BEC with large numbers of atoms. The numbers $q_1, q_2, \ldots$ determine the frequencies of the oscillations of the system's state vector $|\psi(t)\rangle$ and are used to construct the phase POVM by the formulas (5) and (6). The expectation of the relative phase of the state vector at the time t is given by the expectation of $\hat{\theta}$ in the state vector $|\psi(t)\rangle$. The latter can be reconstructed from the measured densities.

As was pointed out, the dependence of the phase on the eigenfrequencies is discontinuous and complicated. In typical systems this means that the dependence of the phase on the parameters in the model is discontinuous. One should not expect that the full complexity of the phase dependence on the parameters can be experimentally demonstrated in a systematic way, because of the impossibility of controlling the parameters with sufficient precision. Nevertheless, comparison of the experimentally determined phase of the state evolution with the theoretical prediction is possible, although more involved than in the case of quantities with smooth dependence on the parameters. Similar problems occur often in controlling the dynamics and testing theories of classically chaotic systems with fractal dependence on the parameters and/or initial conditions [39]. Consider an experiment aimed at monitoring the evolution of the state vector. Parameters of the experiment are fixed to be in some small interval $\Delta_p = (p - \Delta, p + \Delta)$. The evolution of the phase of the state is obtained from the data collected by monitoring the state evolution, and represent the experimental data to be compared with theoretical computation of the phase expectation. Computations are done using a set of parameter values from the above interval Δ_p, first to compute the energy eigenvalues and then the corresponding

phase. The computed phase expectations will be either quite similar to those reconstructed from the experimental data or quite different. In the latter case, the computations should be repeated with another set of parameter values from Δ_p. The shape of experimentally obtained phase distribution suggests the choice of parameter values from Δ_p. Namely, if the experimental data suggest that the phase distribution displays large oscillations then the parameter values from Δ_p that are used for computations should be such that the eigenfrequencies are given by rational numbers with small denominators.

V. DISCUSSION

This section is devoted to a discussion of possible critical comments that might be raised concerning the definition of the normalized phase presented here, its physical meaning and properties. The discussion is to a large extent inspired by the comments [28] on our paper [27], which contains brief exposition of the basic concept treated here.

The physical meaning of the normalized phase studied here should be perhaps stressed again. It is an analogous quantity to the normalized phase of a state point on an orbit of a classical (integrable) system, and represents the relative part of the period undergone by a state vector while it is moving on the orbit in the Hilbert space. Of course, particular more tangible physical meaning of such quantity depends on the concrete physical model, as has been illustrated in the example of 2mBH.

The main difference between the object treated in our paper and that in the remark by Hall and Pegg (HP) [28] is that we study and compare the normalized phases (or normalized age or angle) and HP analyze an absolute age. Consider a periodic system with the period T. Our normalized phase measures the relative part of the total period T undergone by the system during an interval $(0,t)$. In this way the normalized ages of two systems with different periods can be meaningfully compared. There are processes performed by (or with) quantum systems (for example: STIRAP [40], quantum circuits [41] etc...) such that the part of the process undergone by the system, as measured by the normalized phase, and not the actual duration (as measured by the absolute phase), is the only relevant information. Such a process might take quite different time intervals to perform by different systems, but nevertheless one would consider two systems to be in the same phase of the process if the the normalized phases are equal. On the other hand, periodic systems with different frequencies can be used as clocks to measure the same absolute time. In this case the notion of an absolute phase, as a system's observable that measures the absolute time is appropriate. So, both normalized and absolute phase can be defined and have meaningful interpretation.

Incommensurate eigenmodes imply in general quasiperiodic motion whose period can be formally considered as $T = \infty$. Such a system is equally old or young in any particular moment in time. In this sense our result for the normalized phase of a quasiperiodic system is as it should be. Periodic and quasiperiodic motions with different frequencies, but always with bounded orbits, are usually compared by rescaling the motion on a unit circle. Therefore, we computed explicitly the normalized phase observable for periodic motion for all periods, which can and must be rescaled on the unit circle. Then we defined the normalized phase of the quasiperiodic motion as a limit of the corresponding sequence of such normalized phases for periodic motions. The probability distribution over the unit circle that is obtained in the limit is uniform and does not depend on the irrational eigenfrequencies of the limiting quasiperiodic motion. Time, spent by a quasiperiodic system in a subinterval $(\theta_1,\theta_2) \in S^1$ of an orbit and normalized by the infinite period is the measure of this interval given by the normalized phase. This measure does not depend on the angular velocity of motion on the orbit. On the other hand, the expression (21) in Ref. [15] is there considered as a probability distribution on $\mathbf{R}^+$. In order that the expression generates a well-defined functional on some type of function on $\mathbf{R}^+$ one has to consider a special type of norm and the appropriate set of functions, such as the almost-periodic functions. In the case of periodic state motion and for the nondegenerate energy, the two distributions, one on the unit circle and given by our normalized phase and the other on $\mathbf{R}^+$ given by the absolute time are indeed related by the appropriate rescaling. However, in the case of quasiperiodic state motion the expression (21) of Ref. [15] can be considered as a probability functional on the space of almost periodic functions and with the appropriate norm given by the time average. In this sense, the expression (21) of Ref. [15] gives well-defined time averages of almost-periodic functions, with nontrivial and useful properties. In particular, appropriately defined purity displays different properties from the purity of a uniform distribution, as was studied in detail in Ref. [15].

The example provided by HP of a special initial condition leading to a periodic motion in a system with typically quasiperiodic orbits shows just the existence of such special initial conditions. Of course, they are not typical for the considered system with incommensurate eigenmodes neither in the measure theoretic nor in the topological sense.

Discontinuous dependence of the relative phase on the frequency is one of the two main topics of our communication. In particular we show, in general and using the Morse system as an example, how a small perturbation of the spectrum in general implies discontinuous changes of the relative phase. Our results, in fact show much more, i.e., we indicate special sequences of frequencies, namely those corresponding to the successive best rational approximations p_n/q_n of an irrational ν, over which the relative phase varies continuously and approaches the uniform distribution as $p_n/q_n \to \nu$.

Lack of details of the relative phase for a degenerate spectrum in our brief communication [27] has also been criticized by HP. The nonuniqueness of the phase in the degenerate case is treated in detail, and to the best of our knowledge for the first time, in this paper. In particular different sources of nonuniqueness of the phase in the degenerate case have been discussed. This is our second main contribution.

VI. SUMMARY

We have introduced a definition of phase POVM for a system with quite general properties of its energy spectrum. The definition provides objects which satisfy the covariance relation, demanded of the phase observable, for systems with

arbitrary Hilbert spaces, with rationally or irrationally related characteristic frequencies and with possibly degenerate energy spectra.

Dependence of the phase POVM on the characteristic frequencies or the parameters in the Hamiltonian is discussed. It is demonstrated that this dependence is discontinuous in the sense that small variations in the energy eigenvalues leading to small variations of the characteristic frequencies imply large variations in the expectations of the corresponding phase POVM. Due to this discontinuity a sequence of phase POVM for spectra with rational characteristic frequencies all close to an irrational one do not provide good approximations to each other in general. However, if the spectra are characterized by sets of rationals which are close in the Furrey tree of all rationals then the corresponding phase POVMs are also close. Such nontrivial dependence of the phase POVM on the number-theoretic nature of the characteristic frequencies was reported using three-dimensional examples for the first time in Ref. [27], and is discussed and illustrated in more details in the present paper.

Another issue discussed in detail in this paper is the nonuniqueness of the phase POVM for systems with symmetries, i.e., with degenerate energy spectra. Following the discussion of specific examples we proposed a natural procedure that singles out a small number (in some cases just one) of equivalent phase POVM.

Besides of its fundamental theoretical importance, the presented general definition of phase POVM enables one to compare the phases of evolution of different quantum processes.

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