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Phase-Difference Equations: A Calculus for Quantum Revivals

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Abstract—Equations describing the revival times of multimode quantum systems are transformed into a set of phase-difference equations, which are discrete difference equations that describe the phase relationships among the modes of the quantum system at a revival. These equations are developed using an analogy to the differential equations satisfied by polynomials of a continuous variable and serve as a comprehensive toolkit for investigating revival phenomena. We apply these equations to two examples in detail to demonstrate their utility, investigating revivals of selectively populated wavefunctions in the infinite square-well potential and of highly excited wavepackets in arbitrary one-dimensional potentials.

1. INTRODUCTION

Quantum decays and revivals have been studied in an amazing variety of physical systems since the landmark paper by Eberly, Narozhny, and Sanchez-Mondragon that laid the foundation for the field [1]. Decays and revivals were originally predicted in the Rabi oscillations of a two-level atom interacting with a quantized electromagnetic field [1, 2] and are also found, for example, in the classical orbital motion of an atomic electron excited into a circular-orbit wavepacket [3, 4] and in the shape of the wavefunction in an infinitely deep potential well [5, 6]; certain features present in the initial dynamics of these quantum systems decay away over time, only to reappear eventually in time windows broadly called *revivals* (and more specifically classified as *revivals* and *super-revivals*, with corresponding *fractional revivals* and *fractional super-revivals*). Although the feature of the initial state that is lost and later regained and the physics that governs the intervening dynamics depend entirely on the system under investigation, revival phenomena can be studied in a general way that transcends the differences among quantum systems. Amidst such general analyses in the literature (detailed below), the present paper describes a new formalism for investigating revival phenomena that unifies and extends previous efforts and offers a useful tool for future research.

Decays and revivals are generic features of multimode quantum states, which are coherent superpositions of many eigenstates of a quantum system. The constitutive modes slowly walk out of phase with one another and mutually interfere, leading to the decay of the initial quantum state; the revivals are the eventual rephasings of these modes, with partial, or selective, rephasings the source of fractional revival phenomena. The study of revivals, then, is the investigation of how special phase patterns emerge from a complicated multimode interference over time.

Revival phenomena have been predicted or observed in a remarkable range of physical systems that span the current areas of research in quantum mechanics and quantum optics, including the Jaynes–Cummings model of a two-level atom interacting with a quantized monochromatic field [7–11], atomic Rydberg wavepackets [4, 12] including the effects of the quantum defect [13, 14], semiconductor superlattices [15], atoms in gravitational cavities [16, 17], systems with a spin-orbit interaction [18, 19], finite [20, 21] and infinite square wells [6, 22, 23], molecular vibrational wavepackets [24], Bose–Einstein condensates [25–27], classically chaotic systems [28], atomic wavepackets in optical lattices [29], Josephson junctions [30, 31], and angular-momentum coherent states [32]. There has been substantial theoretical work exploring the common features of revival phenomena among quantum systems and investigating revivals [6], fractional revivals [33, 34], super-revivals and longer-term recurrences [35–39], generic signals from multilevel quantum systems [40, 41], and revivals in systems with multiple degrees of freedom [20, 42].

Most of these previous studies of revival phenomena begin with knowledge of the wavepacket revival times, typically found by *ansatz* or by numerical simulation, and then examine the dynamics of the quantum state at these predetermined moments of time. We believe that a robust "calculus" for revival phenomena should be able to predict the revival times from first principles, and this predictive power is the central motivation for and success of the phase-difference equations developed in this paper. These equations arise from a three-step chain of reasoning: First, we identify the physical model for revivals, establishing what feature of the initial dynamics we will search for at later times as constituting a "revival." Second, we extract from this revival model a relationship among the phases of the modes of the quantum state that is satisfied during a revival. Third, we use this phase relationship to determine the revival times for the quantum state. Surprisingly few papers have followed this approach, but such constructive determinations of revival times have been made by Knospe and Schmidt [39] for highly excited wavepackets, by Jie and Wang [43] for fractional revivals, and by Styer [44] for wavefunctions in the infinite square-well potential; here, we show that these disparate studies can be unified with our more general theory.

For a wide array of revival models and physical systems, we find that the phase relationship among the modes at a revival (the second step of our chain of reasoning) has the same general form, which is described by the polynomial dependence on quantum number shown in Eq. (2) below. Using an analogy to the differential equations satisfied by polynomial functions of a continuous variable, we convert this general form into a set of *phase-difference equations* from which the revival times can be readily determined. The goals of this paper are to establish these equations and to demonstrate their use.

1.1. Mathematical Preliminaries

We consider a nonrelativistic quantum-mechanical particle of mass m excited into a coherent superposition of bound-state energy levels in a one-dimensional potential $V(x)$. (We focus on the revival phenomena of particle wavefunctions to be concrete; however, our methods can be used without modification to study revivals associated with the quantized electromagnetic field or with other quantum systems.) The potential is associated with discrete energy eigenvalues E_n (with corresponding frequencies $\omega_n = E_n/\hbar$) and eigenfunctions $\phi_n(x)$, which are found by solving the time-independent Schrödinger equation. At the initial time (taken to be $t = 0$), the amplitude of the wavefunction in the nth energy level is $c_n = \langle\phi_n|\psi(t = 0)\rangle$; then, the wavefunction at time t is described in the energy eigenbasis as

$$\psi(x, t) = \langle x|\psi(t)\rangle = \sum_n \exp[-i\omega_n t]c_n\phi_n(x). \qquad (1)$$

The quantity $\exp[-i\omega_n t]$ is called the *time-evolution exponential*, and its argument $\omega_n t$ is the *dynamical phase* associated with the nth energy level at time t. We adopt the distinction made by Styer [44] and others that the description (1) of the quantum state is generically called a *wavefunction*, whereas the state is specifically called a *wavepacket* to indicate special initial conditions, such as being well-localized in space or well-defined in energy.

We use the mathematical notation that the functional dependence on discrete variables (like the quantum number n) is shown using subscripts, while the dependence on continuous variables (like the coordinate x) is indicated with parentheses.

2. PHASE-DIFFERENCE EQUATIONS

The revival times for quantum wavefunctions can often be identified by solving certain "time eigenvalue" equations. Although the specific form of these eigenvalue equations depends on the particular wavefunction revival model being investigated (as we show in two detailed examples in Sections 3 and 4), broadly speaking the revivals are special moments of time t at which the time-evolution exponential satisfies an equation (either exactly or approximately) in the form

$$\exp[-i\omega_n t] = \exp[-iP_n^{(N)}(t)] \qquad (2)$$

for all quantum numbers n that are pertinent to the wavefunction, where $P_n^{(N)}$ is a polynomial in the quantum number n of order N; that is, revivals are associated with special (polynomial) configurations of the dynamical phases. In the examples below, we approach Eq. (2) with a known, fixed value of the polynomial order N, and we seek both the time eigenvalues t and the polynomial eigenvectors $P_n^{(N)}(t)$ that satisfy the equation. In practice, we are far more interested in the revival times t than in the polynomials $P_n^{(N)}$, and our method of solution takes advantage of this disparity.

Our contribution in this paper is to convert these eigenvalue problems into equations that are more easily solved for the revival times, based on an analogy to the differential equations satisfied by polynomial functions of a continuous variable. These *phase-difference equations* are developed in two steps: First, in Section 2.1, we explore difference equations that describe polynomial functions of a discrete variable n, and, then, in Section 2.2 we apply these difference operators to equations with phase ambiguities that arise from equating the arguments of complex exponentials. Our method of presentation is to develop a useful "toolkit" for the reader rather than to present formal mathematical derivations.

2.1. Finite Difference Equations for Polynomials of a Discrete Variable

Consider a function $\Theta(x, t)$ that depends on continuous variables x and t. In order to determine when Θ is a polynomial in x of order N, we look for values of t for which Θ satisfies the partial differential equation

$$\frac{\partial^{N+1}}{\partial x^{N+1}}\Theta(x, t) = 0 \qquad (3)$$

for all x, since the $(N + 1)$th derivative of an Nth-order polynomial is identically zero. An analogous statement can be made for a function $\theta_n(t)$ that depends on a discrete (integer) variable n and a continuous variable t: the function θ is a polynomial in n of order N when it satisfies the *difference equation*

$$\frac{\Delta^{N+1}}{\Delta n^{N+1}}\theta_n(t) = 0 \tag{4}$$

for all n. The difference operator (also called the first difference) is defined as

$$\frac{\Delta}{\Delta n}\theta_n(t) = \theta_{n+1}(t) - \theta_n(t); \tag{5}$$

the second difference is

$$\frac{\Delta^2}{\Delta n^2}\theta_n(t) = \theta_{n+1} - 2\theta_n(t) + \theta_{n-1}(t), \tag{6}$$

and, in general, the kth difference is defined as k successive applications of the first difference operator,

$$\begin{aligned}\frac{\Delta^k}{\Delta n^k}\theta_n(t) &= \frac{\Delta}{\Delta n}\left[\frac{\Delta}{\Delta n}\left[\cdots\left[\frac{\Delta}{\Delta n}\theta_{n-\lfloor k/2\rfloor}(t)\right]\right]\right] \\ &= \sum_{j=0}^{k}(-1)^{j+k}\frac{k!}{j!(k-j)!}\theta_{n+j-\lfloor k/2\rfloor}(t),\end{aligned} \tag{7}$$

where $\lfloor x\rfloor$ is the largest integer less than or equal to x. The integer argument for θ in Eq. (7) is taken to be $n - \lfloor k/2\rfloor$ instead of n simply to make the resulting expressions as symmetric as possible around n, an aesthetic choice with no physical ramifications. Difference operators (5)–(7) are the discrete analogs to the derivatives of a function of a continuous variable and are used widely in numerical analysis to approximate the derivatives of a function that has been sampled on a grid of equally spaced points [45]. They satisfy sum and product rules similar to those of the derivatives of a function of a continuous variable [46], but, for our present purposes, we consider (4) to be their key attribute.

2.2. *From Time Eigenvalue Equations to Phase-Difference Equations*

In order to extract the revival times from (2), we take the logarithm of both sides of the eigenvalue equation; because of the multiple branches of the logarithm function, this gives

$$\omega_n t = P_n^{(N)}(t) + (\text{multiple of } 2\pi) \tag{8}$$

for all quantum numbers n. The meaning of (8) is that, for a fixed polynomial order N, we seek values of time t at which the dynamical phase $\omega_n t$ broadly follows a polynomial dependence on the quantum number of order N, except that, at each value of n, it may deviate from this polynomial by some integer multiple of 2π.

We can focus our attention on the revival times t and eliminate the unknown polynomial $P_n^{(N)}$ from (8) by applying the $(N+1)$th difference operator to both sides. To understand the result of this operation, first recall from (4) that the $(N+1)$th difference of any polynomial of order N vanishes. Next, note that the difference operator acting on the multiples of 2π is also a multiple of 2π, since difference operators (7) are linear superpositions of function values with integer coefficients. Thus, applying the difference operator transforms (8) into

$$\frac{\Delta^{N+1}}{\Delta n^{N+1}}[\omega_n t] = (\text{multiple of } 2\pi). \tag{9}$$

Equation (9) is called the primary phase-difference equation for wavefunction revivals. It is completely equivalent to the starting eigenvalue Eq. (2) and is a necessary and sufficient condition for revivals.

In addition to the phase-difference Eq. (9), it proves useful to investigate ancillary phase-difference equations that describe necessary, but no longer sufficient, conditions for the revivals. The ancillary equations are found by applying the difference operator an additional j times (for a positive integer j) to the primary equation,

$$\frac{\Delta^{N+j+1}}{\Delta n^{N+j+1}}[\omega_n t] = (\text{multiple of } 2\pi), \tag{10}$$

in analogy to the result from the calculus of a continuous variable that the $(N+j+1)$th derivative of an Nth-order polynomial function exactly vanishes. In principle, the primary Eq. (9) is all that is needed to deduce the revival times for a wavefunction, but, in practice, the ancillary equations help steer us to these solutions. Indeed, in Section 4 we show that the ancillary equations are central to identifying approximate revivals when exact solutions do not exist. We note that equations like (9) have been used to predict revivals in the Jaynes–Cummings model [7, 10, 11], but this past work did not explore the importance of ancillary equations (10) or elevate these equations to a comprehensive toolkit for determining revivals in a broad array of physical systems.

The phase-difference equations are more rigorously stated in terms of congruence algebra from number theory [47, 48] as, for example,

$$\frac{\Delta^{N+1}}{\Delta n^{N+1}}[\omega_n t] \equiv 0 \pmod{2\pi}, \tag{11}$$

where "≡" means "is congruent to." We have found, however, that using the ancillary phase-difference equations largely supersedes the need to perform elaborate calculations using congruence algebra, so we turn to the number-theory notation and framework sparingly.

The remainder of this paper consists of two separate (and self-contained) examples of using the phase-difference equations to identify revival times in quantum systems. The first example (Section 3) emphasizes exact solutions to the revival equations, whereas the second example (Section 4) explores the more physically realistic case of approximate revivals.

3. EXAMPLE 1: POPULATION-DISTRIBUTION DEPENDENCE OF REVIVALS IN THE INFINITE SQUARE WELL

In our first example, we investigate wavefunctions excited in the one-dimensional infinite square-well potential,

$$V(x) = \begin{cases} 0, & |x| \le L/2, \\ \infty, & |x| > L/2, \end{cases} \tag{12}$$

which confines a particle completely to an interval of length L. The discrete energy eigenfrequencies,

$$\omega_n = \frac{\pi^2 \hbar}{2mL^2} n^2 = \frac{2\pi}{T_2} n^2, \tag{13}$$

depend on the square of the quantum number n (for positive integer n), where

$$T_2 = \frac{2\pi}{\omega_1} = \frac{4mL^2}{\pi\hbar} \tag{14}$$

is the time during which the ground state accumulates a 2π dynamical phase. (We write this as T_2 because it is the time scale associated with the n^2 dependence on the quantum number. This notation proves to be more sensible in Section 4 when we associate multiple time scales with the eigenfrequencies.) Rewriting (1) in terms of this time scale, the evolution of a wavefunction in the infinite square well is

$$\psi(x, t) = \sum_n \exp[-i2\pi(t/T_2)n^2] c_n \phi_n(x). \tag{15}$$

By direct substitution into (15), it has been shown [5, 6, 22] that the wavefunction at time $t = T_2$ is the same as at the initial time:

$$\begin{aligned} \psi(x, t = T_2) &= \sum_n \exp[-i2\pi n^2] c_n \phi_n(x) \\ &= \sum_n c_n \phi_n(x) = \psi(x, t = 0). \end{aligned} \tag{16}$$

Thus, time evolution in the infinite square well is periodic with period T_2.

3.1. Physical Model for Revivals

In the infinite square-well potential, we look for revivals of the probability density. We say that a revival occurs at time t when the wavefunction regains its initial form up to a physically insignificant overall constant phase β,

$$\psi(x, t) = \exp[-i\beta]\psi(x, 0), \tag{17}$$

i.e., when the probability densities at the two times are equal:

$$|\psi(x, t)|^2 = |\psi(x, 0)|^2. \tag{18}$$

We combine Eqs. (15) and (17) and use the orthogonality of the energy eigenstates ϕ_n to deduce that, at a probability-density revival, the time-evolution exponential must satisfy

$$\exp[-i2\pi(t/T_2)n^2] = \exp[-i\beta]; \tag{19}$$

then, comparing (2) and (19), we see that revivals are associated with times at which the dynamical phases are constant, independent of the quantum number n.

Note that the periodicity of dynamics in the infinite square well, described by (16), guarantees that there is a probability-density revival at time $t = T_2$, associated with the constant phase $\beta = 0$, for every initial wavefunction. In this example, we show that certain classes of initial wavefunctions have revivals at times earlier than T_2.

3.2. Revival Times as a Function of the Probability Distribution

We wish to examine how the probability-density revival times depend on the energy levels excited by a given wavefunction. To that end, we define a set P containing the quantum numbers of the populated energy levels:

$$P = \{n \,|\, |c_n|^2 > 0\}. \tag{20}$$

Styer [44] recently showed that two particular energy levels j and k in the set P satisfy the condition for probability-density revivals (19) at multiples of the time

$$t_{j,k} = \frac{T_2}{k^2 - j^2}, \tag{21}$$

and, therefore, the first revival time for the wavefunction is the least common multiple (1 cm) of the times given by (21) for all possible pairs of energy levels j and k; this revival time can be written as

$$t = \frac{T_2}{\gcd(k^2 - j^2 \,|\, j, k \in P)}, \tag{22}$$

where $\gcd(S)$ is the greatest common divisor of all of the integers contained in set S [47, 48]. For an arbitrary set P of populated levels, there is no general way to evaluate the denominator in (22). However, for a broad class of excitation sets P that we call *ladder excitations*, we now show that the revival times can be found in closed form using phase-difference equations.

3.3. Revival Times for Ladder Excitations

We consider a wavefunction excited in the infinite square well with a set of populated levels $P = \{b, b + d,$

$b + 2d, \ldots\}$. That is, the quantum numbers n with nonzero population are numbered by $n_j = b + dj$ in terms of a base level b and a level difference d for nonnegative integers j. We refer to such wavefunctions as "ladder excitations" simply because a plot of the population $|c_n|^2$ as a function of quantum number n is equally spaced with spacing d, like the rungs of a ladder.

This selective excitation of the quantum system allows us to disregard energy levels that are not populated by the particular wavefunction. The condition for a revival of such a wavefunction is that the time-evolution exponential satisfies

$$\exp[-i2\pi(t/T_2)(b+dj)^2] = \exp[-i\beta] \tag{23}$$

for all nonnegative integers j. Note that this is the same condition as for the revivals of a fully populated wavefunction in an anharmonic oscillator with discrete energy levels $E_n \propto b^2 + 2bdn + n^2$, so we see that the evolution of a selectively populated quantum state can mimic the dynamics of a different quantum system. (See [49] for an interesting additional example of this general principle, involving the selective excitation of the harmonic-oscillator potential.)

The revivals identified by (23) correspond to times at which the time-evolution exponential is a constant, namely, a polynomial of order $N = 0$ in the index j. This condition is equivalent to the phase-difference equation

$$2\pi(t/T_2)\frac{\Delta}{\Delta j}[(b+dj)^2] = (\text{multiple of } 2\pi), \tag{24}$$

which, after canceling factors of 2π, becomes

$$(t/T_2)\frac{\Delta}{\Delta j}[(b+dj)^2] = (\text{integer}). \tag{25}$$

An ancillary condition for revivals is that the time-evolution exponential satisfies the second difference equation

$$(t/T_2)\frac{\Delta^2}{\Delta j^2}[(b+dj)^2] = (\text{integer}); \tag{26}$$

higher-order ancillary equations offer no further information about the revival times. We reiterate that the revival times that satisfy (25) can be found directly with standard tools from number theory, but it is easier to first consider ancillary condition (26).

Evaluating the second difference Eq. (26), we find that

$$(t/T_2)2d^2 = (\text{integer}), \tag{27}$$

which says that the revival times are given by

$$t = \frac{T_2}{2d^2}R \tag{28}$$

for some integers R. Since (26) is a necessary but not sufficient condition for the probability-density revivals, we cannot simply associate the first revival with $R = 1$. Instead, we substitute (28) into the first difference Eq. (25) to find further stipulations on R; doing so tells us that

$$\frac{R}{2d^2}(2bd + 2jd^2 + d^2) = (\text{integer}). \tag{29}$$

The middle term on the left side of this equation,

$$\frac{2jd^2R}{2d^2} = jR, \tag{30}$$

is an integer, so we eliminate this quantity from both sides of the equation to find that

$$\frac{R(2bd + d^2)}{2d^2} = (\text{integer}). \tag{31}$$

The smallest integer R that satisfies (31) must contain all of the prime factors of $2d^2$ that are not present in $2bd + d^2$; thus, the possible values of R are multiples of

$$R = \frac{2d^2}{\gcd(2d^2, 2bd + d^2)}, \tag{32}$$

and combining (28) and (32), we arrive at the central result of this section, namely, that the revival times for a ladder excitation are

$$t_r = \frac{rT_2}{\gcd(2d^2, 2bd + d^2)} \tag{33}$$

for integer r.

Equation (33) shows that the first revival time ($r = 1$) for a ladder excitation occurs in the interval

$$\frac{T_2}{2d^2} \le t_1 \le T_2, \tag{34}$$

so the level difference d between energy levels excited by the wavefunction places a limit on how much before the time T_2 there can be a revival; the specific revival time within this interval depends on the interplay of the prime factors of the base level b and the level difference d.

The most general case for a ladder excitation is an arbitrary initial wavefunction with population in all energy levels ($b = 1$ and $d = 1$). According to Eq. (33), the first revival of such a fully populated state is at time

$$t_1 = \frac{T_2}{\gcd(2, 3)} = T_2. \tag{35}$$

Although we confirmed in Eq. (16) that all wavefunctions have revivals at this time, here we prove that T_2 is the earliest time at which we are guaranteed to have a probability-density revival in the infinite square well.

The square-well potential has even parity (i.e., $V(-x) = V(x)$), and, thus, the energy eigenstates have definite parity. An arbitrary even-parity wavefunction has population in odd-quantum-number levels (corresponding to the base level $b = 1$ and difference $d = 2$). From Eq. (33), such even-parity states have revivals at multiples of the time

$$t_1 = \frac{T_2}{\gcd(8, 8)} = \frac{T_2}{8}. \tag{36}$$

Similarly, an arbitrary odd-parity wavefunction has population in even-quantum-number levels ($b = 2$, $d = 2$); thus, it has revivals at multiples of the time

$$t_1 = \frac{T_2}{\gcd(8, 12)} = \frac{T_2}{4}. \tag{37}$$

It is interesting to note that an odd-parity state consisting only of energy levels that are odd multiples of two (that is, $b = 2$ and $d = 4$) has its first revival at time $t_1 = T_2/32$, and an odd parity state consisting of energy levels that are multiples of four (that is, $b = 4$ and $d = 4$) revives at multiples of $t_1 = T_2/16$, but a wavefunction that combines both of these subsets into a general odd-parity wavefunction has revivals much less frequently, namely, at multiples of $T_2/4$.

The results presented here offer a constructive proof of statements made in our earlier analysis of dynamics in the infinite square well [22] and generalize the descriptions of these revival times given by Venugopalan and Agarwal [50] and by Styer [44].

4. EXAMPLE 2: REVIVAL PHENOMENA IN HIGHLY EXCITED QUANTUM SYSTEMS

In our second example, we investigate revival phenomena for highly excited wavepackets, spatially localized initial wavefunctions with a large average energy. That is, we focus on quantum states for which the initial spatial extent Δx is much smaller than a characteristic length L associated with particle motion in the potential and the mean quantum number $\bar{n}$ excited by the wavepacket is much larger than the width Δn of the distribution of populated energy states.

It proves useful to describe the dynamics of such wavepackets not with the full description of the eigenfrequencies ω_n but with a simpler approximation valid for the narrow range of energy levels that constitute the wavepacket. To that end, the energy eigenfrequencies of the potential can be recast in a Taylor series centered around the mean quantum number $\bar{n}$ as

$$\omega_n = \omega_{\bar{n}} + 2\pi\left[\frac{(n-\bar{n})}{T_1} + s_2\frac{(n-\bar{n})^2}{T_2} + s_3\frac{(n-\bar{n})^3}{T_3} + \dots\right], \tag{38}$$

in terms of time scales T_j given by

$$\frac{2\pi}{T_j} = \frac{1}{j!}\left|\frac{d^j\omega_n}{dn^j}\right|_{n=\bar{n}}. \tag{39}$$

The constants $s_j = \pm 1$ provide the signs of the derivatives of the eigenfrequencies so that the times T_j are positive, but we need not include a factor s_1 for the linear term since the frequencies are assumed to increase with quantum number. Time evolution (1) and frequency expansion (38) constitute our basic description of the wavepacket dynamics.

For highly excited wavepackets, the time scales T_j generally form a hierarchy [40, 41] such that

$$T_1 \ll T_2 \ll T_3 \ll \dots. \tag{40}$$

This hierarchy has important implications for the time scales pertinent to each stage of wavepacket evolution: for times $t \ll T_{j+1}$, the wavepacket dynamics (1) can be described by approximating the exact eigenfrequencies ω_n in (1) with the quantity $\omega_n^{(j)}$, which is the truncation of expansion (38) to order j.

4.1. Physical Model for Revivals

Early in its evolution ($t \ll T_2$), the wavepacket is described by

$$\begin{aligned}\psi(x,t) &\approx \sum_n \exp[-i\omega_n^{(1)}t]c_n\phi_n(x)\\ &= e^{-i\omega_{\bar{n}}t}\sum_n \exp\left[-i2\pi\left\{(n-\bar{n})\frac{t}{T_1}\right\}\right]c_n\phi_n(x),\end{aligned} \tag{41}$$

and it exhibits the same motion as a wavepacket in a harmonic potential with oscillation frequency $\omega = 2\pi/T_1$. The probability density $|\psi(x, t)|^2$ during this time undergoes periodic motion with period T_1. The quadratic contribution to the eigenfrequencies, neglected in Eq. (41), eventually causes the wavepacket to spread during this harmonic motion, but if the rate of spreading is slow compared with the period T_1, then the wavepacket can move as a localized entity along the trajectory predicted by classical mechanics for several periods before decaying away. This classical nature of highly excited quantum wavepackets makes them ideally suited for investigations into Bohr's Correspondence Principle, which connects the quantum and classical descriptions of motion [51].

At later times ($t \gtrsim T_2$), the dynamics is described by a more complicated interference among the energy levels that comprise the wavepacket. We turn to the initial motion (at times $t \ll T_2$) as our guide for two distinct but closely related models for "revivals" for highly excited wavepackets: (i) revivals of classical motion, which occur during the windows of time when the wavefunction can be written in the form of (41),

$$\psi(x,t) \propto \sum_n \exp\left[-i2\pi\left\{(n-\bar{n})\frac{t}{T_1}\right\}\right]c_n\phi_n(x), \tag{42}$$

characterized by a linear dependence on the quantum number n in the time-evolution exponential; and (ii) revivals of probability density, which occur when the time-advanced probability density is the same as at the initial time,

$$|\psi(x,t)|^2 = |\psi(x,0)|^2, \tag{43}$$

as we considered in Eqs. (17) and (18) for the infinite square well. As elaborated below, we expect classical-motion revivals to correspond to *intervals of time* during which the classical motion of the wavepacket reemerges and probability-density revivals to correspond to specific *instants of time* within the classical-motion revivals, at which the wavepacket passes through its initial location and closely reproduces its initial shape.

The remainder of this example is organized as follows: in Section 4.2, we comment on the role of the mean quantum number $\bar{n}$ in the theory of revivals. In Section 4.3, we convert our two models for revivals of highly excited wavepackets into phase-difference equations. The convention in the literature is to call solutions of models (42) and (43) "revivals" if they occur at times $t \ll T_3$ and to call them "super-revivals" if they occur after the revivals at times $t \ll T_4$; we investigate these two time regimes in Sections 4.4 and 4.5. In Section 4.6 we present a numerical test of our revival predictions. We conclude in Section 4.7 with a brief comment about the phase-difference equations describing fractional revivals.

4.2. The Mean Quantum Number of a Wavepacket

Throughout most of the literature [8, 10–12, 33–41, 43], it is assumed or deduced that the mean quantum number $\bar{n}$ in expansion (38) must be restricted to integer values in order to study revival phenomena. We are against this consensus and show that, although predictions of revival times are simplest when $\bar{n}$ is limited to integer values, this should not be seen as a physical restriction on the wavepacket or as a mathematical limitation on the theoretical formalism. We note that noninteger values of $\bar{n}$ have been considered in two studies of Rydberg wavepackets, by Wals, Fielding, and van Linden van den Heuvell investigating the role of the quantum defect in alkali atoms on the first revival time [14] and by Mallalieu and Stroud exploring semiclassical approximations to the quantum time propagator [52]; here, we extend these results to arbitrary quantum systems and to the super-revival time regime.

We define the mean quantum number $\bar{n}$ implicitly via a statement of the mean energy of the wavepacket,

$$\hbar\omega_{\bar{n}} = \langle E\rangle = \hbar\sum_n |c_n|^2\omega_n, \tag{44}$$

but with quantum systems for which there is no closed-form extension of the energy levels E_n to noninteger values of n, it is sensible instead to compute $\bar{n}$ as the expectation value of the number operator $\hat{n}$ for the wavepacket:

$$\bar{n} = \langle\hat{n}\rangle = \sum_n |c_n|^2 n. \tag{45}$$

Although we do not impose any restrictions on this quantity, we partition it as

$$\bar{n} = \bar{n}_i + \delta\bar{n}, \tag{46}$$

where $\bar{n}_i$ = round($\bar{n}$) is the integer closest to $\bar{n}$ and $\delta\bar{n} = \bar{n} - \bar{n}_i$ is the noninteger remainder. Such partitioning is useful because eigenfrequencies (38) are always evaluated for integer values of the quantum number, and the offset $\delta\bar{n}$ from the integers then plays an important role in the revival-time predictions.

4.3. Phase-Difference Equations

The classical-motion revivals described by Eq. (42) occur when the time-evolution exponential is linear in the quantum number n (a polynomial of order $N = 1$) and, thus, are predicted by the solutions of the second difference equation

$$\frac{\Delta^2}{\Delta n^2}[\omega_n t] = (\text{multiple of } 2\pi). \tag{47}$$

The probability-density revivals of Eq. (43) occur when the time-evolution exponential is constant (independent of the quantum number n) and, thus, are identified from the first difference equation

$$\frac{\Delta}{\Delta n}[\omega_n t] = (\text{multiple of } 2\pi). \tag{48}$$

For times $t \ll T_{k+1}$, we approximate the eigenfrequencies ω_n with the truncated Taylor series $\omega_k^{(k)}$ from (38); then, the primary phase-difference equation for classical-motion revivals is

$$\frac{\Delta^2}{\Delta n^2}\left[\sum_{j=2}^{k} s_j\frac{(n-\bar{n})^j t}{T_j}\right] = (\text{integer}) \quad (t \ll T_{k+1}), \tag{49}$$

and the equation for probability-density revivals becomes

$$\frac{\Delta}{\Delta n}\left[\sum_{j=1}^{k} s_j\frac{(n-\bar{n})^j t}{T_j}\right] = (\text{integer}) \quad (t \ll T_{k+1}); \tag{50}$$

the ancillary higher-order difference equations

$$\frac{\Delta^{r+2}}{\Delta n^{r+2}}\left[\sum_{j=r+2}^{k} s_j \frac{(n-\bar{n})^j t}{T_j}\right] = (\text{integer}) \quad (t \ll T_{k+1}), \tag{51}$$

for positive integer r serve as necessary but no longer sufficient conditions for revivals. Note that the lower limit of the sum in Eq. (51) can be raised to match the order of the difference operator because the discrete differences of lower-order polynomials in the sum identically vanish. For highly excited quantum systems, Eqs. (49) and (50) typically do not have exact solutions, except in the fortuitous cases when the ratios T_j/T_{j+1} of the wavepacket times all form simple, rational fractions. Regardless of such exact solutions, the ancillary equations now provide more than mathematical convenience: they offer a paradigm for approximate revivals in a system governed by multiple time scales T_j ordered by a strong hierarchy.

4.4. Wavepacket Revivals: $t \ll T_3$

For times $t \ll T_3$, there are two time scales relevant to the wavepacket eigenfrequencies:

$$\omega_n \approx \omega_{\bar{n}} + 2\pi\left[\frac{(n-\bar{n})}{T_1} + s_2\frac{(n-\bar{n})^2}{T_2}\right]. \tag{52}$$

We determine the revival times by evaluating the phase-difference equations using this eigenfrequency approximation. Ancillary equations (51) do not provide any information about the revivals in this time regime. The classical-motion revivals are found by evaluating the second difference Eq. (49), which gives

$$2s_2\frac{t}{T_2} = (\text{integer}) \quad (t \ll T_3). \tag{53}$$

As $s_2 = \pm 1$ is an integer, we see that this has solutions

$$t_r = \frac{rT_2}{2} \tag{54}$$

for integer $r \ll 2T_3/T_2$; that is, there are classical-motion revivals at multiples of time $T_2/2$. While this result is well-known, we emphasize that the phase-difference equations allow us to predict the revival times from first principles and without any assumptions about the mean quantum number $\bar{n}$.

Although the classical-motion revival Eq. (49) is only satisfied exactly at discrete instants of time, it is more in the spirit of the physics to view these revivals as intervals centered around the times enumerated by Eq. (54). At times $t = t_1 + \Delta t$ near the first revival $t_1 = T_2/2$, for example, the dynamical phases of the energy levels are given approximately by

$$\omega_n t \approx \omega_{\bar{n}} t + 2\pi\left[(n-\bar{n})\frac{t}{T_1} + s_2(n-\bar{n})^2\frac{t_1}{T_2}\right], \tag{55}$$

where, in the quadratic term, we approximate $(t_1 + \Delta t)/T_2 \approx t_1/T_2$, which is justified by time-scale hierarchy (40) as long as $\Delta t \ll T_2/\Delta n^2$, where we use the width Δn of the distribution of populated energy levels as a typical value for $(n - \bar{n})$. Approximate dynamical phases (55) still satisfy the difference Eq. (47), and, in this sense, the classical-motion revivals can be viewed as lasting for several classical periods T_1 around the revivals given by Eq. (54).

Instead of substituting times (54) directly into the probability-density revival Eq. (50), we use the above time-scale arguments to identify *approximate* solutions to the first difference equation in small intervals of time near revival times (54). That is, we solve the approximate phase-difference equation

$$\frac{\Delta}{\Delta n}\left[\frac{(n-\bar{n})t}{T_1} + s_2\frac{(n-\bar{n})^2 r}{2}\right] = (\text{integer}) \quad (|t - rT_2/2| \ll T_2), \tag{56}$$

obtained by "freezing" the quadratic term at $t = rT_2/2$; this approximation is only justified *a posteriori* by showing that the phase-difference equation does have time solutions that are within a few periods T_1 of the classical-motion revival time $rT_2/2$. Evaluating (56), we find that

$$s_2 r(n-\bar{n}_i) + \frac{t}{T_1} + s_2 r\left\{\frac{1}{2} - \delta\bar{n}\right\} = (\text{integer}). \tag{57}$$

Since s_2, r, n, and $\bar{n}_i$ are all integers, the first term in Eq. (57) is an integer and can be eliminated from both sides of the equation. Writing the unknown integer on the right-hand side as $\bar{c} + c$ (discussed below), the times for the approximate probability-density revivals are

$$t_{c,r} = \left[\bar{c} + c - s_2 r\left\{\frac{1}{2} - \delta\bar{n}\right\}\right]T_1. \tag{58}$$

However, the valid solutions of Eq. (56) must be in the near vicinity of the time $rT_2/2$, so we emphasize this by defining the integer $\bar{c}$ as

$$\bar{c} = \text{round}\left(\frac{rT_2}{2T_1} + s_2 r\left\{\frac{1}{2} - \delta\bar{n}\right\}\right), \tag{59}$$

i.e., the integer that makes $t_{0,r}$ in Eq. (58) as close as possible to the time $rT_2/2$ for $c = 0$. With this definition, the times enumerated by (58) correspond to times at which the wavepacket approximately returns to its original shape during the rth revival, where c is a small integer serving as an index for the classical periods. (Although it is awkward to speak of the "negative-first classical period during the second revival," for example, the integer indices c, r, and s used in this paper may be positive or negative but are generally intended to be small in absolute value.)

4.5. Wavepacket Super-Revivals: $t \ll T_4$

For times $t \ll T_4$, there are three time scales relevant to the wavepacket eigenfrequencies:

$$\omega_n \approx \omega_{\bar{n}} + 2\pi\left[\frac{(n-\bar{n})}{T_1} + s_2\frac{(n-\bar{n})^2}{T_2} + s_3\frac{(n-\bar{n})^3}{T_3}\right]. \quad (60)$$

We determine the revival times by evaluating the phase-difference equations using this eigenfrequency approximation. The ancillary third-difference Eq. (51) tells us that

$$6s_3\frac{t}{T_3} = (\text{integer}) \quad (t \ll T_4), \quad (61)$$

which has solutions

$$t_s = \frac{sT_3}{6} \quad (62)$$

for integer $s \ll 6T_4/T_3$. Following the same rationale as for the revival time regime $t \ll T_3$, here we look for approximate classical-motion and probability-density revivals in the intervals around these times. Appealing to the time-scale hierarchy, we "freeze" the cubic contribution at time $sT_3/6$ and look for solutions to the (approximate) classical-motion revival equation

$$\frac{\Delta^2}{\Delta n^2}\left[s_2\frac{(n-\bar{n})^2 t}{T_2} + s_3\frac{(n-\bar{n})^3 s}{6}\right] = (\text{integer}) \quad (63)$$

for times $|t - sT_3/6| \ll T_3$. Evaluating the second difference and eliminating the integer quantity $s_3\, s(n - \bar{n}_i)$ from the equation, we find

$$2s_2\frac{t}{T_2} - s_3 s\delta\bar{n} = (\text{integer}), \quad (64)$$

and, thus, there are approximate classical-motion revivals in time intervals centered around

$$t_{r,s} = (\bar{r} + r + s_2 s_3 s\delta\bar{n})\frac{T_2}{2} \quad (65)$$

for small integer r, where

$$\bar{r} = \text{round}\left(\frac{sT_3}{3T_2} - s_2 s_3 s\delta\bar{n}\right) \quad (66)$$

is the integer that makes $t_{0,s}$ in (65) as close as possible to the time $sT_3/6$ for $r = 0$.

We identify probability-density revivals by continuing this approximation scheme, namely, by examining the first difference equation

$$\frac{\Delta}{\Delta n}\left[\frac{(n-\bar{n})t}{T_1} + s_2\frac{(n-\bar{n})^2(\bar{r} + r + s_2 s_3 s\delta\bar{n})}{2} + s_3\frac{(n-\bar{n})^3 s}{6}\right] = (\text{integer}) \quad (67)$$

for $|t - t_{r,s}| \ll T_2$, obtained by "freezing" the cubic contribution at time $sT_3/6$ and the quadratic contribution at time $t_{r,s}$ in Eq. (65). Evaluating the first difference and eliminating all integer quantities from the expression, we find (approximate) probability-density revivals at times that solve the equation

$$\frac{t}{T_1} + s_2(\bar{r} + r)\left\{\frac{1}{2} - \delta\bar{n}\right\} + s_3 s\left\{\frac{1}{6} - \frac{\delta\bar{n}^2}{2}\right\} = (\text{integer}) \quad (68)$$

within the restriction $|t - t_{r,s}| \ll T_2$. The probability-density revival times near the rth revival of the sth super-revival are

$$t_{c,r,s} = \left[\bar{c} + c - s_2(\bar{r} + r)\left\{\frac{1}{2} - \delta\bar{n}\right\} - s_3 s\left\{\frac{1}{6} - \frac{\delta\bar{n}^2}{2}\right\}\right]T_1 \quad (69)$$

with

$$\bar{c} = \text{round}\left[(\bar{r} + r + s_2 s_3 s\delta\bar{n})\frac{T_2}{2T_1} + s_2(\bar{r} + r)\left\{\frac{1}{2} - \delta\bar{n}\right\} + s_3 s\left\{\frac{1}{6} - \frac{\delta\bar{n}^2}{2}\right\}\right], \quad (70)$$

for small integers c and r serving as indices for classical periods and revivals, respectively. The times $t_{c,r,0}$ for $s = 0$ predicted by Eq. (69) agree with results (58) for the time regime $t \ll T_3$. Furthermore, when the mean quantum number $\bar{n}$ is restricted to be an integer (thus, $\bar{n}_i = \bar{n}$ and $\delta\bar{n} = 0$), (62) and (65) reduce to the expressions for classical-motion revivals developed by Knospe and Schmidt [39], and (58) and (69) agree with expressions for probability-density revivals found in our earlier work [21].

4.6. Numerical Tests of Revival Predictions

It is important to test if times (69) correspond to approximate probability-density revivals (which tests the time-scale "freezing" approximations used to derive them) and, conversely, if all of the approximate reformations of the wavepacket do indeed correspond

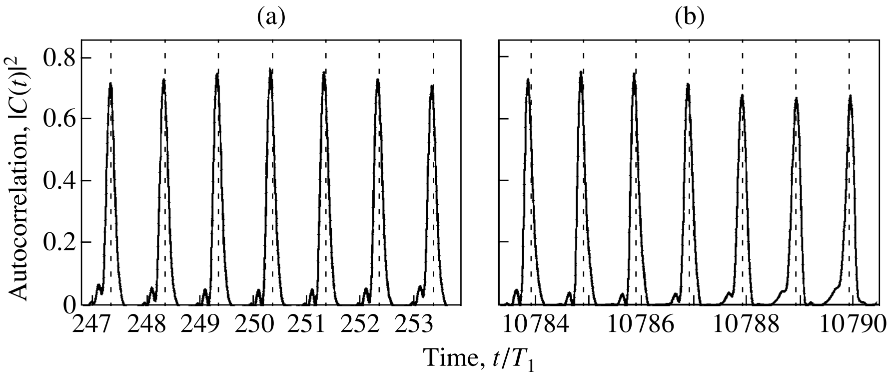

Fig. 1. Tests of predictions for probability-density revival times: Autocorrelation function $|C(t)|^2$ of a circular-orbit wavepacket (with parameters $\bar{n} \approx 250.376$ and $\Delta n = 2$) during (a) the third revival ($r = 3$, $s = 0$) and (b) the fourth revival near the second super-revival ($r = 4$, $s = 2$), for classical motion indices c between –3 and +3. The dashed vertical lines are drawn at times given by Eq. (69), when probability-density revivals are predicted to occur.

to times we have predicted (which tests our paradigm of using the ancillary phase-difference equations to enumerate the approximate probability-density revivals). For this test, we consider the electron in a hydrogen atom excited into a circular-orbit wavepacket [4], a superposition of circular states (hydrogen eigenstates with maximal values of the azimuthal quantum number l and the magnetic quantum number m) described initially by

$$|\psi(t=0)\rangle = \sum_n c_n |n, l = n-1, m = n-1\rangle, \qquad (71)$$

with Gaussian amplitudes

$$c_n = \frac{1}{\sqrt[4]{2\pi\Delta n^2}} \exp\left[-\frac{(n - \langle n\rangle)^2}{4\Delta n^2}\right]. \qquad (72)$$

The eigenfrequencies of the simplest model of the hydrogen atom are

$$\omega_n = -\frac{1}{2n^2} \qquad (73)$$

in atomic units, and with Eq. (39), the wavepacket time scales associated with these eigenfrequencies are

$$T_1 = 2\pi\bar{n}^3, \quad T_2 = \frac{4}{3}\pi\bar{n}^4, \quad T_3 = \pi\bar{n}^5, \quad \text{and} \quad T_4 = \frac{4}{5}\pi\bar{n}^6, \qquad (74)$$

with alternating signs $s_j = (-1)^{j-1}$. Although the circular-orbit wavepacket is excited in the three-dimensional Coulomb potential, eigenfrequencies (73) depend only on the principal quantum number n, so this wavepacket can be viewed as having one degree of freedom and we can apply our revival-time predictions to its dynamics. For our numerical test, we choose $\langle n\rangle = 250.4$ and $\Delta n = 2$ for the parameters of the circular-orbit wavepacket in (72), and, thus, using Eqs. (72) and (73) with our prescription (44), the mean quantum number is taken to be $\bar{n} \approx 250.376$ and, thus, is partitioned as $\bar{n}_i = 250$ and $\delta\bar{n} \approx 0.376$.

A suitable measure of how close the wavepacket is to a probability-density revival at time t is the autocorrelation function

$$|C(t)|^2 = |\langle\psi(t)|\psi(0)\rangle|^2 = \left|\sum_n |c_n|^2 e^{-i\omega_n t}\right|^2. \qquad (75)$$

For exact probability density revival (43), the autocorrelation is equal to unity, but, in general, $0 \le |C(t)|^2 \le 1$, with higher values of autocorrelation corresponding to higher-fidelity incarnations of the initial state. In our test, we computed autocorrelation (75) numerically for times $t \ll T_4$, specifically for times between $t = 0$ and $t = T_4/200$ in steps of $T_1/10^4$. Here, we describe the lessons learned from this numerical test.

First, we find that probability-density revival times (69) do correspond to local maxima of $|C(t)|^2$ in all cases (see Fig. 1), although our theory does not provide an estimate for how rapidly the peaks of $|C(t)|^2$ decrease for increasing values of the indices $|c|$ and $|r|$. For the times $t_{c,r,s}$ predicted by Eq. (69), which correspond to peaks of the autocorrelation satisfying $|C(t)|^2 \ge 70\%$ (chosen arbitrarily), the numerically obtained time values $\tau_{c,r,s}$ that are local maxima of $|C(t)|^2$ agree with our predictions remarkably well; namely, they satisfy $|\tau_{c,r,s} - t_{c,r,s}| < T_1/9$ in all cases and $\langle|\tau_{c,r,s} - t_{c,r,s}|\rangle \approx T_1/28$ on average.

Second, we find that there are peaks of the autocorrelation function that do not correspond to predictions of probability-density revival times; instead, these peaks are signatures of highly asymmetric fractional super-revivals. The fractional revivals that occur at simple fractions of the revival times $rT_2/2$ consist of subpackets of equal size that are symmetrically distributed along a classical period of motion [33, 34]; the subpackets seen during the fractional super-revivals are not, in general, of equal size [36, 37]. Braun and Savichev [38] showed, for example, that, near the time $T_3/12$, there are asymmetric one-half fractional super-revivals consisting of two copies of the initial wavepacket separated by half of a classical period, one with ≈14.6% of the probability and the other with the remaining ≈85.4%. The largest subpacket in an asymmetric fractional super-revival can "trigger" peaks in the autocorrelation function that are not predicted by the revival-time predictions developed above. Nonetheless, we find that every local maxima of $|C(t)|^2$ above 70% for $t \ll T_4$ corresponds either to a probability-density revival (Eq. (69)) or an asymmetric fractional super-revival.

4.7. Fractional Revivals

Although a complete discussion of fractional revivals (and fractional super-revivals) is beyond the scope of the present paper, we comment briefly on how they can be readily examined with phase-difference equations. The fractional revivals of a wavepacket consisting of q subpackets occur when the dynamical phases of nonneighboring quantum levels take on certain polynomial configurations. In terms of a generalized difference operator

$$\frac{\Delta}{\Delta^{(q)}n}\theta_n(t) \equiv \theta_{n+q}(t) - \theta_n(t) \tag{76}$$

that involves indices differing by q, the windows of time for the (classical-motion) fractional revivals are found via the second difference equation,

$$\frac{\Delta^2}{\Delta^{(q)}n^2}[\omega_n t] = (\text{multiple of } 2\pi), \tag{77}$$

and the specific moments of time at which each subpacket passes through the initial wavepacket's location are identified with

$$\frac{\Delta}{\Delta^{(q)}n}[\omega_n t] = (\text{multiple of } 2\pi). \tag{78}$$

5. CONCLUSIONS

We have transformed a class of "time eigenvalue" equations (2) that identify the revival times for quantum wavefunctions into a primary phase-difference equation (Eq. (9)) and a set of ancillary equations (Eq. (10)). The phase-difference equations were motivated by the simple differential equations satisfied by polynomial functions of a continuous variable and were generalized to address the discrete nature of the quantum number n and the phase ambiguities of complex exponentials. We demonstrated the use of these equations in two examples that differed fundamentally in the role of the ancillary equations.

For ladder excitations of the infinite square-well potential (Section 3), we looked for exact probability-density revivals in the form of Eqs. (17) and (18). The ancillary phase-difference Eq. (26) provided a superset of possible revival times, and then the primary Eq. (25) identified which of these times do, indeed, correspond to revivals. Resulting revival-time predictions (33) agreed with and generalized previous results on the revival times of odd- and even-parity wavefunctions.

For highly excited wavepackets (Section 4), we looked for classical-motion revival-time windows and probability-density revival-time instants. Time-scale hierarchy (40) provided a framework for identifying approximate revivals when there need not be exact solutions. The highest order phase-difference equation only operated on the longest time scale in the eigenfrequency spectrum and identified broad time windows during which revivals could occur. Each subsequent lower-order difference equation then addressed dynamics on shorter time scales and designated time subintervals within the broad windows for the revivals; mathematically, this was achieved by "freezing" the high-order polynomial terms when applying lower-order phase-difference equations. In this sense, the revival times are resolved at each wavepacket time scale quasi-independently; this observation was implemented by Knospe and Schmidt, for example, by expressing the unknown (classical-motion) revival time t as

$$t = \rho_1 T_1 + \rho_2 T_2 + \rho_3 T_3 \ldots \tag{79}$$

in terms of independent contributions ρ_j at each time scale [39]. Predictions of classical-motion revival times (54) and (65) and of probability-density revival times (58) and (69) agreed with and generalized previously published results and were found to be highly accurate in a numerical example.

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