Fractional wave-function revivals in the infinite square well

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We describe the time evolution of a wave function in the infinite square well using a fractional revival formalism, and show that at all times the wave function can be described as a superposition of translated copies of the initial wave function. Using the model of a wave form propagating on a dispersionless string from classical mechanics to describe these translations, we connect the reflection symmetry of the square-well potential to a reflection symmetry in the locations of these translated copies, and show that they occur in a ''parity-conserving'' form. The relative phases of the translated copies are shown to depend quadratically on the translation distance along the classical path. We conclude that the time-evolved wave function in the infinite square well can be described in terms of translations of the initial wave-function shape, without approximation and without any reference to its energy eigenstate expansion. That is, the set of translated initial wave functions forms a Hilbert space *basis* for the time-evolved wave functions. [S1050-2947(97)06606-7]

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I. INTRODUCTION

The infinite square-well potential is an important model in quantum mechanics, and insights into the dynamics exhibited in this model speak immediately to a wide range of physical systems. It is a good description for one-dimensional bound-state problems, whenever the confining potential is steeper than that of the parabolically curved harmonic-oscillator potential. It is also an important first approximation to the confining potential seen in semiconductor quantum wells.

It is perhaps surprising that there is new physics in the time evolution of wave functions in a square well. The energy eigenvalues and eigenstates found from solving Schrödinger's equation have simple analytic expressions, and one can readily describe the time evolution of a wave function in this system via its eigenstate expansion. But if we look ahead to Fig. 2, for example, we see that time-evolved wave functions can appear to ''clone'' the initial wave function throughout the well, a phenomenon that cannot be anticipated from such an eigenstate expansion. The primary motivation for this work is to provide a formalism, a foundation, for understanding this behavior.

In this paper, we describe the evolution of a wave function in the infinite square well in terms of full and fractional revivals. We will show that this system is *ideal* for understanding fractional revival phenomena: the fractional revivals in the infinite square well occur to all orders and for any initial wave function, with no stipulations on its initial localization or its energy bandwidth. Fractional revivals are usually thought of as isolated incidents in a quantum system's time evolution, a few special moments in the long-term time dynamics of a carefully excited wave packet. In the infinite square well they allow for a full description of time evolution.

A *revival* of a wave function occurs when a wave function evolves in time to a state closely reproducing its initial form. In its mathematical description, the revival corresponds to phase alignments of nearest-neighbor energy eigenstates that comprise the wave function. Revivals in quantum systems were first studied in the Jaynes-Cummings model, describing a two-level atom interacting with a resonant monochromatic field. Eberly, Narozhny, and Sanchez-Mondragon [1] discovered that the atom's inversion magnitude initially decays away, but near special revival times rises to almost complete inversion before redecaying. Such revivals have been observed experimentally in a micromaser cavity with atomic rubidium [2]. Revivals were also predicted [3] and observed [4] to occur in Rydberg electron wave packets, in which a ''breathing'' motion between the inner and outer classical turning points will lose, then regain, its radial localization. They have also been observed in molecular systems, such as in vibrational wave packets in Na_2 [5].

A *fractional revival* of a wave function occurs when a wave function evolves in time to a state describable as a collection of spatially distributed sub-wave-functions that each closely reproduces the initial wave-function shape. Macroscopic distinguishability or spatial localization among the sub-wave functions has been a major motivation for studying fractional revivals, but should not be seen as a requirement for such a description, as in general the sub-wave-functions overlap in space and interfere. In its mathematical description, the fractional revival corresponds to phase alignments of nonadjacent energy eigenstates that comprise the wave function.

Averbukh and Perelman [6] made a definitive analysis of wave packets formed by highly excited states of quantum systems, and described their fractional revivals, giving a general formalism for understanding earlier results in atomic and nonlinear systems [7]. We will make several references and comparisons to their work. Other theoretical investigations have explored fractional revivals in atomic systems [3,8] and in the Jaynes-Cummings model [9]. More recently fractional revivals have been predicted in other systems, such as in Morse-like anharmonic potentials [10] and by atoms bouncing vertically against a potential wall in a gravitational field [11]. Fractional revivals have been observed in several dif-

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ferent experiments in potassium [12] and rubidium [13], and more recently in vibrational wave packets in Br_2 [14].

In many systems the fractional revivals will in turn undergo decays and revivals. Such *super-revival* effects were studied extensively by Bluhm and Kostelecký [15], and have been applied to understanding the role of the quantum defect in alkali metals [15,16] and the role of initial field statistics in the Jaynes-Cummings model [17]. Experimentally Wals, Fielding, and van Linden van den Heuvell measured the super-revival ''forerunner'' in rubidium [16]. Leichtle, Averbukh, and Schleich [18] recently presented an analytical formalism of multilevel quantum beats to describe wave-packet revivals and super-revivals. The infinite square well does not display super-revival effects, so we will not need this body of research.

Revival experiments with wave packets have thus far focused on atomic and photon cavity systems. It is our hope that the predictions of fractional revival phenomena in the infinite square well might be realized experimentally in semiconductor quantum wells. In recent years there have been tremendous achievements in coherent dynamics in semiconductor systems, including observation of quantum beats in single wells [19] and double wells [20]; the creation [21] and tunability [22] of terahertz radiation from wave packets excited in quantum wells; and the detection [23] and enhancement via laser pulse sequences and pulse shaping [24] of Bloch oscillations in semiconductor superlattices.

In this paper we explore wave-function dynamics in the infinite square well. We begin by giving phenomenological definitions for full and fractional revivals. We do so at the expense of using the specific analytic form of the infinite square well's energy eigenfunctions but at the benefit of gaining insights into the interrelationships among the system's potential, eigenstates, and revival behavior. By proposing that fractional revivals occur in ''parity-conserving form,'' we find a particularly simple and elegant form for an eigenstate expansion of the fractional revivals. With the use of results from number theory, we extend Averbukh and Perelman's analysis [6] to derive phase relationships between sub-wave-functions in the fractional revivals. We end with many probability density graphs to illustrate the wide array of time evolution behavior that is explained with our formalism.

II. INFINITE SQUARE-WELL SYSTEM

The one-dimensional infinite square-well potential confines a particle to a box of width L and is described by

$$V(x)=\begin{cases}0, & |x|\leq L/2\\ \infty, & |x|>L/2.\end{cases} \tag{1}$$

A particle of mass m is placed in this potential. The energy eigenvalues and eigenstates are found by solving the time-independent Schrödinger equation (as in [25]). The discrete energy eigenvalues are

$$E_n=\frac{\pi^2\hbar^2}{2mL^2}\,n^2 \tag{2}$$

for positive integer n. The energy eigenstate wave functions are

$$\phi_n(x)=\begin{cases}\sqrt{\frac{2}{L}}\sin(n\pi x/L), & n \text{ even}\\ & |x|\leq L/2\\ \sqrt{\frac{2}{L}}\cos(n\pi x/L), & n \text{ odd}\\ 0, & |x|>L/2.\end{cases} \tag{3}$$

The energy eigenstates are states of definite parity, as they must be for any system with symmetric potential $V(x)$.

A. Time scales

It has been demonstrated repeatedly (such as in [3,6,15]) that the important time scales of a wave function's evolution are contained in the coefficients of the Taylor series of the quantized energy levels E_n around the mean energy $\overline{n}$,

$$E_{\overline{n}}=E_{\overline{n}}+2\pi\hbar\left[\frac{(n-\overline{n})}{T_{\rm cl}}+\frac{(n-\overline{n})^2}{T_{\rm fr}}+\frac{(n-\overline{n})^3}{T_{\rm sr}}+\cdots\right], \tag{4}$$

where often the zero of energy is shifted to remove the $E_{\overline{n}}$ term. Regrouping the infinite square-well energies (2) in this form gives

$$E_n=E_1n^2=E_1\overline{n}^2+2E_1\overline{n}(n-\overline{n})+E_1(n-\overline{n})^2, \tag{5}$$

and, comparing Eqs. (4) and (5), we relate

$$T_{\rm cl}=\frac{h}{2\,\overline{n}\,E_1}$$

and

$$T_{\rm fr}=\frac{h}{2\,E_1}. \tag{6}$$

That the quantized energy levels (5) are exactly quadratic in n or $(n-\overline{n})$ leads to $T_{\rm sr}\rightarrow\infty$, and so the system shows no super-revival (or higher-order) effects. In contrast to atomic systems, it is important to note that the time scale $T_{\rm fr}$ here does not depend on the mean energy level $\overline{n}$. This will provide us with a ''universal'' time scale for describing wave function evolution that does not depend on the particle's average energy.

B. Time evolution

We write the particle's time $t=0$ wave function in the square well as $\psi(x,t=0)=\psi_i(x)$. We expand this wave function using the energy eigenstate basis

$$\psi_i(x)=\sum_{n=1}^{\infty}c_n\phi_n(x), \tag{7}$$

with

$$c_n=\int_{-\infty}^{\infty}\phi_n(x)\psi_i(x)dx. \tag{8}$$

Using the time scale $T_{\rm fr}=h/E_1$, the time evolution in the energy eigenbasis is found from Schrödinger's equation to be

$$\psi(x,t)=\sum_n \exp[-i2\pi(t/T_{\rm fr})n^2]c_n\phi_n(x). \tag{9}$$

C. Classical trajectories

In Eq. (6) we found that the classical period associated with motion in the square well was $T_{\rm cl}=h/2\overline{n}E_1$. A classical particle with energy E travels at speed $v=\sqrt{2E/m}$. If placed in an infinite square well, such a particle would travel in one direction, rebound elastically off one wall, travel in the opposite direction until rebounding off the far wall, and travel through its starting position, completing one period of classical periodic motion. The round-trip time $T_{\rm rt}$ associated with the periodic motion of the particle is

$$T_{\rm rt}=\frac{2L}{v}=L\left(\frac{2E}{m}\right)^{1/2}. \tag{10}$$

If we take the particle's energy to be $E=E_{\overline{n}}$ and use the quantum-mechanical expression (2) for the energy levels, then we find that $T_{\rm cl}=T_{\rm rt}$, as expected [26]. Using such a description of a classical particle has proven useful for constructing propagators for path-integral solutions to infinite square-well systems [27].

We also can describe the time dynamics in the square well with an analogy to classical wave propagation on a stretched string of length L. We liken the time $t=0$ wave function $\psi_i(x)$ to the initial profile of a stretched string which then propagates without dispersion at speed $v=\sqrt{2E_{\overline{n}}/m}$. The elastic collisions at the infinitely high potential barriers are analogous to perfect reflections from fixed ends of the string. When a wave form propagating on a string reflects at the string ends, it travels in the opposite direction with a π phase change in its amplitude; we will find analogous behavior in the infinite square-well wave function.

A fixed energy E for one-dimensional motion corresponds to two possible velocities, the right- and left-traveling velocities with the same magnitude v. The classical trajectories we will discuss do not lift this ambiguity, and can be taken to be an arbitrary superposition of the initially right-traveling and initially left-traveling classical paths.

III. FULL WAVE-FUNCTION REVIVALS

An *exact wave-function revival* is said to occur when the particle's wave function differs from its time $t=0$ wave function by at most a constant phase; that is, the wave function revival and the original wave function have the same probability density $|\psi_i(x)|^2$. By direct substitution into the energy eigenstate expansion (9), we see that, at time $t=T_{\rm fr}$, the wave function is given by

$$\psi(x,t=T_{\rm fr})=\sum_n \exp[-i2\pi n^2]c_n\phi_n(x)$$
$$=\sum_n c_n\phi_n(x)=\psi_i(x). \tag{11}$$

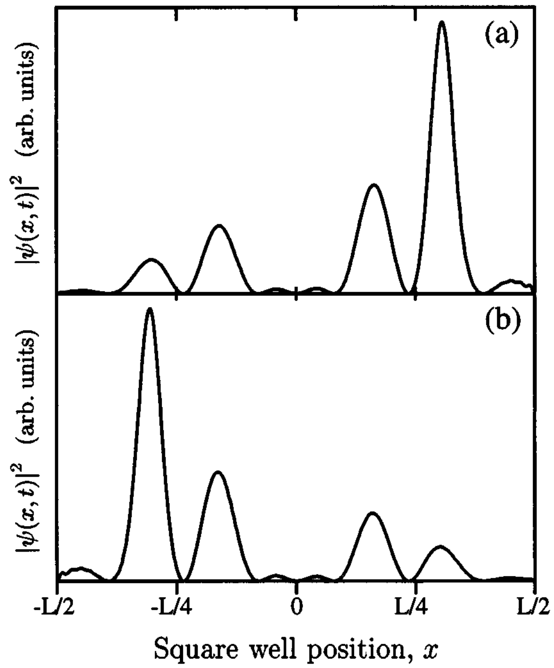

FIG. 1. Probability densities for (a) initial $(t=0)$ and (b) reflected $[t=(1/2)T_{\rm fr}]$ wave functions.

Thus, at time $t=T_{\rm fr}$ there is an exact revival of the wave function. It follows from this that time evolution in the infinite square well is periodic with period $T_{\rm fr}$, that for any time t_0 and integer k,

$$\psi(x,t=t_0+kT_{\rm fr})=\psi(x,t=t_0). \tag{12}$$

For this reason the time $T_{\rm fr}$ can be referred to as the exact revival time or the period of the system. The full revivals and time periodicity of the infinite square-well wave functions were recently discussed by Bluhm, Kostelecký, and Porter [28].

The time $T_{\rm fr}$ is the shortest time for which we are guaranteed to have an exact revival of the initial wave function. There are particular classes of wave functions (such as states of definite parity) that have full revivals at earlier times. This will be illustrated in Sec. V, but a more detailed discussion of such population-dependent revivals will be the subject of a future publication.

Mirror wave-function revivals

Again by direct substitution into the energy eigenstate expansion (9), we see that, at time $t=\frac{1}{2}T_{\rm fr}$ the wave function is given by

$$\psi\left(x,t=\frac{1}{2}T_{\rm fr}\right)=\sum_n \exp[-i\pi n^2]c_n\phi_n(x)$$
$$=\sum_n (-1)^n c_n\phi_n(x)$$
$$=-\psi_i(-x). \tag{13}$$

Thus, at time $t=\frac{1}{2}T_{\rm fr}$ there is a single reflected copy of the initial wave function (see Fig. 1).

For initially well-localized wave packets, the time $t=\frac{1}{2}T_{\rm fr}$ is the first time at which the state regains its initial localization. For revival experiments with Rydberg atomic electron wave packets, this revival of localization is a more important time scale than the exact wave-function revival time, since it also corresponds to a revival of classical periodic motion of the wave packet.

IV. FRACTIONAL WAVE-FUNCTION REVIVALS

An *exact fractional wave-function revival* is said to occur when the particle′s wave function can be written as a superposition of translated initial wave functions. We allow for the possibility that each translated copy has a relative phase difference with the original wave function as we did in Sec. III.

Simply translating the initial wave function is not, in general, compatible with the infinite square-well physical boundary conditions, which require $\psi(x,t)=0$ for $|x|\geqslant L/2$. We address this using the ‘‘wave form on a string’’ analogy: We define the function $\overline{\psi_i}(x,\Delta x)$ to be the wave function found by translating the initial wave function $\psi_i(x)$ a distance Δx in the square well, with any probability amplitude that would be moved out of the well by such a translation is instead reflected back into the well with a π phase change. Translating the wave function a distance $\Delta x=2L$ returns us to the initial configuration, $\overline{\psi_i}(x,\Delta x=\pm 2L)=\psi_i(x)$, so this describes periodic motion in Δx.

Thus, we say there is an exact fractional revival at time t if

$$\psi(x,t)=\sum_{j=1}^{r(t)} A_j(t)\overline{\psi_i}(x,\Delta x=\alpha_j(t)L), \tag{14}$$

where there are $r(t)$ translations of the initial wave function, centered at positions $\alpha_j L$, with amplitudes $|A_j|$ and phases $\arg(A_j)$. It is important to note that at the onset we do not know to what values of time t we must restrict our attention for Eq. (14) to hold. This fractional revival description may only be valid for special times, special ‘‘time eigenvalues’’ of the fractional revival equation. But at these special moments of time we expect Eq. (14) to hold for all values of position x. For this reason we will de-emphasize the time dependence on the right-hand side of this equation, and write the fractional revival definition as

$$\psi(x,t)=\sum_j A_j\overline{\psi_i}(x,\Delta x=\alpha_j L). \tag{15}$$

A. Parity-conserving fractional revivals

The square-well energy eigenstates are states of definite parity, so parity is conserved in time evolution. If the initial wave function $\psi_i(x)$ is an even or odd function of position, parity conservation places a constraint on the form for a fractional revival: if the fractional revival contains a translation term $\overline{\psi_i}(x,\Delta x)$ it must also contain a term $\overline{\psi_i}(x,-\Delta x)$. If $\psi_i(x)$ is a state of definite parity, pairings of the form $[\overline{\psi_i}(x,\Delta x)+\overline{\psi_i}(x,-\Delta x)]$ are the only ones to maintain parity. We define *parity-conserving fractional revivals* as the subset of possible fractional revivals (15) that conserve parity; thus they have the form

$$\psi(x,t)=A_0\psi_i(x)+\sum_j A_j[\overline{\psi_i}(x,\Delta x=\alpha_j L)+\overline{\psi_i}(x,\Delta x=-\alpha_j L)]. \tag{16}$$

We make the ansatz that fractional revivals in the infinite square well are always of this parity-conserving form, even when $\psi_i(x)$ is not a state of definite parity.

B. Energy eigenstate expansion

We extract information on fractional revivals using the surprisingly simple result that the energy eigenstate expansion of a parity-conserving wave-function pair is given by

$$\overline{\psi_i}(x,\Delta x=\alpha L)+\overline{\psi_i}(x,\Delta x=-\alpha L)=2\sum_n \cos(\alpha\pi n)c_n\phi_n(x). \tag{17}$$

The derivation of this expression is shown in the Appendix. We use this to give an energy eigenstate expansion for our posited parity-conserving fractional revivals (16):

$$\psi(x,t)=\sum_n \left\{A_0+2\sum_j A_j\cos(\alpha_j\pi n)\right\}c_n\phi_n(x). \tag{18}$$

Comparing this expression to the energy eigenstate expansion (9), we see that we have a fractional revival at time t when we can write

$$\exp[-i2\pi(t/T_{\rm fr})n^2]=A_0+2\sum_j A_j\cos(\alpha_j\pi\, n). \tag{19}$$

That is, we must be able to write the time-evolution exponential, quadratic in n, in a cosine series, linear in n. Such an expansion, introduced by Averbukh and Perelman [6], is made using the finite Fourier series.

C. Finite Fourier series

A function $f(n)$ whose domain is restricted to the integers ($n\in\mathbb{Z}$) can be written as a finite sum of exponentials if and only if it is r periodic, that is, there is an integer r such that $f(n)=f(n+r)$ for all n. Such a finite sum is called the finite Fourier series. (See [29] for a review of such expansions.)

In our case we identify $f(n)=\exp[-i2\pi(t/T_{\rm fr})n^2]$. The necessary and sufficient condition for this exponential to be a periodic function of the quantum number n is that the time ratio $t/T_{\rm fr}$ must be rational, and we write $t=(p/q)T_{\rm fr}$ for relatively prime integers p and q (that is, p/q forms a simplified fraction). We will refer to p as the *time numerator* and q as the *time denominator*.

The time evolution exponential is an even function of the quantum number n. This allows us to write the finite Fourier series in several different ways:

$$f(n)=\sum_{j=0}^{r-1} A_j\times\begin{cases}\exp[+i2\pi nj/r]\\ \text{or}\\ \exp[-i2\pi nj/r]\\ \text{or}\\ \cos(2\pi nj/r),\end{cases} \tag{20}$$

with

$$A_j=\frac{1}{r}\sum_{n=0}^{r-1} f(n)\times\begin{cases}\exp[+i2\pi nj/r]\\ \text{or}\\ \exp[-i2\pi nj/r]\\ \text{or}\\ \cos(2\pi nj/r).\end{cases} \tag{21}$$

The form of the finite Fourier series (20) has the same form as the sought cosine expansion (19) whenever we are at rational multiples of the revival time, $t=(p/q)T_{\mathrm{fr}}$. This demonstrates that at such times the wave function can be described by a parity-conserving fractional revival. In order to extract the physics from the details of this mathematical formalism, we first need to investigate the properties of the expansion coefficients $\{A_j\}$ (Secs. IV D and IV E) and give results for the period r that appears in the finite Fourier series expression (Sec. IV F) before tying the results together into a concrete physical picture (Secs. IV G and IV H).

D. Expansion coefficient properties and interpretation

From the cosine sum in Eq. (21), we see directly that $A_{j+r}=A_j$. Comparing Eq. (20) with Eqs. (18) and (19), this shows that placing pairs of translated wave functions at $\Delta x=\pm(2j/r)L$ is the same as placing them at $\Delta x=\pm(2j/r)L\pm 2L$, that translation is periodic in the well. Similarly, from Eq. (21) we see that $A_{r-j}=A_j$. Physically this shows that placing pairs at $\Delta x=\pm(2j/r)L$ is the same as placing them at $\Delta x=\mp(2j/r)L$, that we are translating the wave functions in pairs. These two coefficient identities allow us to extend definitions and meanings to coefficients not explicitly included in the finite Fourier series.

E. Shift index relations

In computing the coefficients A_j in Eq. (21) we are summing a periodic function $f(n)$ over a full period. We shift the summing variable from n to $n-k$ (where k is any integer) without changing the result:

$$\begin{aligned}A_j&=\frac{1}{r}\sum_{n=0}^{r-1} f(n)\exp[i2\pi nj/r]\\ &=\frac{1}{r}\sum_{n=0}^{r-1} f(n-k)\exp[i2\pi(n-k)j/r].\end{aligned} \tag{22}$$

By using the explicit form of the time-evolution exponential $f(n)$ it can be shown that this allows us to relate the different coefficients with

$$A_{j+2(p/q)rk}=A_j\exp[i2\pi((p/q)k^2+(j/r)k)]. \tag{23}$$

Since $A_{j+r}=A_j$, we can interpret coefficient indices modulo r. Averbukh and Perelman [6] showed this result for $k=1$. Other values of k allow us to determine the relative phases of the fractional revival pairs.

We recall from number theory that if p and q are relatively prime, p has an integer multiplicative inverse $p_q^{(-1)}$ satisfying $p\times p_q^{(-1)}\equiv 1(\mathrm{mod}\ q)$. While there are no simple closed-form expressions for the smallest possible value of $p_q^{(-1)}$ (in practice one computes the inverse with trial and error), its existence and upper bound are discussed in number theory texts (such as [30]). If we choose $k=p_q^{(-1)}$ the shift index relation becomes

$$A_{j+2(r/q)}=A_j\exp[i2\pi(p_q^{(-1)}/q)((q/r)j+1)]. \tag{24}$$

F. Time-evolution phasor periodicity

At time $t=(p/q)T_{\mathrm{fr}}$, Averbukh and Perelman [6] show that the time-evolution exponential $f(n)=\exp[-i2\pi(p/q)n^2]$ is r-periodic in the quantum number n, with

$$r=\begin{cases}q, & q\not\equiv 0(\mathrm{mod}\ 4)\\ q/2, & q\equiv 0(\mathrm{mod}\ 4).\end{cases} \tag{25}$$

G. Coefficient properties and fractional revivals

We now tie together the results of the previous sections to give general expressions for the finite Fourier series coefficients.

1. Case 1: q is odd

For odd values of the time denominator q, the time-evolution phasor has periodicity $r=q$, and so there are q coefficients $\{A_j\}$ in the finite Fourier expansion. It has been shown [6] that all q coefficients have the same magnitude, $|A_j|=1/\sqrt{q}$. The shift index relation (24) is

$$A_{j+2}=A_j\exp[i2\pi(p_q^{(-1)}/q)(j+1)], \tag{26}$$

which allows us to write coefficients in terms of A_0 for even values of j with

$$A_j=A_0\exp[i2\pi(p_q^{(-1)}/4q)j^2]. \tag{27}$$

We write $A_0=e^{i\phi_0}/\sqrt{q}$ in terms of an unknown phase angle ϕ_0 and known magnitude. Since $r=q$ is odd, exactly one of the indices j or $r-j$ is even. Recalling that $A_j=A_{r-j}$, we can regroup the finite Fourier series as a sum over even indices:

$$f(n)=A_0+\sum_{j=2,4,\ldots}^{2q-2} 2A_j\cos(2\pi nj/q). \tag{28}$$

Comparing Eq. (20) with Eqs. (18) and (19), we see that the wave function can be described as an untranslated copy of the initial wave function, and pairs of translated wave functions with displacements $\Delta x=\pm(j/q)2L$ for even j.

2. Case 2: $q \equiv 2$ (mod 4)

In this case, q is an odd multiple of 2. The time-evolution phasor has periodicity $r = q$ and there are q coefficients $\{A_j\}$ in the finite Fourier expansion. It has been shown [6] that even- and odd-index coefficients are coupled separately; the even coefficients are zero and the the odd coefficients have magnitude $|A_j| = 1/\sqrt{q/2}$. The shift index relation is the same as Eq. (26), which for odd j leads to

$$A_j = A_1 \exp[i2\pi(p_q^{(-1)}/4q)(j^2-1)]. \tag{29}$$

We write $A_1 = e^{i\phi_0}/\sqrt{q/2}$ in terms of an unknown phase. Comparing Eq. (20) with Eqs. (18) and (19), we see that the wave function can be described as pairs of translated wave functions with displacements $\Delta x = \pm (j/q)2L$ for odd j.

3. Case 3: $q \equiv 0$ (mod 4)

In this case, q is a multiple of 4. The time-evolution phasor has periodicity $r = q/2$, and so there are $q/2$ coefficients $\{A_j\}$ in the finite Fourier expansion. It has been shown [6] that all coefficients have the same magnitude, $|A_j| = 1/\sqrt{q/2}$. The shift index relation is

$$A_{j+1} = A_j \exp[i2\pi(p_q^{(-1)}/q)(2j+1)], \tag{30}$$

which for all j gives

$$A_j = A_0 \exp[i2\pi(p_q^{(-1)}/q)j^2]. \tag{31}$$

We write $A_0 = e^{i\phi_0}/\sqrt{q/2}$. Comparing Eq. (20) with Eqs. (18) and (19), we see that the wave function can be described as an untranslated copy of the initial wave function and pairs of translated wave functions with displacements $\Delta x = \pm (4j/q)L$.

H. Summary of fractional revivals

The results in the previous three sections can be combined and written in a unified way. Although our derivation began with the notion of *parity-conserving pairs* of fractional revivals, it is advantageous to rewrite our result using Averbukh and Perelman′s notion of *classical paths*. It is awkward to write a unified answer using the parity-conserving pair form because in case 2 above, the pair displacements always include the translations $\Delta x = \pm L$ which correspond to arriving at the same final location by moving in two different directions.

At times $t = (p/q)T_{\rm fr}$ the wave function in the infinite square well is given by

$$\psi(x, t=(p/q)T_{\rm fr}) = \frac{e^{i\phi_0}}{\sqrt{r}} \sum_{k=0}^{r-1} \exp[i2\pi(p_q^{(-1)}/q)(k+\Delta r)^2] \times \psi_{\rm cl}\left(x, \Delta x = \frac{k+\Delta r}{q} 4L\right). \tag{32}$$

The function $\psi_{\rm cl}$ is an arbitrary superposition of left- and right-translated copies of the initial wave function using wave reflections at the well walls:

$$\psi_{cl}(x,\Delta x) = \Lambda_L \overline{\psi_i}(x, -\Delta x) + \Lambda_R \overline{\psi_i}(x, \Delta x) \tag{33}$$

for any choice of weights satisfying $\Lambda_L + \Lambda_R = 1$. That is, we are writing the wave function as a superposition of classically moving ‘‘string’’ profiles, where the classical path is taken to be an arbitrary mixture of initially left- and right-displaced motions.

The number of subpackets r is given by

$$r(t=(p/q)T_{\rm fr}) = \begin{cases} q/2, & q \text{ even} \\ q, & q \text{ odd,} \end{cases} \tag{34}$$

and the path offset Δr is given by

$$\Delta r(t=(p/q)T_{\rm fr}) = \begin{cases} 0, & q \not\equiv 2 (\text{mod } 4) \\ \frac{1}{2}, & q \equiv 2 (\text{mod } 4). \end{cases} \tag{35}$$

The number-theoretic inverse $p_q^{(-1)}$ is most quickly found by testing the positive integers sequentially, checking for the smallest number satisfying $p \times p_q^{(-1)} \equiv 1$ (mod q). The phase angle ϕ_0 is the only unknown, but exact probability density expressions are obtained without knowing it.

Such a wave function described by Eq. (32) is called the ‘‘p/q fractional revival’’ or the ‘‘fractional revival of order p/q.’’ In this expression, we describe wave function translations covering *twice* the round-trip distance (or in the time domain, twice the classical period) for odd-time denominators, and covering a single classical period for even-time denominators. We see no way to reform Eq. (32), for odd-time denominators in particular, to give a concise phase relationship and describe the motion along *one* round-trip path.

We note that our method to find the relative phases of the sub-wave-functions via the use of the multiplicative inverse of the time numerator, outlined in Secs. IV E and IV G, is immediately generalizable to any quantum system that exhibits fractional revivals. This number theoretic technique has proven to be a useful and insightful method for studying phase interference effects with wave packet fractional revivals.

In a recent publication, Bluhm, Kostelecký, and Porter [28] use numerical autocorrelation calculations to demonstrate the fractional revivals at $\frac{1}{4}T_{\rm fr}$, $\frac{1}{2}T_{\rm fr}$, and $\frac{3}{4}T_{\rm fr}$ without reference to its manifestation in the position representation in the well.

I. Fractional revivals as a Hilbert space basis

Result (32) describes the wave function at times $t = (p/q)T_{\rm fr}$ as translated copies of the initial wave function. We argue that this result can then be extended to completely describe the time evolution of the wave function, for all times t.

From a mathematical point of view, we know from real analysis that the set of times $\{(p/q)T_{\rm fr}\}$ for all relatively prime integer pairs p and q is a dense subset of the time domain: for any choice of time t we can find an arbitrarily close rational multiple of T_{fr}. Wave-function time evolution is continuous in time, $\psi(x,t)\rightarrow\psi(x,t_0)$ uniformly in x as $t\rightarrow t_0$, so finding arbitrarily close rational approximations of time will also recreate the wave function of interest arbitrarily accurately.

From a more physical point of view, we know that any physically realizable state will have a largest energy E_{max} in its energy eigenstate expansion (9), and thus the wave function cannot change significantly in time intervals small compared with $\Delta t\approx\hbar/E_{\mathrm{max}}$.

Using either point of view, we see that the results in Eq. (32) can describe evolution at any time. We are then able to describe time-evolved wave functions in the infinite square well using the set of all translations of the initial wave function $\psi_i(x)$ as a *basis*. The number of translations needed to describe the wave function at a *particular* time is given in terms of the time denominator via the quantity r. The set of all translations needed to describe the wave function at *all* times densely covers the set of all possible translations.

V. PROBABILITY DENSITY PICTURES

The wave functions described in Eq. (32) show a rich array of physical phenomena which we illustrate below. As we wish to emphasize the shape of the wave functions and probability densities and not their scale, the graphs do not have a common dependent axis scale. All graphs superimpose the predictions of the fractional revival description (32) with the results from explicit eigenstate time evolution (9); the two equations agree in all cases to within the precision of the computer calculation.

Let us look at a wave packet initially localized in the center of the well [Fig. 2(a)]. For odd-time denominators q, the wave function is q spatially separated displacements of the initial wave packet [Fig. 2(b)], which alternate across the well between initial and reflected shapes. When the time denominator q is an odd multiple of 2, the wave function is $q/2$ spatially separated copies of the initial wave function [Fig. 2(c)]. When the time denominator q is an even multiple of 2, there are $q/2$ copies of the initial wave function, but the initial and reflected shapes exactly overlap, and the resulting probability densities show strong interference effects [Fig. 2(d)].

When there is not significant overlap between the displaced copies of the wave function, the probability density $|\psi(x,t=(p/q)T_{\mathrm{fr}})|^2$ is determined by the time denominator q, independent of the numerator p. Once we have significant overlap, the relative phases of the overlapping copies is significant and the probability density depends on the time numerator p via its number-theoretic inverse $p_q^{(-1)}$. In Fig. 3 we show probability densities for two different time numerators for the same time denominator, for the on-axis initial wave function shown in Fig. 2(a). Both wave functions in this figure are described by 15 translations of the initial wave function, but due to interference between the translations the two probability densities they look completely different.

If instead we started with a well-localized wave packet that initially is slightly off-center [Fig. 4(a)], the even-time denominator revivals no longer overlap and we see the individual wave-function translations [Fig. 4(b)]. Now, however, the symmetry in the odd-time denominator revivals across the well is lost [Fig. 4(c)], and for even modest time denominator values the initial and reflected shapes will interfere [Fig. 4(d)].

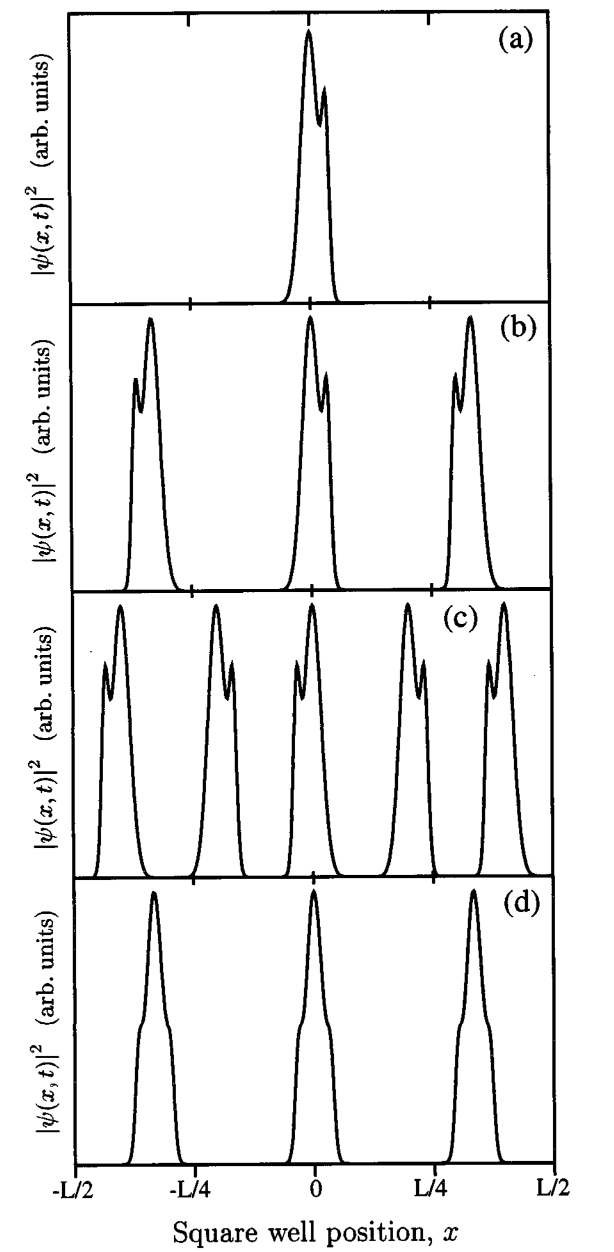

FIG. 2. Initially centered, localized wave function. Probability densities for (a) initial ($t=0$), (b) $t=\frac{1}{3}T_{\mathrm{fr}}$, (c) $t=\frac{1}{10}T_{\mathrm{fr}}$, and (d) $t=\frac{1}{12}T_{\mathrm{fr}}$ wave functions.

Initial wave functions with definite parity are interesting special cases of our theory because the initial and reflected wave forms are indistinguishable. By definition of their parity, such wave functions are centered at the origin. Just as in Fig. 2 we saw interference effects, we see *complete* destructive and constructive interference in states of definite parity.

For even-parity states [as in Fig. 5(a)] there are full revivals of the wave function at multiples of time $t=\frac{1}{8}T_{\mathrm{fr}}$. At times $t=(p/8q)T_{\mathrm{fr}}$ there are q copies of the initial wave

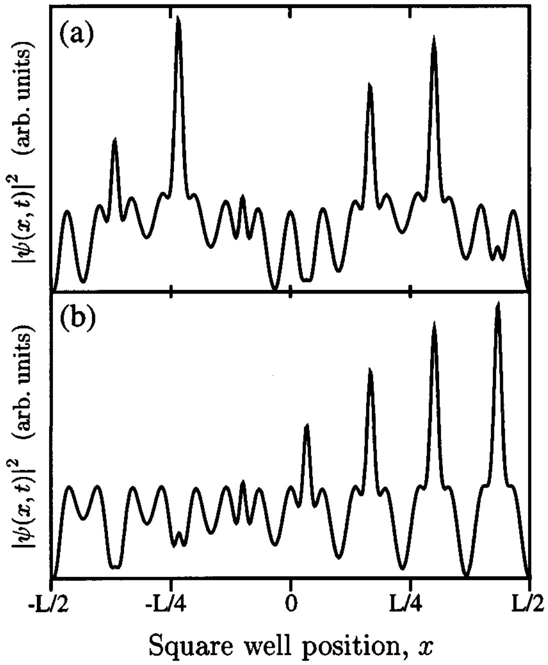

FIG. 3. Initially centered, localized wave function. Probability densities for (a) $t=\frac{1}{15}T_{\rm fr}$ and (b) $t=\frac{4}{15}T_{\rm fr}$ wave functions.

function distributed evenly across the well [Figs. 5(b) and 5(c)].

For odd-parity states [as in Fig. 6(a)], there are full revivals of the wave function at multiples of time $t=\frac{1}{4}T_{\rm fr}$. At times $t=(p/4q)T_{\rm fr}$, for odd values of q there are q translation locations that appear in the probability density [Fig. 6(b)]. For even values of q there are $q/2+1$ translation locations that appear in the probability density [Fig. 6(c)]. For these even q values, we find displacements at $\Delta x=\pm L/2$, where the first half of the sub-wave-function has reflected and constructively interferes with the second half.

The fractional revivals are most striking when the initial wave function is well-localized, but our results are in no way limited to such wave functions. Figure 7 shows a nonlocalized wave function and two of its fractional revivals.

There is an interesting counterpoint to one's usual notions of quantum time evolution in light of the results presented in Eq. (32). We expect that $\psi(x,t+\Delta t)\approx\psi(x,t)$ for ''sufficiently small'' values of Δt, so, for example, we expect

$$\lim_{k\to\infty}\psi(x,t=T_{\rm fr}/10^k)=\psi(x,t=0) \tag{37}$$

This is curious because our result (32) describes the left-hand side of this equation as $\sim 10^k$ translated copies of the initial wave function (and thus the number of translated copies is unbounded as $k\to\infty$), whereas the right-hand side is a single copy of the initial wave function. We show graphs of the asymptotic behavior of the left-hand side for decreasing values of k in Fig. 8.

VI. FINITE SQUARE WELLS

It is impossible to find a physical system that creates a truly infinite confining potential, so we now make some general comments on the evolution of wave functions in a finite well of depth V_0. Finite square wells only support a finite number of bound energy eigenstates. The number of bound states is $n_{\rm max}={\rm int}(2P/\pi)+1]$, where $P=(2mV_0/\hbar^2)^{1/2}L/2$ is the well strength parameter. Solving the time-independent Schrödinger equation for such a well leads to transcendental equations for the energy levels. Via a first-order expansion of such equations, Barker *et al.* [31] showed that a finite square well's energy levels are given by

$$E_n\approx\frac{P^2}{(P+1)^2}\frac{\pi^2\hbar^2}{2mL^2}n^2. \tag{38}$$

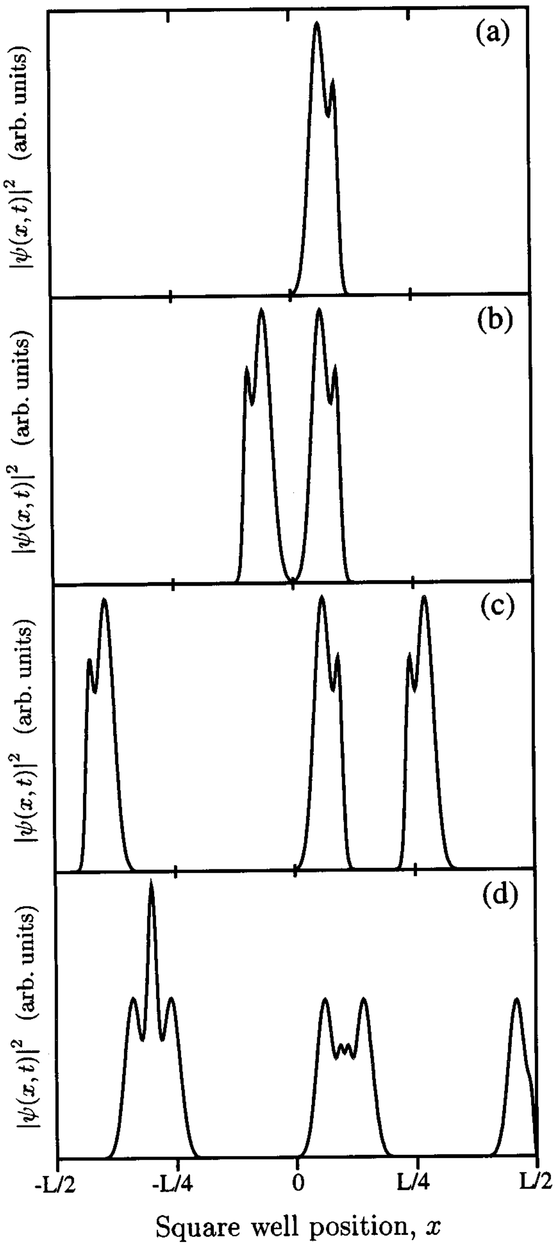

FIG. 4. Initially off-center localized wave function. Probability densities for (a) initial ($t=0$), (b) $t=\frac{1}{4}T_{\rm fr}$, (c) $t=\frac{1}{3}T_{\rm fr}$, and (d) $t=\frac{1}{5}T_{\rm fr}$ wave functions.

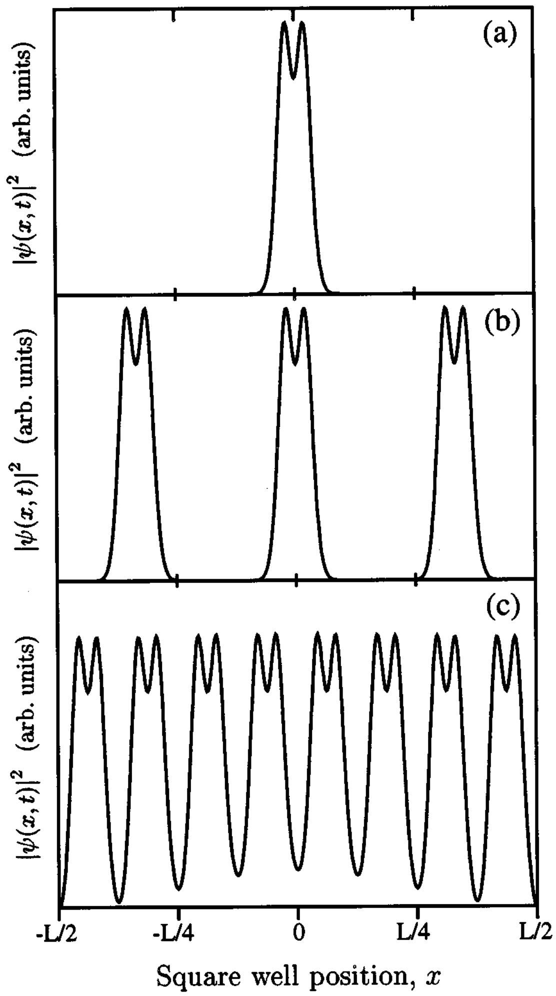

FIG. 5. Even-parity wave function. Probability densities for (a) initial ($t=0$) and full revival ($t=\frac{1}{8}T_{\rm fr}$), (b) $t=\frac{1}{24}T_{\rm fr}$, and (c) $t=\frac{1}{64}T_{\rm fr}$ wave functions.

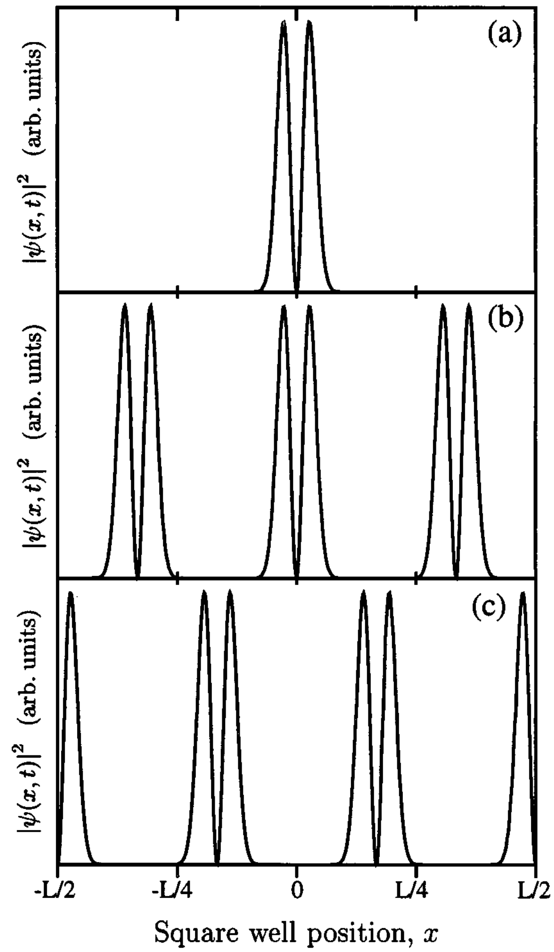

FIG. 6. Odd-parity wave function. Probability densities for (a) initial ($t=0$) and full revival ($t=\frac{1}{4}T_{\rm fr}$), (b) $t=\frac{1}{12}T_{\rm fr}$, and (c) $t=\frac{1}{24}T_{\rm fr}$ wave functions.

These energies are the same as would be found in a larger *infinite* square well of size $L'=(1+1/P)L$. Barker *et al.* also gave a second-order expression for the energies of the finite square well. One could take such an expression, expand it as in Eq. (4), and associate a super-revival time scale $T_{\rm sr}$ with the cubic contribution to the energy levels as a function of the well strength parameter P.

In our treatment we have used the simple classical model of a wave form propagating on an ideal string. In a finite square well this would have to be expanded to describe the evanescent part of the wave function outside the confining well.

VII. SUMMARY AND OUTLOOK

We have found an expression (32) that relates the wave function at rational multiples of a revival time $T_{\rm fr}$ to the initial wave function $\psi_i(x)$ in terms of translations of the initial wave function, treating it as a wave on a string that reflects probability amplitude at the well boundaries. This result holds without approximation, to all fractional revival orders, without limiting the class of initial wave functions or the time ranges considered.

It is no surprise that free time evolution preserves the energy level populations $|c_n|^2$. Far more surprising is that the initial wave function shape, the coherent superposition of energy eigenstates, is in some sense ''remembered'' by the system in its time evolution. Mathematically, Eq. (32) states that the set of initial wave functions translated by rational multiples of the periodic round-trip distance forms a function-space *basis* for the time-evolved wave functions at rational multiples of the revival time $T_{\rm fr}$. This has interesting connections with, and distinctions from, wavelet expansion theory [32] that may deserve more exploration.

In Rydberg atoms, wave packets that exhibit revival and fractional revival behavior need to be excited with considerable care, and a great deal of attention has been given, both theoretically and experimentally, to find the regime in which expansion (4) gives a good description of the pertinent energy levels of the system so that the wave packet will exhibit revival behavior. In this sense the infinite square well is the ideal system for fractional revivals: all wave functions exhibit fractional revivals of all orders just because they were created in a system with such special energy-level spacing.

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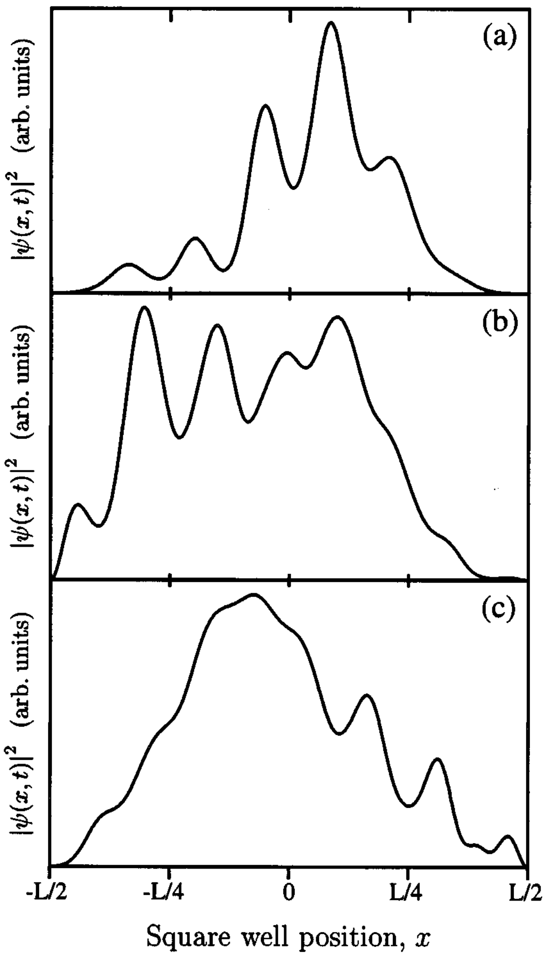

FIG. 7. Initially nonlocalized wave function. Probability densities for (a) initial ($t=0$), (b) $t=\frac{1}{5}T_{\rm fr}$ and (c) $t=\frac{7}{9}T_{\rm fr}$ wave functions.

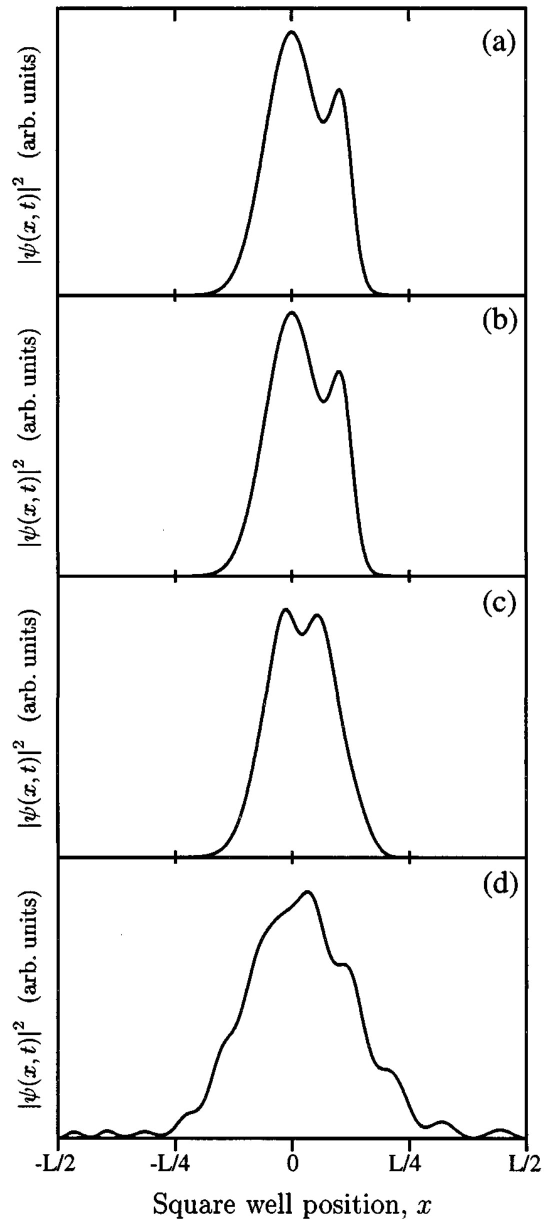

FIG. 8. Initially entered, localized wave function. Probability densities for (a) initial ($t=0$), (b) $t=(1/10^4)T_{\rm fr}$, (c) $t=(1/10^3)T_{\rm fr}$, and (d) $t=(1/10^2)T_{\rm fr}$ wave functions.

APPENDIX: PARITY-CONSERVING FRACTIONAL REVIVAL PAIR EXPANSION

We wish to calculate the overlap integral between a parity-conserving pair of wave-translated wave functions and the nth energy eigenstate. That is, we wish to compute the quantity

$$\int_{-\infty}^{\infty}[\overline{\psi_i}(x,\Delta x=\alpha L)+\overline{\psi_i}(x,\Delta x=-\alpha L)]\phi_n(x)dx. \quad \text{(A1)}$$

We will break the integral up into three separate contributing terms: the translated copies of the initial wave function and the two boundary reflections with π phase shifts. Figure 9 gives an example initial wave function and its translated copies for reference. Although the geometry of this figure would imply translations satisfying $0 \leqslant \alpha L \leqslant L/2$, the result is valid for all αL. For brevity, we will use the notation

$$\mathrm{trig}_n(x)=\begin{cases}\sqrt{\frac{2}{L}}\sin(n\pi x/L), & n \text{ even}\\ \sqrt{\frac{2}{L}}\cos(n\pi x/L), & n \text{ odd.}\end{cases} \quad \text{(A2)}$$

The overlap integral is given by

$$\begin{aligned}\int_{-\infty}^{\infty}&[\overline{\psi_i}(x,\Delta x=\alpha L)+\overline{\psi_i}(x,\Delta x=-\alpha L)]\phi_n(x)dx\\ &=\int_{-L/2}^{L/2}[\psi_i(x-\alpha L)+\psi_i(x+\alpha L)]\mathrm{trig}_n(x)dx\\ &\quad+\int_{L/2-\alpha L}^{L/2}e^{i\pi}\psi_i([L-x]-\alpha L)\mathrm{trig}_n(x)dx\\ &\quad+\int_{-L/2}^{-L/2+\alpha L}e^{i\pi}\psi_i([-L-x]+\alpha L)\mathrm{trig}_n(x)dx. \quad \text{(A3)}\end{aligned}$$

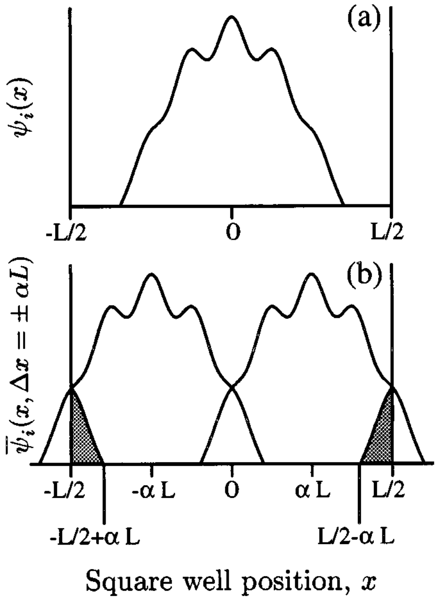

FIG. 9. Sample (a) initial wave function and (b) translated pairs to illustrate the geometry used in the Appendix.

We rewrite the first term as two integrals, each with the initial wave function recentered at the origin:

$$\int_{-L/2}^{L/2} \psi_i(x \pm \alpha L)\mathrm{trig}_n(x)dx$$

$$= \int_{-L/2 \pm \alpha L}^{L/2 \pm \alpha L} \psi_i(x)\mathrm{trig}_n(x \pm \alpha L)dx. \tag{A4}$$

As the initial wave function vanishes for $|x| \geqslant L/2$, the range of integration can be reduced to $-L/2+\alpha L \leqslant x \leqslant L/2$ for the ''positive'' $(+)$ integral and to $-L/2 \leqslant x \leqslant L/2-\alpha L$ for the ''negative'' $(-)$ integral. The second term of Eq. (A3) can be rewritten with the change of variables $L-x-\alpha L \to x$ to center the initial wave function at the origin:

$$\int_{L/2-\alpha L}^{L/2} e^{i\pi}\psi_i([L-x]-\alpha L)\mathrm{trig}_n(x)dx$$

$$= \int_{L/2-\alpha L}^{L/2} \psi_i(x)\mathrm{trig}_n(x+\alpha L)dx. \tag{A5}$$

Similarly, rewriting the third term of Eq. (A3) with the change of variables $-L-x+\alpha L \to x$ leads to

$$\int_{-L/2}^{-L/2+\alpha L} e^{i\pi}\psi_i([-L-x]+\alpha L)\mathrm{trig}_n(x)dx$$

$$= \int_{-L/2}^{-L/2+\alpha L} \psi_i(x)\mathrm{trig}_n(x-\alpha L)dx. \tag{A6}$$

Combining all these results gives a simple expression for the quantity we wish to calculate:

$$\overline{\psi_i}(x,\Delta x=\alpha L)+\overline{\psi_i}(x,\Delta x=-\alpha L)$$

$$= \int_{-L/2}^{L/2} \psi_i(x)[\mathrm{trig}_n(x+\alpha L)+\mathrm{trig}_n(x-\alpha L)]. \tag{A7}$$

Using the explicit expressions for $\mathrm{trig}_n(x)$, one can show that, for all n,

$$\mathrm{trig}_n(x+\alpha L)+\mathrm{trig}_n(x-\alpha L)=2\cos(\alpha\pi n)\mathrm{trig}_n(x). \tag{A8}$$

The remaining integral is our defining equation for the coefficient c_n (8), so we conclude that

$$\overline{\psi_i}(x,\Delta x=\alpha L)+\overline{\psi_i}(x,\Delta x=-\alpha L)=2c_n\cos(\alpha\pi n). \tag{A9}$$

Using the energy eigenfunction orthonormality, this is rewritten as

$$\overline{\psi_i}(x,\Delta x=\alpha L)+\overline{\psi_i}(x,\Delta x=-\alpha L)$$

$$=2\sum_n c_n\cos(\alpha\pi n)\phi_n(x). \tag{A10}$$

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