Piecewise Zero-curvature Solutions
of the One-Dimensional Schrödinger Equation

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Abstract

We discuss the general mathematical condition in one-dimensional time-independent quantum mechanics for a wave function to have zero curvature over an extended region of space and still be a valid wave function. This condition and its solution are not often discussed as part of quantum mechanics texts at any level, yet has interesting consequences for experimental, pedagogical, and theoretical investigations of systems with piecewise-constant potential energy functions. As a detailed example, we solve and visualize the position-space energy eigenstates, including the zero-curvature wave functions, for the double infinite square well. We then present the solutions for several other standard cases in which zero-curvature wave functions are allowed as bound states, scattering states, and as threshold states. These solutions are of interest to supersymmetric quantum mechanics and the procedures we outline can be used to 'design' quantum wells for studies of wave packet dynamics.

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I. INTRODUCTION

One of the standard problems in one-dimensional quantum mechanics is that of the infinite square well (ISW) given by the potential energy function

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{otherwise} . \end{cases} \quad (1)$$

We easily find the time-independent position-space solutions to this problem to be $\psi_n(x) = \sqrt{2/L}\sin(n\pi x/L)$ inside the well, and zero elsewhere. Implementing the boundary conditions yields the following *possible* values for the quantum number, $n = 0, \pm1, \pm2, \ldots$. Since the negative values for n yield the same wave functions as the positive values, apart from an overall phase, they can be omitted without loss of generality. Most textbooks reject the $n = 0$ ($E = 0$) state on the grounds that the wave function, sin(0), does not yield a physical solution. While it is true that an $n = 0$ state is not a valid solution, the process by which this conclusion is reached is incorrect. As pointed out in this Journal [1–3], the $E = 0$ solution to the Schrödinger equation is in fact no longer a sinusoidal function. Instead, this solution has *zero curvature* over the entire width of the well and has the mathematical form $\psi(x) = Ax + B$. This wave function cannot be normalized and still satisfy the boundary and continuity conditions for the ISW, and thus the $E = 0$ solution cannot be an allowed energy eigenstate of the ISW [4].

While the authors of Refs. [1–4] have used the zero-curvature (ZC) case to show that the infinite square well cannot have a zero-energy solution, cases in which ZC solutions are actually valid are seldom considered [5, 6], even though, for example, all of the wave functions for the infinite square well are linear (namely zero) for $x \leq 0$ and $x \geq L$. One related exception is that of the ground state of an infinite well modified with periodic boundary conditions (as considered in Refs. [7] and [8]) or in the related case of the quantum-mechanical rotor defined by the Hamiltonian $\hat{H} = \hat{L}^2/2I$ with $\hat{L} \equiv -(i\hbar)\, d/d\theta$. In these cases, a ZC ground state is present, corresponding to the $m = 0$ angular wave function given by $\Theta_0(\theta) = 1/\sqrt{2\pi}$. As a more advanced example, a linear radial wave function, $u(r)$, naturally occurs in low-energy S-wave scattering from finite potentials [9] used to model low-energy nuclear scattering [10].

In this paper we describe a variety of scenarios in which ZC ($E - V(x) = 0$) wave functions naturally occur over an extended region of space for specially chosen piecewise-constant potential energy functions. In Section II we briefly review solutions of the Schrödinger equation for regions of constant potential energy, including the ZC solution. We describe in Section III the results for the double infinite square well, an infinite well with a symmetric potential energy 'hump' added to it, considering separately the solutions for energies greater than, less than, and equal to the potential energy step. We then briefly examine other related bound-state situations, scattering-state scenarios, and threshold states (states which serve as a boundary between bound and scattering states). These special configurations are often overlooked and, in this sense, extend the set of exactly-solvable problems

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in quantum mechanics. Throughout, we also discuss the pedagogical applications of these solutions.

The procedures we outline can be used to determine specifications for the 'tuning' of quantum wells, like those used in Ref. [11], so ZC wave functions can be another example of the experimental realization of 'designer' quantum wave functions [12–15]. In addition, since the precise knowledge of the entire energy spectrum is crucial to studies of wave packet dynamics, as the time scales of the dynamics are directly related to the energy levels [16], ZC states may play a special role in the dynamics of wave packets in such special wells [17]. Finally, these solutions are also of theoretical interest in supersymmetric quantum mechanics where the zero-energy ZC wave functions can be used to generate supersymmetric partner potentials [6].

Zero-curvature states can serve an important pedagogical purpose as a way to easily extend the standard treatment of piecewise-constant potential energy functions. These special cases help elucidate the connection between the potential energy function, the quantized energy eigenvalue, and the resulting form of the wave function in one-dimensional quantum-mechanical systems [18]. While ZC solutions seem like an intuitively natural interpolation between the much more frequently discussed oscillatory and tunneling solutions, the unfamiliar mathematical form of the one-dimensional Schrödinger equation for these parameters catches many students by surprise [5].

To keep the paper to a reasonable length, many details that are omitted here are included in a longer version which is available online [19] and also at the EPAPS archive [20]. A web site includes a large number of additional images not included in this paper which can be accessed at <http://webphysics.davidson.edu/mjb/zc/>.

II. SOLUTIONS TO THE TIME-INDEPENDENT SCHRÖDINGER EQUATION

The time-independent Schrödinger equation in one dimension in a region where the potential energy function does not change too rapidly with position, and hence can be considered a constant, is:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right]\psi(x) = E\,\psi(x)\ , \qquad (2)$$

which can be written as

$$\left[\frac{d^2}{dx^2} + \frac{2m(E-V_0)}{\hbar^2}\right]\psi(x) = 0\ . \qquad (3)$$

For our analysis, it is convenient to define:

$$k \equiv \sqrt{2mE/\hbar^2}\ , \qquad (4)$$

$$q \equiv \sqrt{2m(E-V_0)/\hbar^2}\ , \qquad (5)$$

and

$$\kappa \equiv \sqrt{2m(V_0-E)/\hbar^2}\ . \qquad (6)$$

In Eq. (3) there are *three* cases to be considered: $E > V_0$, $E < V_0$, and $E = V_0$ (the zero-curvature solution). In these three cases the Schrödinger equation and its solution reduce to:

$$\left[\frac{d^2}{dx^2} + q^2\right]\psi(x) = 0 \rightarrow \psi(x) = A\cos(qx) + B\sin(qx) \text{ or } \psi(x) = A'e^{iqx} + B'e^{-iqx}\ , \qquad (7)$$

$$\left[\frac{d^2}{dx^2} - \kappa^2\right]\psi(x) = 0 \rightarrow \psi(x) = Ae^{\kappa x} + Be^{-\kappa x} \text{ or } \psi(x) = A'\cosh(qx) + B'\sinh(qx)\ , \qquad (8)$$

and

$$\frac{d^2}{dx^2}\psi(x) = 0 \quad \rightarrow \quad \psi(x) = Ax + B\ , \qquad (9)$$

for $E > V_0$, $E < V_0$, and $E = V_0$, respectively. When $E > V_0$, the curvature of the wave function is such that $\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} < 0$ and the wave function is oscillatory (negative curvature for $\psi(x) > 0$ and positive curvature for $\psi(x) < 0$). For $E < V_0$ the curvature of the wave function is such that $\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} > 0$ and hence the wave function curves away from the axis (positive curvature for $\psi(x) > 0$ and negative curvature for $\psi(x) < 0$), and exponentially decays, grows, or does both, depending on boundary conditions. For $E = V_0$, which in general is not considered except as an inflection point between regions of positive and negative curvature, the curvature of the wave function is zero, and the wave function is a constant or is linear.

III. THE DOUBLE INFINITE SQUARE WELL

To illustrate the results of Section II, consider, a double infinite square well (DISW), a symmetric infinite square well with a symmetric potential energy 'hump' added to it as defined by the potential energy function [21, 22]:

$$V(x) = \begin{cases} +\infty & \text{for } x < -b \\ 0 & \text{for } -b < x < -a \quad \text{Region I} \\ +V_0 & \text{for } -a < x < +a \quad \text{Region II} \\ 0 & \text{for } a < x < b \quad \text{Region III} \\ +\infty & \text{for } +b < x \end{cases}\ . \qquad (10)$$

This potential is the piecewise-constant relative of the ISW with repulsive Dirac δ function [23, 24], double finite well [25–28], and smooth double well [29–31] potentials often considered in the literature.

A. $E > V_0$ and $E < V_0$

In order to solve for the energy eigenstates we will separately consider the even- and odd-parity solutions. For the even-parity solution, when $E > V_0$ and already applying the boundary conditions at $-b$ and b, we have for the separate pieces of the wave function

$$\psi_{\rm I} = A\sin(k[x+b]) \ , \tag{11}$$

$$\psi_{\rm II\ even} = B\cos(qx) \ , \tag{12}$$

and

$$\psi_{\rm III} = C\sin(k[x-b]) \ . \tag{13}$$

Matching $\psi_{\rm I}$ and $\psi_{\rm II}$ at $x=-a$ ($\psi_{\rm I}(-a) = \psi_{\rm II}(-a)$ and $\psi'_{\rm I}(-a) = \psi'_{\rm II}(-a)$) we find

$$A\sin(k[b-a]) = B\cos(qa) \tag{14}$$

and

$$kA\cos(k[b-a]) = qB\sin(qa) \ , \tag{15}$$

where matching $\psi_{\rm II}$ and $\psi_{\rm III}$ yields no new information except that $C=-A$. Dividing Eq. (14) by (15), and simplifying, we find the energy-eigenvalue equation

$$q\tan(k[b-a]) = k\cot(qa) \ . \tag{16}$$

A variety of different methods can be brought to bear to find the solutions to this transcendental equation [32–36]. For numerical evaluation, Eq. (16) can be most simply written in terms of the energy by replacing k and q with Eqs. (4) and (5) and using $\hbar = 2m = 1$:

$$\sqrt{E-V_0}\tan(\sqrt{E}[b-a]) = \sqrt{E}\cot(\sqrt{E-V_0}\ a) \ , \tag{17}$$

to solve for E given a particular a, b, and V_0.

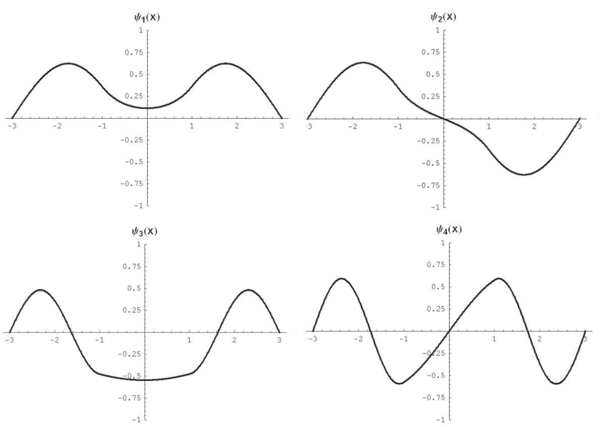

FIG. 1: The first four wave functions (upper pair: $E < V_0$; lower pair: $E > V_0$) for the double infinite square well with $V_0 = 5$. In all of the images $\hbar = 2m = 1$ and $a = 1$ and $b = 3$.

The odd-parity solution proceeds similarly, namely Eqs. (11) and (13) can still be used, but we must replace Eq. (12) with

$$\psi_{\rm II\ odd} = B\sin(qx) \ . \tag{18}$$

Again, matching $\psi_{\rm I}$ and $\psi_{\rm II}$ at $x=-a$ we find that

$$A\sin(k[b-a]) = -B\sin(qa) \tag{19}$$

and

$$kA\cos(k[b-a]) = qB\cos(qa) \ . \tag{20}$$

Due to symmetry, matching $\psi_{\rm II}$ and $\psi_{\rm III}$ at $x=a$ yields no new information except that $C=A$. Dividing Eq. (19) by Eq. (20), and simplifying, we find the energy-eigenvalue equation for odd-parity states:

$$q\tan(k[b-a]) = -k\tan(qa) \ . \tag{21}$$

For $E < V_0$, we again consider the even- and odd-parity solutions separately. For the even-parity solution, Eqs. (11) and (13) are still valid for $\psi_{\rm I}$ and $\psi_{\rm III}$, respectively, but we must use

$$\psi_{\rm II\ even} = B\cosh(\kappa x) \ . \tag{22}$$

Noting that $\cos(i\kappa x) = \cosh(\kappa x)$ and the form of Eqs. (12) and (22), we may find the energy-eigenvalue equation by replacing $q \to i\kappa$ in Eq. (16) to yield

$$\kappa\tan(k[b-a]) = -k\coth(\kappa a) \ . \tag{23}$$

The odd-parity solution proceeds similarly, but with

$$\psi_{\rm II\ odd} = B\sinh(\kappa x) \ . \tag{24}$$

Now noting that $\sin(i\kappa x) = i\sinh(\kappa x)$ and the form of Eqs. (18) and (24), we may find the energy-eigenvalue equation by simply replacing $q \to i\kappa$ in Eq. (21) to yield

$$\kappa\tan(k[b-a]) = -k\tanh(\kappa a) \ . \tag{25}$$

The first four wave functions for a DISW ($a=1$, $b=3$, and $V_0=5$) are shown in Figure 1. For $E > V_0$, the wave functions of a DISW can have some unexpected features, such as the special cases in which there is an antinode at $x = \pm a$ which yields the same maximum amplitude for the wave function across the well [37]. This is approximately the case for the $n=3$ and $n=4$ states shown. Otherwise when the *wiggliness* or *curviness* of the wave function changes across regions due to changes in the potential energy function, the amplitude must also change [38].

B. $E = V_0$

To find a well with a ZC state ($E = V_0$), we proceed much like before, considering even and odd states separately. For the even states we can use Eqs. (11) and (13) which are still valid for $\psi_{\rm I}$ and $\psi_{\rm III}$, respectively, but in Region II we must use

$$\psi_{\rm II\ even} = B\ , \tag{26}$$

which has no slope. Matching $\psi_{\rm I}$ and $\psi_{\rm II}$ at $x = -a$, we find

$$A \sin(k[b-a]) = B \tag{27}$$

and

$$kA \cos(k[b-a]) = 0\ , \tag{28}$$

which yields an energy-eigenvalue equation that can be solved analytically

$$\cot(k[b-a]) = 0 \ \rightarrow\ k[b-a] = n\pi/2\ , \tag{29}$$

for odd integer n (which correspond to even-parity states). Since $E = V_0$, this is also the condition on V_0 for a ZC state to exist. Eq. (29) yields an analytic result for V_0 since the matching of the even-parity solutions at $x = \pm a$ must occur at an antinode of $\psi_{\rm I}$ and $\psi_{\rm III}$, because the wave function is flat in Region II. For these states, therefore, there are $n/4$ 'wavelengths' of the wave function in Regions I and III, respectively.

When the wave function is odd, $\psi_{\rm II}(0) = 0$, and the wave function in Region II must be:

$$\psi_{\rm II\ odd} = Bx\ . \tag{30}$$

Matching $\psi_{\rm I}$ and $\psi_{\rm II}$ at $x = -a$ for an odd-parity wave function, we find

$$A \sin(k[b-a]) = -Ba \tag{31}$$

and

$$kA \cos(k[b-a]) = B\ , \tag{32}$$

which yields the energy-eigenvalue equation:

$$\tan(k[b-a]) = -ka\ . \tag{33}$$

Again since k is related to the energy via Eq. (4), and since $E = V_0$, this is also a condition on V_0 such that there is a ZC state.

Zero-curvature solutions are, therefore, only possible for special 'tuned' DISWs with suitable values of V_0, a, and b, *and* the quantum number, n. It is easy to conclude that for a DISW there exists either one or (more likely) zero ZC states in the energy spectrum. The first four possible zero-curvature wave functions corresponding to four different DISWs ($a = 1$, $b = 3$, and $V_0 = 0.61685$, 1.30979, 5.55165, and 6.46935, respectively) are shown in Figure 2.

In addition to the comparison of these wave functions in position space, it is also straightforward to Fourier transform these solutions into momentum space. We refer the reader to Refs. [19, 20] for details of the momentum-space calculations in the DISW case. In Ref. [5] the asymmetric infinite square well momentum-space calculations are done in detail including a discussion of the relationship between the form of the momentum-space wave function and the different regions of the well.

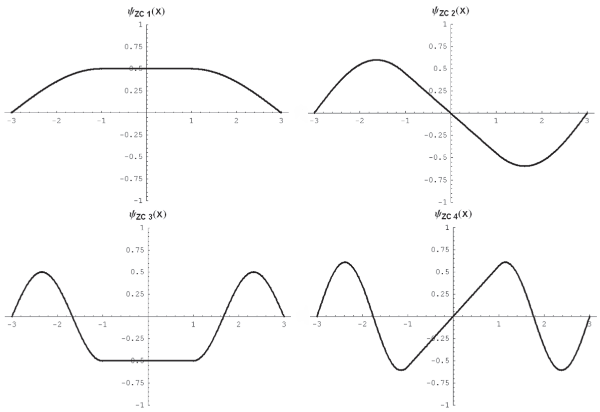

FIG. 2: The first four ZC wave functions for the double infinite square well with V_0 that satisfy Eq. (29) and Eq. (33). In all of the images $\hbar = 2m = 1$ and $a = 1$ and $b = 3$.

IV. OTHER VARIANTS OF THE ISW

A. Symmetric Finite Square Well within ISW

The potential energy well for this case is the same as Eq. (10) except that in Region II, $V_0 < 0$ [39]. For this ZC and also zero-energy case, which is the only case we will consider here, note that the solutions will be very different than those of the previous Section. We again consider the even and odd solutions separately. For $E = 0$ the even solutions that satisfy the boundary conditions at $-b$ and b correspond to the following wave function pieces:

$$\psi_{\rm I} = A[x+b]\ , \tag{34}$$

$$\psi_{\rm II\ even} = B \cos(qx)\ , \tag{35}$$

and

$$\psi_{\rm III} = C[x-b]\ . \tag{36}$$

Matching $\psi_{\rm I}$ and $\psi_{\rm II\ even}$ at $x = -a$, we have the energy-eigenvalue equation:

$$\cot(qa) = q[b-a]\ . \tag{37}$$

For the odd-parity solution when $E = 0$, we use $\psi_{\rm II\ odd} = B\sin(qx)$ and the energy-eigenvalue equation becomes

$$\tan(qa) = -q[b-a]\ . \tag{38}$$

Since $E = 0$, $q = \sqrt{2m|V_0|/\hbar^2}$, and thus Eqs. (37) and (38) are conditions on $|V_0|$ such that a ZC solution can exist. An example of the first four possible zero-curvature wave functions for four different infinite wells with added finite wells ($a = 1$, $b = 3$, and $V_0 = -0.42676$, -3.37308, -10.8393, and -23.19233, respectively) are shown in Figure 3.

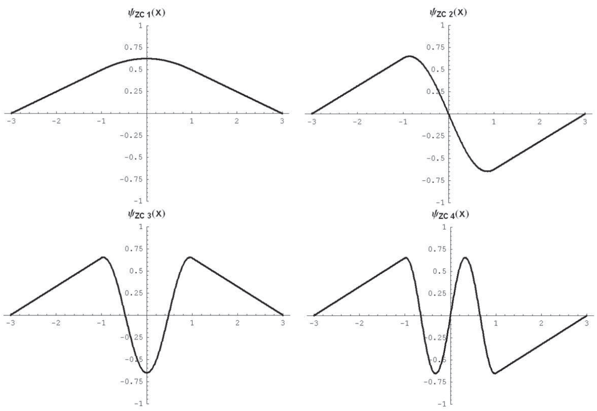

FIG. 3: The first four ZC wave functions for four different infinite square wells with an additional potential energy well, $V_0 < 0$ that satisfy Eq. (37) and Eq. (38). In all of the images $\hbar = 2m = 1$ and $a = 1$ and $b = 3$.

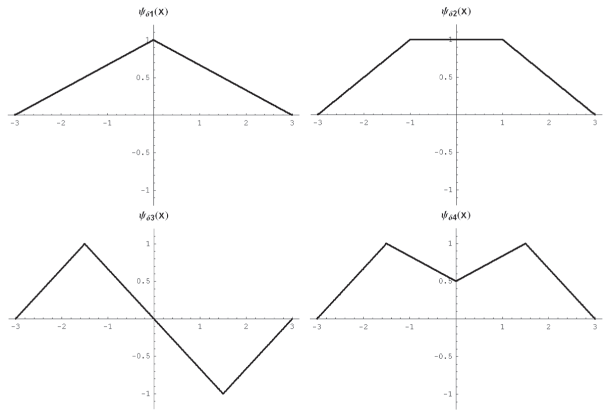

FIG. 4: The unnormalized ZC wave functions corresponding to four different Dirac delta function potentials added to a symmetric ISW. In all of the images $\hbar = 2m = 1$ and $b = 3$.

B. Symmetric ISW with Dirac Delta Functions

A logical extension of the previous discussion is to replace the finite barrier or well with one or more Dirac delta functions. We begin by considering a single attractive Dirac delta function at the origin of a symmetric ISW with walls at $x = -b$ and $x = b$, so that $V(x) = \alpha\delta(x)$ with $\alpha < 0$. While this scenario has been considered before theoretically [40–43], and is related to experimental scenarios in which a potential energy 'spike' inserted in a quantum well is modeled by a Dirac delta function [14, 15], our approach differs in that we tune α so that a 'pure' ZC solution (of zero energy) arises.

For example, if we add to the ISW, $V_{\delta_1} = -\frac{2}{b}\,(\frac{\hbar^2}{2m})\,\delta(x)$, the additional potential energy function splits the well into two regions: Region I ($x < 0$) and Region II ($x > 0$). Assuming a ZC wave function exists, it must be that $\psi_{\rm I}(x) = A(x+b)$ and $\psi_{\rm II}(x) = -A(x-b)$ after we apply the boundary conditions and match the wave functions at $x = 0$. We must next ensure that the wave function has the proper discontinuity in its slope at the origin due to the Dirac delta function. In general, we must have that

$$\psi'(x_{0_+}) - \psi'(x_{0_-}) = \alpha\left(2m/\hbar^2\right)\,\psi(x_0)\,. \qquad (39)$$

We find that our chosen V_{δ_1} satisfies this requirement for our ZC wave function. This ZC, triangle-shaped wave function was shown as a limiting case of an analysis that used supersymmetric quantum mechanics in Ref. [43].

There are an endless number of combinations of Dirac delta functions that when added to the ISW result in a ZC wave function. For example consider the additions of $V_{\delta_2} = -\frac{3}{2b}\,(\frac{\hbar^2}{2m})\,[\,\delta(x+b/3) + \delta(x-b/3)\,]$ and $V_{\delta_3} = -\frac{4}{b}\,(\frac{\hbar^2}{2m})\,[\,\delta(x+b/2) + \delta(x-b/2)\,]$ which along with the ZC solution to V_{δ_1} (and the following V_{δ_4}) are depicted in Figure 4.

In addition to starting with the ZC wave function, we can also proceed in the *opposite* direction: write any 'pure' piecewise zero-curvature (single-valued) wave function and determine the potential that must be added to the ISW. Such a problem is called a working-backwards or a Physics Jeopardy problem [44]. As an example of this process, consider the "M"-shaped, ZC wave function in Figure 4 and determine V_{δ_4}. A quantitative result is possible from direct measurement of the wave function slopes, wave function values at the kinks, the positions of the kinks, and Eq. (39). Answer: $V_{\delta_4} = -\frac{3}{b}\,(\frac{\hbar^2}{2m})\,[\,\delta(x+b/2) - \frac{4}{3}\delta(x) + \delta(x-b/2)\,]$.

We also note that the wave functions in Figure 4, and their relatives, are valid despite the fact that they are obviously 'kinky.' The fact that kinky wave functions can be valid is often lost in most introductory texts on quantum mechanics. In fact, wave functions must be smooth *only* if their corresponding potential energy functions are 'well behaved.' It turns out that only infinite walls (such as in the boundaries of the ISW) and Dirac delta functions behave badly enough to correctly generate kinks in the wave functions. For example, a comparison of the upper-left-hand image of Figure 4 (corresponding to V_{δ_1}) to the upper-left-hand image of Figure 3 shows that the 'softening' of the potential (the replacement of the attractive Dirac delta function with a finite well in an ISW) removes the kink.

V. SCATTERING SOLUTIONS

A. Step Potential

We define the step potential as

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \quad \text{Region I} \\ V_0 & \text{for } x > 0 \quad \text{Region II} \end{cases}\,. \qquad (40)$$

For $E = V_0$, in Region I we have the usual scattering-state wave function of: $\psi_{\rm I}(x) = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)}$. In Region II the wave function must be finite as $x \to \infty$, and we therefore have $\psi_{\rm II}(x) = De^{-i\omega t}$. Matching $\psi_{\rm I}$ and $\psi_{\rm II}$ at $x = 0$ and at $t = 0$ (since once the boundary condition is satisfied, it is always satisfied), we have $A + B = D$ and $Aik - Bik = 0$. We find from these two equations that $A = B = 2D$, which guarantees that we have 100% reflection despite the existence of a finite $\psi_{\rm II}$ as $x \to \infty$. This is due to the fact that the wave function in Region II is not spatially varying (and thus it does not have a spatially varying phase, despite its temporally varying phase) in this region. Therefore the probability current density is zero here, which supports the result for the transmission and reflection coefficients.

B. Finite Barrier

The finite barrier is defined as

$$V(x) = \begin{cases} 0 & \text{for } x < -a \quad \text{Region I} \\ +V_0 & \text{for } -a < x < +a \quad \text{Region II} \\ 0 & \text{for } x < a \quad \text{Region III} \end{cases} . \tag{41}$$

For $E = V_0$,

$$\psi_{\rm I} = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)} , \tag{42}$$

$$\psi_{\rm II} = (Cx + D)\, e^{-i\omega t} , \tag{43}$$

and

$$\psi_{\rm III} = Fe^{i(kx-\omega t)} . \tag{44}$$

Matching $\psi_{\rm I}$ and $\psi_{\rm II}$ at $x = -a$ and at $t = 0$ we find

$$Ae^{-ika} + Be^{ika} = -Ca + D \tag{45}$$

and

$$ikAe^{-ika} - ikBe^{ika} = C . \tag{46}$$

Matching $\psi_{\rm II}$ and $\psi_{\rm III}$ at $x = a$ we have

$$Ca + D = Fe^{ika} \quad \text{and} \quad C = ikFe^{ika} . \tag{47}$$

After simplifying, we find a transmission coefficient of $T = |F/A|^2 = 1/(1+k^2a^2)$. This direct calculation agrees with the limiting case of $E \to V_0$ for the $E > V_0$ and $E < V_0$ solutions of the transmission coefficient which is often left as a homework problem [45].

VI. THRESHOLD STATES

A. Finite Square Well

We define the finite square well as

$$V(x) = \begin{cases} 0 & \text{for } x < -a \quad \text{Region I} \\ -|V_0| & \text{for } -a < x < a \quad \text{Region II} \\ 0 & \text{for } x < +a \quad \text{Region III} \end{cases} . \tag{48}$$

When we have tuned the well such that $E = 0$, we have the possible wave function pieces

$$\psi_{\rm I} = Ax + B , \tag{49}$$

$$\psi_{\rm II} = C\sin(qx) + D\cos(qx) , \tag{50}$$

and

$$\psi_{\rm III} = Fx + G , \tag{51}$$

where $q = \sqrt{2m|V_0|/\hbar^2}$. For the zero-curvature (and zero-energy) case, because $\psi_{\rm I}$ and $\psi_{\rm III}$ must be finite at $x = \mp\infty$, respectively, we must have $\psi_{\rm I} = B$ and $\psi_{\rm III} = G$. Note that the boundary conditions of the threshold state at $x \to \pm\infty$ means that the wave function does not vanish, instead it must be a constant. If there was any slope in the wave function, at $x \to \pm\infty$ the wave function would not be finite.

The choice of $\psi_{\rm II}$ depends on the parity of the wave function. When the wave function is even, $\psi_{\rm II\ even} = D\cos(qx)$, the energy-eigenvalue equation yields analytic solutions:

$$\tan(qa) = 0 \to qa = (n-1)\pi/2 \quad (n = 3, 5, 7, \ldots) , \tag{52}$$

while when the wave function is odd, $\psi_{\rm II\ odd} = C\sin(qx)$, and we have

$$\cot(qa) = 0 \to qa = (n-1)\pi/2 \quad (n = 2, 4, 6, \ldots) , \tag{53}$$

which both agree with the standard, non-ZC solution when one considers what is required to add another bound state to the well [46]. In general, if a particular $|V_0|$ and a satisfy either Eq. (52) or (53), a slight increase in either $|V_0|$ or a will result in the threshold state becoming another bound-state solution.

We can combine Eqs. (52) and (53) to find a general condition for a zero-curvature solution to occur: $|V_0| = (n-1)^2\pi^2\hbar^2/2m(2a)^2$ where $n = 2, 3, 4, \ldots$, which has a form similar to that of the energies of an ISW of length $2a$. In addition, to match the flat wave functions in Regions I and III, there are $n/2$ 'wavelengths' of the wave function in Region II. The first four threshold states for four different finite wells are shown in Figure 5. Note that the *lowest lying* of these possible threshold states, $n = 2$, is an *odd-parity solution* since there will always be at least one bound state (which is itself an even-parity state) in the finite square well. These results agree with the results presented in Ref. [17] in which the poles of the S matrix for the finite square well were analyzed for bound, threshold, and scattering states.

Perhaps the most interesting pedagogical implication of teaching with these threshold states, whether one discusses scattering states before or after bound states, is that ZC threshold states can serve as a concrete illustration of how the boundary conditions at $x \to \pm\infty$ can be consistently considered. As mentioned earlier in regard to 'kinky' wave functions, many textbooks overstate the

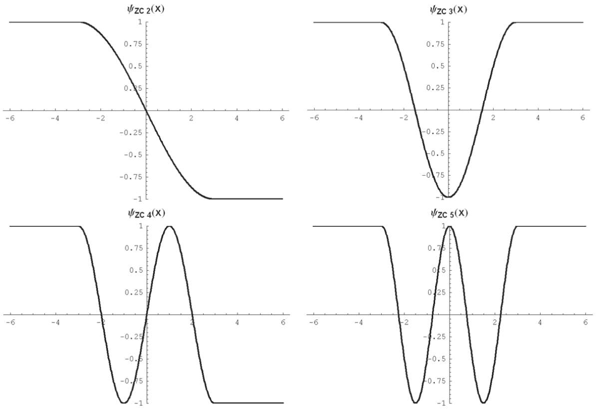

FIG. 5: The first four ZC threshold wave functions for finite square wells with $|V_0| = (n-1)^2\pi^2\hbar^2/2m(2a)^2$. In all of the images $\hbar = 2m = 1$ and $a = 3$.

restrictions on the wave function, and boundary conditions are another example of this. Textbooks tend to imply that bound-state wave functions must go to zero as $x \to \pm\infty$, yet scattering states clearly do not abide by this 'rule.' This dichotomy can confuse students, especially when bound states are considered first [47].

In a more consistent approach, one can require a single constraint on all states: that $P(x) \equiv |\psi(x)|^2$ is *finite* as $x \to \pm\infty$. In one dimension, this constraint forces bound-state wave functions to asymptotically approach zero, forces threshold-state wave functions to asymptotically approach a finite constant, and forces scattering-state wave function amplitudes to asymptotically approach a finite constant. When calculating probabilities and expectation values, one must use localized states in which $\psi(x) \to 0$ as $x \to \pm\infty$ such that $\int_{-\infty}^{+\infty} P(x)\, dx < \infty$, whether localized by virtue of the potential energy function (bound states), superposition (free-particle wave packets), or both (bound-state wave packets). When calculating transmission and reflection coefficients, which require ratios of probability current densities and hence ratios of absolute squares of wave functions, one is free to use non-localized states, such as scattering states, where the wave functions need not be normalizable, but instead must remain finite at $x \to \pm\infty$ [48].

B. Half Finite/Half Infinite Well

We define the potential energy function as

$$V(x) = \begin{cases} +\infty & \text{for } x < 0 \\ -|V_0| & \text{for } 0 < x < a \quad \text{Region I} \\ 0 & \text{for } x < +a \quad \text{Region II} \end{cases} . \quad (54)$$

For the zero-curvature (and zero-energy) case, $\psi_{\rm I} = A\sin(qx)$ and $\psi_{\rm II} = D$, since the wave function in Region II cannot have an x dependence and be finite at infinity. Matching $\psi_{\rm I}$ and $\psi_{\rm II}$ at $x = a$ gives the energy-eigenvalue equation with the analytic solutions:

$$\cot(qa) = 0 \quad \to \quad qa = n\pi/2 \;\; (n = 1, 3, 5, \ldots) . \quad (55)$$

Using $q = \sqrt{2m|V_0|/\hbar^2}$ in Eq. (55), yields the condition for these threshold states: $|V_0| = n^2\pi^2\hbar^2/2m(2a)^2$ where $n = 1, 3, 5, \ldots$. For these states, there are $n/4$ 'wavelengths' of the wave function in Region I. For $n = 1$, this equation is also the condition for the first bound state to occur. Unlike the finite well, this well does not always support a bound state. If $|V_0| = \pi^2\hbar^2/2m(2a)^2$, there will be a threshold state with one-quarter 'wavelength' inside the well, while when $|V_0| > \pi^2\hbar^2/2m(2a)^2$, this threshold state becomes a bound state.

The form of this potential can be used as a radial potential for a simple model of low energy neutron-proton scattering. The previous results can be used if one makes the substitution that $x \to r$ and $\psi(x) \to u(r)$ where $u(r) = r\psi(r)$. There is also a one-to-one correspondence of the Schrödinger equations in x and r, $\left[d^2/dr^2 + 2m(E - V_0)/\hbar^2 \right] u(r) = 0$, since in low-energy scattering, only the S-wave ($l = 0$) contributes. For the general ZC zero-energy solution in Region II we can write $u(r) = A - l_s^{-1} r$, where l_s is called the scattering length. Bound states occur for positive l_s, threshold states for $l_s = \infty$, and unbound states for negative l_s.

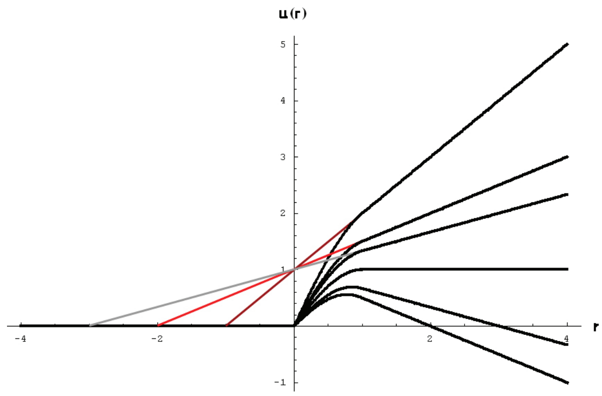

FIG. 6: Six $E = 0$ states of six different strength (V_0) half-infinite/half-finite square wells are shown. The states are ZC states in Region II with differing scattering lengths due to the differing potentials. The linear parts of the negative scattering length solutions are carried backwards to show the crossing with the r axis.

As an illustrative example, consider the six $E = 0$ states of six different strength (V_0) half-infinite/half-finite square wells shown in Figure 6. The wave functions are ZC states of the form $u(r) = A\sin(qx)$ in Region I ($0 < r < a$), and in Region II ($r > a$) of the form: $u(r) = 1 - r/l_s$ where, for simplicity, the constant in the ZC solution has been chosen to be one. Given a scattering length (or V_0), matching the wave function at $r = a$ yields the transcendental equation for the energy (or the scattering length): $\tan(qx) = q(1 - l_s)$. The scattering length determines where the wave function crosses the r axis (for negative scattering lengths the linear part of the wave function is continued backwards toward the r axis). The scattering lengths depicted are -1, -2, -3, ∞, 3, and 2, respectively.

VII. CONCLUSION

We have outlined several one-dimensional quantum mechanics problems in which zero-curvature solutions to the time-independent Schrödinger equation are valid. These position-space wave functions are easily determined and visualized and can be thought of as extending the set of exactly-solvable problems in quantum mechanics. Numerous other piecewise-constant potential energy functions with ZC solutions can be created, for either theoretical or experimental [11] investigations. For example, an ISW with two potential energy steps can be 'tuned' to yield a wave function with oscillatory, zero curvature, and exponential forms in the three different regions. Such states can serve the pedagogical purpose of introducing the relationships between solutions and boundary conditions; specifically that wave functions must tend towards a finite constant at $x \to \pm\infty$. In addition, the pure ZC wave functions of Figure 4 can help illustrate the relationship between kinetic and potential energies when 'kinky' wave functions naturally occur [6].

Acknowledgments

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APPENDIX A: ADDITIONAL DETAILS FOR THE DISW WITH $E < V_0$

Here we show the complete derivation of the transcendental equation for $E < V_0$ shown briefly in Section IIIA. Again we consider the even- and odd-parity solutions separately. For the even-parity solution when $E < V_0$, Eqs. (11) and (13) are still valid for ψ_{I} and ψ_{III}, respectively, but we must use

$$\psi_{\mathrm{II\ even}} = B\cosh(\kappa x)\ . \tag{A1}$$

Matching ψ_{I} and ψ_{II} at $x = -a$ we find

$$A\sin(k[b-a]) = B\cosh(\kappa a)\ , \tag{A2}$$

and

$$kA\cos(k[b-a]) = -\kappa B\sinh(\kappa a)\ . \tag{A3}$$

Matching ψ_{II} and ψ_{III} at $x = a$ yields no new information except $C = -A$. Dividing Eq. (A2) by (A3), and simplifying, we find the energy-eigenvalue condition

$$\kappa\tan(k[b-a]) = -k\coth(\kappa a)\ . \tag{A4}$$

The odd-parity solution proceeds similarly, namely Eqs. (11) and (13) are still valid, but we must replace Eq. (A1) with

$$\psi_{\mathrm{II\ odd}} = B\sinh(\kappa x)\ . \tag{A5}$$

Matching ψ_{I} and ψ_{II} at $x = -a$ we find

$$A\sin(k[b-a]) = -B\sinh(\kappa a)\ , \tag{A6}$$

and

$$kA\cos(k[b-a]) = \kappa B\cosh(\kappa a)\ . \tag{A7}$$

Matching ψ_{II} and ψ_{III} at $x = a$ yields no new information except $C = A$. Dividing Eq. (A6) by (A7), and simplifying, we find the energy-eigenvalue condition

$$\kappa\tan(k[b-a]) = -k\tanh(\kappa a)\ . \tag{A8}$$

APPENDIX B: DISW IN MOMENTUM SPACE

The wave functions in momentum space are straightforward to calculate from the position-space wave functions via the Fourier transformation:

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\psi(x)\,e^{-ipx/\hbar}\,dx\ . \tag{B1}$$

By using the wave functions from Section III, momentum-space wave functions can be written as

$$\begin{aligned}\phi(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{a}^{+b}\psi_{\mathrm{III}}(x)\,e^{-ipx/\hbar}\,dx\\ &+\frac{1}{\sqrt{2\pi\hbar}}\int_{-a}^{+a}\psi_{\mathrm{II}}(x)\,e^{-ipx/\hbar}\,dx\\ &+\frac{1}{\sqrt{2\pi\hbar}}\int_{-b}^{-a}\psi_{\mathrm{I}}(x)\,e^{-ipx/\hbar}\,dx\ ,\end{aligned} \tag{B2}$$

such that $\phi(p) \equiv \phi_{\mathrm{I}}(p) + \phi_{\mathrm{II}}(p) + \phi_{\mathrm{III}}(p)$. Given the form of the position-space wave function discussed in Section III, it is clear that for $E < V_0$, $E = V_0$, and $E > V_0$ the momentum-space wave functions in Regions I and III will be identical (with the exception of an overall sign for even-parity $\phi_{\mathrm{III}}(p)$ which comes from an overall sign in the even-parity position-space wave functions relative to the odd position-space wave functions). The momentum-space wave functions in Regions II, however, will all be different. We therefore begin with the calculations for Regions I and III.

In Region I the position-space wave function is always of the form

$$\psi_{\mathrm{I}} = A\sin(k[x+b])\ , \tag{B3}$$

where the overall normalization constant, A, must be determined based on the state.

We find two terms from the Fourier transform of Eq. (B3):

$$\phi_{\mathrm{I}(\pm)}(p) = \pm\frac{A}{\sqrt{2\pi\hbar}}\left(\frac{(b-a)i}{2}\right)e^{+ipb/\hbar}e^{-i\Delta_{(\pm)}}\left[\frac{\sin(\Delta_{(\pm)})}{\Delta_{(\pm)}}\right], \tag{B4}$$

where $\Delta_{(\pm)} \equiv (p \pm \hbar k)(b-a)/2\hbar$.

In Region III the position-space wave function, apart from an overall sign, is always of the form

$$\psi_{\mathrm{III}} = A\sin(k[x-b]) . \tag{B5}$$

We again find two (similar-looking) terms:

$$\phi_{\mathrm{III}(\pm)}(p) = \pm\frac{A}{\sqrt{2\pi\hbar}}\left(\frac{(b-a)i}{2}\right)e^{-ipb/\hbar}e^{+i\Delta_{(\pm)}}\left[\frac{\sin(\Delta_{(\pm)})}{\Delta_{(\pm)}}\right]. \tag{B6}$$

Given that these two wave functions will always appear in the overall momentum-space wave function, it is convenient to consider the combinations:

$$\Phi_{\mathrm{even}(\pm)}(p) = \mp\frac{A(b-a)}{\sqrt{2\pi\hbar}}\sin(pb/\hbar - \Delta_{(\pm)})\left[\frac{\sin(\Delta_{(\pm)})}{\Delta_{(\pm)}}\right] \tag{B7}$$

and

$$\Phi_{\mathrm{odd}(\pm)}(p) = \pm\frac{A(b-a)i}{\sqrt{2\pi\hbar}}\cos(pb/\hbar - \Delta_{(\pm)})\left[\frac{\sin(\Delta_{(\pm)})}{\Delta_{(\pm)}}\right], \tag{B8}$$

where $\Phi_{\mathrm{even}(\pm)}(p) = \phi_{\mathrm{I}(\pm)}(p) - \phi_{\mathrm{III}(\pm)}(p)$ and $\Phi_{\mathrm{odd}(\pm)}(p) = \phi_{\mathrm{I}(\pm)}(p) + \phi_{\mathrm{III}(\pm)}(p)$. From these forms, it is clear that as the energy of the eigenstate and therefore k increases, the momentum-space probability densities become more noticeably peaked at $p = \pm\hbar k$.

1. Region II: $E > V_0$

For $E > V_0$ in Region II, we consider the even and odd wave functions separately. For the even-parity wave function

$$\psi_{\mathrm{II\ even}} = A\left[\frac{\sin[k(b-a)]}{\cos(qa)}\right]\cos(qx) , \tag{B9}$$

we find two terms:

$$\phi_{\mathrm{II\ even}(\pm)}(p) = \frac{Aa}{\sqrt{2\pi\hbar}}\left[\frac{\sin[k(b-a)]}{\cos(qa)}\right]\left[\frac{\sin(\delta_{(\pm)})}{\delta_{(\pm)}}\right] , \tag{B10}$$

where $\delta_{(\pm)} \equiv (p \pm \hbar q)a/\hbar$. The odd-parity solution proceeds similarly, but with

$$\psi_{\mathrm{II\ odd}} = -A\left[\frac{\sin[k(b-a)]}{\sin(qa)}\right]\sin(qx) , \tag{B11}$$

and again we find two terms:

$$\phi_{\mathrm{II\ odd}(\pm)}(p) = \mp\frac{Aia}{\sqrt{2\pi\hbar}}\left[\frac{\sin[k(b-a)]}{\sin(qa)}\right]\left[\frac{\sin(\delta_{(\pm)})}{\delta_{(\pm)}}\right] . \tag{B12}$$

From these forms, it is clear that as the energy of the eigenstates, and therefore q, increase, the momentum-space probability densities become more noticeably peaked at $p = \pm\hbar q$.

2. Region II: $E < V_0$

For $E < V_0$, we again consider the even- and odd-parity solutions separately. We use

$$\psi_{\mathrm{II\ even}} = A\left[\frac{\sin[k(b-a)]}{\cosh(\kappa a)}\right]\cosh(\kappa x) , \tag{B13}$$

and we find two terms:

$$\phi_{\mathrm{II\ even}(\pm)}(p) = \frac{Aa}{\sqrt{2\pi\hbar}}\left[\frac{\sin[k(b-a)]}{\cosh(\kappa a)}\right]\left[\frac{\sinh(\xi_{(\pm)})}{\xi_{(\pm)}}\right] , \tag{B14}$$

where $\xi_{(\pm)} \equiv (\kappa \pm ip/\hbar)a$. The odd-parity solution proceeds similarly, but with

$$\psi_{\mathrm{II\ odd}} = -A\left[\frac{\sin[k(b-a)]}{\sinh(\kappa a)}\right]\sinh(\kappa x) , \tag{B15}$$

and again we find two terms:

$$\phi_{\mathrm{II\ odd}(\pm)}(p) = \pm\frac{Aa}{\sqrt{2\pi\hbar}}\left[\frac{\sin[k(b-a)]}{\sinh(\kappa a)}\right]\left[\frac{\sinh(\xi_{(\pm)})}{\xi_{(\pm)}}\right] . \tag{B16}$$

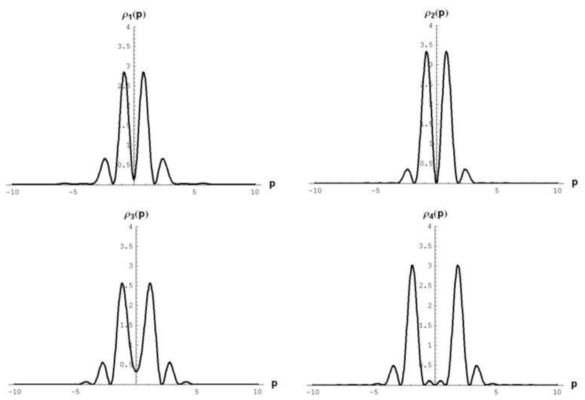

FIG. 7: The first four momentum-space probability densities (upper pair: $E < V_0$; lower pair: $E > V_0$) for the double infinite square well with $V_0 = 5$.

Figure 7 shows the first four momentum-space probability densities of the same DISW corresponding to the images in Figure 1.

3. Region II: $E = V_0$

For the even states we use

$$\psi_{\mathrm{II\ even}} = A\sin[k(b-a)] , \tag{B17}$$

and we find:

$$\phi_{\mathrm{II\ even}}(p) = \frac{2Aa}{\sqrt{2\pi\hbar}}\sin[k(b-a)]\left[\frac{\sin(pa/\hbar)}{(pa/\hbar)}\right] . \tag{B18}$$

When the wave function is odd, the wave function in Region II is:

$$\psi_{\mathrm{II\ odd}} = -A\sin[k(b-a)]x , \tag{B19}$$

and we find:

$$\phi_{\text{II odd}}(p) = \frac{2Aia^2}{\sqrt{2\pi\hbar}} \sin[k(b-a)] \left[\frac{\sin(pa/\hbar)-(pa/\hbar)\cos(pa/\hbar)}{(pa/\hbar)^2}\right] . \tag{B20}$$

From these forms, it is clear that the momentum-space probability densities should have a noticeable peak at $p=0$.

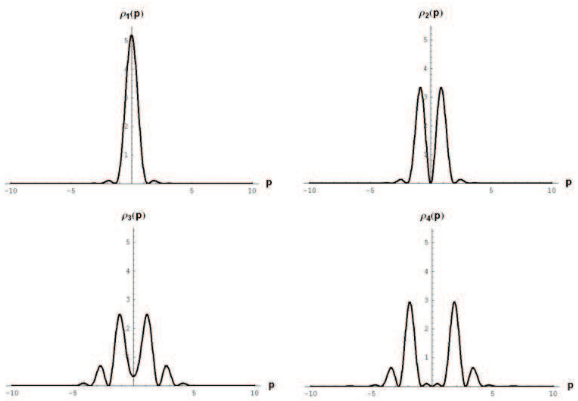

FIG. 8: The first four ZC momentum-space probability densities for the double infinite square well with V_0 that satisfy Eq. (29) and Eq. (33).

In Figure 8 the first four ZC momentum-space probability densities of the same DISWs corresponding to the images in Figure 2 are shown. Note that while one expects large peaks around $p=0$ due to the zero-curvature nature of the wave function in position space, these peaks do not occur for these states. The energy of these states is relatively low, and hence there is a noticeable 'interference' between the parts of the momentum-space wave functions that correspond to $E > V_0$ and $E = V_0$.

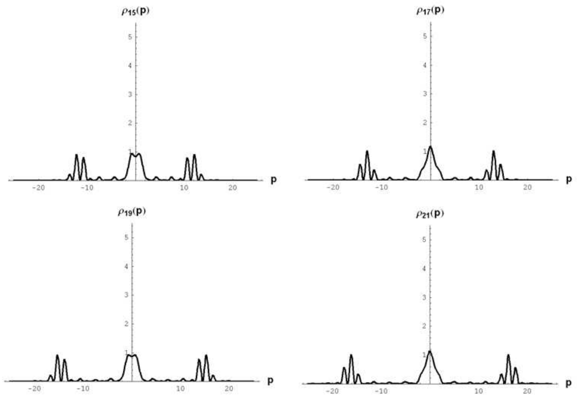

FIG. 9: Four large n (15,17,19,21) ZC momentum-space probability densities for the double infinite square well with V_0 that satisfy Eq. (29) and Eq. (33).

4. Large-n ZC Momentum-space Images

In order to better visualize the effect of the ZC state in momentum space, Figure 9 shows several large-n momentum-space probability densities. For these states, there are again large peaks around $p=0$ corresponding to the zero-curvature nature of the wave function in position space. Since the energy of these states is relatively high, there is less noticeable 'interference' between the parts of the momentum-space wave functions that correspond to $E > V_0$ and $E = V_0$.

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[47] As a further example, this discussion is complicated in three dimensions in cylindrical and spherical coordinates by the volume element. For example, the R_{n0} wave functions of the Coulomb problem are not zero at $r = 0$, but $u_{n0}(r) \equiv rR_{n0}$ are. This is why one often sees the definition $P_{nl}(r) \equiv |u_{nl}(r)|^2$ used.
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