Chapter 12
Infinite Well States
And
Dynamics

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Now for the saga of prisoner M, a tiny mass trapped in a maximum-security prison made of infinite potential walls! This is the simplest Schrodinger model besides the Bohr orbitals discussed in Chapter 9, in fact it is subset contained within the Bohr problem. The infinite well provides a setting for introducing expectation values of energy and dipole transition and it helps clarify concepts of uncertainty and Fourier dynamics (revivals) introduced previously. This maximum-security prison prepares one for the other lesser-or-minimum-security prisons such as finite square well, oscillator, and Coulomb whose discussions occupy later Chapters. It will seem like all the particles spend most of their time in jail. Schrodinger analysis does seem to encourage a lot of recidivism!
Chapter 12. Infinite Well States and Dynamics

12.1 Infinite-Well Wavefunctions

Suppose a potential that is zero only in a finite well region of width $W$ between walls at $x=0$ and $x=W$. Outside $V(x)$ is made extremely high so it is effectively an infinite prison that makes the mass $M$ inside to bounce back and forth forever between the walls. Poor prisoner $M$!

(a) Eigenstate wavefunctions

However, eigenwaves for $M$ in the prison may not be so different from what they may have been before the walls were put up. The difference now is that $\psi$ must be a standing wave like the lowest plot of Fig. 11.4.1, and the energy must be such that points $x=0$ and $x=W$ lie under wave nodes. If the wave is zero in the walls it must be zero at the walls. These are the infinite square-well boundary conditions.

$$\psi_{\text{in well}}(x) = A_+ e^{ikx} + A_- e^{-ikx} = \begin{cases} 
0 & \text{for } x=0, \text{ or } A_+ + A_- = 0 \\
0 & \text{for } x=W, \text{ or } A_+ e^{ikW} + A_- e^{-ikW} = 0
\end{cases} \quad (12.1.1a)$$

Solving gives amplitude conditions and quantization conditions for sine standing wave eigenfunctions.

$$A_+ = -A_- \quad kW = n\pi \quad \text{or} \quad k = n\pi/W \quad (12.1.1b)$$

$$\langle x|\epsilon_n \rangle = \psi_n(x) = A \sin(k_n x) = A \sin\left(\frac{n\pi x}{W}\right) \quad (n=1,2,3,\ldots) \quad (12.1.1c)$$

These are plotted in Fig. 12.1.1 on the three lowest energy eigenvalue levels to which they belong.

$$\epsilon_n = \frac{\hbar^2}{2M} k_n^2 = \frac{\hbar^2 n^2 \pi^2}{2MW^2} = \left(1^2, 2^2, 3^2, \ldots, n^2\right) \frac{\hbar^2}{8MW^2} \quad (12.1.1d)$$

![Fig. 12.1.1 Asleep in prison. Infinite square well standing waves have stationary envelopes.](image)

Imposition of boundary conditions (12.1.1b) on prisoner $M$ causes severe restrictions. The infinite continuum of energy and $k$-values is reduced to a discrete semi-infinite spectrum like the Bohr spectrum sketched in Fig. 7.1.1. However, unlike a Bohr or free-space spectrum, double energy degeneracy is
halved; only singlet sine waves remain while all cosine waves, including the \( n=0 \) state, are forbidden. This rules out moving or galloping wave eigenstates. Recall that zero-quanta were forbidden for the optical cavity (the "photon prison") in Fig. 6.3.7. Imprisoned spectra start counting with \( n=1 \), and the very first energy level is non-zero and called a zero-point energy. For the infinite square well it is \( \frac{\hbar^2}{8MW^2} \).

(b) Superposition wavefunctions

While none of the \( \langle x | \psi_n \rangle \) waves in Fig. 12.1.1, by themselves, move any but their invisible phases, combinations like \( \alpha \langle x | \psi_1 \rangle + \beta \langle x | \psi_2 \rangle \) do appear to bounce back and forth at a "beat" frequency equal to the difference \( |\omega_m - \omega_n| \). For example, consider a wave state \( \langle x | \Psi(t) \rangle \) that is a 50-50 combination

\[
\langle x | \Psi(t) \rangle = \langle x | \psi_1 \rangle \langle \psi_1 | \Psi(t) \rangle + \langle x | \psi_2 \rangle \langle \psi_2 | \Psi(t) \rangle = \langle x | \psi_1 \rangle (e^{i\omega_1 t}) + \langle x | \psi_2 \rangle (e^{i\omega_2 t}) \tag{12.1.2}
\]

of the first two waves \( \langle x | \psi_1 \rangle \) and \( \langle x | \psi_2 \rangle \) in Fig. 12.1.1. Its envelope "sloshes" at a beat frequency of

\[
\omega_{\text{beat}} = \omega_2 - \omega_1 = \frac{2^2 - 1^2}{h} \frac{\hbar^2}{8MW^2} = 3 \frac{2\pi \hbar}{8MW^2} = 3\omega_1 \tag{12.1.3}
\]

as shown below in Fig. 12.1.2. Poor \( M \) is up and pacing back and forth in the cell. No rest for the wicked!

\[ \text{Fig. 12.1.2 Exercise in prison. Infinite square well eigensolution combination "sloshes" back and forth.} \]

It is important to clearly visualize the dynamics of a combination wave such as is plotted in Fig. 12.1.2. If, at time \( t=0 \), the two components of (12.1.2) were in phase, the combination wave would be the sum of \( \psi_1(x) + \psi_2(x) \) that is biased or "sloshed" to the left side of the cell. Half a beat-period later the sum becomes a difference as slower \( \psi_1(x) \) falls \( \pi \) behind \( \psi_2(x) \) to give \( -\psi_1(x) + \psi_2(x) \) "sloshed" to the right.
Because $\langle x | \Psi(t) \rangle$ is a combination of $\langle x | \psi_1 \rangle$ and $\langle x | \psi_2 \rangle$ it seems reasonable that $M$ has a kinetic energy that lies somewhere between the allowed quantum levels $\varepsilon_1$ and $\varepsilon_2$ of its component eigenstates as drawn in Fig. 12.1.2. Roughly speaking, $M$ is somewhere between sleeping on the floor ($\varepsilon_1$) and sleeping in the first excited state or second level ($\varepsilon_2$). A quantum system is not restricted to its energy eigenvalues, "quanta" $\varepsilon_m$ are just values at which it can "sleep" or "play dead." It may have any energy between its $\varepsilon_m$ values and have it in many ways, as long as it stays "awake!" This generalized energy is called the energy expectation value $\langle \varepsilon \rangle$ and will be defined shortly.

Suppose poor sleepless $M$ is really pacing back and forth along the full width $W$ of the cell. In fact, he stops well short of each wall when pacing at low energy, and only really "smacks" the cell wall when he's really mad and pacing at high energy. Precise definition of this uses the position expectation value $\langle x \rangle$ to be defined shortly along with that of energy. But, if we assume $M$ paces at the beat frequency (12.1.3) and at a constant speed $v$ (he is, after all, on a flat $V=0$ prison floor in between the walls) and covers a distance $2W$ in one beat period then he will have an average speed of about

$$
v = \frac{2W}{\tau_{\text{beat}}} = \frac{2W \omega_{\text{beat}}}{2\pi} = \frac{3h}{4MW},
$$

(12.1.4a)

and an approximate energy of

$$
E = \frac{1}{2} M v^2 = \frac{1}{2} M \left( \frac{3h}{4MW} \right)^2 = \frac{9h^2}{48MW^2},
$$

(12.1.4b)

that is, $2^{1/4}$ of the quantum ground state (zero-point) energy $\varepsilon_1$, and a little shy of half way between $\varepsilon_1$ and $\varepsilon_2$, which is $2^{1/2}$, the exact value as we'll see soon. Now let's see if we can figure out exactly what prisoner $M$ is up to! (Cons must be watched precisely even while incarcerated.)

(c) Energy expectation values

Prisoner $M$ "wakes up" and "paces" when in a combination state of at least two eigenstates such as

$$
|\Psi(t)\rangle = |\psi_1\rangle \langle \psi_1 | \Psi(t) \rangle + |\psi_2\rangle \langle \psi_2 | \Psi(t) \rangle = \alpha(t)|\psi_1\rangle + \beta(t)|\psi_2\rangle
$$

(12.1.5a)

where coefficients $\langle \psi_1 | \Psi(t) \rangle = \alpha(t) = \alpha(\theta) e^{-i\omega_1 t}$ and $\langle \psi_2 | \Psi(t) \rangle = \beta(t) = \beta(\theta) e^{-i\omega_2 t}$

(12.1.5b)

preserve normalization, that is

$$
|\alpha(t)|^2 + |\beta(t)|^2 = 1.
$$

(12.1.5c)

Indeed, they should, since $|\alpha(t)|^2$ (or $|\beta(t)|^2$) is the probability for prisoner $M$ to be found sleeping on the floor-level-$\varepsilon_1$ (or first bunk level-$\varepsilon_2$, respectively) if the warden wanders by with his flashlight. We have been assuming that $M$ has only enough strength to get up to the first bunk. Bad assumption, perhaps, and we will modify it shortly.

However, if $M$ is confined to the two lowest levels then his energy may be easily computed by summing the probabilities for being in each level times the energy of the level.

$$
E_{\text{average}} = \langle E \rangle_{\Psi} = \sum_{n=1}^{2} \left( \text{Energy of state } n \right) \left( \text{Probability of state } n \right)
$$

$$
= \sum_{n=1}^{2} \left( \varepsilon_n \langle \psi_n | \Psi \rangle \langle \Psi | \psi_n \rangle \right)
$$

(12.1.6)

For this case the sum reduces to
\[ \langle E \rangle_{\Psi} = \varepsilon_1 |\alpha|^2 + \varepsilon_2 |\beta|^2 \left( = \frac{\varepsilon_1 + \varepsilon_2}{2} = \frac{5\varepsilon_1}{2} \right) \text{ for: } \alpha = \frac{1}{\sqrt{2}} = \beta, \]  

(12.1.7)

or for a 50-50 combination, exactly \(2^{1/2}\) times the quantum ground state (zero-point) energy \(\varepsilon_1\), and exactly half way between \(\varepsilon_1\) and \(\varepsilon_2\). So our previous estimate of \(2^{1/4}\) for \(M\)'s energy was a little bit low.

The general formula for energy expectation is (12.1.6) summed over all eigenstates.

\[
E_{\Psi \text{average}} = \langle E \rangle_{\Psi} = \sum_{n=1}^{\infty} \varepsilon_n \langle \varepsilon_n | \Psi \rangle^* \langle \varepsilon_n | \Psi \rangle = \sum_{n=1}^{\infty} \varepsilon_n \langle \Psi | \varepsilon_n \rangle \langle \varepsilon_n | \Psi \rangle
\]

(12.1.8a)

Notice that conjugation axiom-2 makes this sum into a matrix element of the spectral decomposition of the Hamiltonian \(\mathbf{H}\) operator in terms of its eigenvector ket-bras \(|\psi_m\rangle\langle \psi_m | = |\varepsilon_m\rangle\langle \varepsilon_m | \).

\[
E_{\Psi \text{average}} = \langle E \rangle_{\Psi} = \langle \Psi | \mathbf{H} | \Psi \rangle, \text{ where: } \mathbf{H} = \sum_{n=1}^{\infty} \varepsilon_n |\varepsilon_n \rangle \langle \varepsilon_n |
\]

(12.1.8b)

This is the "professional" formula for the energy expectation value of any state \(|\Psi\rangle\). It goes along a similar formula for "existence" or number expectation value based on the completeness axiom-4.

\[
N_{\Psi \text{average}} = \langle N \rangle_{\Psi} = \langle \Psi | \mathbf{1} | \Psi \rangle = \langle \Psi | \Psi \rangle, \text{ where: } \mathbf{1} = \sum_{n=1}^{\infty} |\varepsilon_n \rangle \langle \varepsilon_n |
\]

(12.1.9a)

The latter is just a simple "bed-count" of prisoner(s) \(M\). Here, it had better be equal to "1" or the warden is going to be in big trouble. This is, after all, an infinitely maximum-security prison! Later, we will consider more realistic prisons that are not so escape-proof. For this one, however, we assume there is exactly one prisoner and that sets the norm or normalization of all the states \(|\varepsilon_m\rangle\) and \(|\Psi\rangle\).

\[
\langle \varepsilon_m | \varepsilon_m \rangle = 1 = \langle \Psi | \Psi \rangle
\]

(12.1.9b)

Normalization of base-eigenstates is required by orthonormality axiom-2 but not necessarily for general combination states like \(|\Psi\rangle\).

(d) Position expectation values

While prisoner \(M\) paces back and forth in state \(|\Psi\rangle\) we can imagine (the warden) wanting to know his position in that dark cell with as much accuracy as possible. However, this is a quantum prison with all the problems and strange behavior introduced so far. Chief among these is the fact that quantum theory has nothing to say about individual observations of prisoner \(M\). Let us all say this again for emphasis: "About each observation, quantum theory tells you nothing!..zip!..nada!..diddley-squat!..fuggedaboudit!" To a classicist warden, quantum mechanics might seem like not a theory at all,..just sheer rubbish!

What saves quantum mechanics is sheer numbers and its statistical predictions. To be useful, quantum theory needs thousands and thousands of prison cells each with a prisoner \(M\) in state \(|\Psi(t)\rangle\). (This is apparently a goal of many modern politicians.) Or else, a single prisoner \(M\) has to be put in cell state \(|\Psi(t)\rangle\) and analyzed over and over again for each value of time \(t\). (The social-psychological approach.)

Fortunately for quantum theory, photons, electrons, and other atomic particles are relatively cheap and plentiful so massively sequential or parallel experiments are easily done. So we may accumulate huge statistical distributions to check a quantum theory. For example, in the case of prisoner \(M\) in state \(|\Psi\rangle = |\Psi(t)\rangle\) it is possible to accurately predict the position expectation value \(\langle x \rangle\) defined as follows.

\[
x_{\Psi \text{average}} = \langle x \rangle_{\Psi} = \langle \Psi | \mathbf{x} | \Psi \rangle, \text{ where: } \mathbf{x} = \int_{-\infty}^{\infty} dx |x \rangle \langle x |
\]

(12.1.10a)
Like \( \langle E \rangle \) and \( \langle x \rangle \) is based on the spectral decomposition of position operator \( x \) which yields

\[
x_{\Psi} \text{average} = \langle x \rangle_{\Psi} = \langle \Psi \vert x \vert \Psi \rangle = \int_{-\infty}^{\infty} dx \langle x \vert \Psi \rangle \langle x \vert \Psi \rangle = \int_{-\infty}^{\infty} dx \langle \Psi \vert x \rangle \langle x \vert \Psi \rangle^* = \int_{-\infty}^{\infty} dx \Psi^* (x) x \Psi(x)
\]

(12.1.10b)

This is the sum \( \int dx \) over position \( x \) times the probability \( \langle x \vert \Psi \rangle \langle x \vert \Psi \rangle = \Psi^* (x) \Psi(x) \) for each position. Moreover, the functional spectral decomposition yields the functional position expectation value \( \langle f(x) \rangle \)

\[
\langle f(x) \rangle_{\Psi} = \langle \Psi \vert f(x) \vert \Psi \rangle = \int_{-\infty}^{\infty} dx \langle \Psi \vert f(x) \vert \Psi \rangle = \int_{-\infty}^{\infty} dx f(x) \langle \Psi \vert x \rangle \langle x \vert \Psi \rangle = \int_{-\infty}^{\infty} dx f(x) \Psi^* (x) \Psi(x)
\]

(12.1.10c)

This includes as a special case the number expectation value.

\[
\langle N \rangle_{\Psi} = \langle \Psi \vert \hat{N} \vert \Psi \rangle = \int_{-\infty}^{\infty} dx \langle \Psi \vert x \rangle \langle x \vert \Psi \rangle = \int_{-\infty}^{\infty} dx \langle \Psi \vert x \rangle \langle x \vert \Psi \rangle^* = \int_{-\infty}^{\infty} dx \Psi^* (x) \Psi(x)
\]

(12.1.10d)

The latter is \( x \)-representation of the "bed-count" of prisoner(s) \( M \), and it had better be equal to "1" here in the "maximum-security" case every time the warden looks.

\[
\langle N \rangle_{\Psi} = 1 = \int_{-\infty}^{\infty} dx \Psi^* (x) \Psi(x)
\]

(12.1.10e)

In other words, in a "strict" prison we demand unit normalization of all states.

The above equations provide the means for developing a complete statistical analysis of the prisoner \( M \) population and dynamics. \( \langle f(x) \rangle \) formulas give the values and time behavior not only of the average or mean position \( \langle x \rangle \) of prisoner(s) \( M \) each time the warden uses his flashlight, but also the (possibly time-dependent) mean square \( \langle x^2 \rangle \), mean-cube \( \langle x^3 \rangle \), and so forth. These are "moments" that will warm the heart of the coldest statistician, and the body count \( \langle N \rangle = \langle x^0 \rangle \) is just another precious moment.

There's more. A similar formulation (12.1.10) gives the momentum operator \( p \) and its moments \( \langle p^0 \rangle, \langle p \rangle, \langle p^2 \rangle \), and distributions. This yields statistics about where the prisoner was going when caught each time by the glare of the warden's hated flashlight.

(e) Position moments: Dipole matrices

Evaluation of position expectation values \( \langle \Psi \vert x \vert \Psi \rangle \) or moments \( \langle \Psi \vert f(x) \vert \Psi \rangle \) can be done in any basis. The energy eigenfunction basis is one possibility. Using its completeness gives

\[
\langle x \rangle_{\Psi} = \langle \Psi \vert x \vert \Psi \rangle = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \langle \Psi \vert e_m \vert \Psi \rangle \langle e_m \vert x \vert e_n \rangle \langle e_n \vert \Psi \rangle
\]

(12.1.11)

This will require some dipole matrix elements \( \langle e_m \vert x \vert e_n \rangle \) that may be evaluated in the coordinate \( \vert x \rangle \)-basis. First, the \( x \)-completeness relation is used twice to expand both sides of the matrix element. Then the \( x \)-eigenvalue relation \( \vert x \rangle = x \vert x \rangle \) and orthonormality \( \langle x' \vert x \rangle = \delta(x'-x) \) are used.

\[
\langle e_m \vert x \vert e_n \rangle = \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dx \langle e_m \vert x' \rangle \langle x' \vert x \rangle \langle x \vert e_n \rangle
\]

(12.1.12a)

The \( \delta(x'-x) \) kills one integral. Wavefunctions (12.1.1c) are inserted.

\[
\langle e_m \vert x \vert e_n \rangle = \int_{-\infty}^{\infty} dx \langle x \vert e_m \rangle^* \langle x \vert e_n \rangle = \frac{1}{\text{norm.}} \int_{-\infty}^{\infty} dx x \sin k_m x \sin k_n x
\]

(12.1.12b)

Finally, the normalization constant \( \text{norm.} \) needs to be found using (12.1.10e).
Ignoring these gives the necessary off-diagonal dipole matrix elements.

Our failure to heed symmetry bothers us with (m=n)-terms of \( \sin(0)/0 \) that just give the \( W/2 \) in (12.1.13). Ignoring these gives the necessary off-diagonal dipole matrix elements.
Fourier analysis of wave packets. We return to that next.

Choice for moment functions are shape analysis will require many higher moments. Instead, descriptor of the morphology of prisoner \( M \) next Section 12.2 is devoted to putting \( M \) on a diet and slimming him down somehow.

Also, the sloshing lump is so fat it takes up half the cell and cannot get very close to the wall "slosh" amplitude is only about 25% of \( \omega_0/2 \).

Poor prisoner \( M \) ! His quantum pacing is restricted to 18% of his cell width from the center. If you look at the plot in the center of Fig. 12.1.2, it seems to be evidence of such cruel and unusual penury. The peak's "slosh" amplitude is about 25% of \( W \) and it has a "tail" on the opposite side that reduces \( \langle x \rangle \) even more. Also, the sloshing lump is so fat it takes up half the cell and cannot get very close to the wall without deforming significantly. (Prison life has fattened prisoner \( M \). Maybe the food is not so bad.) The next Section 12.2 is devoted to putting \( M \) on a diet and slimming him down somehow.

Moments of morphology

It should be clear that the position expectation value \( \langle \Psi \mid x \rangle \langle x \mid \Psi \rangle \) by itself is a rather incomplete descriptor of the morphology of prisoner \( M \). For a Newtonian particle, it’s all you need, but for a quantum wave it only gives the centroid of a wavepacket blob that can take on many shapes and sizes. Instead, shape analysis will require many higher moments \( \langle \Psi \mid x^m \rangle \langle x^m \mid \Psi \rangle \) or moment functions \( \langle \Psi \mid f(x) \rangle \langle x \mid \Psi \rangle \). An obvious choice for moment functions are \( f(x) = \sin mx \), the eigenfunctions themselves, but that leads back to Fourier analysis of wave packets. We return to that next.
12.2 Wave Packet Shape and Dynamics

By combining more and higher energy eigenstates it becomes possible to slim down the wavefunction of prisoner $M$ to the point that he can approach arbitrarily close to either wall. But, then something else happens to severely affect his new slim figure. It is called wavepacket dynamics.

Before we discuss the ruinous effects of wavepacket spreading, let's see how slim we can make the wave function. In principle, we can make it infinitely thin, provided we could pay for the energy needed to make a Dirac delta-wavefunction $\Psi(x) = \delta(x-a)$. Such an anorexic shape will require exercising prisoner $M$ to the extreme and will have extraordinary side effects.

A key to this extraordinary slenderizing is $|x\rangle$-orthonormality and $|\varepsilon_n\rangle$-completeness

$$\delta(x-a) = \langle x|a\rangle = \sum_{n=1}^{\infty} \langle x|\varepsilon_n\rangle \langle \varepsilon_n|a\rangle = \sum_{n=1}^{\infty} a_n \sin k_n x , \quad (12.2.1a)$$

where the constant coefficients

$$a_n = \langle \varepsilon_n|a\rangle = (2/W) \sin k_n a \quad (k_n = n\pi/W) \quad (12.2.1b)$$

depend on the position ($0 < a < W$) where we would like to put this "slim-jim" wonder-wave. Note that it can't stand exactly at the walls because $\sin k_n a$ goes to zero for $a = 0$ and $a = W$, but it can get close.

This is a situation that happens quite often in continuum quantum theory. The sum (12.2.1) is infinite and discrete and makes an infinitely sharp feature in a bounded continuum. Here you get what you pay for, and no one can afford the time or energy it takes to make prisoner $M$ infinitely thin. So (12.2.1) becomes an approximate or truncated sum that just stops when we tire of summing. A 30 term truncation of (12.2.1a) for ($a=0.2W$) is shown in Fig. 12.2.1. (It is scaled down by a factor of 30.)

Fig. 12.2.1 Greetings from prisoner $M$! Initial wavepacket combination (12.2.1) of 30 energy states.

Now let’s see what happens if we pay for a few more terms! We’ll redo the pulse wave analysis that was done for optical waves in Chapter 5 equation (5.3.5).
(a) Uncertainty relation and 'Last-in-First-out' effect

By summing over 100 levels the profile of the prisoner M wave becomes quite svelte, as seen in Fig. 12.2.2. The ultimate shape of this kind of delta function is beginning to emerge. About its center, it has a distinctive shape of the elementary diffraction function \( \sin \frac{kx}{\lambda} \) that is seen often in spectral theory.

You can derive this shape approximately by converting the \( k_n \)-sum (12.2.1) into a \( k \)-integral.

\[
\Psi(x) = \frac{2}{W} \sum_{n} k_n a \sin k_n x = \frac{2}{W} \int_{0}^{K_{\text{max}}} \frac{\Delta n}{\Delta k} \sin ka \sin kx = \frac{2}{W} \frac{K_{\text{max}}}{\pi} \int_{0}^{\frac{\pi}{K_{\text{max}}}} dk \sin ka \sin kx
\]

The approximate result is a function that wiggles just as much as the maximum \( k \)-value \( K_{\text{max}} \) allows.

\[
\Psi(x) \approx \frac{2K_{\text{max}}}{\pi} \int_{0}^{\frac{\pi}{K_{\text{max}}}} \frac{1}{\pi} dk \cos k(x-a) - \cos k(x+a)
\]

You might call this the "last-in-first-out" effect. The last \( K_{\text{max}} \)-value dominates while the lesser values get "smothered" by interference with neighboring values above and below them. Note that \( \Psi(x) \) peaks at \( x=a \) and plummets to zero on either side at \( x=a \pm \Delta x \) with half-width \( \Delta x \) inversely related to \( K_{\text{max}} \) by

\[
\sin K_{\text{max}}(\Delta x) = 0, \quad \text{which implies:} \quad (\Delta x)K_{\text{max}} = \pm \pi, \quad \text{or:} \quad \Delta x = \pm \pi / K_{\text{max}}.
\]

This is another example of the celebrated Heisenberg uncertainty relation which estimates the product of widths \( \Delta x \) and \( \Delta k \) (or \( \Delta p = h \Delta k \)) of coordinate and wavevector (or momentum) distributions.

\[
\Delta x \cdot |K_{\text{max}}| = \Delta x \cdot \Delta k = \pi \quad \text{or:} \quad \Delta x \cdot \Delta p = \pi \hbar = h/2
\]

Simply stated: the more accurately the warden determines M's position or where prisoner M is, the less he knows about M's momentum or where he's going. Crudely stated: a fat prisoner M mostly sits around like a big couch potato and only sloshes his beer gut like Fig. 12.1.2. A thin prisoner M like Fig. 12.2.2 is a high energy "bundle of nerves" or wavepacket which, as we will see next, is about to explode like a bomb!
(b) Wavepacket explodes! (Then revives)

Prisoner M's svelte figure doesn't last. In an instant he is blown all over his cell as shown in Fig. 12.2.3. M's one-hundred energy states or ten thousand zero-point energy units $\varepsilon_1$ ($\varepsilon_{100} = 100^2 \varepsilon_1$) go about two miles high if the $\varepsilon_1$ level is a foot off the cell floor. So it's not surprising that M goes off with a bang!

Time is given in terms of a fundamental unit of time that is the period $\tau_1$ of the slowest phasor belonging to ground or "zero-point" level in Fig. 12.2.2. The fundamental zero-point period $\tau_1 = 1/\nu_1$ is

$$\tau_1 = \frac{2\pi}{\omega_1} = \frac{2\pi h}{\varepsilon_1} = \frac{h}{\hbar^2 / 8MW^2} = \frac{8MW^2}{h}$$

(12.2.6)

Notice in Fig. 12.2.3 the highest ($n=100$) energy wave which was "last-in" is now "first-out" and makes a group "shock" wave that races across the cell toward the right wall at $x=W$. The speed of that wave is the group velocity or classical particle velocity at the highest energy $\varepsilon_{100}$. The $\varepsilon_n$-level classical velocity is

$$V_n = \frac{d\omega_n}{dk} = \frac{d\varepsilon_n}{h} = \frac{h^2}{2M} = \frac{h^2k_n}{2M} = \frac{h\pi}{MW} = \frac{h\pi}{2MW}$$

(12.2.7)
Related to this is the \( \varepsilon_n \)-level classical round trip time \( T_n(2W) \) or the time for the "particle" or "shock" wave associated with quantum level \( \varepsilon_n \) to go distance \( 2W \) back and forth across a width-\( W \)-cell.

\[
T_n(2W) = \frac{2W}{V_n} = \frac{2MW^2}{hn} = \frac{1}{2n} \frac{8MW^2}{h} = \frac{\tau_1}{2n} 
\]

(12.2.8)

The time sequence in Fig. 12.2.3 shows the group going a distance of \( 0.8W \) from \( x=0.2W \) to \( x=W \) in a time \( 0.002\tau_1 \) or 0.8 of the \( \varepsilon_n \)-level classical one-way trip time \( T_n(W) \) for a "particle" to cross the cell once.

\[
T_n(W) = T_n(2W) / 2 = \frac{\tau_1}{4n} \quad (0.0025 \tau_1 \text{ for: } n=100) \quad (12.2.9)
\]

The "break-away" wave speeding at \( V_{100} \) to the right in Fig. 12.2.3 is due to the "last-in-first-out" \( k \)-value \( K_{\text{max}} = k_{100} \) which shapes the initial wave pattern in Fig. 12.2.2 according to (12.2.3) and gives the break-away "shock" of 100 half-waves per cell width \( W \) moving under a smooth group envelope. Its front end reflects from \( x=W \) at \( t=0.0020\tau_1 \) and starts to make a jagged interference envelope. The left break-away wave reflects from \( x=0 \) immediately, after which its interference envelope stretches like an accordion.

There is something else quite wonderful. According to (12.2.8), the fundamental zero-point period \( \tau_1 \) is exactly enough time for a "particle" or group wave in the \( \varepsilon_n \)-level to make \( 2n \) round trips.

\[
\tau_1 = 2nT_n(2W) = \frac{8MW^2}{h} 
\]

(12.2.10)

So, in one fundamental period \( \tau_1 \) the ground \( \varepsilon_1 \)-level particle makes 2 round trips, the first excited \( \varepsilon_2 \)-level particle makes 4 round trips, the next excited \( \varepsilon_3 \)-level particle makes 6 round trips, ...and the 100-th excited \( \varepsilon_{100} \)-level particle makes 200 round trips, all in exactly the same time \( \tau_1 \).

Prisoner \( M \) may look like he is exploding randomly, but he is executing a dance whose timing would be the envy of the Moscow Ballet! After 50 round-trips across the stage, \( M \)'s wave performs a partial revival as it piles up into an upside down-delta function around \( x=0.8W \). Then, after 100 round trips \( M \) undergoes a full revival and "unexplodes" into his original spike at \( x=0.2W \), as seen in Fig. 12.2.4.

\[
t = 0.5000\tau_1 = 1.5\tau_{\text{beat}}
\]

\[
t = 1.0000\tau_1 = 3.0\tau_{\text{beat}}
\]

Fig. 12.2.4 Revival for prisoner \( M \). Exploded wavepacket in Fig. 12.2.3 re integrates twice per \( \tau_1 \) period.

The wave packet of the energized \( M \) performs its perfect wavefunction revival in a time that is three times the beat period of the low energy "couch-potato" combination in Fig. 12.1.2. The high energy
revival is of the wavefunction. The low energy combination in Fig. 12.1.2 only revives its probability envelope in $\tau_1/3$. It still takes a full $\tau_1$ to get the wavefunction back to the initial shape.

The full wavefunction revival is a consequence of the integral values of the energy spectrum (12.1.1d) shown in Fig. 12.1.1. As will be shown, it is closely related to the Bohr revivals discussed in Chapter 9. All eigenphases complete an integral number of complete $2\pi$ rotations in the time $\tau_1$ it takes the lowest phasor to complete a single $2\pi$ rotation. So all phases return to initial settings at exactly $\tau_1$, as does the envelope or probability distribution made from their sum. More remarkably, the envelope can perform full or partial revivals in even shorter times while performing a kind of "dance of deltas" as in Fig. 12.2.5. Here the initial delta is put in the exact center ($x=0.5W$) instead of at $x=0.2W$, and this gives a beautiful series of $q$ kaleidoscope deltas at rational relatively prime time fractions ($p/q$) of $\tau_1$. Views at periodic fractional times are called stroboscopic pictures. To understand this kaleidoscopic and stroboscopic behavior we review how it happens for Bohr orbitals that also have a quadratic spectrum.

![Fig. 12.2.5 The "Dance of the deltas." Mini-Revivals for prisoner M's wavepacket envelope function.](image)

We shall see that this behavior is closely related to the Bohr-revivals in Fig. 5.6.5 of Ch. 5.

(c) Bohr rotor waves: Relation to square well waves

Now suppose that prisoner $M$ is moved (because of good behavior and his stunning dance moves) from his width-$W$ cell into a less restrictive environment consisting of a circle of circumference $L=2\pi R$.
and radius $R$, that is, to a Bohr-rotor. Bohr rotor wavefunctions and levels were first plotted in Fig. 7.1.1. The equation for their energy eigenvalues was first given by (5.6.10) in Chapter 5 and is repeated below.

\[ E_m = \hbar \omega_m = \left( \frac{\hbar k_m}{2M} \right)^2, \text{ where: } p_m = \hbar k_m = \hbar \frac{2\pi}{L} m \ (m=0, \pm 1, \pm 2, \cdots) \]  
\[ \text{(12.2.11a)} \]

Notice that, like (12.1.1d), the energy values are also quadratic in the Bohr rotor quantum number $m$.

\[ E_m = \frac{\hbar^2}{2M} k^2 = \frac{2\hbar^2 m^2 \pi^2}{ML^2} = \left( 0, 1^2, 2^2, 3^2, \ldots \text{or } m^2 \right) \frac{\hbar^2}{2ML^2} = \frac{\hbar^2 m^2}{2MR^2} \]  
\[ \text{(12.2.11b)} \]

In fact the Bohr rotor momentum or wavevector and energy are the same for a given quantum number $m$ if the circumference $L$ is twice the linear cell width $W$, that is $L = 2W$ as shown in Fig. 12.2.6.

To better understand the relation between an infinite square well and a Bohr rotor we sketch in Fig. 12.2.6 one example of each system arranged so that their eigensolutions match as closely as possible. The square well in Fig. 12.2.6a has a width $W$ that is exactly half the length $L = 2W$ of the Bohr rotor in Fig. 12.2.6b. The sine wave solutions of the Bohr rotor are arranged so that their wavefunctions on the front half-range $(0 < \chi < W)$ or $(0 < \phi < \pi)$ are identical to the square-well waves in the same region of Fig. 12.2.6a. The Bohr-rotor cosine waves, including the $(m=0)$-wave, are plotted with dashed lines of Fig. 12.2.6b but are absent from the square well in Fig. 12.2.6a. The remaining Bohr-rotor sine waves are identical in form, momentum, and energy to the infinite square-well sine wave solutions in the front range $(0 < \phi < \pi)$ only. Note that the rotor has a zero-quantum state with zero energy and a constant wavefunction $\Psi_0 = A \cos 0x = A$. The fundamental frequency for the Bohr waves is equal to the difference between the first and zero-th levels. This equals the first beat frequency and the first frequency eigenvalue, as follows.

\[ \omega_{\text{beat}} = \omega_1 - \omega_0 = \frac{E_1 - E_0}{\hbar} = \frac{1^2 - 0^2}{\hbar} \frac{\hbar^2}{2ML^2} = \frac{\hbar}{2ML^2} = \frac{\hbar}{2MR^2} = \omega_1 \]  
\[ \text{(12.2.12)} \]

This is the same as the fundamental $\omega_1$ for the linear cell of width $W=L/2$. The fundamental time unit is

\[ \tau_1 = \frac{2\pi}{\omega_1} = \frac{2ML^2}{\hbar} = \frac{8MW^2}{\hbar}. \]  
\[ \text{(12.2.13)} \]

The time $\tau_1$ above and in (3.2.25) is enough time for two round trips of total length $4W=2L$ up and down a linear cell, or as we will see, for a rotor to go a distance $2L$ or twice around circumference of length $L$.

Excited Bohr energy levels are doubly degenerate because there are negative as well as positive values of the $m$-quantum number in (12.2.1). This means that the full $U(2)$ freedom of choice for standing, moving, and galloping waves exists at each excited level. (The ground $m=0$ level is the one exception. It has only a single constant wave of zero energy and momentum; the penultimate "couch-potato" of the quantum world; asleep on its circular sofa and snoring at zero frequency. The infinite square-well prison allows no such luxury!)
Fig. 12.2.6 Comparison of eigensolutions for (a) Infinite square well, and (b) Bohr rotor.
All waves in the frontrange \((0<x<W)\) of the Bohr-rotor system can be made to duplicate exactly what happens to the infinite-square-well in its front range. In order to do this, the waves in the back range \((-W<x<0)\) of the Bohr-rotor (where all infinite-square-well waves vanish) must be perfectly inverted copies of the waves in the front range \(\Psi(x\pm W)=-\Psi(x)=\Psi(-x)\) since sine waves are odd to inversion.

Both the rotor and infinite-well have quadratic \(\omega_m=\omega_0 m^2\) spectra. To understand infinite-well revivals we first review the less restrictive Bohr system. Complex \(e^{im\phi}\) waves are actually simpler than \(\sin m\phi\) waves of the well. A delta function of Bohr angle \(\phi = 2\pi x/L\) uses ortho-completeness axioms 3 and 4.

\[
\psi_{\phi_0}(\phi) = \delta(\phi-\phi_0) = \langle \phi | \phi_0 \rangle = \sum_{n=-\infty}^{\infty} |n| \langle n | \phi_0 \rangle
\]

This is a "spike" at position \(x=x_0=\phi_0 L/2\pi\). In terms of the Bohr orbital waves, \(\delta(\phi-\phi_0)\) becomes

\[
\psi_{\phi_0}(\phi) = \delta(\phi-\phi_0) = \sum_{n=-\infty}^{\infty} \frac{e^{in\phi}}{\sqrt{2\pi}} \frac{e^{-in\phi_0}}{\sqrt{2\pi}} = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} e^{in(\phi-\phi_0)}
\]

Each amplitude \(\langle n | \phi_0 \rangle\) is a preset constant, but eigenfunction \(\langle \phi | n \rangle\) or eigenket \(|n\rangle\) has eigenfrequency \(\omega_n\).

\[
|n(\psi)| = e^{-i\omega_n t} |n(0)| = e^{-i\omega_n t} |n\rangle, \text{ or: } \langle \phi | n(t) \rangle = e^{-i\omega_n t} \langle \phi | n \rangle = e^{-i\omega_n t} \langle \phi | n \rangle
\]

Level-\(n\) has energy \(\varepsilon_n = \hbar \omega_n\). Inserting this into (12.2.14a) gives the time behavior of a delta wave.

\[
\psi_{\phi_0}(\phi,t) = \sum_{n=-\infty}^{\infty} \frac{e^{i(n-\omega_n t)}}{\sqrt{2\pi}} \frac{e^{-i\omega_n t}}{\sqrt{2\pi}} = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} e^{i(n-\omega_0 t - n^2 \omega_1 t)}
\]

NOTE: only the state factor \(\langle \phi | n \rangle\) gets the Planck time-phase factor \(e^{-i\omega_n t} = e^{-i\omega_1 t}\) while the coefficient \(\langle n | \phi_0 \rangle\) is fixed by the initial \(x_0\)-position state's overlap with the eigenstate \(|n\rangle\) at initial time \(t=0\).

It is impossible excite an infinite number of levels. (Even a hundred is costly.) We may arbitrarily cut off the sum at some value \(n=N_{\text{CUT}}\) (such as \(N_{\text{CUT}}=30\) in Fig. 12.2.1), or we may multiply the terms by a weighting or windowing function \(W(n)\) that vanishes for high \(n\). Let us consider some possibilities.

(1) "Boxcar windows": Wavepackets that go "Bang!"

Consider first a square window or "Boxcar" weight function. It is the same as a simple cut-off.

\[
\psi_{\phi_0}(\phi,t) = \sum_{n=-\infty}^{\infty} W(n)e^{i(n-\omega_0 t - n^2 \omega_1 t)} \text{ where: } W(n) = \begin{cases} A & \text{if: } |n| \leq N_{\text{CUT}} \\ 0 & \text{if: } |n| > N_{\text{CUT}} \end{cases}
\]

A sharp cut-off by a boxcar window produces a ringing \(\sin x/x\) wavefunction as described in (12.2.3). Such a wave goes off with a "bang" like the one shown earlier in Fig. 12.2.3. Fig. 12.2.7 shows the magnitude \(|\Psi(x,t)|\) of a Bohr-rotor equivalent wave with \(N_{\text{CUT}}=16\) plotted using shading at each space-point \(x\) (horizontal axis) and time \(t\) (vertical axis). The white regions correspond to nodal regions in which the destructive interference of the 16 excited waves gives probability that is small or zero. Interference patterns begin to develop after the left-and-right-moving shock fronts meet each other at the opposite side \((x=\pm\pi)\) of the Bohr-rotor ring space. The group velocity of the fastest \((m=N_{\text{CUT}})\) waves is for \((m>>1)\).

\[
V_{\text{group}}(m) = \frac{d\omega_m}{dk_m} = \frac{d\omega_m}{dm} \frac{dm}{dk_m} = \frac{\hbar}{2M} \frac{d}{dm} \left( \frac{2\pi m}{L} \right)^2 = \frac{\hbar 2\pi}{2\sqrt{2\pi m} L} = \frac{L}{2\pi} \frac{2m}{\tau_1} = 2N_{\text{CUT}}
\]
Fig. 12.2.7 (a) Initial evolution for $\Delta x = 0.03$ and $\Delta m = 16$ "boxcar" wavepacket for Bohr rotor.

The maximum $V_{\text{group}}$ is 32 Bohr $L$-laps per Bohr time units $\tau_1$, or 1/2 circumference $L$ in $1/64$-th $\tau_1$. The interference starts in Fig. 12.2.7 at time fraction $1/64$ just before $t/\tau_1 = 1/50$. Then a series of fractional revivals are seen starting at time fraction $1/32$ which is enough time for the fastest waves to make a full circle. The $1/32$ revival has 16 zeros (or peaks), the $1/16$ revival has 8 zeros (or peaks), the $1/14$ revival
that the Fourier transform of a Gaussian
The remaining variable factor
A(Δm,φ) = \sum_{m=-∞}^{∞} e^{-(mΔm/2φ)^2} \int_{-∞}^{∞} dk e^{-\left(k/\Delta m\right)^2} = \sqrt{\pi} Δm (12.2.7e)

The remaining variable factor \(e^{-(Δm/2φ)^2}\) is a Gaussian function of angle \(φ\) or position \(x\). It is remarkable

That is, at \(φ=±Δφ\), function \(e^{-(Δφ/2)^2}\) becomes \(e^{-1}\). Also for the Gaussian \(e^{-(mΔm)^2}\) the parameter \(Δm\) is the

\(HWeM\) of the momentum distribution. \((HWeM_m=Δm)\) Equating \(e^{-(Δφ)^2}\) to \(e^{-(Δm/2φ^2)}\) in (12.2.7d) relates

half-width \(HWeM_m=Δm=LΔk/2π\) of momentum \(m\) or wavevector \(k\) to the half width \(HWeM_φ=Δφ=2πΔx/L\) of angle \(φ\) or position \(x\). (This re-derives uncertainty relations (5.3.7) and (9.3.15).)
Fig. 12.2.8 (a) Initial evolution for $2\Delta x = 0.04$ and $\Delta m = 16$ "Gaussian" wavepacket for Bohr rotor.

$$\Delta m = \frac{2}{\Delta \phi} = \frac{1}{(\pi \Delta)} \text{ or: } \Delta \phi \Delta m = 2 = \Delta x \Delta k$$ (12.2.8)
This is a Gaussian uncertainty relation to be compared with the uncertainty product $\Delta x \Delta k = \pi$ of a "box-car" window in (12.2.5). The Gaussian seems "less uncertain" than the box-car by a factor $2/\pi$, but one has to be careful when being so precise about imprecision! It's a little like comparing apples and oranges.

Often we use full-widths instead of half-widths. Fig. 12.2.8 shows Full-Width-at-(1/e)-th-Maximum ($FWeM = 2HWeM$), or twice the half-width of both the position and momentum Gaussian.

$$FWeM_\phi = 2\Delta \phi, \quad FWeM_m = 2\Delta m \quad (12.2.9)$$

Given momentum quanta excitation of $\Delta m = m_{HWeM} = 16$ or a full momentum width of $FWeM_m = 2\Delta m = 32$ we use (12.2.8) to derive the angular full width $FWeM_\phi$ in units of $2\pi$.

$$FWeM_\phi = 2\Delta \phi = \frac{4}{HWeM_m} = \frac{8}{FWeM_m} = \frac{8}{32} = \frac{1}{8\pi} 2\pi \quad (12.2.10)$$

This predicts $8\pi = 25.1$ packet full-widths fit in the full $2\pi$ circle. This is shown at the bottom of Fig. 12.2.8 for $2\Delta m = 32$. Each packet's angular half-width $HWeM_\phi = \Delta \phi = 2\pi \Delta$ is only $\Delta = 2\%$ of a full $2\pi$.

The subsequent evolution of the Gaussian packet in Fig. 12.2.8 is also to be contrasted with that of the box-car packet in Fig. 12.2.7. The box-car wave explodes with a ringing "Bang," but the Gaussian wave gently expands with little or no wrinkling or change of shape until its two oppositely moving "feet" meet at $\phi = \pm \pi$ on the other side of the ring. The $m$-component waves with $\Delta m = m_{HWeM} = 16$ have group velocity $2m = 32$ by (12.2.16). So they circle the ring in $(1/32)\tau_1$ or go half-way in $(1/64)\tau_1$ at which time the two speeding "feet" first meet each other.

But, the $m = 16$-component waves aren't the fastest "feet" in this distribution. The $m$-distribution in the lower left hand part of Fig. 12.2.8 shows higher $m = 17, 18, 19, ...$ have amplitudes that are less than $(1/e)$ but significant all the way up to $m = 30$ or 31. Each of these "feet" will meet at $\phi = \pm \pi$ earlier than $(1/64)\tau_1$. So, interference wrinkles due to $m = ...25, 26, 27, ...$ are visible in Fig. 12.2.8 already at $(1/100)\tau_1$.

Finally, by $(1/32)\tau_1$ the $m = 16$ components have made a complete circle so their "feet" meet at origin ($\phi = \pm 2\pi$), and they are staging a fractional revival as a wave having 16 miniature peaks.

By $(1/16)\tau_1$ (near top of Fig. 12.2.8) there is a revival in a wave having 8 miniature Gaussian peaks with 8 long flat nodal regions in between the peaks. As we will see, this is due mainly to the $m = \pm 8$ "feet" and the $m = \pm 16$ "feet" combining. Shortly afterwards, at $(1/15)\tau_1$ there is a revival in a wave having 15 miniature Gaussian peaks followed closely at $(1/14)\tau_1$ by a wave having 7 miniature Gaussian peaks, and so on until the figure stops at $(1/10)\tau_1$ with a 5 peak revival plotted at the top.
The space-time plot of the Gaussian packet in Fig. 12.2.8 has many of the same patterns that are seen in the boxcar packet in Fig. 12.2.7. However, the Gaussian patterns have a clarity and linearity that is obscured in the boxcar patterns. An explanation based upon $C_N$ phases giving the patterns of lines in Fig. 12.2.8 goes to the heart of quantum symmetry and dynamics. This was given in Chapter 9.

(d) Brief history of revival structure and dynamics

Quantum revivals like classical chaos and fractals are a class of phenomena that many saw but few observed. Each has required modern computer simulations and graphics to make a convincing case for their existence. Each of these phenomena is important because they illuminate inadequacies of Newtonian calculus or continuum analysis and favor discrete algebraic-number-theoretic theory.

The term revival is a coinage by Joe Eberly to describe unexpected rephasing that appeared in 1976 computer studies of atom-quantum field theory. For the next two decades there were sporadic reports of revival phenomena including fractional revivals in quantum treatments of much simpler systems such as rotors and anharmonic vibrators or Rydberg orbitals. The first explanations in 1989 of fractional revival phenomena involved a particle in an infinite square well ("particle-in-a-box"). Finally, in 1996 and 1997, Berry, Schleich and others used the square well simulations to plot "quantum fractal" landscapes and "quantum carpets" which clearly showed that revivals are a phenomena that is begging to be fully understood.

We have given two ways to understand the phenomena. The first uses phase and group velocity of wave zeros and the Farey arithmetic analysis of fractal circle maps in Section 9.3. The second uses cyclic ($C_N$) group theory and discrete Fourier analysis of Section 9.4. The latter elucidates fractal revival structure while the former illuminates quantum phase behavior. Together they show how wave symmetry and fractal wave behavior are two sides of the same coin.

Now we consider some of the features that are peculiar to the infinite square well.
12.3 Infinite Well Dynamics vs. Bohr Waves

The infinite square-well is a subset of the Bohr rotor system. As shown in Fig. 12.2.6, the square well width $W$ takes up the front half ($0<\phi<\pi$) or ($0<x<W$) of the Bohr ring whose circumference of $L=2W$ and angular range of $2\pi$ ($-\pi<\phi<\pi$) is twice that of the well. The back half of the Bohr ring, where angle $\phi$ is negative ($-\pi<\phi<0$), is an inpenetrable region for the square-well. The Bohr system has energy-degenerate ($E_m=E_1(\pm m)^2$) sine and cosine wave eigenstates $\sin(m\phi)$ and $\cos(m\phi)$, where a quantum number $m=0,1,2,3,...$ of wavelengths must fit in one Bohr lap length $L$. In contrast, the square-well can only keep the sine standing waves for $m=1,2,3,...$from the Bohr set. But, the square-well energy spectrum is the same except it is no longer degenerate. Also, the $E_0$-level is missing. The square-well system gets to keep only the odd or antisymmetric ($-$)-states which flip their sign if the angle $\phi$ is reversed. ($\phi\rightarrow -\phi$) These are the sine standing waves from the Bohr set, excluding $m=0$.

$$\sin(-m\phi)=-\sin(m\phi) \quad (12.3.1)$$

For the square well, all waves are pinned to zero at origin ($\phi=0$) and at the other side of the well ($\phi=\pi$). Beyond, those points lies the inpenetrable negative-$\phi$ region where all square well waves must vanish.

$$\Psi^\text{well}_m(\phi) = 0 \quad \text{for} \; \phi<0. \quad (12.3.2)$$

This zeroing by (12.3.2) seems inconsistent with anti-symmetry conditions (12.3.1). To sort this out, one might need another lesson in Schrodinger wave mechanics.

(a) The Bohr image-wave

It turns out that the Bohr system will reproduce the dynamics of the square-well system in the well region (postive $\phi$ or $x$ between 0 and $W=L/2$) if we use only its sine wave states that satisfy the anti-symmetry condition (12.3.1). If the two systems are using the same waves and the same spectrum, that is, the same eigenvalues and eigenfunctions, then they must have the same dynamics wherever eigenwaves and spectra are the same.

Still it seems inconsistent that square-well has its wave supressed in the negative-$\phi$ region, while the Bohr system is running a negative image wave in that region in order “fake” the dynamics in the well. Will not the image wave “leak” out of the negative region and spoil the Bohr’s reproduction in the well?

The buck stops here!

To understand image waves we must take symmetry conditions and associated boundary conditions seriously. Antisymmetry about $\phi=0$ implies the wave is zero at $\phi=0$, that is, $\Psi=-\Psi$ implies that $\Psi=0$. And, a wave zero at even one point cannot “leak” or transmit anything through that point. The buck stops there! Any energy or wave action that is in the well region stays there and the same applies to the nether region.

Perhaps, the coupled pendulum analogy will make this clear. If you weld even one pendulum so it cannot move, then you create an inpenetrable wall between the regions on either side. Now one side may “party-on” as loud as they want, and the occupants on the other side will never hear a peep!

This applies to standard 1D-Schrodinger wave dynamics which is analogous to waves in pendulums coupled only to nearest neighbors through the $S$-amplitude or effective mass coefficient in (11.5.6). It does not apply to hyper-Schrodinger dynamics which has additional next-nearest coefficients.
Such hyper-Schrödinger equations have \( x \)-derivatives of fourth or higher order which might allow waves to “hop” over one “dead-point” and bypass a single zero boundary point. Blocking hyper-waves requires a zero of the wave and its first derivative and its second derivative, and so forth, depending on the order of the coupling.

**b) Flipped revivals**

Well-wave pulses include flipped revivals such as shown in Fig. 12.2.4. The example shown there is the half-time revival of the Bohr image wave as sketched below in Fig. 12.3.1(c).

The Bohr rotor uses its sine-waves in (b) to copy a wave-packet (a) in the square-well region between \( \phi = 0 \) and \( \phi = \pi \). This gives rise to an image wave in (b) on the other side of the origin. Creation of a Bohr packet that only existed on the right hand (positive) side would require the use of its sines and cosines, the latter of which are not available in the square-well’s set of eigenfunctions. At half-time each of the Bohr wavepackets revive on the opposite side of the ring at an angle \( \pi \) away from whence they started in Fig. 12.3.1(d). The square well sees a Bohr image’s revival. It’s flipped in sign.
Can this be seen as a passage of the wavepackets through the supposedly inpenetrable wall that has been set up at origin? No! That is a Newtonian idea. Either wave motion would not change if the two sides were put a mile apart. Prisoner $M$ has not escaped from either half-cell. He is a Schrödinger cat!

(b) Cloned revivals

A phenomenon related to both Bohr and square-well revivals is that of wave profile cloning. We shall see that cloning wavefunctions is problematic; it would violate uncertainty relations for one thing. But, a fractional revival such as the 1/3-time revival at the top of Fig. 12.2.5 has a probability distribution $\Psi^*\Psi$ or wave magnitude $|\Psi|$ that is copied quite perfectly, three times in a row. The phases inside each wavepacket are clearly different from the original and each other. Revival peak phases are precisely given by the $C_3$ revival phases in the $(t=1/3)$-row of the Fig. 9.4.2(c). Examples are detailed in Fig. 12.3.2 below.

(left peak phase $=-30^\circ$, main peak phase $=90^\circ$, right peak phase $=-30^\circ$)  \hspace{1cm} (12.3.3)

All this makes sense if you imagine a wave line is made up of a set of $C_N$-symmetric coupled pendulums where $N$ is an enormous with lots of factors. We might “pluck” just one of these pendulums to make an “almost-Dirac-delta” function which clones itself. More likely, we pluck out an arbitrary pulse shape to make a combination of several “almost-Diracs” which then spawn cloned copies according to a schedule given in a $C_N$-revival table like Figures 9.4.2 and 9.5.3.

The important thing to remember is that each of the $N$ starting points, that is, each of the $N$ “quantum dots” is equivalent. Revivals starting from one point look the same as they would starting off down the line somewhere; the whole schedule just shifts accordingly. As a result, low order revivals of narrow packets are usually cloned quite perfectly. The clones are not so perfect if one of them overlaps with a neighbor as will happen if the initial packet is too wide or the revival has too many copies.

Another thing to remember is that the real line is composed of all possible fractions $m/N$ and so a wavepacket function is plucking not just many pendulums but many overlapping sets of many pendulums. The resulting cacophony washes out many of the finer interference effects and helps to make the profiles better copies of the original. But, as seen in the details of Fig. 12.3.2, the phases inside the profiles vary from point to point and from clone to clone in a complicated way.
Fig. 12.3.2 Examples of a 1/3-period revival for excitation numbers (a) $N=6$, (b) $N=24$, and (c) $N=32$. 

(a) $N=6$, $\nu=1$, $r=2$, $\rho=0$, $\rho=1$, $\rho=2$. 
(b) $N=24$, $\nu=1$, $r=8$, $r=16$, $r=0$. 
(c) $m=0$ to 32 excitation.
Problems for Chapter 12.

Zero-point-zero
12.1.1 The zero point energy (ZPE) of the infinite well is a feature not seen in the Bohr spectrum. Or is it? Discuss.
(a) If the cell width is increased how does the ZPE behave?
(b) What would the ZPE be for a cell of two equal dimensions? (square) three dimensions? (cube)

Cell pacing 9-to-5
12.1.2 It was noted after Eq. (3.3.25) that the maximum dipole "pacing" amplitude \(\langle x \rangle\) (\(\langle e x \rangle\) is called an electric dipole or \(E1\) moment) of \(M\) was only 18% of cell width \(W\) for a 50-50 excitation of the lowest two levels \(m=1\) and \(m=2\). Does this increase if we excite to higher levels? Consider the following cases. (Caution! Some are trick questions.) Find maximum or saturated \(E1\) moment \(\langle e x \rangle / W\) for :
(a) 50-50 excitation of levels \(m=1\) and \(m=5\).
(b) 50-50 excitation of levels \(m=1\) and \(m=10\).
(c) 50-50 excitation of levels \(m=4\) and \(m=5\).
(d) 50-50 excitation of levels \(m=4\) and \(m=10\).
(e) 50-50 excitation of levels \(m=9\) and \(m=10\).
(f) 50-50 excitation of levels \(m=9\) and \(m=5\).

Current events
12.1.3 Consider the momentum or current dipole (or \(M1\)) operator \(p\) and its expectation values \(\langle p \rangle\).
(This is related to the magnetic \(M1\) dipole operator \(e/M\) \(p\).)
(a) Derive a formula for the \(\langle m|p|n\rangle\) matrix elements in the square well eigenbasis.
(b) Derive the time dependent expectation \(\langle p(t) \rangle\) for a 50-50 excitation of levels \(m=1\) and \(m=2\).
Compare time plot of \(\langle p(t) \rangle\) with \(\langle x(t) \rangle\) derived in Sec. 12.2. Discuss.

More poles
12.1.4 Consider the electric quadrupole (or \(E2\)) operator \(e x^2\) and its expectation values \(\langle e x^2 \rangle\).
(This is related to the 2-photon transition operator \(e^2 x^2\).)
(a) Derive a formula for the \(\langle m|x^2|n\rangle\) matrix elements in the square well eigenbasis. (You might use the fact that \(\langle m|x^2|n\rangle = \sum_{\ell} \langle m|x \ell|n\rangle \langle \ell|x|n\rangle\) to check you results.)
(b) Find maximum expected \(E2\)-moment \(\langle e x^2 \rangle\) for 50-50 excitation of levels \(m=1\) and \(m=2\).
(c) Find maximum expected \(E2\)-moment \(\langle e x^2 \rangle\) for 50-50 excitation of levels \(m=1\) and \(m=3\).

Uncertain uncertainty
12.2.1 Compare the “boxcar-window” spectral uncertainty relation (12.2.5) for a boxcar wave \(\Psi_{Box}\) to (9.3.15) for a Gaussian-window wave \(\Psi_{Gauss}\). Consider the definition of standard deviation \(\Delta q = \sqrt{\left[q - \langle q \rangle\right]^2}\) where:
\(f(q) = \langle \Psi | f(q) | \Psi \rangle\).
(a) Derive \(\Delta x\) and \(\Delta k\) for each wave. (Give numerical examples if analytic result is problematic.)
(b) Which is more certain? Discuss.

First-in last-out
12.2.2 The “"last-in-first-out” principle involved the \(k\)-integral (12.2.3) from 0 to \(K_{max}\).
(a) Does a “"first-in-last-out” principle apply for a lower limit: \(K_{min}\) to \(K_{max}\)? Discuss effect on initial pulse shape.
(b) Discuss how a lower limit \(K_{min}\) affects the uncertainty \(\Delta x\) of initial pulse.
(c) Discuss how a lower limit \(K_{min}\) affects the waveforms that emerge from the initial wave.
Cloning around

12.3.1. Suppose the initial wave $|\Psi(0)|$ and $\text{Re} \Psi(0)$ are the same at $t=0$. ($\text{Im} \Psi(0)$ is identically zero.) Use the $C_2$ and $C_3$ revival schedules in Fig. 9.4.1-2 to sketch $|\Psi(t)|$, $\text{Im} \Psi(0)$, and $\text{Re} \Psi(t)$ in each of the boxes below.