Wave Packet Revivals in the Asymmetric Infinite Square Well.

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ABSTRACT: Wave packets in an infinite square well (ISW) experience perfect quantum revivals at periodic intervals. In the asymmetric infinite square well (AISW) a potential step within the well breaks the symmetry of the ISW, perturbing the energy eigenvalues and preventing perfect revivals. Second-order perturbation theory for the AISW shows that the even-numbered eigenstates and the odd-numbered eigenstates should have different revival times. Therefore a wave packet composed of only even-numbered eigenstates should experience partial revivals at a different time then a wave packet composed of only odd-numbered eigenstates. We examine the numerically calculated auto-correlation function of even and odd sub wave packets. We find clear evidence for different revival times within a certain parameter regime. We also find that this difference in odd and even revival times is a leading cause in the poor revivals of the AISW.

Introduction

In the infinite square well (ISW),

$$V(x) = \begin{cases} \infty, & x \le -a \\ 0, & -a < x < a \\ \infty, & x \ge a, \end{cases}$$

a wavepacket will have a periodic motion. It will initially disperse but after a fixed period (known as the revival time) it will return to its initial state. So, for a given wave packet Ψ(x,0) in the ISW, we know that if m is an integer and τ_{rev} is the revival time, then

$$|\Psi(x,0)|^2 = |\Psi(x, m\tau_{rev})|^2 .$$

This effect is referred to as a wave packet revival. The ISW experiences perfect wave packet revivals. The revival time for a wave packet peaked on the nth eigenstate in any system is given by

$$\tau_{rev} = 4\pi \left| \frac{d^2 E_n}{dn^2} \right|^{-1} .$$

For the ISW we have

$$E_n = \frac{\pi^2 \hbar^2 n^2}{2m(2a)^2} \rightarrow \tau_{rev} = \frac{16ma^2}{\pi\hbar}.$$

Adding a small step in potential halfway through the ISW results in the asymmetric infinite square well,

$$V(x) = \begin{cases} \infty, & x \le -a \\ 0, & -a < x < 0 \\ V_0, & 0 \le x < a \\ \infty, & x \ge a. \end{cases}$$

Wave packets in the AISW do not have perfect revivals. We used perturbation theory and numerical calculations to explain why this potential step causes the perfect wave packet revivals of the ISW to become the imperfect wave packet revivals of the AISW.

Perturbation Theory Solutions for the AISW

Perturbation theory can be used to find the energy corrections for the AISW. First-order time independent perturbation theory gives the following formula for the energies of the AISW:

$$E_n \approx \frac{\pi^2 \hbar^2 n^2}{2m(2a)^2} + \frac{V_0}{2}.$$

To first order the energies of the AISW are just the ISW energies plus a constant. This will change the overall phase of the wave functions in the AISW, but will not change any of the revival properties. So first order perturbation theory predicts perfect revivals. Examining the second order energy corrections, however, sheds more light on the situation. Assuming that we're dealing with wave packets constructed of high energy (large *n*) states, the energies of the AISW to second order are

$$E_n \approx \frac{\pi^2 \hbar^2 n^2}{2m(2a)^2} + \frac{V_0}{2} + \frac{\gamma m V_0^2 (2a)^2}{8\pi^2 \hbar^2 n^2},$$

where

$$\gamma = \begin{cases} 3, & n \text{ is even} \\ -1, & n \text{ is odd.} \end{cases}$$

So second order perturbation theory predicts a different revival time for even-numbered eigenstates compared to odd-numbered eigenstates. This means that a wave packet composed of only even-numbered states will have a different revival time than a wave packet composed of only odd-numbered states. It also means that a wave packet composed of both even-numbered and odd-numbered states may experience poor revivals because the even-numbered eigenstates are out of phase with the odd-numbered eigenstates. That is, when the "even" part of the wave packet is ready to revive, the "odd" part isn't and vice versa. For specific parameter values we find clear evidence for this effect.

Wave Packet

We examined revivals in the AISW for a Gaussian wave packet with initial state

$$\Psi(x,0) = \left(\frac{1}{\alpha^2 \hbar^2 \pi} \right)^{1/4} \exp\left[\frac{-ip_0(x-x_0)}{\hbar} - \frac{(x-x_0)^2}{2\alpha^2\hbar^2} \right],$$

where our units are defined such that

$$\hbar = 1, \; m = 1/2, \; a = 3, \; x_0 = -a/2, \text{ and } \alpha = 1/4.$$

The probability density for the initial wave packet is shown below. If we increase p_0 the wave packet will still have the same initial probability density, but the wave packet will be built from higher energy eigenstates. We can determine the eigenstate, or value of *n*, at which the wave packet is peaked by simply squaring the value of p_0.

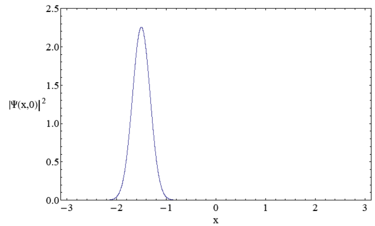

Figure 1. A plot of the wave packet we examined.

To maximize the relative difference between even and odd revival times we chose V_0 = .25 and looked at wave packets peaked at energies corresponding to *n* = 3, 25, and 50. This poster shows the results for a wave packet peaked on the *n* = 3 state, but similar behavior was found for the *n* = 25 and *n* = 50 cases.

Comparing Full Wave Packet Autocorrelation to Subpackets

To examine the revivals of this wave packet we computed the autocorrelation function:

$$A(t) = \int_{-a}^{a} \Psi^*(x,0)\Psi(x,t)dx.$$

When *A(t) = 1* the wave packet matches up perfectly with its initial probability density. So spikes in the autocorrelation function that approach *A(t) = 1* indicate perfect or near-perfect revivals. When we plot the autocorrelation function for our full wave packet (see Figure 2) we find that as *t* increases the revival peaks deteriorate. Our perturbation theory analysis suggests one possible reason for this deterioration: the even and odd revivals are out of sync.

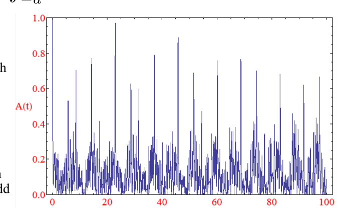

Figure 2. Autocorrelation function plot of the full wave packet.

To examine this hypothesis we divided the full wave packet into subpackets composed of only even-numbered or only odd-numbered eigenstates. We then computed the autocorrelation function for each of these subpackets. The results are shown in Figures 3 and 4.

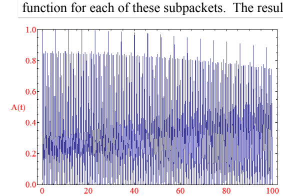

Figure 3. Autocorrelation function of the only even-numbered eigenstates subpacket.

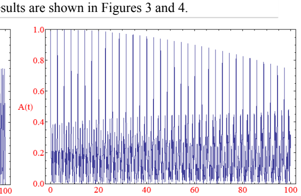

Figure 4. Autocorrelation function of the only odd-numbered eigenstates subpacket.

Though not perfect, the even and odd subpackets exhibit much better revivals than the full wave packet. This can be viewed as evidence that the full wave packet revivals are deteriorating as the even and odd subpackets gradually get out of sync. To thoroughly examine what's happening to the full wave packets, it's necessary to look at the even subpacket, the odd subpacket and the full wave packet on the same plot.

Figure 5 shows the autocorrelation function of the full, even, and odd wave packets near the time of the second full revival. Note that this plot shows obvious evidence of a different revival time for even and odd subpackets. We also see that the peak in the full wave packet autocorrelation function is between the peaks of the even and odd autocorrelation functions and that the full wave packet peak is shorter than the even and odd peaks. This provides evidence that the difference in even and odd revival times contributes to the deterioration of the full wave packet revivals.

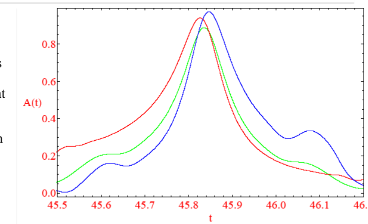

Figure 5. A plot of the full wave packet autocorrelation (green) vs. the odd subpacket autocorrelation (red) vs. the even subpacket autocorrelation (blue) during a time frame that corresponds to the second revival for the full wave packet.

Direct Revival Time Comparison for Even and Odd Subpackets

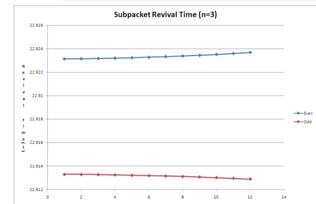

Figure 6. Even subpacket revival time vs. odd subpacket revival time.

Figure 6 is a direct comparison of the numerically calculated revival times for even and odd subpackets. Revival times are calculated by computing the time difference between consecutive full revival peaks in the autocorrelation function. There is a clear difference in the revival times of approximately 0.01 time units. Again, this strongly suggests that one reason for the deterioration of the revivals in the full wave packet is that the even and odd portions of the wave packet get out of sync as time passes.

Other Findings and Future Research

We found results similar to those for the *n = 3* wave packet in wave packets centered on the *n = 25* and *n = 50* states. In both of these cases the full wave packet showed deteriorating revivals due, in part, to the even and odd subpackets getting out of sync.

Another factor that affects wave packet revivals in the AISW is the fact that the revivals times are not integer multiples of the so-called classical period. The classical period describes the time it takes for the peak of the wavepacket to complete one full circuit within the well, irrespective of any changes in the wave packet's shape. In the ISW the revival times occur at multiples of the classical period, ensuring that the wave packet is in the correct location within the well when it experiences a revival. In the AISW this relationship no longer holds and the wave packet may be in a different part of the well when it reaches a revival time. As the revival times and classical periods get further out of sync the revivals of even and odd subpackets will deteriorate. We believe this is the reason for the deterioration of revivals shown in Figures 3 and 4, but more research is required to show this quantitatively.

References

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