# Coherent polychotomous waves from an attractive well

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An effect of a wave-packet scattering off an attractive one-dimensional well is found numerically and analytically. For a wave packet narrower than the width of the well, the scattering proceeds through a quasi-bound state of almost zero energy. The wave reflected from the well is a polychotomous (multiple-peak) monochromatic and coherent train. The transmitted wave is a spreading smooth wave packet. The effect is strong for low average speeds of the packet, and it disappears for wide packets. [S1050-2947(99)02409-9]

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This paper deals with the classical textbook exercise of a wave packet interacting with an attractive well [1]. Despite being a thoroughly studied example of quantum scattering for plane-wave stationary states, the effect to be presented here for wave packets was yet to be found.

A one-dimensional attractive well can either reflect or transmit a wave. Reflection and transmission coefficients are the simplest scattering amplitudes. They can easily be calculated for a square well by using plane waves and elementary continuity conditions. The analysis of the exact time development of a packet, as well as the treatment of realistic well shapes, is however reserved for numerical treatment.

We show here that wave-packet scattering possesses an intriguing aspect: Packets that are narrower than the well width initially, resonate inside it, generating a reflected wave that is coherent and monochromatic in amplitude, a polychotomous wave train.

Polychotomous (multipeak) waves are observed when a superintense laser field focuses on an atom [2]. Ionization is hindered and the wave function is localized, in spite of the presence of the strong radiation field. The wave packet representing the excited electron eventually spreads and the degree of localization and/or ionization depends on the parameters of the radiation field. The above effect appears when the external field operates on a bound state.

We will describe here a similar and quite unexpected phenomenon when a wave packet scatters off an attractive well. Localization of the reflected waves will be also found. These waves spend a large amount of time spreading out of the scattering region. The speed of the reflected wave is independent of the initial average energy of the packet. It is completely generated by a bound state of almost zero binding energy. The well acts as a resonator that emits a coherent wave, but, only backwards.

The effect may be tested in back-angle nuclear reactions and ion traps. The effect is analogous to lasing inside a cavity; the well becomes then the most natural laser available.

Consider a minimal uncertainty wave packet traveling from the left with an average speed $v$, initial location $x_0$, mass $m$, wave-number $q=mv$, and initial width $\delta$;

$$\psi=C\exp\left(iq(x-x_0)-\frac{(x-x_0)^2}{4\delta^2}\right) \quad (1)$$

impinging on an attractive well located at the origin, with depth $A$ and width $w$. For the sake of simplicity we use a Gaussian well, but the results are not specific to the type or shape of the well,

$$V(x)=-A\exp\left(-\frac{x^2}{w^2}\right). \quad (2)$$

We solve the Schrödinger equation for the scattering event in coordinate space taking care of unitarity. We use the method of Goldberg *et al.* [3], that proved to be extremely robust and conserves the wave normalization with an error of less than 0.01%, even after hundreds of thousands of time-step iterations. We have verified that the solutions actually solve the equation with extreme accuracy by explicit substitution. Other simple discretization methods of resolution such as Runge-Kutta, leapfrog, etc., are unstable for this type of equation; they violate unitarity.

We study the scattering of an impinging packet with $\delta=0.5$ and a well width of $w=1$. We also use a large mass $m=20$ in order to prevent the packet from spreading too fast [1]. Figures 1 through 4 show pictures of the reflected and transmitted waves after long periods of time for various initial velocities. The ripples at the left and right ends of the figures are due to reflection from the boundaries.

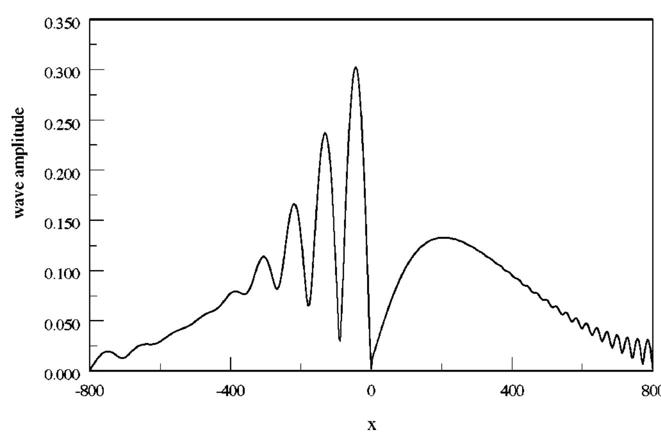


FIG. 1. Wave amplitude as a function distance $x$ for an initial wave packet of width $\delta=0.5$ starting at $x_0=-10$ impinging upon a well of width, $w=1$ and depth $A=1$ after $t=5000$; the initial average momentum of the packet is $q=0.2$.

 

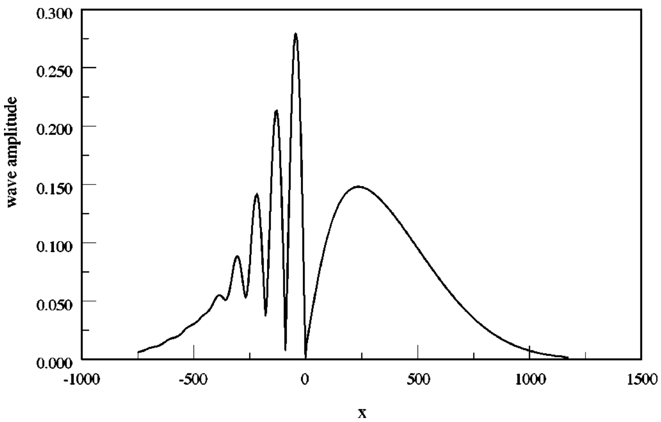


FIG. 2. Same as Fig. 1 but for an initial momentum $q=0.6$.

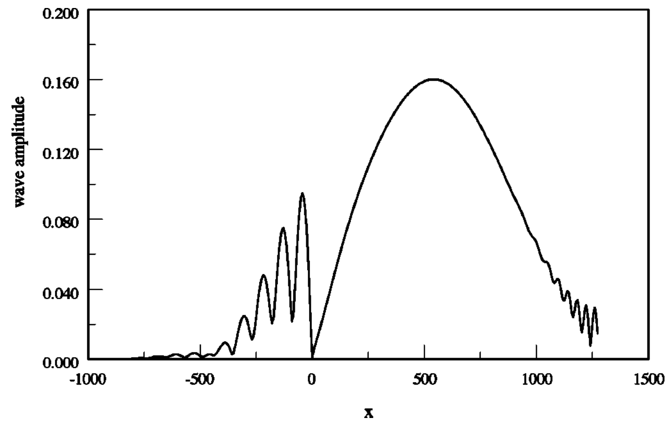


FIG. 4. Same as Fig. 1 but for an initial momentum $q=2.2$.

We would have expected a smooth packet for each of the reflected and transmitted waves. This is not the case in the figures. A polychotomous (multiple-peak) wave recedes from the well. For low velocities corresponding to average packet energies less than half the well depth, several peaks in the reflected wave show up. Simple inspection reveals that the distance between the peaks is constant. The reflected wave is propagating with an amplitude of the form

$$C(x)\approx e^{-\lambda|x|}\sin^2(kx). \tag{3}$$

The exponential drop is characteristic of a bound-state solution inside the well. The parameters λ and $k$ are independent of the initial velocity, but depend on time. The wave spreads and its amplitude diminishes, as expected. We have checked that the polychotomous behavior continues for $t\rightarrow\infty$ without modification.

The only possible explanation for both the coherence and independence of the reflected wave on the initial energy is that it must be generated by a resonant phenomenon inside the well. Figure 5 shows the excitation of the resonance inside the well for an initial velocity of $v=0.05$. The same picture arises for the different velocities. The resonance is a quasibound state. The energy of the bound state is the closest it can be to zero. If we borrow the bound-state conditions from the case of a square well for even and odd states,

$$k'\tan(k'w)=k \quad \text{for even states,}$$

$$k'\cot(k'w)=-k \quad \text{for odd states,} \tag{4}$$

where $k'=\sqrt{2m(A+E)}$, $E$ is the energy of the bound state, $A$ is the depth of the well, and $k=\sqrt{2m|E|}$; we find for $k\approx 0$, $k'w=n\pi$ for even states and $k'w=(2n+1)\pi/2$ for odd states.

For the parameters used here $k'\approx 2\pi$. This is the wave number that can be read off by inspecting Fig. 5. (Note that the figure displays the absolute value of the wave.) The bound-state condition is indeed operative. We may further put this in evidence, by modifying the mass of the packet to $m\approx 11$. For this mass, the bound-state condition is satisfied only with an odd state for which $k'w\approx 3\pi/2$. Figure 6 reveals that the condition is again correct.

The state excited inside the well is a quasibound state that decreases in amplitude as a function of time (decays) emitting energy to both sides of the well. However, its shape remains constant even at extremely large times. In a particulate point of view, the resonance in the well produces a coherent bunch of particles. Both the particulate aspect and the wave aspect through the modulation of the wave amplitude are still present.

The real and imaginary parts of the packet inside the well follow the trend of the amplitude depicted in the figures, their separate amplitudes do not always coincide, and their phases may differ as time passes. These differences may be

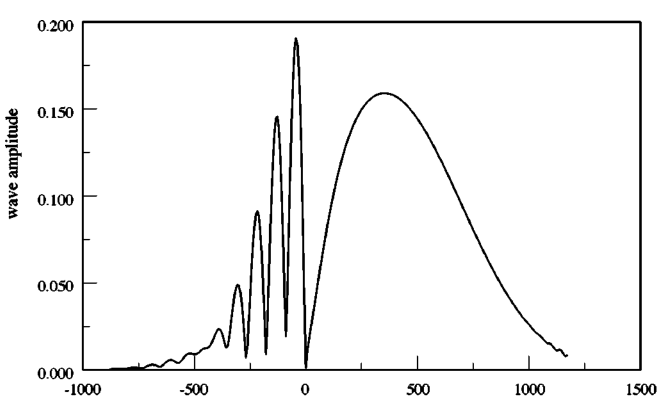


FIG. 3. Same as Fig. 1 but for an initial momentum $q=1.4$.

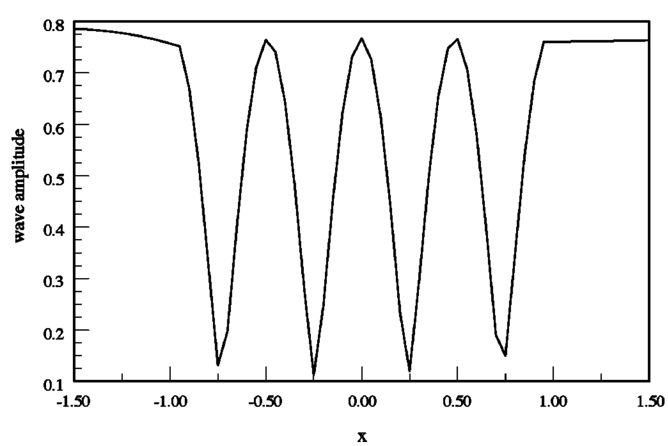


FIG. 5. Same as Fig. 1, for an initial momentum q=1 showing the resonance inside the well and for t=200, at which the resonance is fully developed

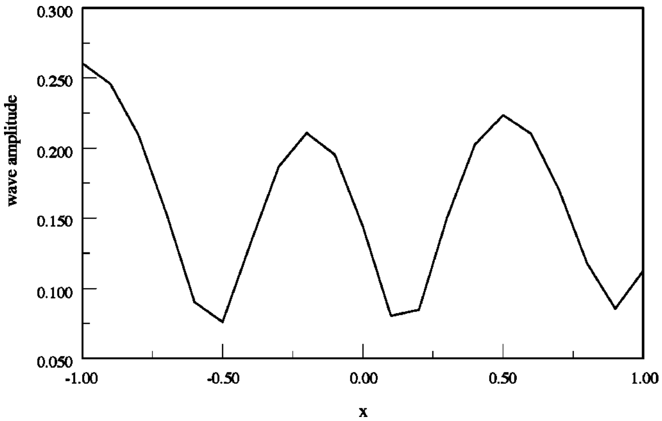


FIG. 6. Same as Fig. 5, but for a mass $m=11$.

traced back to the nonresonant components of the scattering that show up as a background under the peaks of the reflected waves. This nonresonant background is generated by the coupling to the infinite tower of free modes in the well and to the other bound states besides the dominant one at zero energy.

From Figs. 1–4, it is clear that the reflected coherent wave becomes less and less noticeable as we increase the initial energy of the wave packet. For average packet energies of the order of *A*, the well depth, the reflected wave is negligible but it still shows a tiny coherent train. The fact that the wave number of the reflected wave is independent of speed (as well as packet amplitude) suggests that it is also constrained by the resonance condition. Trial and error lead us to a simple formula. We find that the condition for the reflected wave number at the time of formation (later it will decrease due to packet spreading) is $4kw=\pi$.

The transmitted packet travels at a different velocity than that of the coherent reflected packet. It may be easily read out from the graphs following the development in time or by taking a large enough time for which the well is far behind. The reflected packet travels with a constant speed of $v=k(t_{formation})/m$. The speed can be found by evaluating the effective center-of-mass $\mathbf{X}$,

$$X_{refl}=\int_{-\infty}^{-w}dx\, x|\psi(x)|^2, \tag{5}$$

where the wave function is properly normalized to 1. Using the above equation one finds that the reflected wave center of mass recedes with a constant speed of approximately $v=0.03$ independent of the initial speed of the incident packet, while the transmitted wave rides away with a velocity slightly higher than the initial packet average velocity, and it is determined by overall energy conservation.

The polychotomous effect disappears when the wave packet is broader than the well. Figure 7 shows the standard reflected and transmitted waves as usually seen in the literature [3] for a wave packet of $\delta=2$ much greater than the well width of $w=1$. No coherent reflected wave is seen.

We have also investigated other types of wells, such as a Lorentzian well, a square well, etc., and found the same phenomena described here. The shape and average velocity of the receding packet does, however, depend on the depth and shape of the well. Moreover, the effect is independent of the shape of the packet as long as it is narrower than the well width. We have used square packets, Lorentzian packets, linear exponential packets, etc., with analogous results.

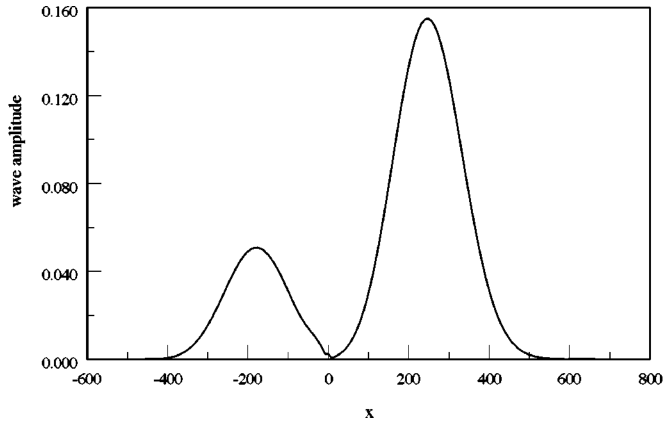


FIG. 7. Same as Fig. 1 but a wave packet of width $\delta=2$ and $q=1$.

In order to check the effect analytically we resort to the simplest packet, namely, a square packet

$$\psi(x)=e^{iq(x-x_0)}\Theta(d-|x-x_0|), \tag{6}$$

where $d$ is half the width of the packet, $x_0$ is the initial position, and $q$ is the wave number. The wave impinges on a square well located at the origin, whose width is $2a$ and depth $V_0$,

$$V(x)=-V_0\Theta(a-|x|). \tag{7}$$

This case is solvable using the techniques of Ref. [4]. The method is appropriate only for packets with sharp edges, which terminate at a certain point. It consists of integrating the Fourier amplitude of the wave using a contour in the complex momentum plane that avoids the poles of the scattering matrix corresponding to the bound states. For each momentum, one uses the appropriate stationary scattering state for the square well. The integral reads

$$\psi(x,t)=\int_C \phi(x,p)a(p,q)dp, \tag{8}$$

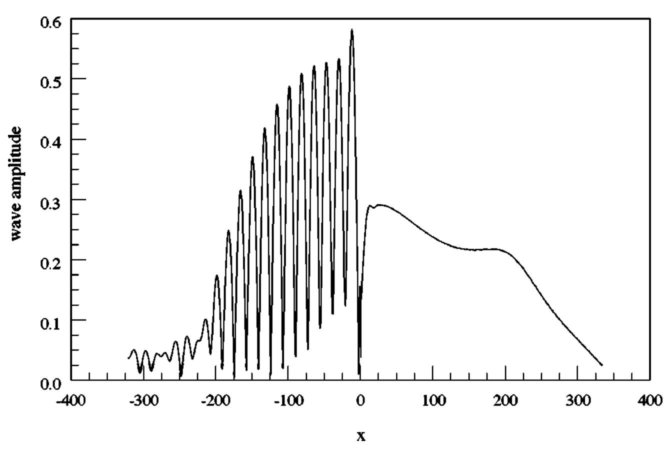


FIG. 8. Theoretical calculation for a square initial-packet scattering off a square well for $t=1000$.

where $C$ is a contour that goes from $-\infty$ to $+\infty$ and circumvents the poles that are on the imaginary axis for $p < i\sqrt{2mV_o}$ by closing it above them. $\phi(x,p)$ is the stationary solution to the square-well scattering problem for each $p$ and $a(p,q)$ is the Fourier transform amplitude for the initial wave function with average momentum $q$. Figure 8 shows the results of Eq. (8) for the reflected and transmitted waves for scattering of an initial wave packet with average momentum $q=1$, packet width $d=0.5$, and well parameters $V_0 = 1$, $a=1$ initially far away from the well at $x_0=-10$ (an essential condition for the integral to converge). The reflected wave shows exactly the same polychotomous behavior as the numerical simulations. The effect is general; even the packet amplitude is unimportant.

Although our treatment here is one-dimensional, it should apply also for the case of zero angular momentum in three dimensions with little change. Backward nuclear scattering is one possible experimental setting for the effect described here. The effect may serve as a method to determine nuclear well depths (or radii) by merely registering the dead time between bunches in the reflected wave beam. The effect may also be tested in atomic collisions at backward angles and in ion traps.

The only stumbling block for the detection of the mentioned coherent multiple-peaked waves representing the fluxes of particles is the production of narrow wave packets of particles, which is beyond present accelerator capabilities.

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