Excitation of a harmonic oscillator by unipolar rectangular radiation pulses

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An analysis of the excitation of classical and quantum harmonic oscillators by unipolar pulses in a rectangular time profile has been carried out. For a quantum oscillator, the probability of excitation is determined depending on the parameters of the problem. The transition from the case of extremely short pulses, when the excitation is determined by the electrical area of the pulse, to long pulses, for which the main factor is the pulse energy, is traced. At the same time, a significant difference was found in the conditions for the applicability of the sudden perturbation approximation in the cases of classical and quantum oscillators.

Introduction

The model of a harmonic oscillator, both classical and quantum, describes well a number of physical processes, including molecular vibrations (unless high vibrational levels [1] are excited). For a quantum oscillator, the nonrelativistic Schrödinger equation has an exact solution closely related to the solution of the classical equation of motion, at an arbitrary kind of external force and time dependence of the oscillator frequency (see original articles [2–6], the contents of which are summarized in monograph [7]). The result, of course, depends significantly on the type of time dependence of these quantities.

Recently, significant progress has been made in obtaining very short laser pulses, recognized by the awarding of the Nobel Prizes in 1999 ([8] femtosecond durations) and 2023 ([9] attosecond pulses). Of particular interest, in our opinion, are extremely short unipolar or quasi-unipolar pulses due to their unidirectional (for the entire duration of a pulse) effect on electric charges (see original articles [10–16], reviews [17–19] and a chapter in monograph [20]). Although some properties of unipolar pulses have already been discussed more than 60 years ago [21], discussions about the very possibility of existence of such pulses are still ongoing [22,23]. In our opinion, there is convincing theoretical and experimental evidence for the existence of such pulses and their propagation in coaxial waveguides [20]. The acuteness of the discussion is reduced by the fact that there are no essential differences between the effect on microobjects of a strictly unipolar pulse and a pulse with an extended weak front of pulses of opposite polarity and/or a pair of widely spaced unipolar pulses with a total zero electrical area.

The purpose of the present work is to analyze the excitation of a harmonic oscillator by a unipolar pulse with a rectangular time profile and to compare the classical and quantum descriptions of such excitation. This will make it possible to trace the transition from extremely short to longer pulses. Note that the excitation of a quantum harmonic oscillator has been considered on the basis of the exact solution and the solution in the sudden perturbation approximation [24,25] in numerous studies [26–31]. The problem considered in this paper allows us to clarify the conditions of applicability of the sudden perturbation approximation. We also point out that the possibility of controlling the shape and obtaining unipolar or quasi-unipolar pulses with a near-rectangular time profile is demonstrated theoretically in [32–35].

Classical oscillator

The equation of motion of a classical harmonic oscillator with unit mass under the action of external force $f(t)$, which can be identified with electric field strength E, has the following form:

$$d^2x/dt^2 + \omega^2 x = f(t). \tag{1}$$

Here, x is the displacement of the oscillator relative to the equilibrium position in the absence of force and ω is the frequency of free oscillations. Before the start of the external force pulse $(t < 0)$, the oscillator is in the equilibrium position, $x(0) = 0$, $dx/dt(0) = 0$.

A single pulse with a rectangular time profile with duration τ and amplitude A has „pulse area" (understood as electrical area) $S_f = \int f(t)dt = A\tau$ and energy $W_f = A^2\tau$. During a pulse $(0 < t < \tau)$, the solution (1) describes a

harmonic oscillation near the displaced equilibrium position:

$$x(t) = \frac{A}{\omega^2}[1 - \cos(\omega)] = 2\frac{A}{\omega^2}\sin^2\left(\frac{\omega t}{2}\right). \quad (2)$$

By the end of a pulse $(t = \tau)$, the oscillator gains energy

$$W = 2\frac{A}{\omega^2}\sin^2\left(\frac{\omega\tau}{2}\right). \quad (3)$$

For a fixed force amplitude A and increasing pulse duration τ, the energy of the oscillator changes periodically between a maximum value of $W_{max} = 2\frac{A}{\omega^2}$ at $\tau = \left(N + \frac{1}{2}\right)T_{osc}$, where $T_{osc} = \frac{2\pi}{\omega}$ is the period of free oscillation of the oscillator and N is an integer, and a minimum value of $W_{min} = 0$ corresponding to complete stopping of the oscillator in the equilibrium position at $\tau = NT_{osc}$. In terms of pulse energy,

$$W = 2\frac{W_f}{\omega^2\tau}\sin^2\left(\frac{\omega\tau}{2}\right) = \frac{W_f}{\omega^2\varphi}\sin^2\varphi, \quad (4)$$

where $\varphi = \omega\tau/2$. Extrema of the oscillator energy at a fixed pulse energy and increasing pulse duration are reached at φ values that are the solutions of transcendental equation $\tan\varphi = 2\varphi$. The first and main maximum is realized at $\varphi \approx 1.17$. Energy minima $W_{min} = 0$ again correspond to the oscillator stopping at $\tau = NT_{osc}$.

For pulses of duration much shorter than the period of the oscillator,

$$\tau \ll T_{osc}, \quad (5)$$

its final energy, as can be seen from (3), is completely determined by the electrical area of a pulse: $W = \frac{1}{2}(A\tau)^2 = \frac{1}{2}S_E^2$. This corresponds to the approximation of sudden perturbations where a pulse is so short that its duration is not sufficient for the position of the oscillator to shift, and the whole effect of the pulse on it is reduced to the transmission of a mechanical momentum proportional to the electrical area of the pulse. It is noteworthy that in the classical description, condition (5) is the only condition for the applicability of the sudden perturbation approximation, regardless of the amplitude or energy of the excitation pulse.

Oscillator excitation by multiple rectangular pulses can be examined in a similar way. The difference is the change in initial conditions for the next pulse due to the effects of previous pulses.

Quantum oscillator

The Schrödinger equation for a quantum harmonic oscillator excited by external force $f(t)$ for wave function $\psi(x, t)$ in the atomic system of units (unit charge and mass of the electron, $e = m = 1$, and reduced Planck's constant $\hbar = 1$) has the following form:

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}\omega^2 x^2\psi - fx\psi. \quad (6)$$

Here, x is the coordinate, and the rest of the notation is as above.

In the absence of an external force, before the arrival of a pulse $(t \to -\infty)$ and after its termination $(t \to +\infty)$, stationary states of the free oscillator are described by an equidistant energy spectrum and wave functions of the form [7]

$$\psi_n(x, t) = \varphi_n(x)\exp\left[-i\left(n + \frac{1}{2}\right)\omega t\right],$$

$$\varphi_n(x) = \left(\frac{1}{2^n!}\sqrt{\frac{\omega}{\pi}}\right)^{1/2}\exp\left(-\frac{1}{2}\omega x^2\right)H_n\left(\sqrt{\omega}x\right). \quad (7)$$

Here, $n = 0, 1, 2, \ldots$ is the state number and H_n are Hermite polynomials. Transitions between these levels occur during a pulse. The probability of transition from level n to level m within the entire pulse duration is given by the expression [7]

$$W_{mn} = \frac{n_<!}{n_>!}\nu^k\left(L_{n_<^k}\right)^2\exp(-\nu), \quad (8)$$

where L_n^k are generalized Laguerre polynomials, $n_< = \min(m, n)$, $n_> = \max(m, n)$, and $k = |n - m|$. In particular, the probabilities of the oscillator remaining in the ground state W_{00} after a pulse and its excitation W_{exc} are

$$W_{00} = \exp(-\nu), \quad W_{exc} = 1 - W_{00} = 1 - \exp(-\nu). \quad (9)$$

The main parameter in (8) and (9) is dimensionless quantity ν, which depends on the type of function $f(t)$. For a rectangular pulse with the above characteristics,

$$\nu = \nu_0\left\{4\sin^2\frac{\omega\tau}{2} + \left[\frac{A}{\omega^2}\omega\tau + \left(1 - \frac{A}{\omega^2}\right)\sin(\omega\tau)\right]^2\right\}, \quad (10)$$

where $\nu_0 = \frac{A^2}{2\omega^3}$. For extremely short pulses (condition (5)) in the lowest approximation,

$$\nu = \frac{(A\tau)^2}{2\omega} = \frac{S_f^2}{2\omega}. \quad (11)$$

The dependence of the probability only on the electrical area of a pulse corresponds to the sudden perturbation approximation.

With the next term of the expansion of (10) in small parameter $\omega\tau$ taken into account,

$$\nu = \frac{S_f^2}{2\omega}\left[1 - \frac{1}{3}\left(\frac{1}{4} + \frac{A}{\omega^2}\right)(\omega\tau)^2\right]. \quad (12)$$

The correction term depends not only on the electrical area of a pulse, but also on its duration. It is small under the condition

$$\frac{1}{3}\left(\frac{1}{4} + \frac{A}{\omega^2}\right)(\omega\tau)^2 \ll 1. \quad (13)$$

Inequality (13) is violated at sufficiently large pulse amplitudes, i.e., at large displacements of the mean oscillator position A/ω^2. Requirement (5) of smallness of the pulse duration is then insufficient to justify the sudden perturbation approximation. Physically, it implies that at large pulse amplitudes, the oscillator is displaced by appreciable distances during a pulse. Thus, the non-point nature of the quantum oscillator, which, in contrast to a point classical oscillator, is characterized by a spatially distributed wave function, becomes significant. And this violates the conditions of applicability of the sudden perturbation approximation in the case of a quantum oscillator.

For pulses with durations markedly longer than the oscillation period of the free oscillator ($\omega\tau \gg 1$),

$$\nu = \frac{W_f^2}{2\omega^5}. \tag{14}$$

In this case, the degree of oscillator excitation is determined not by the electrical area of a pulse, but by its energy.

Figure 1 shows the dependence of the probability of excitation (W_{exc}) of a quantum oscillator from its initial ground state on the pulse duration (more precisely, on dimensionless quantity $\omega\tau$, which has the meaning of „number of periods" of free oscillations of the oscillator during a pulse) calculated by formulae (9) and (10) at different values of parameter A/ω^2. As in the case of the classical oscillator, this dependence is not periodic. The „quantum" difference is the fact that the minima do not fall to zero, contradicting the sudden perturbation approximation (except for the trivial case $\omega\tau = 0$. It can also be seen that as pulse amplitude A increases, the excitation probability approaches unity. These results confirm the possibility of creating level population inversion by pumping with extremely short pulses.
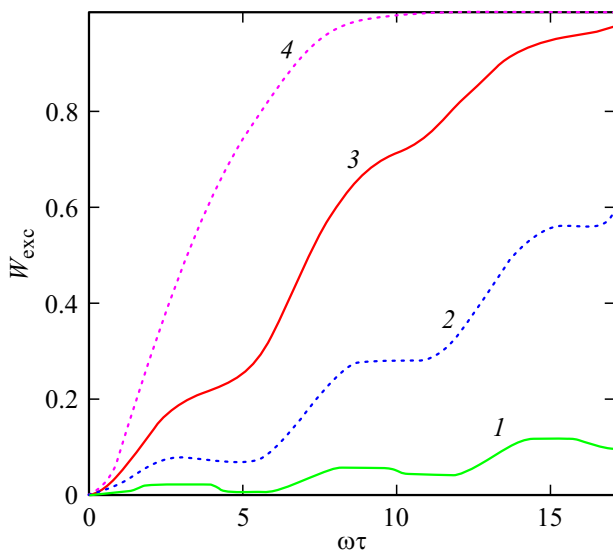
Figure 1. Dependence of oscillator excitation probability W_{exc} on excitation pulse duration τ. Parameters: $\omega = 0.1$; $A = 0$ (curve *1*), 0.05 (*2*), 0.07 (*3*), and 0.1 (*4*).
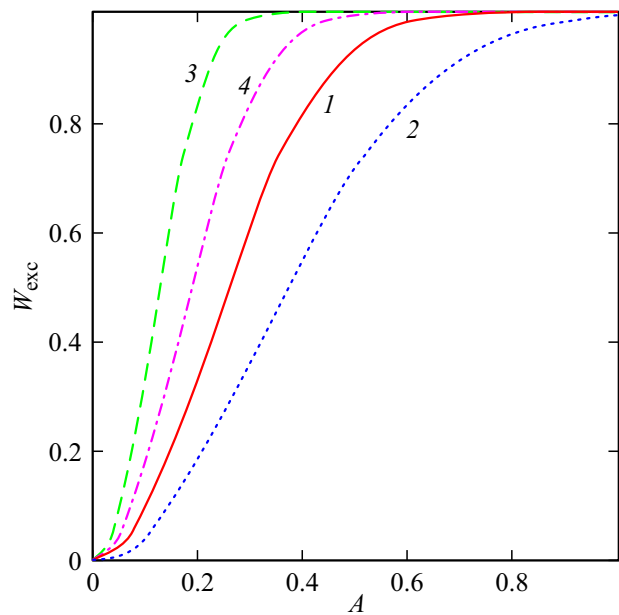
Figure 2. Dependence of the oscillator excitation probability (exact (curves *1* and *3*) and in the sudden perturbation approximation (*2*, *4*)) on amplitude A of the excitation pulse at $\omega\tau = 0.1$ (*1, 2*) and 0.2 (*3, 4*).

Figure 2 illustrates a comparison between the „exact" expression for the excitation probability and its counterpart in the sudden perturbation approximation. The difference is quantitative in nature and evident at intermediate values of pulse amplitude. This fact allows us to define the scope of application of the above approximation.

Discussion and conclusion

Thus, while the approximation of sudden perturbations is applicable in the case of a classical oscillator if just the requirement of smallness of the perturbation pulse duration in comparison with the characteristic period of the oscillator is fulfilled, an additional restriction on the perturbation amplitude arises for a quantum oscillator. Taken together, these conditions reduce to the requirement of smallness of changes in the potential energy of the oscillator during a pulse. The difference in the applicability conditions of the approximation for classical and quantum oscillators is due to the fact that the former is point-like and the latter is spatially distributed. It appears that this conclusion is also true for other objects modelled by harmonic oscillators.

Another conclusion, also of a general character, is the transition from the electrical area of a pulse (as a major factor of excitation efficiency) at short durations to the energy of that pulse for longer pulses. These conclusions were obtained outside the framework of perturbation theory, which extends the scope of their applicability.

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Conflict of interest

The author declares that he has no conflict of interest.

Appendix. Derivation of formula (10)

We use the notation from [7] and the method of solving the Schrödinger equation given there for a rectangular pulse with amplitude A and duration τ. To do this, we return to the equation of motion of a classical oscillator (1), where x is replaced by η, for function $f(t) = A$ at $0 < t < \tau$ and 0 outside of this time interval. Let us assume that at $t < 0$ $\eta = \exp(i\omega t)$. Within the $(0, \tau)$ interval, the solution of equation $d^2\eta/dt^2 + \omega^2\eta = A$ is the expression

$$\eta(t) = \frac{A}{\omega^2} + \exp(i\omega t) - \frac{A}{\omega^2} \cos(\omega t). \qquad (A1)$$

We now find the value of d:

$$d = \frac{iA}{\sqrt{2\omega}} \int_0^\tau \eta(t)dt = \frac{A}{\sqrt{2}\omega^{3/2}} \left\{ -2\sin^2\frac{\omega\tau}{2} \right.$$

$$\left. + i\left[\frac{A}{\omega^2}\omega\tau + \left(1 - \frac{A}{\omega^2}\right)\sin(\omega\tau)\right] \right\}. \qquad (A2)$$

Finally, the calculation of $\nu = |d|^2$ yields expression (10).

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