Stabilization of atoms in a strong field and the Kramers–Henneberger approximation

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The stabilization of a quantum system in a strong electromagnetic field is investigated by means of numerical integration of the time-dependent Schrödinger equation. The results of the numerical calculations are compared with calculations and analytical estimates based on the Kramers–Henneberger model in order to establish the limits of the applicability of the latter. The effect of the rise time of a laser pulse on attaining the stable regime is studied. © *1994 American Institute of Physics.*

I. INTRODUCTION

At the present time there is wide interest in the stabilization of atoms in an external intense light field due to the reduction in the ionization rate as the intensity of the laser light increases.[1–3] In the literature it is customary to distinguish two possible mechanisms for suppressing ionization, operating in different parameter ranges of the laser light:

a) destructive quantum interference of the amplitudes of the transitions to the continuum from a group of closely spaced quantum states;[4,5]

b) the formation of an electron wave packet oscillating with large amplitude in the external electric field and hence weakly interacting with the atomic core, which reduces the probability of photon absorption.[6,7]

The main results relating to the stabilization effect are usually derived at present using the Kramers–Henneberger (KH) approximation.[7–10] However, despite the wide use of this approach for solving specific problems, the actual region of applicability of the Kramers–Henneberger approximation has been little studied. Consequently, there is considerable interest in comparing information derived using this approximation with the results of "numerical experiments" in order to sharpen the physical picture of the proces by which the quantum system is stabilized in a strong electromagnetic field and to determine the range of applicability of the KH approximation.

In the present work the Kramers–Henneberger formalism is used to treat the effect of stabilization in a one-dimensional quantum system with a short-range potential. The results are compared with calculations based on direct numerical integration of the time-dependent Schrödinger equation for a quantum system in the field of an electromagnetic wave. The relation between the rise time of the wave electric field and the occurrence of stabilization is investigated.

2. THE KRAMERS–HENNEBERGER APPROXIMATION

Physically the KH approximation is based on going over to a noninertial coordinate system oscillating like a free electron in the field of the electromagnetic wave (the Kramers coordinate system[11]):

$$x' = x - a_e \cos \omega t, \tag{1}$$

where $a_e = eE_0/m\omega^2$ is the amplitude of the oscillatory motion of the electron and E_0 and ω are the amplitude and frequency of the wave field. We go over to this coordinate system using the time-dependent unitary transformation

$$\psi_{\mathrm{KH}}(x',t) = S(t)\psi(x,t), \tag{2}$$

where

$$S(t) = \exp\left\{ \frac{i}{\hbar} \int_{-\infty}^{t} H_{\mathrm{int}}(t)dt \right\},$$

and $H_{\mathrm{int}}(t)$ is the operator of the interaction between the electron and the wave electromagnetic field.

In the dipole approximation in the dE gauge this operator takes the form

$$H_{\mathrm{int}}(t) = -exE_0 \cos \omega t. \tag{3}$$

In the Kramers coordinate system the Schrödinger equation for the electron wave function $\psi_{\mathrm{KH}}(x',t)$ can be written in the form

$$i\hbar \frac{\partial \psi_{\mathrm{KH}}}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_{\mathrm{KH}}}{\partial x^2} + V(x' + a_e \cos \omega t)\psi_{\mathrm{KH}}(x',t), \tag{4}$$

where $V(x)$ is the atomic potential. Thus, the atom-field interaction is reduced to a time-dependent shift in the argument of the potential.

Expanding the potential $V(x' + a_e \cos \omega t)$ in a Fourier series we find

$$V(x' + a_e \cos \omega t) = \sum_{n=-\infty}^{\infty} V_n(x',a_e)e^{in\omega t}, \tag{5}$$

where

$$V_n(x',a_e) = \frac{1}{2\pi} \int_0^{2\pi} V(x' + a_e \cos \omega t)e^{-in\omega t} d(\omega t). \tag{6}$$

The Kramers–Henneberger approximation consists of neglecting all modes in (4) except the zeroth mode $n=0$. As a result, the motion of the electron in the atomic potential in the presence of the variable wave field reduces to the prob-

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lem of the Schrödinger equation with a time-independent potential $V_0(x,a_e)$ (the Kramers–Henneberger potential):

$$i\hbar \frac{\partial \psi_{\rm KH}}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi_{\rm KH}}{\partial x^2} + V_0(x,a_e)\psi_{\rm KH}(x,t). \qquad (7)$$

Here and in what follows we omit the prime.

The modes $V_n(x,a_e)$ are taken to be small, so that they can be treated as perturbations:

$$\delta V(x,a_e,t) = V(x+a_e\cos\omega t) - V_0(x,a_e). \qquad (8)$$

In the potential $V_0(x,a_e)$ there exists a system of time-independent and therefore stable (with respect to ionization) states. Being in one of these states is the essence of the stabilization phenomenon. The key question in this approach is when it is justified to neglect the harmonics $V_n(n\neq 0)$ in (4). The analysis in Refs. 6, 7, 12, and 13 shows that for high frequencies (formally, infinite frequencies) and intensities these terms vanish, i.e., the electron "sees" only the time-averaged potential. In Ref. 7 it was postulated that the necessary condition for the applicability of the Kramers–Henneberger approximation is the inequality

$$\hbar\omega \gg \varepsilon_1^{\rm KH}, \qquad (9)$$

where $\varepsilon_1^{\rm KH}$ is the energy of the ground state in the KH potential. In the alternative approach in which in the right-hand side of the inequality (9) the energy of the ground state in the original potential appears, rather than in the Kramers–Henneberger potential. As will be clear from what follows, our calculations provide no support for this point of view.

3. NUMERICAL EXPERIMENTS TO OBSERVE ATOMIC STABILIZATION

In recent years direct integration of the time-dependence Schrödinger equation has been actively employed to study the dynamics of an atomic system in an electromagnetic wave field.[14] Numerical experiments designed to study the stabilization effect have been carried out repeatedly both for the smoothed Coulomb potential[15,16] and for short-range potentials.[17–20] These treatments have shown that for a given radiation frequency there exists a critical intensity above which the stability of the atomic system against further disruption increases.

In Refs. 17–19 the photodisruption mechanism in a strong field and atomic stabilization due to the formation and spreading of a rapidly oscillating wave packet were analyzed in detail. The conditions under which this regime occurs were determined: strong fields, low frequencies, and short rise times for the pulse. It was shown that as the rise time of the pulse increases the regime in which free expansion and oscillations of the wave packet occur is replaced by one in which Kramers–Henneberger stabilization occurs in the model. The physical meaning of the stabilization is that the atomic potential limits the spreading of part of the wave packet when it becomes larger than the electron oscillation amplitude a_e. The model of almost-free oscillations of the electron wave packet was also treated in Ref. 20, where it was shown to yield good agreement with the results of numerical experiments.

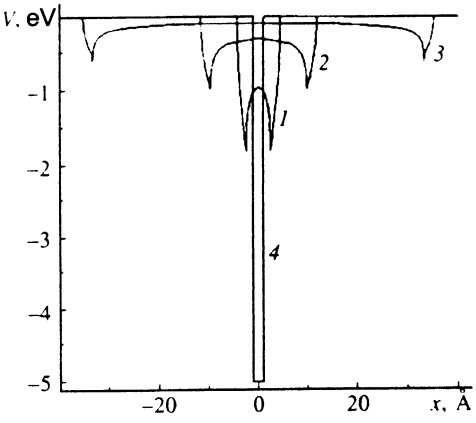


FIG. 1. The Kramers–Henneberger potential for laser radiation intensity (W/cm^2) *1*—10^{14}; *2*—10^{15}; *3*—10^{16}; *4*—the initial atomic potential.

4. ONE-DIMENSIONAL MODEL OF THE ATOMIC SYSTEM

As the atomic potential we will consider a square-well potential

$$V(x) = \begin{cases} -V_0, & |x| \leqslant d/2, \\ 0, & |x| > d/2, \end{cases}$$

with parameters $V_0=5$ eV, $d=2$ A. This well has a single bound state with energy $\varepsilon_1=-2.55$ eV and wave function $\varphi_1(x)$, determined as the eigenvalue and eigenfunction of the atomic potential $H_0=-(\hbar^2/2m)d^2/dx^2+V(x)$. Figure 1 displays the Kramers–Henneberger potential for this atom for different values of the intensity and $\hbar\omega=2.5$ eV. At high intensities ($P>10^{14}$ W/cm^2) it has a typical two-well shape (the distance between the wells is equal to $2a_e$). This is the typical shape of the KH potential and does not depend on the specific properties of the atom.[2,19] The number of states in the KH potential increases as a function of intensity. For example, for an intensity $P=10^{16}$ W/cm^2 in the potential $V_0(x,a_e)$ there exist five time-independent states with energies $\varepsilon_1^{\rm KH}=\varepsilon_2^{\rm KH}=-0.152$ eV, $\varepsilon_3^{\rm KH}=-0.09$ eV, $\varepsilon_4^{\rm KH}=-0.055$ eV, $\varepsilon_5^{\rm KH}=-0.01$ eV. The position of the two lowest energy levels, corresponding to the time-independent state in the KH potential as a function of intensity, are shown in Fig. 2. The spatial distributions of the probability density $\rho_i^{\rm KH}(x) = |\Psi_i^{\rm KH}|^2$ $(i=1,...,5)$ for $P=10^{16}$ W/cm^2 are shown in Fig. 3. It is noteworthy that the two lowest states are degenerate and the distributions $\rho_i^{\rm KH}(x)$ for them are the same.

In this model the harmonics $V_n(x,a_e)$ can be calculated analytically, and the perturbation $\delta V(x,a_e,t)$ in the region $x\in(-a_e-d/2, a_e+d/2)$ assumes the form

$$\delta V(x,a_e,t) = -\frac{|V_0|}{\pi}\sum_{n=1}^{\infty}(-1)^n \times[\sqrt{1-\xi_1^2}U_{n-1}(\xi_1)\delta(\xi_1) - \sqrt{1-\xi_2^2}U_{n-1}(-\xi_2)\delta(\xi_2)]\begin{Bmatrix}\cos n\omega t \\ \sin n\omega t\end{Bmatrix}. \qquad (10)$$

Here

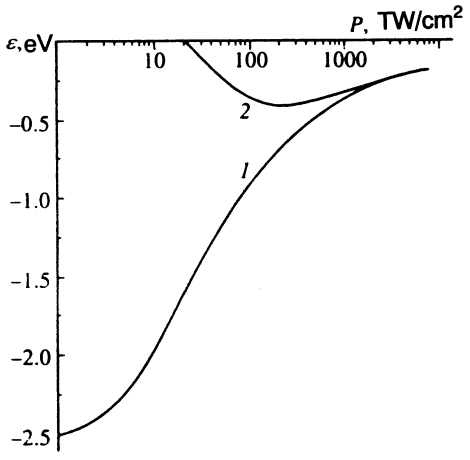


FIG. 2. Position of the ground (*1*) and first excited (*2*) states in the KH potential as a function of the radiation intensity.

$$U_n(\xi)=\frac{\sin((n+1)\arccos\,\xi)}{\sin\,\xi}$$

are Chebyshev polynomials of the second kind[21] with arguments $\xi_{1,2}=(d/2\mp x)/a_e$ and

$$\delta(\xi)=\begin{cases}1, & \xi^2<1,\\ 0, & \xi^2>1.\end{cases}$$

In Eq. (10) $\cos(n\omega t)$ corresponds to even values of n and $\sin(n\omega t)$ to odd values.

5. DYNAMICS OF AN ATOMIC SYSTEM IN A WAVE FIELD WITH CONSTANT INTENSITY

We will assume that at $t=0$ the system is in the ground state of the Kramers–Henneberger potential. Our calculations reveal that in the range of values $P=10^{14}$–10^{16} W/cm^2 the rate at which the initial state is destroyed falls off as the laser intensity increases, i.e., one can speak of the stabilization of the quantum system with respect to ionization. Note that condition (9) is satisfied in this range of intensities: thus, e.g., for $P=10^{14}$ W/cm^2 we have $|\varepsilon_1^{KH}|\simeq 0.9$ eV. On the other hand, under the conditions of our calculations the photon energy is somewhat smaller than the ionization potential of the system. The presence of stabilization in this situation is evidence in favor of the validity of the criterion (9). As an example of the evolution of a quantum system in time, in Fig. 4 we show the time dependence of the populations of

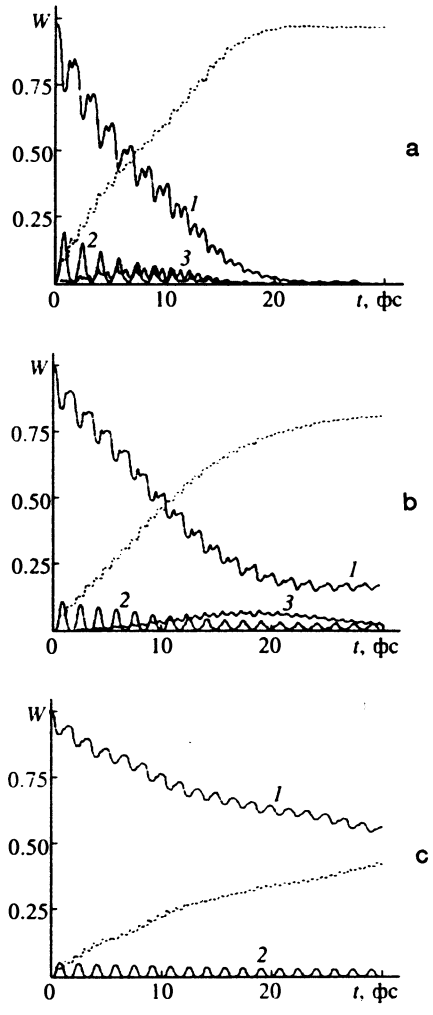


FIG. 4. Time dependence of the populations of the ground state (*1*), first excited state (*2*), and third excited state (*3*) in the KH potential. The broken trace is the probability for transition to the continuum. The radiation intensities (in W/cm^2) are a—10^{15}; b—$3\cdot 10^{15}$; c—10^{16}.

the ground state and two lowest excited states in the KH potential, together with the probabilities for transition to the continuum for different field intensities, derived from exact solution of (4). These results show that as the intensity increases the contribution of the harmonics $V_n(x,a_e)$ to the full potential $V(x+a_e\cos\omega t)$ drops off. The space-time evolution of the probability density $\rho(x,t)$ for $P=10^{16}$ W/cm^2 is shown in Fig. 5a. Figure 5b displays $\rho(x,t)$ for the same field

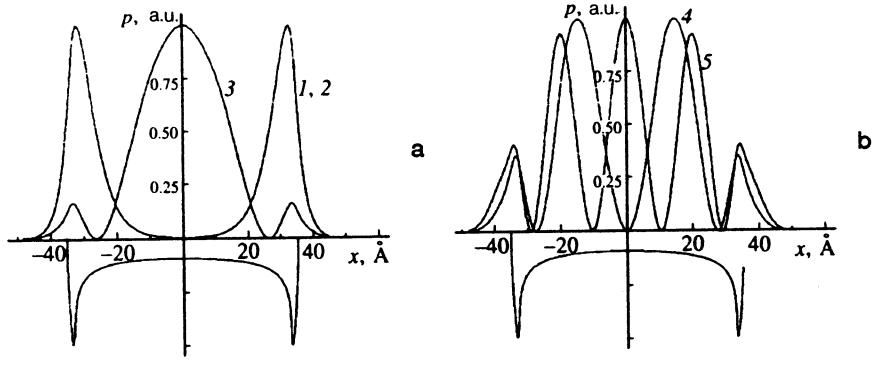


FIG. 3. Spatial distributions of the probability density in the time-independent states of the KH potential for $P=10^{16}$ W/cm^2.

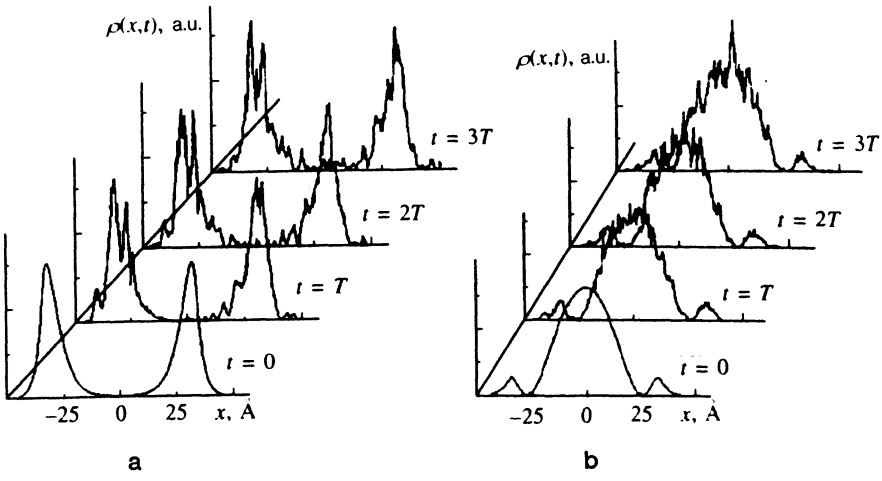


FIG. 5. The space-time evolution of the probability density $\rho(x,t)$ for $P=10^{16}$ W/cm^2. The initial state corresponds to the ground state (a) and third state (b) in the KH potential (T is the laser field period, $T=2\pi/\omega$).

intensity, but for the case in which the system is initially in the third state of the KH potential. As can be seen, this state also exhibits great stability.

In order to determine the contribution of the various harmonics $V_n(x,a_e)$ of the ionization process, we performed numerical solution of Eq. (7), retaining the harmonics $V_i(x,a_e)$, $i=1,2,3,...$ on the right-hand side. It was found that as the intensity increased and the ionization rate decreased the number of harmonics which must be retained in (7) grows. Thus, for $P=10^{14}$ W/cm^2 it suffices to treat just two terms V_1 and V_2; for $P=10^{15}$ W/cm^2 the three harmonics ($i=1,2,3$) contribute only 50% of the total ionization probability. In the case $P=10^{16}$ W/cm^2, however, these three harmonics contribute a mere 20–25% to the probability of transition to the continuum.

This property of the ionization process can readily be understood in terms of perturbations in the form of the operator $\delta V(x,a_e,t)$. Regarding δV as a perturbation about the Hamiltonian

$$H_{KH}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V_0(x,a_e),$$

we can write an expression for the transition probability per unit time from the initial state $\Psi_1^{KH}(x)$ to the continuum:

$$W_p\cong\frac{2\pi}{\hbar^2}\sum_{n=1}^{\infty}|V_{0k}^{(n)}|^2\frac{m}{\hbar k_n}. \tag{11}$$

Here

$$V_{0k}^{(n)}=\int\Psi_1^{KH}(x)V_n(x,a_e,t)e^{ik_nx}dx \tag{12}$$

is the matrix element coupling the initial state and the continuum state, which by virtue of the condition $\hbar\omega\gg|\varepsilon^{KH}|$ can be represented as a plane wave; k_n is determined from the condition

$$\frac{\hbar^2k_n^2}{2m}=n\hbar\omega-|\varepsilon^{KH}|\cong n\hbar\omega. \tag{13}$$

Assuming that the wave function Ψ_1^{KH} is a smoothly varying function of position in comparison with V_n and $\exp(ik_nx)$, we can easily find from (11) and (12) that

$$W_p\cong\pi B\frac{|V_0|}{2\hbar}\sum_{n=1}^{\infty}\frac{J_n^2(k_na_e)}{n^2k_na_e}\frac{\sin^2 k_na}{(k_na)^2}\frac{1}{1+\alpha}, \tag{14}$$

where $B=2m|V_0|a^2/\hbar^2$, $a=d/2$, $\alpha=a/a_e$.

A similar expression was obtained previously for the photoionization probability of a quantum system in Ref. 22 using the Keldysh–Faisal–Reiss approximation.

In weak fields when $\alpha\ll1$ holds, it suffices to retain one term $n=1$ of the series in Eq. (14), whereupon $W_p\sim P$, which corresponds to the usual perturbation theory for single-photon transitions. In the opposite limit $\alpha\gg1$ we have

$$W_p\sim1/a_e^2\sim1/P. \tag{15}$$

This dependence of the probability ionization from the KH state in the stabilization regime agrees with the results of exact numerical calculations (see Fig. 5). The dependence $W(P)$ in the form (15) was also obtained previously in Ref. 20 in the model of nearly free expansion of the electron wave packet.

Expression (14) enables us to estimate the number of harmonics that need to be taken into account in the perturbation δV for different values of the intensity. Noting the property of Bessel functions

$$|J_n(x)|\ll1 \quad \text{for} \quad x>n,$$

we can anticipate that the contribution to (14) comes from terms for which

$$k_na_e\geqslant n. \tag{16}$$

Condition (16) can be rewritten in the form

$$n\leqslant\varepsilon_e/\hbar\omega,$$

where ε_e is the electron vibrational energy in the field of the electromagnetic wave. It is well known[22,23] that the parameter $N=\varepsilon_e\hbar\omega$ determines the number of peaks in the spectrum of the subthreshold ionization. These calculations therefore demonstrate that the number of harmonics excited in connection with photoionization is correlated with the photoelectron spectrum.[2] In particular, for $P=10^{16}$ W/cm^2 we find from (16) that $n\simeq10$.

Our analytical expressions also enable us to establish the relationship between stabilization of a quantum system in a wave field and the effect of high-frequency harmonic generation.[2] Specifically, the nth mode $V_n(x,a_e)$ of the potential induces oscillations of the dipole moment of the system, and consequently emission at the frequency $n\omega$. Increasing the number of modes $V_n(x,a_e)$ that must be retained as the radiation intensity increases thus leads to an increase in the number of harmonics generated.

6. STABILIZATION AND FINITE PULSE RISE TIME

Thus far we have considered the effect of stabilization for a constant radiation intensity. From the practical standpoint it is important to take into account the finite rise time of a laser pulse and to determine the probability that an electron will undergo a transition from a time-independent state of the atomic Hamiltonian to a time-independent state of the KH potential, and then (when the pulse is turned on) to the initial state.

It is well known that when the wave electric field is turned on discontinuously an electron feels a shove and acquires an energy in directed motion on the order of the vibrational energy of an electron in the wave field. The absolute value of this energy is dependent on the phase of the electric field at the time it is turned on. In the range of intensities treated above, this quantity is greater than the ionization potential of the atom, i.e., the jolt can cause ionization of the atom and destroy stability. On the other hand, when the intensity increases slowly the duration of the stage in which the KH approximation is unsuitable is increased: the harmonics $V_n(x,a_e)$ $(n\geqslant 1)$ lead to ionization of the atom before the stabilization regime is attained. The maximum ionization rate will occur when a wave field with the "atomic" value $E_a\simeq V_0/ea$ is reached (the corresponding atomic intensity is $P_a=cE_a^2/8\pi\simeq 8\cdot 10^{13}$ W/cm^2). From these comments it follows that there exists an optimum rise time for the laser pulse in order to achieve the stabilization regime.

Let us consider the transition of the quantum system from the initial time-independent atomic state to a state of the KH potential when the amplitude of the wave electric field increases linearly:

$$E_0(t)=\mathbb{E}_0 t/\tau_f, \tag{17}$$

where τ_f is the length of time used for the yield to rise to the value $\mathbb{E}_0$.

The probability W_i for excitation of the different states of the KH potential when the field is turned on according to Eq. (17) has been calculated by expanding the solution of the Schrödinger equation in the KH approximation

$$i\hbar\frac{\partial\psi_{KH}}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi_{KH}}{\partial x^2}+V_0\left(x,\frac{eE_0(t)}{m\omega^2}\right)\psi_{KH}(x,t) \tag{18}$$

in the eigenfunctions of the time-independent states $\psi_i^{KH}(x)$ of the KH potential:

$$W_i(t)=|\langle\psi_{KH}(x,t')|\Psi_i^{KH}(x)\rangle|^2. \tag{19}$$

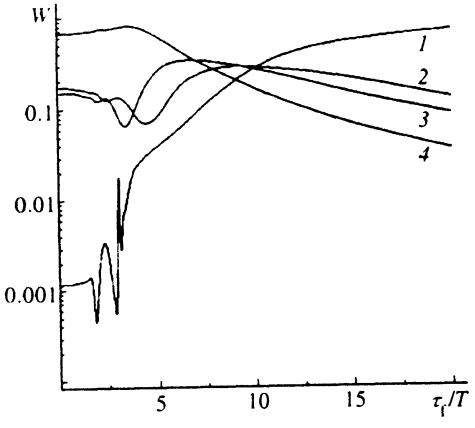


FIG. 6. Probabilities for occupation of the states $i=1,3,5$ in the KH potential (traces 1,2,3, respectively) as functions of the rise time of the pulse, calculated in the KH approximation. Trace 4 is the ionization probability. The radiation intensity is 10^{16} W/cm^2.

The wave functions of the initial state for Eq. (18) was determined by solving the eigenvalue problem for the atomic Hamiltonian.

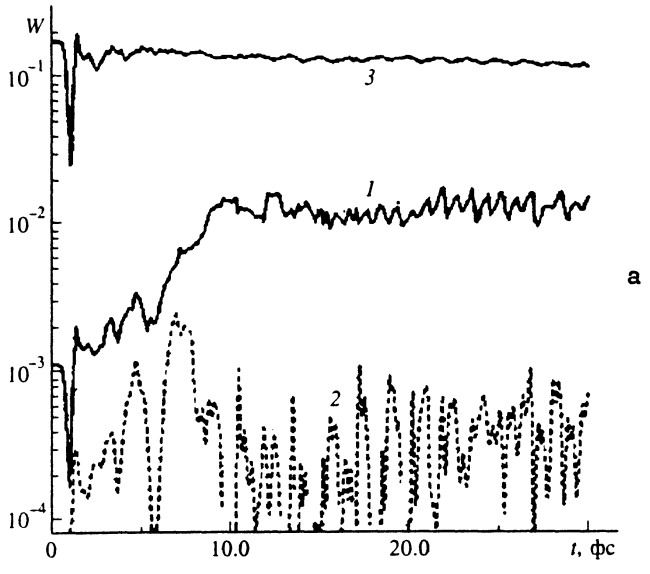
The probabilities for occupation of the states $i=1,3,5$ (characterized by even wave functions) as a function of the rise time τ_f are shown in Fig. 6. For long times τ_f, corresponding to an adiabatically slow increase in the field, the system goes over preferentially to the ground state of the KH potential, and the probabilities for occupation of the other states and for ionization are exponentially small. In the range of values $\tau_f=(2-6)T$ the $W_i(\tau_f)$ curves exhibit resonances, whose origin is not completely clear.

As already noted, when the field is turned on slowly and the harmonics $V_n[x,a_e(t)]$ are not taken into account, Eq. (18) yields erroneous results. The solution of the general equation (4) for the electric field

$$E(t)=E_0(t)\sin\omega t=\begin{cases}\mathbb{E}_0\dfrac{t}{\tau_f}\sin\omega t, & t<\tau_f,\\ \mathbb{E}_0\sin\omega t, & t\geqslant\tau_f\end{cases} \tag{20}$$

allows us to determine the evolution of $\psi_{KH}(x,t)$ when the laser field is turned out as well as the populations of the various KH states in the potential $V_0(x,e\mathbb{E}_0/m\omega^2)$. The time evolution of the three lowest states for $\tau_f=6T$ and $\tau_f=14T$ is shown in Fig. 7. The case $\tau_f=6T$ corresponds to stabilization of the system in the third KH state, while for $\tau_f=14T$ the system goes principally to the ground and first excited states of the KH potential. In the stabilization regime the decrease in the population of the states with $i=1,2$ is accompanied by an increase in the population of the third state.

There is considerable interest in determining the optimum rise time for the laser pulse, corresponding to the greatest probability for $\mathbb{W}=\Sigma_i W_i$ for exciting the set of KH states. Calculations of this quantity for the leading edge of the pulse determined by (20) are given in Fig. 8. The function $\mathbb{W}(\tau_f)$ is nonmonotonic, which is related to the preferential population of the various KH states for different values of τ_f. The absolute maximum, corresponding to $\tau_f=4T$ and $5T$, is determined mainly by the transition of the system to the third



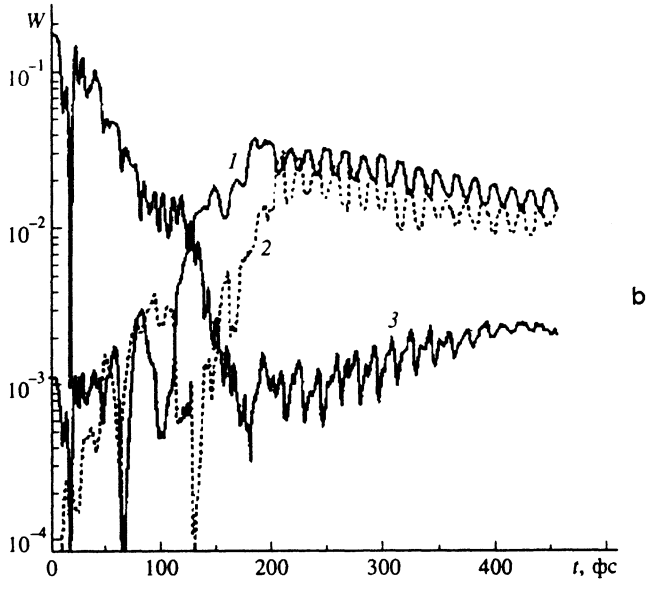


FIG. 7. Time dependence of the population of the three lowest states of the KH potential $V_0(x, eE_0/m\omega^2)$ when the electric field varies according to Eq. (20) for τ_f=6T (a) and τ_f=14T (b). The radiation intensity is 10^{16} W/cm^2.

time-independent state of the KH potential, while the maximum for $\tau_f = 12T$ and $13T$ occurs as a result of the transition to the degenerate states $i=1,2$. The same figure shows the function $\mathbb{W}(\tau_f)$ found in the Kramers–Henneberger approximation (18). In the region $\tau_f \leqslant 4T-5T$ the exact solution and the calculation in the KH approximation agree qualitatively with one another. For long rise times the quantity W calculated in the KH approximation increases, which is related to the adiabatic nature of the increase in the electric field. An exact calculation shows that $\mathbb{W}(\tau_f)$ goes to zero for long times: the ionization takes place before the stabilization regime occurs.

Thus, these calculations show that the optimum pulse rise time is $\simeq$5T. In this case the total probability for population of the time-independent states in the KH potential is 20–25%.

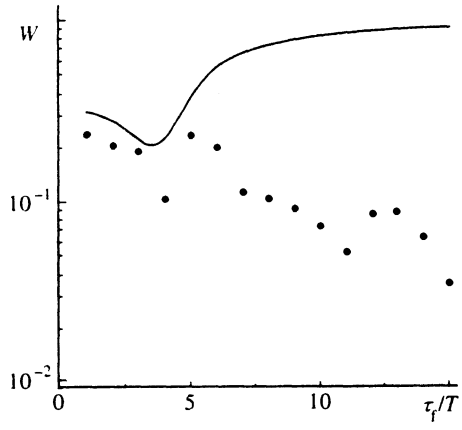


FIG. 8. Probability for excitation of a set of time-independent states in the KH potential as a function of the rise time of the pulse. The solid trace is the calculation using the KH approximation; the points are an exact calculation. The radiation intensity is 10^{16} W/cm^2.

Similar investigations should be carried out also for the trailing edge of the pulse. For the case of a wave field amplitude that falls off linearly one would expect that the system is most likely to return to the bound state of the atomic potential for $\tau_f \simeq 5T$.

7. CONCLUSION

The calculations described in this work show that the stabilization regime in the Kramers–Henneberger model sets in for intensities in the range $\sim 10^{14}$–10^{16} W/cm^2, when somewhat more closely spaced energy states exist in the KH potential. Consequently, we can expect that the mechanism of destructive quantum interference[4,5] and the Kramers–Henneberger model constitute different aspects of the description of an atom in a strong light field.

Under our conditions an increase in the radiation intensity above 10^{16}3 W/cm^2 should result in the loss of atomic stabilization due to the appearance of a relativistic drift effect.[19] This estimate can easily be carried out by comparing the magnetic component $F_M = e/cv\mathrm{H}$ of the Lorentz force (where $v \simeq eE/m\omega$ is the electron velocity) and the intraatomic force $F_A \simeq |V_0|/d$ acting on the electron. In this connection it is impermissible to talk about the effect of stabilization in the dipole approximation in the range of intensities up to 10^{19} W/cm^2 (see, e.g., Ref. 2).

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