Electron photocapture into the bound state of a short-range potential in a strong laser field

E. A. Volkova and A. M. Popov

Nuclear Physics Research Institute, M. V. Lomonosov Moscow State University
(Submitted 31 January 1994)
Zh. Eksp. Teor. Fiz. **105**, 1559–1565 (June 1994)

We examine the scattering of an electron wave packet by a short-range potential in an electromagnetic field by numerically solving the one-dimensional time-dependent Schrödinger equation. We study transitions from the continuum to discrete bound states under the influence of an electromagnetic wave over a wide range of parameters describing the radiation and the electron wave function.

Direct numerical solution of the time-dependent Schrödinger equation for a quantum system in the field of an electromagnetic wave has recently become one of the commonest ways to investigate elementary processes in a laser radiation field. Here the emphasis has principally been on the photoionization of atoms or negative ions—that is, on processes that can be described as a transition from a discrete bound state to the continuum.[1–6] This process can also be reversed so as to consider an electromagnetic field-induced transition from an initial continuum state (or group of states) to a final discrete bound state. Depending on the nature of the potential, such a process amounts either to stimulated photorecombination or stimulated photoattachment of an electron to a neutral atom.

The formation of a bound state of a quantum-mechanical system stimulated by a strong electromagnetic field was addressed in Refs. 7 and 8 using perturbation theory in a study of the induced formation of mesoatoms and mesomolecules, and in resonant atomic scattering of electrons in an external electromagnetic field.

Electron capture into a bound state of some potential in an external electromagnetic field was first studied via direct numerical solution of the time-dependent Schrödinger equation by Grobe *et al.*,[9] who modeled the scattering of an electron by a one-dimensional potential that simulated the negative hydrogen ion H^- (ionization potential ≈ 0.75 eV). They solved for the evolution of an electron wave packet in time and space, and determined the dynamical behavior of the probability of detecting an electron in a bound state. Grobe *et al.*[9] also pointed out the resemblance between the scattering of an electron by a potential in an electromagnetic field and photodissociation: in both cases, the electron wave packet oscillates within the region affected by the potential, leading to transitions among the various states of the discrete and continuous spectrum.

Electron scattering was also considered[8] in a short-range potential subject to a strong laser field, and it was shown that under certain circumstances, in addition to transitions among continuum states (stimulated bremsstrahlung), transitions to discrete states (electron photocapture into a bound state) are also important.

The present paper describes the numerical modeling of electron photocapture into a bound state when the electron is scattered by a short-range potential. We derive the dependence of the photocapture probability on the intensity and frequency of the electromagnetic radiation, and on the initial parameters of the electron wave packet. We compare our results with those of Grobe *et al.*[9]

As in our previous work,[10,11] we have restricted the treatment to a one-dimensional model of electron photocapture into a bound state, with the electron wave packet being scattered by a potential in the presence of an external electromagnetic field. Atomic scattering of the electron is then described by the Schrödinger equation

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x)\psi(x,t)-eE(t)x\psi(x,t), \tag{1}$$

where $V(x)$ is the atomic potential, $E(t)=E_0\cos(\omega t)$ is the electric field due to the electromagnetic wave, and ω is its frequency.

As in Ref. 10, we chose the atomic potential $V(x)$ to be a rectangular well of width $d=2$ Å and depth $V_0=-5$ eV; a well of this size will have a single bound state at $\varepsilon_1=-2.55$ eV. The field intensity of the electromagnetic wave was varied over the range $P=10^{11}$–10^{13} W/cm^2, and the photon energy was $\hbar\omega=2.5$–5 eV. The initial state ($t=0$) was assumed to be a Gaussian wave packet,

$$\varphi_0(x)=\frac{1}{\sqrt{a\sqrt{\pi}}}\exp\left(\frac{i}{\hbar}p_0x\right)\exp\left(-\frac{1}{2}\frac{(x-x_0)^2}{a^2}\right), \tag{2}$$

where p_0 is the mean momentum, a is the packet's half-width, and x_0 is the particle's mean spatial coordinate. Equation (2) describes an electron moving toward positive x at a mean speed $v_0=p_0/m$. Note that the assumed time dependence of the wave electric field strength does not lead to any additional directed velocity over and above v_0. An electron in the state (2) does not have a precisely defined energy: for $p_0\gg\hbar/a$, the mean energy is $\varepsilon_0=p_0^2/2m$.

We have assumed in our calculuations that $\varepsilon_0=1$–8 eV and $a=10$–60 Å. The duration of the scattering process $\tau_s\approx 2a/v_0$ is such that $\omega\tau_s\gg 1$ holds over the full range of both parameters, i.e., the electron interacts with the atomic potential over many periods of the wave field.

We used the finite-element method to solve the Schrödinger equation over a region of size $L=600$–700 Å with a cubic approximation for ψ at each element, following the

 1063-7761/94/060840-04$10.00

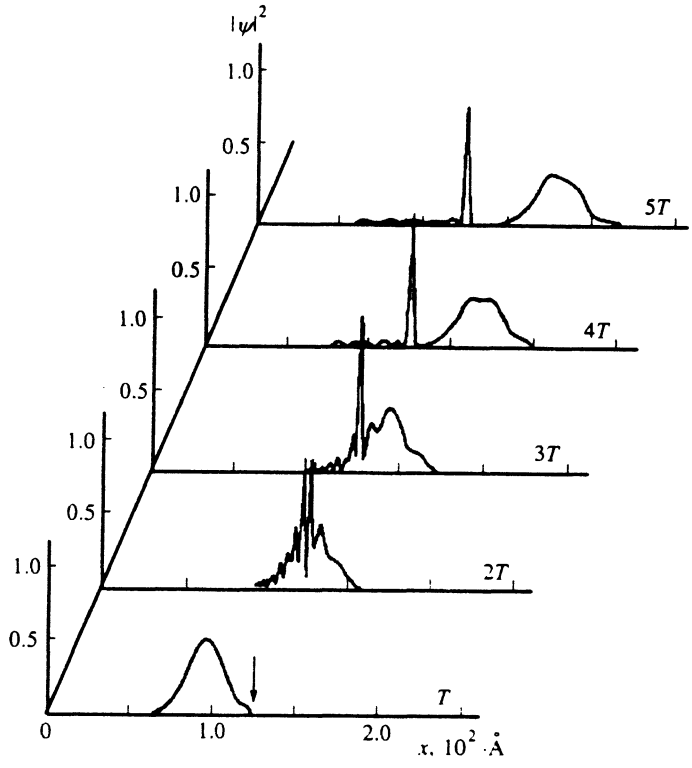

FIG. 1. Space-time evolution of $|\psi|^2$ in electron scattering by a potential in the field of an electromagnetic wave ($\hbar\omega=2.5$ eV, $P=10^{13}$ W/cm^2). Parameters of the initial wave packet are $\varepsilon_0=2$ eV, $a=20$ Å. The arrow indicates the position of the potential well.

approach described in Ref. 11. The computational region was subdivided nonuniformly in such a way that the greatest precision was achieved in calculating the wave function within a region ≈ 100 Å in extent centered on the atomic potential. We artificially attenuated the solution near the boundaries of the spatial grid so as to "eat away" at the wave function and avoid reflections. This made it possible, as required, to study the evolution of an electron trapped in a discrete bound state over times exceeding the electron transit time for the spatial grid, L/v_0. In integrating the equation, the temporal step size ranged from 0.01 to 0.02 of the period of the laser field $T=2\pi/\omega$.

Figure 1 shows the typical evolution in time and space of an electron wave packet scattered by an atom in the field of an electromagnetic wave. The wave packet separates into three parts—a transmitted part, a reflected part, and a part "stuck" in the well. The latter corresponds to the wave function of the bound state in the well. As we noted above, this state has energy -2.55 eV, so photocapture in the present case ($\hbar\omega=2.5$ eV) is accompanied by the emission of two field quanta.

To analyze the numerically modeled solution of the one-dimensional time-dependent Schrödinger equation, we expanded the wave function $\psi(x,t)$ in eigenfunctions of the atomic Hamiltonian. The probability of finding the electron in the bound state of the well is then

$$W(t)=\left|\int \psi^*(x,t)\varphi_1(x)\exp\left(-\frac{i}{\hbar}\varepsilon_1 t\right)dx\right|^2, \qquad (3)$$

where $\varphi_1(x)$ is the eigenfunction of the atomic Hamiltonian corresponding to energy ε_1.

Typical calculated probabilities $W(t)$ for an electron with energy $\varepsilon_0=2$ eV to be captured into the bound state in a field with intensity $P=10^{13}$ W/cm^2 are shown in Fig. 2 for photon energies $\hbar\omega=2.5$ eV and $\hbar\omega=5$ eV. In the case

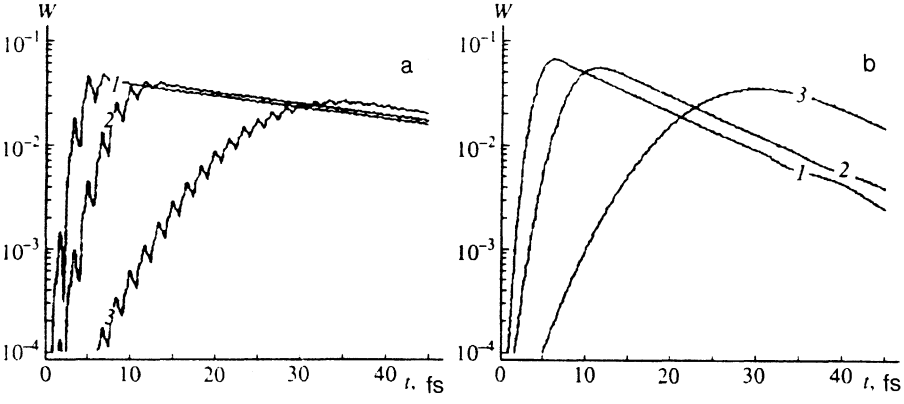

FIG. 2. Probability of electron detection in a bound state as a function of time during potential scattering. Photon energy is a) $\hbar\omega=2.5$ eV or b) $\hbar\omega=5$ eV. The half-width of the initial wave packet is *1*) 10 Å, *2*) 20 Å, *3*) 60 Å. Electron energy is $\varepsilon=2$ eV, and radiative intensity is $P=10^{13}$ W/cm^2.

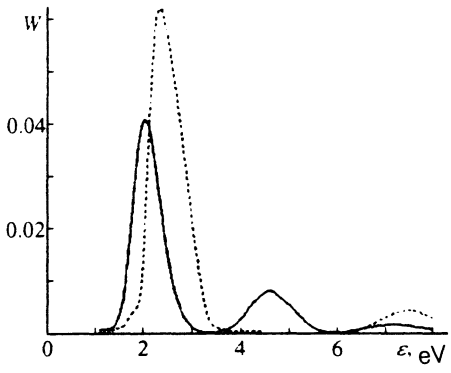

FIG. 3. Probability of photocapture into a bound state as a function of electron energy ($P=10^{13}$ W/cm^2). The continuous curve represents $\hbar\omega=2.5$ eV, the dashed curve $\hbar\omega=5$ eV. The half-width of the initial wave packet is 20 Å.

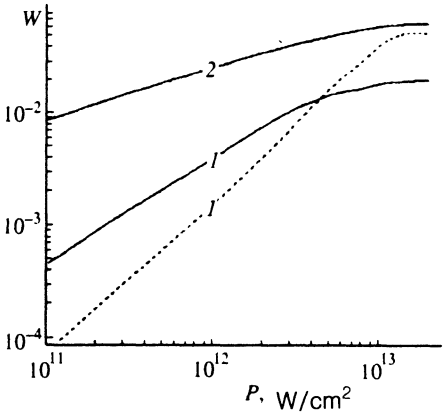

FIG. 4. Probability of photocapture as a function of radiative intensity: *1*) $\hbar\omega=2.5$ eV, *2*) $\hbar\omega=5$ eV. Continuous curve, $\varepsilon=2$ eV; dashed curve, $\varepsilon=2.5$ eV. The half-width of the initial wave packet is 20 Å.

considered, the maximum photocapture probability is $W_0\approx 0.05$–0.06, which is somewhat less than Grobe *et al.*[9] computed in similar fashion for the probability of detecting an electron in a bound state. We believe that the discrepancy is not a fundamental one, but is merely related to the fact that a number of parameters, such as the size of the potential well, the frequency of the laser field, and the resonance energy of the scattered electron, have different values.

After scattering has ceased, W decreases monotonically and exponentially as a result of photoionization, the reverse process, as shown by Fig. 2:

$$\ln W(t)=\ln W_0-\frac{t-t_{\max}}{\tau_d}. \tag{4}$$

Here $t_{\max}$ is the time required for bound-state occupancy to reach its maximum value W_0, and τ_d is its characteristic decay time, which depends on the frequency and intensity of the radiative excitation. For the cases shown in Fig. 2, τ_d is approximately 90 fs for $\hbar\omega=2.5$ eV and 27 fs for $\hbar\omega=5.0$ eV. The estimates indicate that the time scales and their ratio are consistent with photodissociation of the bound state as a result of the one-photon ($\hbar\omega=5.0$ eV) and two-photon ($\hbar\omega=2.5$ eV) photoelectric effect.

Grobe *et al.*[9] derived a time dependence for the probability of detecting an electron in the well after the cessation of scattering that looks much like (4), and that corresponds to $\tau_s\ll\tau_d$. For $\tau_s\gg\tau_d$, the bound state decays more rapidly than it is repopulated, and in the limit $\tau_s\gg\tau_d$, the dynamical behavior of the bound-state population depends on the probability of detecting a scattered electron within the effective range of the potential.[9] Under the conditions considered here, the duration of scattering—over the full parameter range—was less than the photodissociation time, and therefore the bound state decayed exponentially. Oscillations of the bound-state population while a wave packet traverses the potential well are also worth noting. Those oscillations are graphically obvious in Fig. 2a, and are associated with transitions between discrete bound states and a group of continuum states lying an integral number of quanta $\hbar\omega$ higher in energy. Photocapture is then most likely at resonance:[9]

$$\varepsilon=|\varepsilon_1|+n\hbar\omega+\varepsilon_e, \tag{5}$$

where $\varepsilon_e=e^2E_0^2/4m\omega^2$ is the oscillatory energy of an electron in the field of the electromagnetic wave, which shifts the boundary of the continuum, n is an integer equal to $n_{\min}$ or greater ($n\geqslant n_{\min}$), and $n_{\min}$ is the minimum number of photons required to couple a continuum state to a discrete bound state. Under the present conditions, $n_{\min}=2$ for radiation with $\hbar\omega=2.5$ eV and $n_{\min}=1$ for $\hbar\omega=5$ eV. Figure 3 shows the photocapture probability as a function of the energy of the scattered electron ($P=10^{13}$ W/cm^2) for $\hbar\omega=2.5$ eV and 5 eV. Here and below, the figures show the maximum probability of the bound state being occupied, which is attained by the end of the scattering process. The curves display clearcut maxima spaced by $\hbar\omega$ that correspond to the n-photon resonance (5). The peaks for $\hbar\omega=2.5$ eV and 5 eV fail to coincide here, a consequence of the ponderomotive energy that appears in (5). Note that peaks corresponding to the emission of more than $n_{\min}$

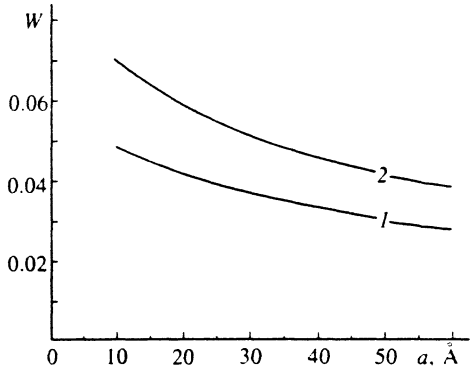

FIG. 5. Probability of capture into a bound state as a function of the half-width of the initial wave packet ($P=10^{13}$ W/cm^2): *1*) $\hbar\omega=2.5$ eV, $\varepsilon=2$ eV; *2*) $\hbar\omega=5$ eV, $\varepsilon=2.5$ eV.

photons are suppressed, since the photon multiplicity parameter $N=\varepsilon_e/\hbar\omega$, which determines the probability of the process,[10,11] satisfies $N<1$ in the present case.

Figure 4 shows the calculated electron photocapture probability as a function of radiative intensity. One characteristic feature of these curves is the saturation of W when the intensity reaches $P\geqslant 10^{13}$ W/cm^2. This saturation is probably related to the rise in photoionization in the electromagnetic radiation field as the discrete bound state becomes populated. The rise in electron oscillatory energy, which leads to a gradual change in the resonance energy given by (5), must also be taken into account. It is precisely this circumstance that has a bearing on the features of the $W(P)$ curves obtained at $\hbar\omega=2.5$ eV and electron energies of 2.0 and 2.5 eV. In the intensity range $P\ll 5\times 10^{12}$ W/cm^2, the oscillatory energy can be neglected, and the 2.5 eV electron energy satisfies the two-photon resonance condition essentially exactly. When the intensity satisfies $P\approx 10^{13}$ W/cm^2, the oscillatory energy is approximately 0.25 eV, thereby reducing the two-photon resonance energy.

It should be pointed out that photocapture in fields much stronger than those considered here, leading to suppression of electron photodissociation in a superstrong optical field, is a problem of interest in its own right.[4-6,12] Such a system undergoes so-called dichotomization of the electron wave function, which can be treated in the Kramers–Henneberger approximation.[13] In a superstrong field, it is therefore more correct to consider photocapture into Kramers–Henneberger states, which determine the stationary states of the atom+electromagnetic field system, an approach taken in Ref. 14. It must be borne in mind, however, that when the Kramers–Henneberger approximation actually describes the stationary states of an atom in an electromagnetic field accurately, photocapture into those states should be completely suppressed. Electron scattering due to atoms in a superstrong field therefore requires further study.

To conclude, we briefly discuss the way in which the electron photocapture probability depends on the extent of the original wave packet. This dependence is shown in Fig. 5 for a Gaussian wave packet with half-width $a=10$–60 Å; the function decreases monotonically over the range $a\gg d=2$ Å. This results from a decrease in the probability of detecting the scattered electron within the effective range of the atomic potential, and a consequent decrease in the transition probability from the continuum to a discrete bound state. In analyzing actual experiments, the simulation results must be averaged over the parameters of individual electron wave packets.

[1] J. Javanainen, J. H. Eberly, and Q. Su, Phys. Rev. **A36**, 3430 (1988).
[2] Q. Su, J. H. Eberly, and J. Javanainen, Phys. Rev. Lett. **64**, 862 (1990).
[3] W. G. Greenwood and J. H. Eberly, Phys. Rev. **A43**, 525 (1991).
[4] R. Grobe and M. V. Fedorov, Phys. Rev. Lett. **68**, 2552 (1992).
[5] R. Grobe and M. V. Fedorov, J. Phys. **B26**, 1181 (1993).
[6] R. Grobe and M. V. Fedorov, Laser Phys. **2**, 265 (1993).
[7] D. F. Zaretskii, V. V. Lomonosov, and V. A. Lyul'ka, Zh. Eksp. Teor. Fiz. **77**, 867 (1979) [Sov. Phys. JETP **50**, 437 (1979)].
[8] A. D. Gazazyan and R. G. Unanyan, Zh. Eksp. Teor. Fiz. **85**, 1553 (1983) [Sov. Phys. JETP **58**, 903 (1983)].
[9] R. Grobe, D. G. Lappas, and J. H. Eberly, Phys. Rev. **A43**, 388 (1991).
[10] E. A. Volkova, A. M. Popov, and O. B. Popovicheva, Fiz. Plazmy **18**, 1558 (1992) [Sov. J. Plasma Phys. **18**, 807 (1992)].
[11] E. A. Volkova, A. M. Popov, and O. B. Popovicheva, Zh. Eksp. Teor. Fiz. **102**, 496 (1992) [Sov. Phys. JETP **75**, 263 (1992)].
[12] E. A. Volkova and A. M. Popov, Zh. Eksp. Teor. Fiz. **105** (1994), in press.
[13] K. Burnett, V. C. Reed, and P. L. Knight, J. Phys. **B26**, 561 (1993).
[14] R. Grobe and J. H. Eberly, Phys. Rev. **A47**, 719 (1993).

Translated by Marc Damashek