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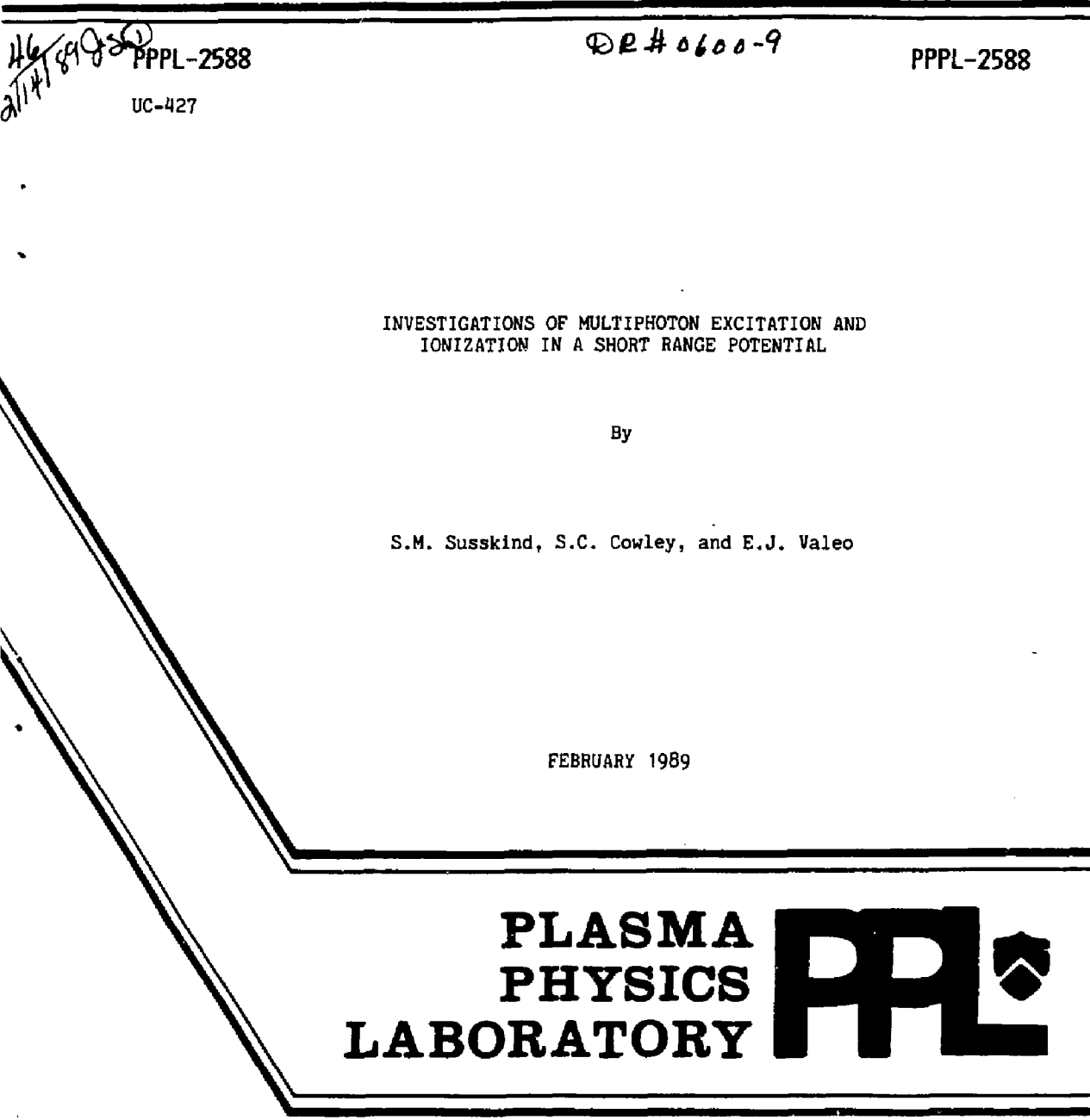
By

S.M. Susskind, S.C. Cowley, and E.J. Valeo

FEBRUARY 1989



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Investigations of Multiphoton Excitation and Ionization in a Short Range Potential*

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Abstract

We introduce an approach to the study of excitation and ionization for a system with a short range potential. In particular, analytical and numerical results are presented for the multiphoton ionization rate, under strong field conditions, of an electron confined by a δ-function potential.

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I. Introduction

Recently, there has been an increase of interest in the study of methods to calculate the excitation and ionization of atoms in the presence of strong electromagnetic fields. This interest stems from the availability in the laboratory of very powerful lasers capable of delivering a focused intensity on the order of and beyond the typical intensity felt by an electron in the atom ($\sim 10^{16}$Watt/cm^2). Such strong fields make the problem of calculating rates non-perturbative in character whereas traditional methods, which are based on a perturbation expansion in the applied field over the atomic field, $F/F_{\rm atom}$, are of limited applicability.

In many of the experiments the photon energy ω (we adopt atomic units everywhere) is much smaller than the typical ionization potential I_p (or the typical energy difference between the atomic levels of interest, ΔE). For instance, for a CO_2 laser $\omega = 0.1$ eV and for a Nd laser $\omega \simeq 1$ eV, but ionization potentials are usually tens of eV. Clearly, one way to proceed is to formulate a theory in which ω/I_p (or $\omega/\Delta E$, for excitation) is treated as small.[1] Note that, for small fields, I_p/ω ($\Delta E/\omega$) is roughly the number of photons involved in the ionization (excitation). This type of approach was pioneered by Keldysh,[2] who studied the ionization of a hydrogen atom. Perelomov, Popov, and Terentev[3] in an alternative way studied the ionization of an electron from a δ-function potential. Several authors[4,5] have studied the excitation of a two-level system when $\omega/\Delta E$ is considered a small parameter. Non-perturbative methods should eventually provide a way of studying the competition between excitation and ionization and understanding the possibility of obtaining in the laboratory population inversions due to multiphoton pumping, between levels with an energy difference in the X-ray region.[6]

In recent experiments on the ionization of atoms the outcoming electron was analyzed in energy.[7,8] Several features like ponderomotive corrections to the ionization potential and above-threshold ionization, where the electron absorbs more than the minimum number of photons necessary for ionization, were observed. These features were already predicted qualitatively in the above-mentioned approaches.

The purpose of the present work is to examine some aspects of the strong field, many-photon limit in a class of models that represents the atom (or energy levels of interest) with model potentials consisting of a sum of δ-functions. The analytic results given here are derived using a new method which is asymptotically correct when the number of photons goes to infinity. The results are quite good, however, for a few photons. We compare some analytic results with direct numerical integration of the equations. The agreement is good.

II. The Model

We will represent our atom by the following binding potential:

$$V(x) = -\sum_{i=1}^{M} B_i\,\delta(x - x_i)\,. \tag{1}$$

$V(x)$ is clearly a short-range potential and has the following properties: 1)The number of bound states that it can have lies between 1 and M (number of δ-functions). 2)It has a continuum spectrum for all energies above zero. 3)By adjusting the parameters B_i and x_i we can make the energy levels of the model coincide with any M levels of a real atom we are interested in studying. We will concentrate here in presenting our numerical and analytical results for the simplest potential of this class, the one δ-function potential ($M = 1$) studied by Perelomov *et al.* This potential has one bound state and a continuum and hence will allow us to study ionization. Detailed derivations of the formulas will be presented elsewhere. We will also relegate the study of the next simpler member of the class of potentials (1), M=2, in which the competition between excitation and ionization already can be studied, to a future publication.

III. Multiphoton Ionization in a Delta function potential

A. Analytical Treatment

We are going to study, then, an electron bound by the potential

$$V(x) = -B\,\delta(x)\,. \tag{2}$$

This potential has only one bound state, of energy $-B^2/2$ ($I_p = B^2/2$), where the electron is going to be at $t = 0$. We will subject this system to the linearly polarized field (we choose to work in the $F \cdot x$ gauge)

$$V_{\rm ext} = Fx\cos(\omega t)\,, \tag{3}$$

F is the amplitude of the applied field (all the expressions will be given in atomic units). Schrödinger's equation for this system is then

$$i\frac{\partial\psi(x,t)}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi(x,t)}{\partial x^2} - B\,\delta(x)\,\psi(x,t) + Fx\,\cos(\omega t)\,\psi(x,t)\,. \tag{4}$$

It proves to be more convenient to work with the following integral form of Eq. (4).

$$\psi(x,t) = \psi_0(x,t) - \frac{i^{1/2}}{\sqrt{2\pi}}\int_0^t \frac{dt'}{\sqrt{(t-t')}}\int_{-\infty}^{\infty} dx'\,\exp[iS_a(x,t;x',t')]\,V(x')\,\psi(x',t')\,. \tag{5}$$

The inhomogeneous term is the wavefunction $w_0(x,t)$ which coincides with the bound state at $t=0$ and which at later times evolves with the Hamiltonian of the electron in the external field only. The factor $\exp(iS_{cl})/\sqrt{2\pi i(t-t')}$ is the Green's function[9] for, and $S_{cl}(x,t;x',t')$ is the classical action of, an electron subject to the potential (3) which starts at x',t' and ends at x,t. In our case $V(x')$ is given by Eq. (2) and then the x' integral is straightforward. Specializing the equation to $x=0$, we obtain an integral equation, now in time only, for $\chi(t)=\psi(0,t)$:

$$\chi(t)=\chi_0(t)-\frac{i^{1/2}B}{\sqrt{2\pi}}\int_0^t\frac{dT}{\sqrt{T}}\exp[iS(t,t-T)]\,\chi(t-T)\,. \tag{6}$$

where $S(t,t-T)=S_{cl}(0,t;0,t-T)$ and is given by

$$S(t,t-T)=\frac{1}{2T}[x_0(t)-x_0(t-T)]^2-\frac{1}{2}\int_{t-T}^{t}d\tau\,\dot{x}_0^2(\tau)\,. \tag{7}$$

$x_0(t)$ is the classical position of an electron subject to the external field only.

Note that we have eliminated in this way the space dependence from the problem. From the solution $\chi(t)$ of Eq. (6), we can reconstruct $\psi(x,t)$ by means of Eq. (5). However, this is unnecessary for computing the ionization rate.

We look for a solution of the integral equation (6) in the eikonal form

$$\chi(t)=\exp\Big[i\int_0^t\Omega(\tau)d\tau\Big]\,, \tag{8}$$

where $\mathrm{Re}\,\Omega(\tau)$ is the eigenvalue of the bound state plus its a.c. shift and $\mathrm{Im}\,\Omega(\tau)$ is half of the instantaneous ionization rate. With this form of the solution we can calculate, basically by a steepest descents method in the complex T-plane, the time-averaged ionization rate w. The assumptions used in the derivation are that the number of photons be large, $B^2/2\omega\gg 1$, and at the same time $\gamma^2\ll$ number of photons, where $\gamma=\omega B/F$ is Keldysh's parameter. The result is

$$\begin{aligned}w=&\frac{2}{\pi}\gamma^2F\sum_{p\geq\nu}k_p^{-1}\Big[\beta^2-\frac{4k_p^2\gamma^4}{B^2}\Big]^{-1/4}\\&\times\exp\Big\{-\frac{B^2}{\omega}\Big[\Big(1-\frac{k_p^2}{B^2}-\frac{1}{2\gamma^2}\Big)v_0-\frac{1}{2\gamma}\Big(\frac{3k_p}{B}v_1-u_1\Big)\Big]\Big\}\times\Big\{1+(-1)^p\\&\times\cos\Big\{\frac{B^2}{\omega}\Big[\Big(1-\frac{k_p^2}{B^2}-\frac{1}{2\gamma^2}\Big)u_0+\frac{1}{2\gamma}\Big(\frac{3k_p}{B}u_1-v_1\Big)+\frac{1}{2}\arctan\Big(\frac{2k_p\gamma^2}{B\beta}\Big)\Big]\Big\}\Big\}\,,\end{aligned} \tag{9}$$

where the u_0,v_0 have the following definitions:

$$u_0=\arccos\sqrt{\frac{\alpha}{2}+\sqrt{\frac{\alpha^2}{4}+\gamma^2}}\,;\quad v_0=\mathrm{arcsinh}\sqrt{-\frac{\alpha}{2}+\sqrt{\frac{\alpha^2}{4}+\gamma^2}}\,. \tag{10}$$

with α defined by $\alpha = 1 - \gamma^2 - k_p^2\gamma^2/B^2$, and u_1, v_1 defined by

$$u_1 = \sqrt{\frac{\beta}{2} + \sqrt{\frac{\beta^2}{4} + \frac{k_p^2\gamma^4}{B^2}}}\,; \quad v_1 = -\sqrt{-\frac{\beta}{2} + \sqrt{\frac{\beta^2}{4} + \frac{k_p^2\gamma^4}{B^2}}}\,. \tag{11}$$

and β defined by $\beta = 1 + \gamma^2 - k_p^2\gamma^2/B^2$.

Note that $k_p^2/2$ is the kinetic energy of the electron ejected by absorbing p-photons which satisfies the energy conservation relation

$$-\frac{B^2}{2} - \frac{F^2}{4\omega^2} + p\omega = \frac{k_p^2}{2}\,. \tag{12}$$

in which $-B^2/2$ is the ionization potential of the atom in the absence of the external field, and $-F^2/4\omega^2$ is the correction to the ionization potential due to the field, the so-called ponderomotive shift.

The sum in formula (9) expresses the fact that the rate is a sum of processes involving the absorption of an integer number p of photons, where $p \geq \nu \equiv B^2/2\omega + F^2/4\omega^3$. This is the so-called above-threshold ionization.[7,8]

If we expand Eq. (9) up to k_p^2/B^2; that is, to first order in the kinetic energy of the ejected electron over the 'bare' ionization potential, we obtain the expression for w due to Perelomov, Popov, and Terentev[3]:

$$w = \frac{2F}{\pi}\frac{\gamma^2}{(1+\gamma^2)^{1/2}}\exp\Big\{-\frac{B^2}{\omega}\Big[(1+\frac{1}{2\gamma^2})\mathrm{arcsinh}\gamma - \frac{1}{2\gamma}\sqrt{1+\gamma^2}\Big]\Big\}$$
$$\times \sum_{p\geq\nu}^{\infty}\Big[1 + (-1)^p\cos\Big(\frac{2Bk_p}{\omega\gamma}\sqrt{1+\gamma^2}\Big)\Big]\frac{1}{k_p}\exp\Big[\frac{k_p^2}{\omega}(\frac{\gamma}{\sqrt{1+\gamma^2}} - \mathrm{arcsinh}\gamma)\Big]\,. \tag{13}$$

The two formulas, Eqs. (9) and (13), are qualitatively the same but differ substantially in cases where the higher terms beyond the first are important; that is, towards the tunneling limit in Keldysh's nomenclature ($\gamma \simeq 1$ or lower).

B. Numerical Treatment

We have developed a code that solves the integral equation (6), by advancing in time the wave function at $x = 0$; that is $\psi(0,t) = \chi(t)$. From it, one could reconstruct the wave function $\psi(x,t)$ using Eq. (5). However, we are only interested here in calculating the average ionization rate. The average decay rate of $|\chi(t)|^2$ is the ionization rate; this can be obtained from a plot of $\ln|\chi(t)|^2$ versus time. The results obtained from the code are compared with the analytic results of Eq. (9) in Figs. 1 and 3 for a variety of cases. In Fig. 1, the logarithm of the ionization rate

w given by Eq. (9) is plotted against the logarithm of the relative field $F/F_{\rm atom}$. The range of intensities in the graph corresponds in hydrogen to $1.6 \cdot 10^{14}\,{\rm W\,cm^{-2}}$ to $1.2 \cdot 10^{15}\,{\rm W\,cm^{-2}}$. The atomic field seen by the electron in the bound state of the potential (2) is $F_{\rm atom} = B^3$. We choose for the calculations a value of $B = 1.59$ a.u., which corresponds to $I_p = 1.27$ a.u. By choosing the photon energy $\omega = 0.5$ a.u., we have that the number of photons necessary to reach the continuum is $\lfloor I_p/\omega \rfloor - 1 = 3$ for small fields (the notation $\lfloor\ \rfloor$ denotes 'integer part of'). As the ponderomotive term $F^2/4\omega^2$ starts to increase by going to higher field amplitudes, we see a dramatic change in the slope of the log-log curve. This change corresponds to the transition from a 3-photon process to a 4-photon process because the field is so high that the corrected ionization potential is larger by one photon energy than the 'bare' ionization potential and the system requires one more photon to ionize. One can verify that the two slopes in Fig. 1 are in a 3 to 4 ratio. The dots in the figure indicate the results of a numerical evaluation of the integral equation (5) to obtain $\chi(t)$. We determine w from the average slope of the plot of $\ln|\chi(t)|^2$ versus t. An example of this kind of plot is shown in Fig. 2. Each dot in Fig. 1 is determined in this way from the $|\chi(t)|^2$ versus t plots for the different values of F. We can see that the comparison between the asymptotic result and the numerical result is very good, even for the small number of photons involved (remember that the analytical result is better the larger the number of photons).

In Fig. 3, we do the same comparison between analytical and numerical ionization rates but for a photon energy of $\omega = 0.25$ a.u. Now, the 'bare' atom needs 7 photons to ionize and, as we can see from the figure, the number of photons needed goes up to 15 for the higher fields in the graph. We can see also a lot of structure due to the change in character, from p to $p-1$ photons, in the ionization with relatively little change in the field. The numerical results reproduce this structure. For the lowest field values, where the ionization rate is so low that an average slope has to be computed over longer running times of the code, the numerical evaluation is inaccurate.

IV. Acknowledgments

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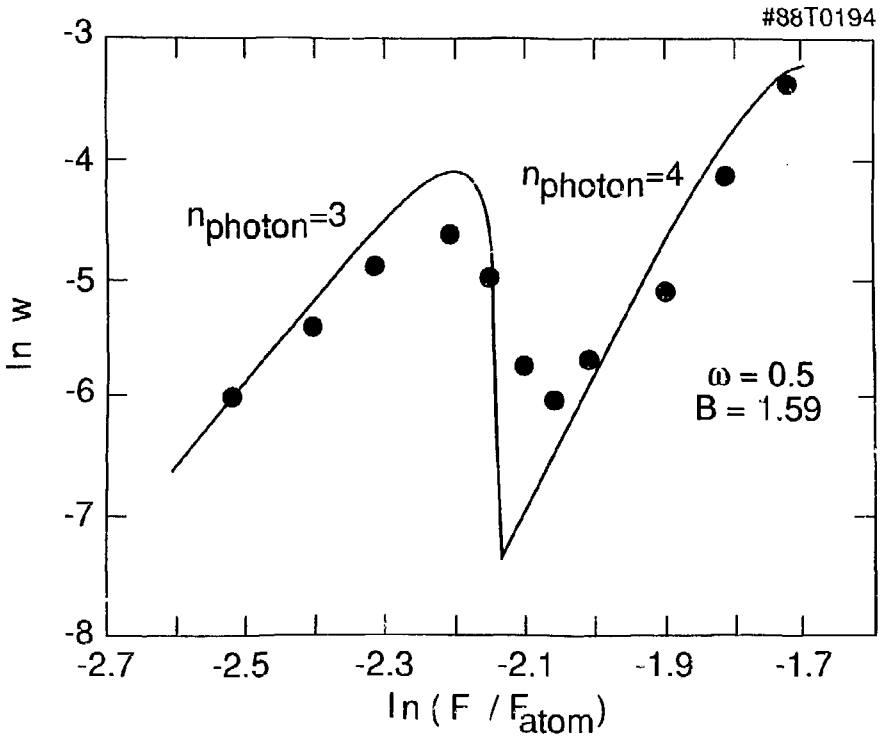
Figures

FIG. 1. Log-log plot of the ionization rate w versus the strength F of the time dependent field normalized to the 'atomic field strength' $F_{atom} = B^3$. The curve is an evaluation of the asymptotic formula Eq. (9). The dots are results obtained from a direct numerical solution of integral Eq. (5). For the parameters chosen, $\omega = 0.5$, $B = 1.59$, substitution into Eq. (12) shows the minimum number of potons required for ionization as $F \to 0$ is 3. As $\ln(F/F_{atom})$ increases beyond $\simeq -2.1$, an additional photon is required because of the increasing 'ponderomotive potential' F^2 [illegible].

FIG. 2. Natural logarithm of $\chi(t)^2$, which is the probability that the electron remains at the origin, versus time t, obtained from a direct numerical solution of Eq. (5).

FIG. 3. Log-log plot of the ionization rate versus the relative field as described in Fig. 1, except that ω has been reduced to 0.25, so that the minimum number of photons required for ionization is now 7 and increases to 15 at the maximum field strength.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-3
-4
-5
-6
-7
-8
ln w
-2.7
-2.5
-2.3
-2.1
-1.9
-1.7
ln (F / F atom)
n photon=3
n photon=4
ω = 0.5
B = 1.59

Fig. 1

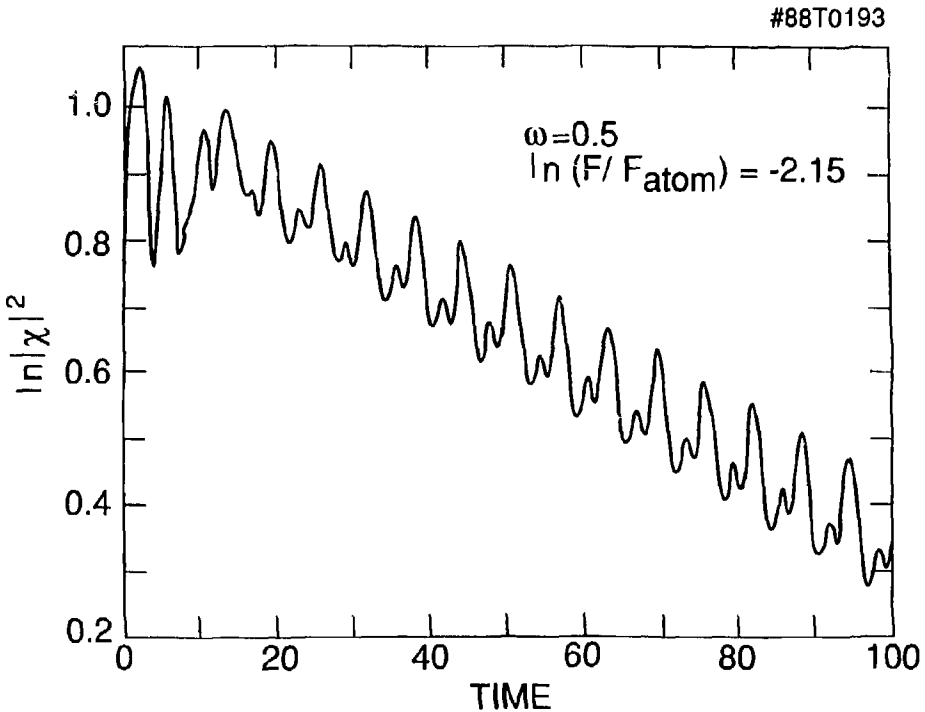
#88T0193
ω=0.5
ln (F/ F_atom) = -2.15
ln|χ|²
1.0
0.8
0.6
0.4
0.2
0
20
40
60
80
100
TIME

Fig. 2

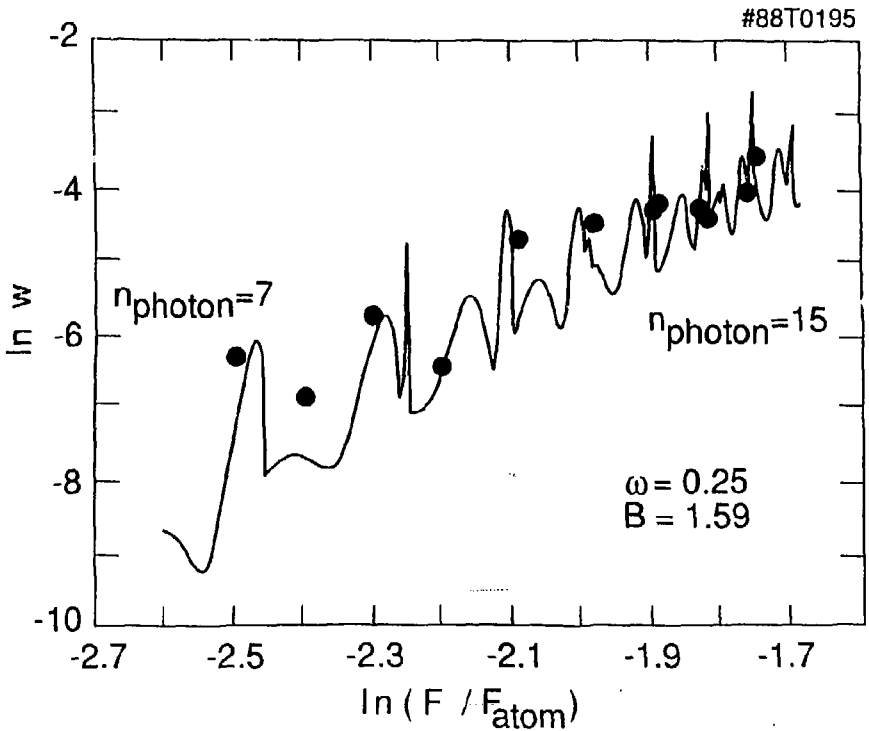
#88T0195
-2
-4
-6
-8
-10
ln w
n_{photon}=7
n_{photon}=15
ω = 0.25
B = 1.59
-2.7
-2.5
-2.3
-2.1
-1.9
-1.7
ln (F / F_{atom})

Fig. 3

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