# First iteration within the high-frequency Floquet theory of laser-atom interactions

M. Marinescu [1] and M. Gavrila [1,2]
[1] *Institute for Theoretical Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138*
[2] *FOM–Institute for Atomic and Molecular Physics, Kruislaan 407, 1098 SJ, Amsterdam, The Netherlands*
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The high-frequency Floquet theory (HFFT) of laser-atom interactions solves the space-translated version of the Schrödinger equation by an iterative procedure, leading to corrections of increasing order in the inverse photon energy. The lowest-order approximation (high-frequency limit) has been often evaluated before, but its accuracy at finite frequencies has not been established. To explore this issue we have computed the corrections yielded by the first-order iteration to the energy levels, and the ionization rates of a one-dimensional atomic model with a Gauss attractive potential. We have then compared, at frequencies above the field-free ionization potential $|W_0|$, the HFFT results with those of a full Floquet calculation. We show that the agreement is substantially improved by the inclusion of the HFFT corrective terms. The agreement is good at all intensities for photon energies larger than several times $|W_0|$. Even when the photon energy is marginally larger than $|W_0|$ the discrepancies vanish at sufficiently high intensities.

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## I. INTRODUCTION

The high-frequency Floquet theory (HFFT) of laser-atom interactions is a version of the Floquet approach specifically adapted to treat the high-frequency $\omega$ case. In addition, the theory is convenient to handle the case of high intensities, of the order of the atomic unit or higher. Originally developed in the contest of laser-modified scattering (by Gavrila and Kaminski [1]), it was thereafter extended to ionization (by Gavrila [2]; see also [3]).

As opposed to the standard Floquet approach, based on the Schrödinger equation for the laboratory frame [4], the HFFT proceeds from the equivalent ''space-translated'' version of the Schrödinger equation [5], pertaining to the oscillating ''Kramers frame.'' A corresponding Floquet system of equations is derived for this frame that yields the complex quasienergies of the atomic states $E=W-i(\Gamma/2)$. As usual, $W$ is interpreted as the energy level of the state and $\Gamma$ as its total ionization rate. The HFFT solves the Floquet system by successive iterations, leading to results of increasing order in $(1/\omega)$. General *a priori* arguments indicate that this iteration procedure should converge at high enough $\omega$ [6]. The lowest approximation (the high-frequency limit) of the theory contributes to $W$ only. The first iteration gives a complex correction $\Delta E^{(1)}$, containing a contribution $\Delta W$ to $W$, and yields the first nonvanishing contribution to $\Gamma$.

The high-frequency limit of the HFFT has predicted an exotic structure for atoms and molecules in superintense fields, e.g., for the hydrogen atom [7], the hydrogen negative ion [8], the hydrogen molecular ion [9]. Ionization rates for the hydrogen atom have been evaluated based on the formula for $\Gamma$ given by the first iteration; this has led to the discovery of ''adiabatic stabilization'' [10]. On the other hand, although the formal expression for $\Delta W$ was derived long ago (see Ref. [2] and Ref. [3], Sec. IV), because of its complexity, no attempt has been made to evaluate it so far. Moreover, the previous results being valid at high frequencies, it was not clear what errors were involved when applying them at the lower, currently available experimental frequencies.

Results from the full Floquet theory have confirmed the HFFT predictions for the energy levels and ionization rates. This was first the case with Floquet calculations done for one-dimensional (1D), short-range potential models: Bhatt, Piraux, and Burnett [11] have used a polarization potential, while Bardsley, Szöke, and Comella [12], and more recently Yao and Chu [13], have used Gaussian potentials. Satisfactory confirmation has come also from three-dimensional (3D) calculations on hydrogen by Dörr, Potvliege, Proulx, and Shakeshaft [14a]; Dörr. Burke, Joachain, Noble, Purvis, and Terao-Dunseath [14b]; and Dimou and Faisal [15]. Although, in both 1D and 3D cases, the frequencies considered were not really high, the agreement was encouraging for the level shifts, but it was only qualitative for the ionization rates. In the latter case the comparison was handicapped by the fact that the Born approximation had been made for the final electron in the HFFT calculation of $\Gamma$, which is a severe limitation at lower electron (photon) energies [16]. Consequently, it was not clear whether the discrepancy for $\Gamma$ was due to the contribution of neglected higher orders in the HFFT or to the Born approximation.

It is therefore of substantial interest to evaluate accurately the first-order correction $\Delta E^{(1)}$ yielded by the HFFT for realistic 3D cases. This would give better quantitative results in the high-frequency, high-intensity regime, where Floquet calculations based on expansions in spherical harmonics encounter convergence problems. Moreover, it should shed light on the convergence of the iteration scheme of the HFFT.

In order to assess the feasibility of this program, we are exploring here the case of a 1D model atom. Such models have yielded valuable information on the physics of laser-atom interactions and on the directions to pursue in full-fledged 3D computations. The field-free potential of our model has been chosen to be of the attractive Gauss form, a prototype of a smooth short-range potential and, to some extent, representative of a negative ion [17]. The same potential has been used by Yao and Chu in their Floquet studies

 

[13] and also by Fearnside, Potvliege, and Shakeshaft in their study of shadow states [18]. The advantage of such a 1D model is that not only can the corrected high-frequency approximation of the HFFT be calculated with relative ease, but even the full Floquet calculation needed for comparison is within reasonable limits of difficulty. For comparing the two calculations we shall consider only energies $\omega$ larger than the unperturbed binding energy of the initial state (single-photon ionization is possible). The alternative case, when several photons are needed for ionization, cannot be handled by the HFFT in its present form and leads to different physics.

In Sec. II we recall the basics of the HFFT and present some developments relevant to our study. In Sec. III we describe the numerical methods used for computing $\Delta W$ and present an algorithm for 1D full Floquet calculations. The results for the energy levels and the ionization rates are given and discussed in Sec. IV. We conclude that the corrections obtained from the first iteration of the HFFT improve substantially the lowest-order approximation of the theory (high-frequency limit).

## II. HIGH-FREQUENCY FLOQUET THEORY DEVELOPMENTS

The HFFT proceeds from the ''space-translated'' form of the Schrödinger equation, which reads, in the 1D case (a.u. are used throughout) [3]

$$[\tfrac{1}{2}P^2+V(x+\alpha(t))]\Psi=i\frac{\partial\Psi}{\partial t}. \tag{1}$$

$V(x)$ is the potential of the unperturbed model-atom problem. For a monochromatic field $\alpha(t)$ can be chosen as

$$\alpha(t)=\alpha_0\cos\omega t, \quad \alpha_0=I^{1/2}\omega^{-2}. \tag{2}$$

The Floquet ansatz is used to find solutions describing steady multiphoton ionization from a state of quasienergy $E$:

$$\psi(x,t)=e^{-iEt}\sum_n \phi_n(x)e^{-in\omega t}. \tag{3}$$

Insertion into Eq. (1) yields the system of coupled equations for the Floquet components $\phi_n$:

$$[\tfrac{1}{2}P^2+V_0-(E+n\omega)]\phi_n=-\sum_m^{m\neq n} V_{n-m}\phi_m, \tag{4}$$

where $V_n(\alpha_0;x)$ are the Fourier components of $V(x+\alpha(t))$. Since $V(x)$ is real and assumed to be even $[V(x)=V(-x)]$, we have

$$V_n(-x)=(-1)^nV_n(x), \quad V_{-n}(x)=V_n(x). \tag{5}$$

These conditions lead to the possibility of finding solutions with (generalized) parity $P=0$ (even) or 1 (odd), defined by $\phi_n(-x)=(-1)^{P+n}\phi_n(x)$ for all $n$.

We are interested in determining resonance state solutions of the Floquet system describing constant rate multiphoton ionization, e.g., see Ref. [3], Sec. III. For a short-range potential and parity $P$, thee are characterized by the resonance (Siegert) boundary conditions

$$\phi_n^P(x)\to\begin{cases} f_n\exp(ik_nx) & \text{for } x\to\infty \\ (-1)^{P+n}f_n\exp(-ik_nx) & \text{for } x\to-\infty, \end{cases} \tag{6}$$

where $k_n=\pm[2(E+n\omega)]^{1/2}$ and $E$ is the complex quasienergy to be determined. The signs of the square roots should be chosen such that

$$\mathrm{Re}k_n>0, \quad \mathrm{Im}k_n<0 \quad \text{for open channels;}$$

$$\mathrm{Re}k_n<0, \quad \mathrm{Im}k_n>0 \quad \text{for closed channels.} \tag{7}$$

HFFT represents a procedure of successive approximations within the full Floquet theory embodied by Eqs. (4)–(7), valid at high frequencies. It is achieved by carrying out successive iterations on the system Eq. (4), each iteration introducing corrections of higher order in $1/\omega$; see Ref. [3], Sec. IV. To *lowest (zeroth) order* in $1/\omega$ (the high-frequency limit $\omega\to\infty$) and at fixed $\alpha_0$ [19], only the component $\phi_0$ of Eq. (3) survives. $E$ and $\phi_0$ reduce approximately to an eigenvalue $W_0$ and an eigenfunction $u_0$ of the Schrödinger equation

$$(H-W_0)u_0=0, \quad H\equiv\tfrac{1}{2}P^2+V_0(\alpha_0;x), \tag{8}$$

which replaces Eq. (4) in this limit. As $W_0(\alpha_0)$ is real, the states of the high-frequency limit are stable (nonionizing). Moreover, $W_0(\alpha_0)$ is independent of $\omega$ at all $\alpha_0$ (intensities). The 3D version of this equation was solved for a number of physical systems [7–9].

At large $\alpha_0$ the eigenstates of Eq. (8) undergo ''dichotomy'' (similarly to the 3D atomic states in a field of linear polarization; see Ref. [7] and Ref. [3], Sec. V). The meaning of this is that, at given large $\alpha_0$, the wave functions of the lower-lying states in the energy spectrum split into two nonoverlapping parts, concentrated around the points $x=\pm\alpha_0$. As a consequence, an even-odd (gerade-ungerade) degeneracy sets in: the lowest-lying even and odd pair of energies coalesce, followed by the next higher-lying pair, etc.

The first iteration of the HFFT yields the *first-order corrections* in $1/\omega$ to the previous result. The correction to $W_0$ is complex and given by [see Ref. [2], Eqs. (38)–(40) and, for more details, Ref. [3], Eqs. (101)–(105)]

$$\Delta E^{(1)}=\sum_{m\neq0}\langle u_0|V_mG(W^{(m)}+i\epsilon)V_m|u_0\rangle, \tag{9}$$

where $G(E)$ is the Green's operator associated to the Hamiltonian Eq. (8); we have denoted $W^{(m)}\equiv W_0+m\omega$. All energies $W^{(m)}+i\epsilon$ lie on the physical sheet of the Green's operator $G(E)$, either on the negative real axis, if $W^{(m)}<0$, or infinitesimally above the positive-energy continuum cut, if $W^{(m)}>0$.

$\Delta E^{(1)}$ can be decomposed as

$$\Delta E^{(1)}=\Delta W-i(\Gamma/2), \tag{10}$$

$$\Delta W=\sum_{m\neq0}\langle u_0|V_m\mathscr{P}[(W^{(m)}-H)^{-1}]V_m|u_0\rangle, \tag{11}$$

$$\Gamma = 2\pi \sum_{m \neq 0} \langle u_0 | V_m \delta(W^{(m)} - H) V_m | u_0 \rangle, \tag{12}$$

where $\mathscr{P}$ and $\delta$ are the principal part and delta operators. $\Gamma$ can also be written as [20(a)]

$$\Gamma = 2\pi \sum_{m>0} \sum_{P} |\langle u^P_{k_m} | V_m | u_0 \rangle|^2. \tag{13}$$

The summation over $m$ should now be performed over all open channels $m>0$. The summation over $P$ extends over the two continuum wave functions $u^P_{k_m}$, with definite parity $P$, belonging to the twofold degenerate energy subspace $W^{(m)}$; they are assumed to be normalized in the energy scale [20(b)].

*A priori* arguments indicate that the HFFT iteration procedure in general, and the equations above in particular, should be valid if the following high-frequency condition is satisfied (see Ref. [3], Sec. IV D):

$$\omega \gg |\bar{W}_0(\alpha_0)|, \tag{14}$$

where $|\bar{W}_0(\alpha_0)|$ is an average excitation energy from the ground state. In general this will be of the order of magnitude of the binding energy of the ground state *in the field* (i.e., at the value of the field at which the ionization takes place). We emphasize that there are no restrictions on $\alpha_0$, as long as condition Eq. (14) is satisfied [21]. It is not clear, however, how large the errors involved actually are at values of $\omega$ satisfying only approximately the condition. Nevertheless, as the energies of all bound states of Eq. (8) vanish in the limit of large $\alpha_0$, it is obvious that the larger $\alpha_0$, the better the HFFT will apply at any frequency.

The high-frequency condition Eq. (14) is confirmed by the fact that, when satisfied, the correction $\Delta E^{(1)}$, Eqs. (9)–(13), is small. For $\Gamma$, Eq. (13), this is due to the increasingly rapid oscillations of $u^P_{k_m}$ as $k_m$ and $\omega$ tend to $\infty$. For $\Delta W$, we shall prove it by extracting the dominant behavior in $(1/\omega)$.

By inserting in Eq. (11) the completeness equation $S_\sigma |u_\sigma\rangle\langle u_\sigma| = I$, we may write

$$\Delta W = \sum_{m>0} \mathscr{P} S_\sigma \frac{2(W_0 - W_\sigma)}{(W_0 - W_\sigma)^2 - m^2\omega^2} \times \langle u_0 | V_m | u_\sigma \rangle \langle u_\sigma | V_m | u_0 \rangle. \tag{15}$$

Based on Eq. (14), this can be approximated by

$$\Delta W \cong \frac{2}{\omega^2} \sum_{m>0} \frac{1}{m^2} S_\sigma (W_\sigma - W_0) \langle u_0 | V_m | u_\sigma \rangle \langle u_\sigma | V_m | u_0 \rangle, \tag{16}$$

provided that the sum $S_\sigma$ converges. By taking into account that $|u_\sigma\rangle$ and $|u_0\rangle$ are eigenstates of $H$, symmetrizing the result, and reusing the completeness equation, we get

$$\Delta W \cong \frac{1}{\omega^2} \sum_{m>0} \frac{1}{m^2} \langle u_0 | [V_m, [H, V_m]] | u_0 \rangle. \tag{17}$$

With $P_x \equiv -i\partial/\partial x$, we have

$$[H, V_m] = -\{P_x V_m\} P_x - \tfrac{1}{2}\{P_x^2 V_m\}, \tag{18}$$

where a curly bracket indicates that the $P_x$ operator it contains acts only on the function inside it. This leads to

$$[V_m, [H, V_m]] = -[V_m, \{P_x V_m\} P_x] = -\{P_x V_m\}^2. \tag{19}$$

Finally,

$$\Delta W \cong \frac{1}{\omega^2} \sum_{m>0} \frac{1}{m^2} \left\langle u_0 \left| \left[ \frac{\partial V_m}{\partial x} \right]^2 \right| u_0 \right\rangle. \tag{20}$$

For the nonsingular potential we are considering, the expectation values contained here are finite and Eq. (20) displays indeed the dominant order of $\Delta W$ with respect to $(1/\omega)$ [22]. Thus, whatever the state $u_0$, $\Delta W \to 0$ as $\omega \to \infty$, and $\Delta W > 0$.

## III. ATOMIC MODEL AND COMPUTATION

The field-free Gauss potential we have considered is [13,18]

$$V_G(x) = -0.270\,35 \exp[-(x/2)^2]. \tag{21}$$

This potential has only one bound state, of energy $W_0(0) = -0.1327$. Its parameters were chosen so as to describe the behavior of the extra electron in the (field-free) $Cl^-$ ion [17].

We have carried out two computations, one to determine the corrected HFFT quasienergies, the other to determine their exact Floquet counterparts. In both cases the Numerov algorithm was applied. As parity is conserved [see Eq. (5)] it is sufficient to consider the interval $x \geqslant 0$ if the adequate parity condition is imposed at the origin.

The *determination of the corrected HFFT quasienergies*, based on Eqs. (10)–(13), requires the evaluation of bound and continuum eigenstates of Eq. (8), as well as of the associated Green's function. Bound-state eigenfunctions were determined by the following procedure. The bounded exponential solution existing in the asymptotic region $x>0$ for a trial value of the parameter $E$ was propagated inward. The necessary and sufficient condition that this solution $u$ be an eigenfunction is that it have parity. By denoting its values at points $x = \pm h$ of the grid, where $h$ is the step, by $u_{\pm 1}$, the parity condition was imposed by requiring that

$$l(E) = 0 \quad \text{where } l(E) \equiv u_{-1} - (-1)^P u_{+1} \ (P = 0,1). \tag{22}$$

$E$ was varied until Eq. (22) was satisfied.

For continuum states $u^P_k(x)$, the integration is started in the vicinity of the origin with the proper parity condition satisfied: $u_{-1} = (-1)^P u_{+1}$. The phase shift $\delta^P_k$ and the normalization constant are then determined by matching asymptotically to the analytical form

$$u^P_k(x) \underset{x \to +\infty}{\to} (\pi k)^{-1/2} \cos\left( kx + \delta^P_k - P\frac{\pi}{2} \right). \tag{23}$$

$u^P_k(x)$ is normalized in the energy scale, as required by Eq. (13) [20(b)]. The computation of $\Gamma$ is straightforward.

We evaluate the level shift $\Delta W$ by applying the Dalgarno-Lewis method [23]. By introducing the notation

$$|\chi_{k_m}\rangle = \mathscr{P}[(W^{(m)}-H)^{-1}]V_m|u_0\rangle, \tag{24}$$

Eq. (11) can be written

$$\Delta W = \sum_{m\neq 0} \langle u_0|V_m|\chi_{k_m}\rangle. \tag{25}$$

The function $\chi_{k_m}$ satisfies the inhomogeneous equation

$$\left[\frac{1}{2}\frac{d^2}{dx^2}-(V_0-W^{(m)})\right]\chi_{k_m} = +2V_m u_0 \tag{26}$$

and boundary conditions following from Eq. (24). The operator $\mathscr{P}[(W-H)^{-1}]$ contained in Eq. (24) is the standing-wave Green's operator

$$\tilde{G}(W) \equiv \tfrac{1}{2}[G(W+i\epsilon)+G(W-i\epsilon)] = \mathscr{P}[(W-H)^{-1}]. \tag{27}$$

The associated Green's function can be expressed in terms of the exact continuum solutions $u_k^P(x)$ of Eq. (8) for energy $W>0$ as

$$\begin{aligned}\tilde{G}(x,x';W) = {} & \pi\tan(\delta_k^0-\delta_k^1) \\ & \times[u_k^0(x)u_k^0(x')-u_k^1(x)u_k^1(x')] \\ & -\frac{\pi}{\cos(\delta_k^0-\delta_k^1)} \\ & \times[u_k^0(x_>)u_k^1(x_<)-u_k^1(x_>)u_k^0(x_<)].\end{aligned} \tag{28}$$

The asymptotic behavior of $\chi_{k_m}$ then follows from Eqs. (24) and (28). Concerning its behavior at the origin, we note that when $\tilde{G}(W)$ is applied to a function of given parity it yields a function of the same parity. As $V_m u_0$ has definite parity [both $u_0$ and $V_m$ have definite parities; see Eq. (5)], this will hold also for $\chi_{k_m}$ and should be implemented at $x=0$.

In the computation of Eq. (25) the sum was truncated by $|m|\leqslant 6$. The accuracy of this truncation depends on $\alpha_0$; the relative error on $\Delta W$ is less than $10^{-6}$ at $\alpha_0=10$, and less than $10^{-3}$ at $\alpha_0=30$.

For the *determination of the full Floquet quasienergies*, we need to solve the (truncated) system of coupled second-order differential equations Eq. (4), which can be cast into the form

$$\left[\mathbf{I}\frac{d^2}{dx^2}-\mathbf{Q}(x)\right]\mathbf{\Phi}(x)=0. \tag{29}$$

Here $\mathbf{\Phi}(x)$ is a column with $N$ components and

$$\mathbf{Q}(x)=2[\mathbf{V}(x)-E\mathbf{I}], \tag{30}$$

where $\mathbf{V}(x)$ is the $N\times N$ matrix

$$\mathbf{V}_{nm}=V_{n-m}(x)-n\omega\delta_{nm}. \tag{31}$$

The solution has a complex character because of the resonance boundary conditions Eq. (6) imposed. The integration was started in the asymptotic region $x>0$, with a set of $N$ linearly independent columns $\mathbf{\Phi}(x)$ satisfying the boundary conditions Eqs. (6) and (7) for a trial value of $E$. The column solutions were propagated inward with the Numerov algorithm. When grouping the columns into an $N\times N$ matrix $\mathbf{\Psi}$, at the $n$th step the linear system of complex equations has to be solved:

$$(\mathbf{I}-\mathbf{T}_{n-1})\mathbf{\Psi}_{n-1}=(2\mathbf{I}+10\mathbf{T}_n)\mathbf{\Psi}_n-(\mathbf{I}-\mathbf{T}_{n+1})\mathbf{\Psi}_{n+1}, \tag{32}$$

where $\mathbf{T}_n=(h^2/12)\mathbf{Q}_n$ and $\mathbf{\Psi}_n$ denotes the value of $\mathbf{\Psi}$ at step $n$. The resonance eigensolution $\mathbf{\Phi}_E(x)$ of Eq. (29) is a linear combination of the columns contained in the matrix $\mathbf{\Psi}$, i.e.,

$$\mathbf{\Phi}_E(x)=\mathbf{\Psi}(x)\mathbf{R}, \tag{33}$$

where $\mathbf{R}$ is a column of constants [24]. However, in order that $\mathbf{\Phi}_E(x)$ be an eigensolution it is necessary and sufficient that it have well-defined parity (as defined in Sec. II). The parity condition can be expressed by the requirement of the vanishing of the column $\mathscr{S}(E)$, defined by

$$\mathscr{S}(E)\equiv\mathbf{\Phi}_{-1}-\mathbf{P}\mathbf{\Phi}_1=(\mathbf{\Psi}_{-1}-\mathbf{P}\mathbf{\Psi}_1)\mathbf{R}=0; \tag{34}$$

here $\mathbf{P}$ is the parity matrix, having only diagonal elements consisting alternatively of $\pm 1$, with the parity of the field-free state in the $n=0$ channel. Equation (34) represents a homogeneous system of linear equations, the compatibility of which yields the condition that $E$ be a quasienergy:

$$\mathscr{E}(E)\equiv\det(\mathbf{\Psi}_{-1}-\mathbf{P}\mathbf{\Psi}_1)=0. \tag{35}$$

Starting from an initial choice, new values of $E$ were selected by a fast optimization library routine until Eq. (35) was satisfied.

Because of the special nature of the resonance boundary conditions Eq. (6), by which some of the Floquet components are increasing exponentially at large $x$, whereas others decrease exponentially, during the propagation of the solution matrix $\mathbf{\Psi}$, its columns tend to become linearly dependent, leading to strong numerical instabilities. In order to avoid them, following Friedman, Jamieson, and Preston [25], we have applied to $\mathbf{\Psi}$ from time to time a Gram−Schmidt orthogonalization procedure, so that the linear independence of its columns remains preserved [26]. Moreover, we have used a Johnson-type [27] rescaling for each column of $\mathbf{\Psi}$ separately. This consists of dividing all elements of the column by the absolute value of its largest component, when larger than some prescribed value (e.g., $10^5$), in order to keep all components within a reasonable range of magnitude. With these refinements our integration method is very stable even at large values of $\alpha_0$ and with a relatively large number of channels. Its only restriction appears to be the computation time, which increases with $\alpha_0$ [because the starting value of $x$ has to be larger than $\alpha_0$, to accommodate for the size of the lobe of $(\Phi_E)_0$ located around $+\alpha_0$, and a larger number of iterations is required]. We have carried out the computations for $\alpha_0$ up to 30 (see Sec. IV) and in some cases up to 40 (not shown).

As for our HFFT calculation, we have routinely limited the number of channels to $|n| \leq 6$, i.e., 13 channels in all. To assess the accuracy of this truncation we have studied the convergence of the values of $E$ as the number of channels was increased to 19 (at this point the calculation becomes rather time consuming). The additional channels included were all open, as the change in $E$ when adding closed channels is quite small in comparison to adding open ones. From this comparison we infer that the relative accuracy of our truncation is better than $10^{-6}$ for both $W$ and $\Gamma$ at $\alpha_0 = 1$ and all $\omega$ considered. At $\alpha_0 = 10$ the errors on $W$ are at the level of 1% or smaller, decreasing with $\omega$, as expected. The error on $\Gamma$ is at the level of several percent ($\Gamma$ is in general much smaller than $W$). The errors are slightly higher at $\alpha_0 = 20$. As a different check on our calculation, we have obtained essentially identical numerical replicas (within accuracies like the ones just mentioned) of our $W_0(\alpha_0)$ curves, shifted by $+\omega$ or $-\omega$ [28].

Finally, we mention that the computation time required to evaluate the HFFT result, Eqs. (8) and (10)–(12), at given $\alpha_0$ is about 10 times shorter than that of the corresponding full Floquet result, Eq. (4). In the HFFT case most of the time is spent for the calculation of the $V_n$, whereas in the full Floquet case this represents a small fraction of the time required by the solution of the differential equations.

## IV. RESULTS AND DISCUSSION

In order to compare the quasienergies given by the corrected HFFT and the full Floquet theory, we have chosen only photon energies larger than the binding energy of the ground state of the field-free potential $\omega > |W_0|$. The values are $\omega = 0.14$, 0.236 (photon energy of the ArF laser), and 0.5. Note that the first value $\omega = 0.14$ is extremely unfavorable for the application of the HFFT according to the high-frequency condition Eq. (14), as it leads, in the absence of the field, to a ratio $R$ of photon energy to binding energy equal to only 1.05. For the other two cases considered, the ratio $R$ is, respectively, 1.78 and 3.8.

Our results for the energy levels $W$ and the total ionization rates $\Gamma$ are contained in Figs. 1–3. As apparent from Figs. 1 and 3(a), although the potential $V_0$ supports only one bound state at small $\alpha_0$, "light-induced" excited states materialize at various ($\omega$-dependent) values of $\alpha_0$. The first two of these states have been found before in Ref. [13] and a study of the appearance of the first one was made in Ref. [18]. The occurrence of light-induced states had, however, been signaled previously, originally for short-range potentials [11,12] and then also for physical systems such as H [14] and $H^-$ [8].

We have found a third light-induced state at $\alpha_0 > 25$; the second and third states are shown for $\omega = 0.236$ in Fig. 3(a). Whereas the ground state is the lowest representative of the even-parity manifold, the first light-induced state is the lowest of the odd-parity manifold. The second induced state has even parity and the third is odd. Note that the lowest even and odd states coalesce energetically at large $\alpha_0$. This is a manifestation of the even-odd degeneracy for the eigensolutions of Eq. (8), mentioned in Sec. II, which in turn is a consequence of the dichotomy of the eigensolutions. Likewise, higher induced states will coalesce in pairs (even and

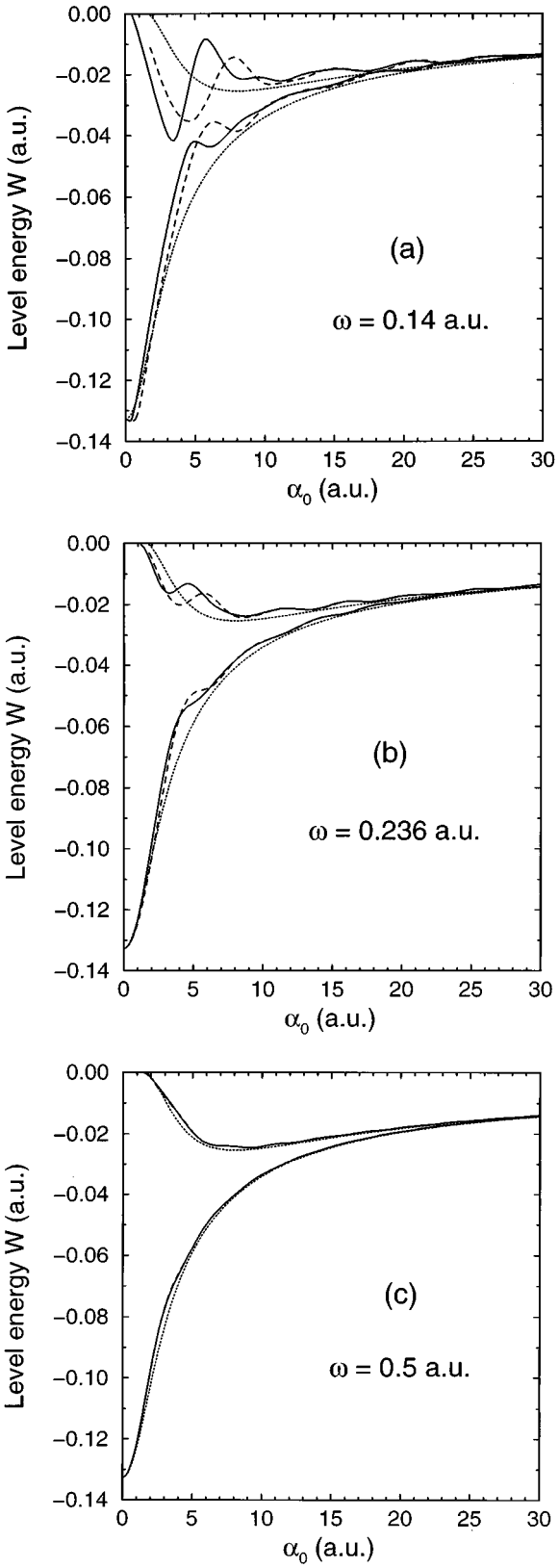


FIG. 1. Energy-level $W$ dependence on $\alpha_0$ at different $\omega$: (a) $\omega = 0.14$ a.u., (b) $\omega = 0.236$ a.u., and (c) $\omega = 0.5$ a.u. Shown are the results of three calculations for the ground state and the first light-induced excited state. Continuous curves: exact Floquet results, from Eq. (4); dotted curves: high-frequency limit results of the high-frequency Floquet theory (HFFT), from Eq. (8); dashed curves: first-order corrected HFFT, from Eqs. (8) and (11).

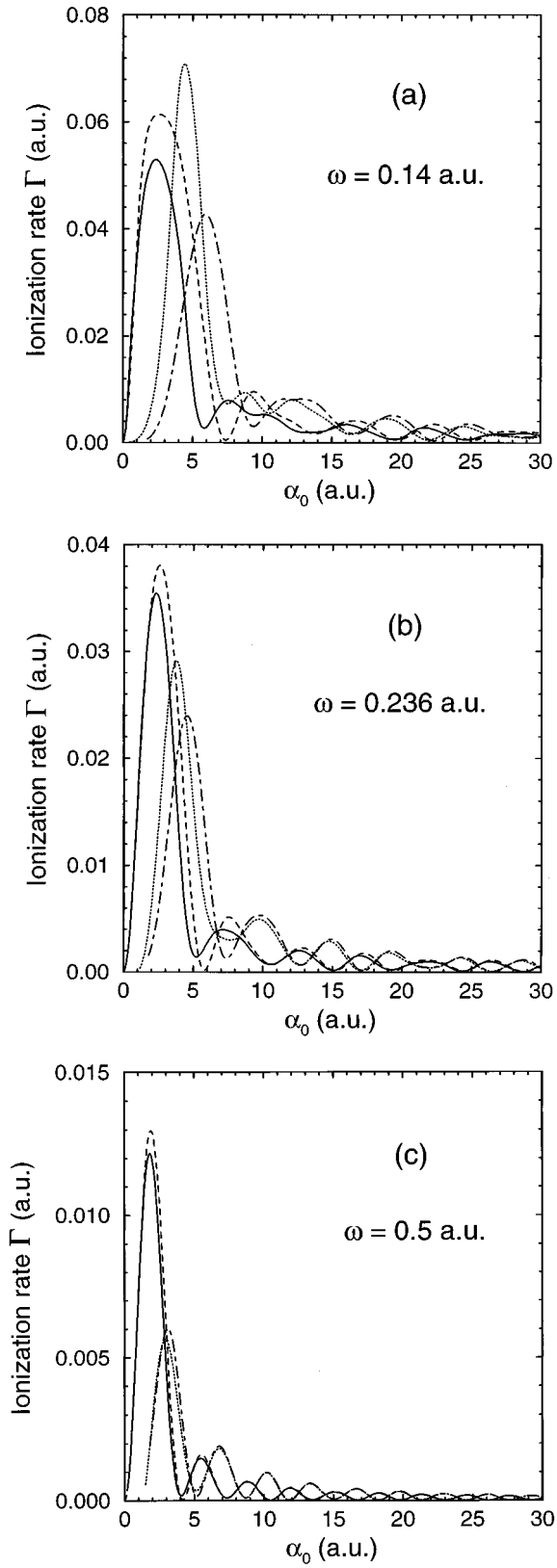


FIG. 2. Total ionization rate $\Gamma$ dependence on $\alpha_0$ for the ground state and the first light-induced excited state, at the same $\omega$ as in Fig. 1. Two curves are shown for each state, the exact Floquet result from Eq. (8) and the lowest-order HFFT result from Eq. (13). Continuous curve: ground state, exact Floquet; dashed curve: ground state, HFFT; dotted curve: excited state, exact Floquet; chain curve: excited state, HFFT.

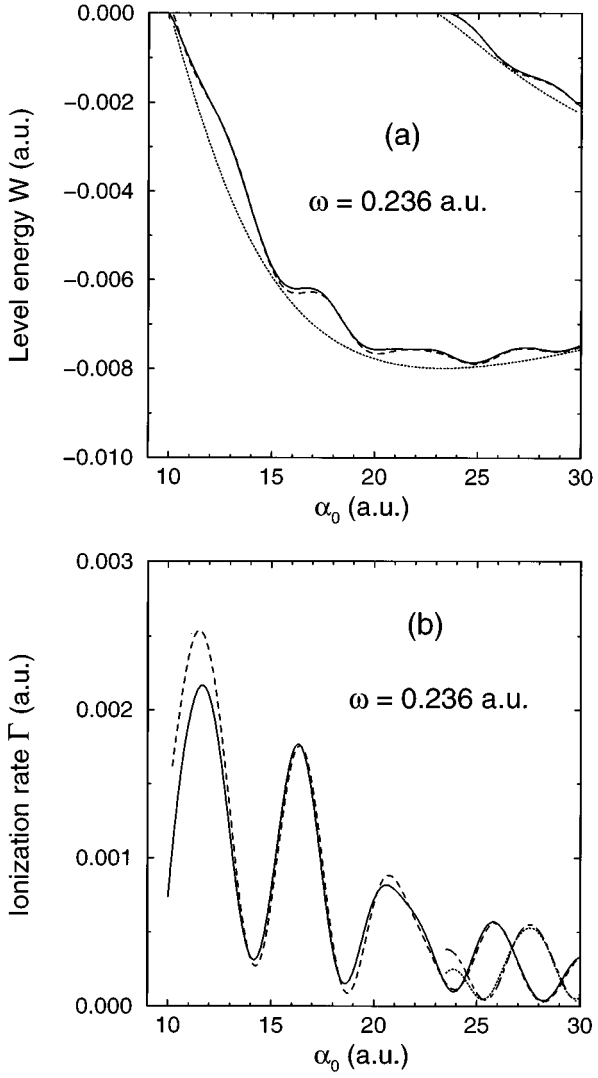


FIG. 3. Results for the energy levels and ionization rates of the second and third light-induced excited states at $\omega = 0.236$ a.u. (a) contains three results for the energy $W$ of each state. Continuous curves: exact Floquet results; dotted curves: high-frequency limit of the HFFT; dashed curves: first-order corrected HFFT. (b) contains two rates $\Gamma$ for each state. Continuous curve: second state, exact Floquet; dashed curve: second state, HFFT; dotted curve: third state, exact Floquet; chain curve: third state, HFFT.

odd); however, for the two states in Fig. 3(a) this happens at higher values of $\alpha_0$ than we have considered.

Figures 1 and 3(a) contain three curves for each of the levels considered: one represents the level according to the high-frequency limit equation [Eq. (8)], the second includes the high-frequency correction $\Delta W$ [Eq. (11)], and the third gives the full Floquet calculation. As apparent, already the high-frequency limit result $W(\alpha_0)$ [Eq. (8)], gives in all cases the global dependence on $\alpha_0$ of the exact Floquet result. Inclusion of the correction $\Delta W(\alpha_0, \omega)$ substantially improves the agreement in that now the corrected energy curve acquires the same undulations as the Floquet result, in some cases shifted in $\alpha_0$, but in others coinciding with the Floquet result.

More specifically, the agreement is enhanced at all $\alpha_0$ by

increasing $\omega$, which confirms the high-frequency character of the theory. On the other hand, for any $\omega$, at large $\alpha_0$ the agreement becomes complete, even if there were discrepancies at lower $\alpha_0$. This is because, as mentioned in Sec. II, the ratio $R$ of the photon energy to the binding energy of the ground state becomes larger. Thus, even in our most unfavorable case $\omega=0.14$, good visual agreement sets in at about $\alpha_0=25$, where $R\cong 8.7$. For $\omega=0.236$ and 0.5 very good agreement sets in for all states in Figs. 1(b) and 3(a) starting at about $\alpha_0=10$, where $R$ is approximately 7.6. For higher frequencies, such as $\omega=0.5$, there is excellent agreement already at $\alpha_0=0$ [28].

Moreover, note that whenever the agreement of the corrected HFFT calculation agrees well with the exact Floquet calculation [i.e., the condition Eq. (14) is well satisfied], both lie *above* the high-frequency limit result given by Eq. (8). This means that $\Delta W>0$, as predicted by Eq. (20).

Figures 2 and 3(b) contain the results for $\Gamma$. For each of the two lowest-lying states we give in Fig. 2 two curves: one is the HFFT result based on Eq. (13), the other the exact Floquet result. Since the HFFT formula used represents the lowest-order approximation within the theory for $\Gamma$, it cannot be expected to fare too well, especially at lower $\omega$. The shape of the curves is, nevertheless, the same for both calculations, although sometimes shifted in $\alpha_0$. Here too the agreement improves with increasing $\omega$ and ends up by being complete at large enough $\alpha_0$.

As has been noted before [13], this model displays stabilization against ionization, similarly to that found in the 3D case of the hydrogen atom [10,3]: $\Gamma$ tends to zero as $\alpha_0$ increases, albeit in an oscillatory manner. The reasons for the oscillatory behavior here, and its absence in the 3D case, were discussed in Ref. [13]. We agree with that analysis, but we conclude that this is a feature of 1D models (it exists also in the case of the "soft" Coulomb potential) and shall not pursue the issue further.

In Fig. 4 we compare at $\omega=0.236$ the HFFT result Eq. (13) for $\Gamma$, the corresponding Born approximation, and the exact Floquet result. [The HFFT Born approximation is obtained by replacing in Eq. (13) $u^P_{k_m}(x)$ by the asymptotic form Eq. (23) with $\delta^P_k=0$.] As apparent, the Born approximation worsens the agreement of the HFFT result with the exact Floquet result, in particular at large $\alpha_0$ [30]. We therefore expect that future HFFT calculations of $\Gamma$ for atomic hydrogen, done without the Born approximation, will substantially improve the agreement with the full Floquet calculations of Refs. [14] and [16].

On the example of this model we now comment on the capability of the full stationary Floquet theory to describe physical situations (i.e., agree with wave-packet dynamics). It has been emphasized that a necessary condition is that the value of $\Gamma$ be sufficiently small (see Ref. [31] and Ref. [3], Sec. III B) such that $\Gamma \ll W^{(N)}$, where $W^{(N)}$ is the kinetic energy of the slowest ionized electron ($N$ is the minimal number of photons required for ionization, in our case $N=1$). This is required in order that the asymptotic channel momenta $k_n$ ($n\geqslant N$) in Eq. (6) be quasireal and hence quasiobservable. From Figs. 1(b), 1(c), 2(b), and 2(c), it follows that the condition is fairly well satisfied for the ground state at $\omega=0.236$ and 0.5 and for $\alpha_0$ outside the interval $0.5<\alpha_0<5$, where $\Gamma$ has its largest maximum; however, even on this interval $\Gamma$ is smaller than $W^{(1)}$. For $\omega=0.14$, on the other hand, $\Gamma$ becomes larger than $W^{(1)}$ around $\alpha_0=2$ [see Figs. 1(a) and 2(a)] and therefore Floquet theory becomes totally inadequate in this vicinity. Nevertheless, it is plausible that even under these circumstances (when no constant ionization rate can be defined), the lifetime calculated according to $\tau=(1/\Gamma)$ will be indicative of that obtained from wave-packet dynamics. Note that all light-induced states materialize in this model with rather small $\Gamma$ (long lifetimes), such that the condition for the validity of the Floquet description is fairly well satisfied [32]. For a physical system in this situation this would imply that the light-induced state would be apt to leave an observable signature in selected experiments.

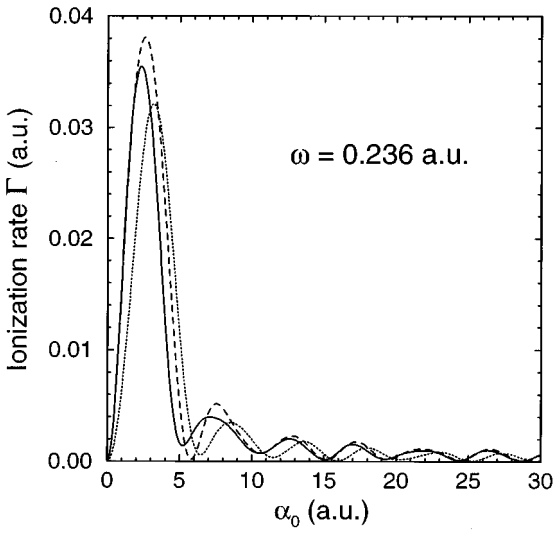


FIG. 4. Comparison of $\Gamma$ values for the ground state at $\omega=0.236$ a.u. according to the Born approximation of the HFFT result (dotted curve), the unapproximated HFFT result (dashed curve), and the exact full Floquet result (continuous curve).

We finally consider the numerical accuracy of our computation, by comparing it to those of Yao and Chu [13] and Fearnside, Potvliege, and Shakeshaft [18], at $\omega=0.236$, a case considered also by these authors. Our results agree well at the graphical level, with those in Figs. 2–4 of Ref. [13] for $W$ and $\Gamma$. Some numerical results were given in Table I of Ref. [13] for $\Gamma$ that can be compared to ours. For $\alpha_0=2.25$, 5.25, 7.0, 10.4, and 12.7, we find, respectively, $\Gamma=3.5384\times10^{-2}$, $1.3844\times10^{-3}$, $3.9526\times10^{-3}$, $7.3553\times10^{-4}$, and $2.0155\times10^{-3}$. The agreement is to within less than 0.1% for the first value, but only to within about 2% for the following ones [33]. Also, the agreement with Fig. 1 of Ref. [17], representing the case of small values $\alpha_0$, is good at the graphical level.

*In conclusion*, our investigation of the first iteration within the high-frequency Floquet theory has shown that the correction it yields to the energy levels of the lowest-order approximation (high-frequency limit) substantially improves the agreement with the exact Floquet result at lower frequencies. This illustrates the potential of the HFFT and is an incentive to calculate the correction for the realistic case of one-electron atoms, where a larger-scale computation is

needed, but nevertheless simpler than a full-fledged Floquet calculation.

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[19] Recall that in the HFFT, $\omega$ and $\alpha_0$ are independent parameters.

[20] (a) Equation (13) is the 1D analog of Eq. (113) of Ref. [3]. (b) For continuum normalization in the energy scale see E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1970), Chap. 6, Sec. 3.

[21] The condition $\alpha_0^2\omega \gg 1$, mentioned in Ref. [1] and reproduced by others [e.g., K. Burnett *et al.*, J. Phys. B **26**, 561 (1993)], has proven to be superfluous.

[22] The argument fails in the case of the 3D hydrogen atoms in a field of linear polarization. There the procedure would lead to an equation similar to Eq. (20), but containing the average of $(\nabla V_m)^2$. Because all $V_m$ for the Coulomb case behave like $r^{-1/2}$ in the neighborhood of the points $\pm\alpha_0\mathbf{e}$ (where $\mathbf{e}$ is the polarization vector), the averages are divergent. This means that the order of $\Delta W$ is higher than $\omega^{-2}$; it is, in fact, $\omega^{-2}\ln^2\omega$; see Ref. [3], Sec. IV D.

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[29] This was to be expected as, at small $\alpha_0$ and sufficiently high $\omega$, the HFFT results agree with those of the lowest-order perturbation theory which, on the other hand, agrees with Floquet theory.

[30] It is known that the Born approximation gives larger errors for the ionization amplitudes when Coulomb-tail potentials are involved [such as $V_0$ for the hydrogen atom; see Ref. [10(a)]] than in the case of short-range potentials; e.g., see J. G. Cordes

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[33] This is possibly due to a different truncation of the Floquet system in the two calculations. Our calculation was done with 13 channels, symmetrically disposed with respect to $n=0$ (i.e., $|n|\leqslant 6$), whereas that in Ref. [13] was done with up to ten (unidentified) channels.