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Ionization by an Oscillating Field: Resonances and Photons

To the memory of Pierre Hohenberg

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Abstract

We describe new exact results for a model of ionization of a bound state in a 1d delta function potential, induced by periodic oscillations of the potential of period $2\pi/\omega$. In particular we have obtained exact expressions, in the form of Borel summed transseries for the energy distribution of the emitted particle as a function of time, ω and strength α of the oscillation of the potential. These show peaks in the energy distribution, separated by $\hbar\omega$, which look like single or multi-photon absorption. The peaks are very sharp when the time is large and the strength of the oscillating potential is small but are still clearly visible for large fields, and even for time-periods of a few oscillations. These features are similar to those observed in laser induced electron emission from solids or atoms (Phys Rev Lett 105:257601, 2010). For large α the model exhibits peak-suppression. The ionization probability is not monotone in the strength of the oscillating potential: there are windows of much slower ionization at special pairs (α, ω). This shows that ionization processes by time-periodic fields exhibit universal features whose mathematical origin are resonances which pump energy into the system represented by singularities in the complex energy plane. All these features are proven in our simple model system without the use of any approximations.

Keywords Ionization · Schroedinger equation

1 Introduction

When light of frequency ω shines on a metallic surface or on a gas of atoms one observes the emission of electrons. This photo-electric effect is generally described to leading order along the lines in which Einstein first explained the phenomena in 1905 [1,2]: an electron absorbs n photons, thought of as "localized light particles", acquiring a kinetic energy $K = n\hbar\omega - E_b$,

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where E_b is the minimum energy necessary to eject the bound electron from the metal or atom.

To study the ionization process quantitatively elucidating its dependence on the parameters of the field and of the target, one generally does computations "semi-classically" c.f. [2–9]. That is, one considers the electromagnetic field produced by the laser as a continuum non-quantized field; see however [10–15]. The emission process is described by the time-dependent solutions of a time-dependent non-relativistic Schrödinger equation

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = (H_0 + V(x,t))\psi. \tag{1}$$

Here H_0 describes the Hamiltonian of the reference system, e.g. a hydrogen atom, with both bound and free states and $V(x,t) = V(x, t + 2\pi/\omega)$ represents a classical oscillatory field, started at $t = 0$. The latter is represented as a vector potential or, in the length gauge, a dipole field, e.g. $V(x,t) = e\,E \cdot x\, \sin \omega t$ [4,13].

Starting with an initial state $\psi(x, 0) = u_b(x)$, a bound state of H_0 with energy $-E_b$, $\psi(x,t)$ is then represented as a superposition of the initial bound state and of the generalized eigenstates of H_0 with momentum $\hbar k$, $u(k, x)$, i.e. asymptotically free scattering states of the emitted electron:

$$\psi(x,t) = \theta(t) e^{iE_b t} u_b(x) + \int_{\mathbb{R}^d} \Theta(k,t) u(k,x) e^{-i\hbar^2 k^2 t/2m}\, dk \tag{2}$$

where d is the spatial dimension of the system and we have assumed that there is only one (relevant) bound state.

The different terms in (2) specify the states of the system at $t \geq 0$: $|\theta(t)|^2$ is the probability at time t that the particle is still in its bound state and $|\Theta(k,t)|^2$ is the probability density of finding the ionized electron in the (quasi) free state with momentum $\hbar k$ and energy $\hbar^2 k^2/2m$. The unitarity of the evolution then gives $|\theta(t)|^2 + \int_{\mathbb{R}^d} |\Theta(k,t)|^2 dk = 1$.

When $\hbar\omega > E_b$, first order perturbation theory in the strength of V (used very judiciously) yields, for "long times", emission into states $u(k, x)$ with $\hbar^2 k^2/2m + E_b = \hbar\omega$. This is interpreted as representing the absorption of one photon even though it is known that perturbation theory is not valid for "very long times".

The clever use of first order perturbation theory also yields Fermi's golden rule of exponential decay of $|\theta(t)|^2$ from the initial bound state. To deal with the case of transitions caused by "n photons", which one observes as "peaks" in noisy emission data [1], one needs in principle to go to n'th order perturbation theory. This is very complicated, so it is almost never attempted in practice. Instead one uses the so called strong field approximation due to Keldysh and others [1,7,8]; see e.g. the analytical results in [16]. These are basically uncontrolled approximations which however give qualitative good results. For $\alpha = m\omega$ with m integer, usual quantum mechanics perturbation theory does not apply and $|\theta(t)|^2$ has power-law decay.

Description of the model To gain a clearer picture of how resonances from a time-periodic potential give rise to peaks in the emitted energy distributions which look similar to n photon absorption, it is desirable to obtain an exact solution of the Schrödinger equation for arbitrary t, ω and strength of V. To this end we investigated in [17] and [18] a very simple 1d model system with $H_0 = -\frac{\partial^2}{\partial x^2} - 2\delta(x)$ and $V(x,t) = -2\alpha \sin(\omega t)\delta(x)$ leading to the time dependent Schrödinger equation

$$i\psi_t = -\psi_{xx} - 2\,(1 + \alpha \sin \omega t)\; \delta(x)\, \psi \tag{3}$$

where we use units $\hbar = 2m = 1$.

The Hamiltonian H_0 has a single bound state $u_b(x) = e^{-|x|}, \quad x \in \mathbb{R}$, with energy $-E_b = -1$, and continuum states

$$u(k,x) = \frac{1}{\sqrt{2\pi}}\left(e^{ikx} - \frac{e^{i|kx|}}{1+i|k|}\right), \quad x, k \in \mathbb{R} \tag{4}$$

The attractive δ function in H_0 might imitate the potential seen by an electron in a negative ion and and has been studied extensively before [19–21].

The oscillatory part is, however, distinct from an oscillatory electromagnetic field with a dipole-type potential, in particular we have no tunneling. Nevertheless, as already noted, our model yields results on the ionization rates and energy distributions of the emitted particles which are similar to those produced by more realistic $V(x,t)$ and seen in numerical experiments [3].

In [17] $\theta(t)$ was proven to go to zero as $t \to \infty$. Its form for small α was obtained by a combination of analytic results and numerics, and shown to have many features similar to those obtained experimentally for the ionization of hydrogen-like atoms in a microwave electric field. There was however no computation of $\Theta(k,t)$. In this paper we present the physical content of new results for these quantities obtained via new techniques described in [18]. These show rigorously, for the first time we believe, resonances in the energy distribution $|\Theta(k,t)|^2$ which correspond to multiphoton absorption for both short and long times. They also show existence of regions in the (α, ω) parameter space where the decay of $|\Theta|^2$ is of power type for physically relevant times. These are based on exact expressions in the form of multi-instanton expansions [18].

While this model is clearly a caricature of reality, both as far as H_0 and V are concerned, exact solutions of toy models often bring out underlying universal features which explain real behavior. We believe this to be the case here.

The underlying mathematical structure of ionization by an oscillating field shows poles and branch points in the complex energy plane which give rise to resonances that look like photons. These singularities yield a complex behavior of the survival probability. For a generic amplitude and frequency this probability decays exponentially for a long time, eventually switching to a power law. Surprisingly, many features are clearly visible even after a few periods, see Fig. 5.

The motion of singularities in the complex plane as the parameters change leads to what we will call "windows of stabilization", ranges of α, ω in which ionization is substantially slowed down. The mechanism is possibly distinct from the large laser pulse stabilization described in [22]. The model also exhibits subexponential decay for special parameters and other unexpected phenomena, see below. This phenomenon is mathematically explained at the end of the next section.

2 Results

Using the Laplace transform of Θ, $\hat{\Theta}(k,p) = \mathcal{L}(\Theta) = \int_0^\infty \Theta(k,t)e^{-pt}dt$, it was shown in [18] that the functions $\Theta(k,t)$ and $\theta(t)$ have Borel summable transseries (multi-instanton) expansions in t valid for all $t > 0$, for all α, ω. The transseries for Θ has the form

$$\Theta(k,t) = \Theta(k,\infty) + \sqrt{\frac{2}{\pi}}\frac{|k|}{1-i|k|}e^{i(1+k^2)t}\sum_{n\in\mathbb{Z}}\left(r_n e^{p_n t} + e^{-in\omega t}\sum_{j\geq 3}\frac{c_{nj}}{t^{j/2}}\right) \tag{5}$$

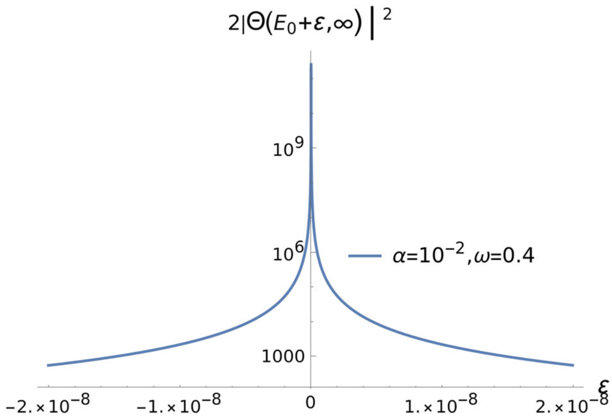


Fig. 1 Three-photon ionization: log-plot of $2|\Theta(k,\infty)|^2$ as a function of $\varepsilon = k^2 - E_0$, $E_0 = 0.1999\ldots$, where $\omega = 0.4$, $\alpha = 0.01$

where $p_n = -\gamma + in\omega$, $\gamma > 0$, $n \in \mathbb{Z}$. This corresponds to an array of poles of $\hat{\Theta}(k, p)$ in the left half p-plane (the energy space rotated by $\frac{\pi}{2}$) at distance γ from the imaginary line. The poles represent resonances and the residues are Gamow vectors [23,24].

Also

$$\Theta(k,\infty) = \frac{i}{\sqrt{2\pi}} \frac{|k|}{1 - i|k|} \left[1 + i(1+k^2)\hat{\theta}\left(-i(1+k^2)\right)\right] \tag{6}$$

where $\hat{\theta} = \mathcal{L}(\theta)$ and $k^2 = E$ is the energy of a particle with wave vector k.

For small α and $\omega > 1$, $\Theta(k, t)$ has the explicit leading order

$$\Theta(k,t) = \frac{(2\pi)^{-\frac{1}{2}}|k|\alpha}{i|k| - 1} \left[\frac{2\omega + ip_0}{(1+k^2+\omega)(1+k^2-\omega-ip_0)} \right. \\ \left. + \frac{e^{-i\omega t} e^{(p_0+i+ik^2)t}}{1+k^2-\omega-ip_0} - \frac{e^{i\omega t} e^{(p_0+i+ik^2)t}}{1+k^2+\omega-ip_0}\right](1+o(\alpha)) \tag{7}$$

It follows that, for $\alpha \to 0$, after $t \to \infty$, Θ becomes a delta function at $k^2 = \omega - 1$. There is a similar behavior for $\omega < 1$, the delta function now occurring at $k^2 = m\omega - 1$, where m is the smallest integer such that $m\omega > 1$. This is illustrated in Fig. 1 where we display the very sharp peak for $\alpha = .01$, $\omega = .4$ (so $m = 3$). There is a (Stark) shift of order $\alpha^2 = 10^{-4}$. The shape is close to a Lorentzian.

There are also other sharp peaks in $2|\Theta(k,\infty)|^2$ for small α, located close to energies $E = n\omega - 1$, $n \geqslant m$. This is shown in Fig. 2 where we also see that the peaks for $(n+1)\omega$ are smaller than those for $n\omega$ by a factor of α^2.

For larger α, in Fig. 3 we show $2|\Theta(k,\infty)|^2$ for $\omega = .51$, $\alpha = 1$. The peak near zero corresponds to 3-"photon" ionization: because of the Stark shift we do not see the 2 photon peak. Because of this and the prefactor $\frac{k^2}{k^2+1}$ in the probability, the first peak gets suppressed; in realistic experiments this phenomenon is called "peak suppression" [1].

Despite the Stark shift the spacing between the peaks remains close to ω. The fact that α is large permits us to see that many peaks: one can distinguish peaks corresponding up to 8-photon absorption. As we see from Figs. 3 and 4, these peaks are of comparable magnitude when α is large.

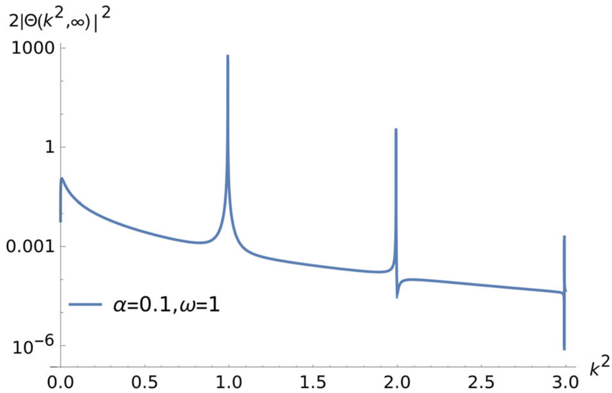


Fig. 2 Energy spectrum for $\omega = 1$ and $\alpha = 0.1$

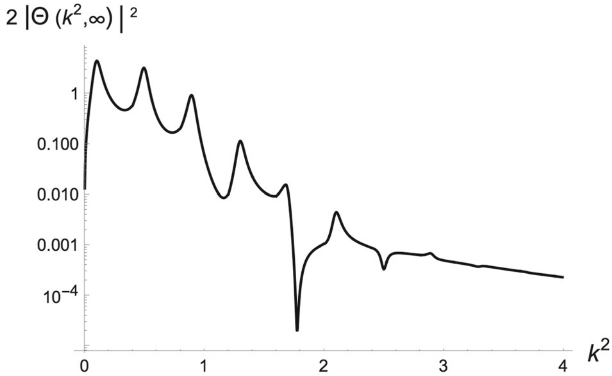
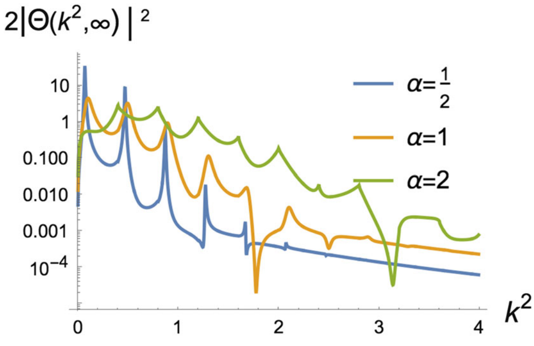


Fig. 3 Log plot of $2|\Theta(k, \infty)|^2$ as a function of $k^2 = E$ for $\alpha = 1$ and $\omega = 0.51$

Fig. 4 Log plots of $2|\Theta(k, \infty)|^2$ as a function of $k^2 = E$ for $\omega = 0.5$ and $\alpha = 1/2, 1, 2$



As α increases even further, the poles move away from the imaginary line, hence the peaks flatten, and power law decay becomes dominant. This is seen in the log plots in Fig. 4 showing how the peaks broaden when α gets large: they essentially disappear for $\alpha \gtrsim 3$. Here too we see that the distance between the peaks is almost independent of α. This is also seen in Fig. 5, where for finite times the peaks broaden and get smaller. They are however still visible when t is of the order of a few periods. The reason for this is that for t not too

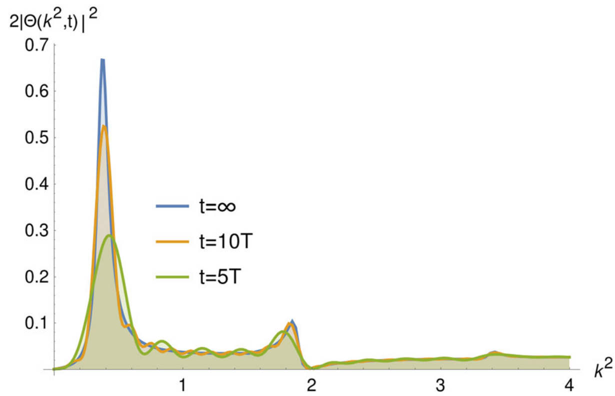


Fig. 5 $2|\Theta(k,t)|^2$ as a function of k^2 for $\omega = 1.51$, $\alpha = 0.5$ at $t = 5T, 10T, \infty$, where $T := \frac{2\pi}{\omega}$. The peaks are obvious after only 5 oscillations

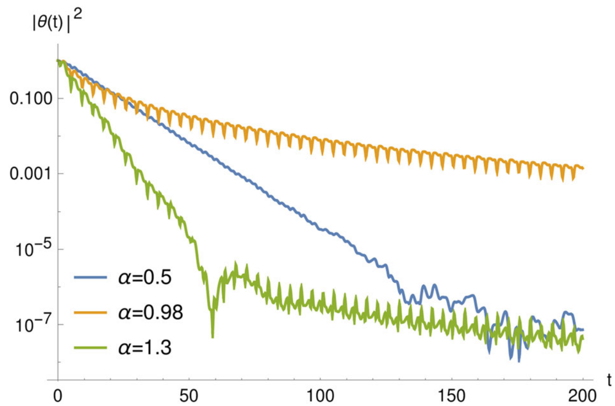


Fig. 6 Log plot of $|\theta(t)|^2$ for $\omega = 1.51$ at $\alpha = 0.5$, $\alpha = 0.98$ (power-law decay), and $\alpha = 1.3$

large, $\Theta(k;t) - \Theta(k;\infty)$ decays exponentially (at the rate, $e^{-\mathrm{Re}\, p_0 t}$), and thus the limiting profile is visible after only a few oscillations if α is not too small.

In Fig. 6 we show several graphs of $|\theta(t)|^2$, the survival probability versus t. For $\alpha = 0.5$ the Fermi Golden rule is clearly visible, for all relevant times. At larger times, the t^{-3} behavior kicks in, again mixed with oscillations, as predicted by the multi-instanton expansions. At $\alpha = .98$ we observe a stabilization window: the decay is power-like and thus slower, except at very short times. Stabilization amplitude results in more than five orders of magnitude reduced ionization at $t = 200$ relative to a smaller amplitude. At $\alpha = 1.3$ the log-plot shows an initial exponential behavior, followed by a rough dip when the exponential and polynomial parts become comparable, resulting in some cancellations, after which the behavior becomes polynomial, with oscillations.

Another interesting phenomenon which is noted even for small amplitudes, especially those close to stabilization windows, is the presence of small oscillations superimposed over the decay profile.

Decay versus windows of stabilization Generally, a time-independent Hamiltonian has, in energy-space representation, poles corresponding to eigenvalues and a branch point at

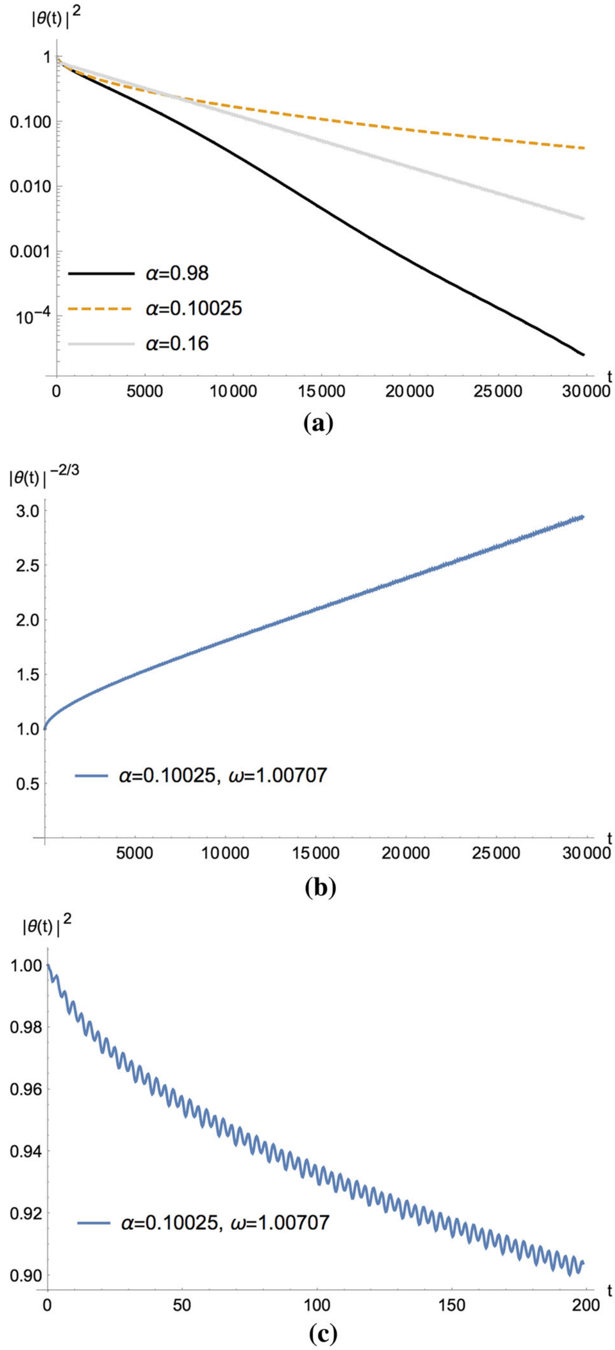


Fig. 7 Small field stabilization window. **a** Log-plot of $|\theta(t)|^2$ up to $t = 310^4$. The slowest decay is for $\alpha = 0.10025$ when the poles and branch points are aligned, and it is power-like. **b** $|\theta(t)|^{-2/3}$: power law decay of $|\theta|^2$. **c** Shorter time detail

zero. As a result of a time-periodic forcing of amplitude α and frequency ω the branch point becomes an ω-spaced array on the real line, while each pole becomes an ω-spaced array of poles in the lower half-plane. These poles induce large, smooth peaks on the real line, while the branch-points-caused peaks are much smaller in size, except for special values of (α, ω) when the poles and branch points are aligned. Generically, due to smoothness, including around the large peaks, the Fourier transform needed for returning from the (x, E) to the (x, t) representation decays exponentially. However, when the poles and branch points are aligned, the smoothness of the peaks is destroyed and the decay is much slower, resulting in a stabilization window. This is seen in Fig. 7a–c for $\omega = 1.00707106,\ \alpha = 0.10025$. It is useful to note here that although α is small, perturbation theory does not apply. Fermi's golden rule based on perturbation theory predicts exponential decay of the survival probability as seen for neighboring values of α in the Fig. 7a instead of a power-law, as in Fig. 7b.

We note that the alignment of poles and branch cuts occurs at the pairs (α, ω) where there is a transition between n and $n + 1$ photon-requirement for ionization.

3 Concluding remarks

Behavior of $\boldsymbol{\theta}$, $\boldsymbol{\Theta}$ for large $\boldsymbol{t}$. The explicit transseries expansions in [18] used in the above figures are essentially obtained by pushing the inverse Laplace transform contour in the left half plane, collecting residues (resulting in small exponentials) and Hankel contours around branch cuts, which are in fact Borel sums of asymptotic series in powers of $t^{-1/2}$, with leading power $t^{-3/2}$. For small α, $\Theta(k, t)$ and $\theta(t)$ have exact expressions in α for all t, provided that certain sums in the exponentials are kept in the exponent as in (7). On the other hand, a pure power series expansion in α, as used in classical perturbation theory, converges only for t up to order $\alpha^{-1}|\log \alpha|$. There are exceptions to this convergence, as illustrated above.

All the above results do not use perturbation theory but agree with it when the latter is applicable. We obtained the plots of Θ and θ by numerically taking the inverse time Laplace transform of $\hat{\Theta}(k, p)$ for moderate time, and then by using a stationary phase calculation. Various features of $|\Theta(k, t)|^2$ are similar to those observed in experiments [1].

This model exhibits small field "windows of stabilization" phenomena, which, based on the mathematical explanation and our experience with the analytic properties of the solutions of one-particle Schrödinger equations with periodic forcing, we believe should be universal in this class of models. This suggests numerical tests to see whether such a phenomenon is present in more realistic models. It is to be noted that the smaller the field, the narrower the window of stabilization is.

A more direct connection between our model and the "photon" picture can be made via Floquet theory [25]. Using a suitable representation for the laser field in a cavity one can describe the absorption of n (non-localized) photons by an atom in terms of the solution of a Schrödinger equation. We shall consider the connection between our results and this formalism in a future work [26].

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