Nonperturbative time dependent solution of a simple ionization model

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Joint work with Ovidiu Costin and Joel L. Lebowitz

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Ionization

Ionization is the process by which an atom or a molecule acquires a negative or positive charge by gaining or losing electrons.

The interaction of atoms and molecules with sufficiently strong laser fields leads to ionization.

In general, analytic solutions are not available, and the approximations required for manageable numerical calculations do not provide accurate enough results.

We solved mathematically a simple model used in physics, in which the atom is represented by a delta-function.

General model

The Schrödinger equation: (units s.t. $\hbar = 2m = 1$)

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

- H_0 describes the time-independent system
- the laser field is modeled by a time periodic potential:

$$V(t,x) = V(t + 2\pi/\omega, x) \quad (\text{e.g. } V(t,x) = E \cdot x \sin \omega t)$$

The initial condition is a bound state $\psi(x,0) = u_b(x)$ of H_0, corresp. to the energy $-E_b$. Expanding in generalized eigenstates, assuming u_b is the only effective bound state, the evolution is given by

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

$|\theta|^2$ = the probability of finding the particle in the eigenstate $u_b(x)$
$|\Theta(k,t)|^2$ = the probability density of the ionized electron in "quasi-free" states (continuous spectrum) with energies k^2.
The evolution is unitary hence $|\theta(t)|^2 + \int_{\mathbb{R}^d} |\Theta(k,t)|^2\,dk = 1$

If $\theta(t) \to 0$ as $t \to \infty$, we say that the system ionizes completely.

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Our model

Reference Hamiltonian H_0 (well understood, Cycon et. al. 1987)

$$H_0 = -\frac{\partial^2}{\partial x^2} - 2\delta(x), \quad x \in \mathbb{R} \tag{3}$$

It has a single bound state

$$u_b(x) = e^{-|x|}$$

Its generalized eigenfunctions:

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

We add a parametric harmonic perturbation: $V(x,t) = -2\alpha \sin \omega t \, \delta(x)$

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Our type of results

Schrödinger equation:

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

describing the ionization of a model atom by an oscillating potential.
Studied before by O. Costin, J.L. Lebowitz, A. Rokhlenko 2000, '01, '08.
It has surprisingly many *features in common with those observed* in the ionization of real atoms and emission by solids, subjected to microwave or laser radiation.
We solve this model for all values of the parameters (non-perturbative).
To go beyond previous investigations we needed new mathematical methods and we provide a complete and rigorous analysis.
We obtained a Borel-resummed transseries (multi-instanton expansion) for ψ, for ionization probability, and energy distribution of the emitted electrons, valid for all values of α, ω, t.
The "photonic" picture shows up, e.g. strong peaks of $|\Theta(k,t)|^2$ for small α and $\omega \in \left(\frac{1}{n}, \frac{1}{n-1}\right)$.

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Previous results:

$$\theta(t) = 1 + 2i\int_0^t \varphi(s)ds, \quad \Theta(k,t) = \sqrt{\frac{2}{\pi}}\frac{|k|}{1-i|k|}\int_0^t \varphi(s)\,\mathrm{e}^{i(1+k^2)s}\,ds$$

where φ satisfies the integral equation

$$\varphi(t) = \alpha\sin\omega t\left(1 + \int_0^t \varphi(s)\eta(t-s)ds\right)$$

with $\eta(s) = \frac{2i}{\pi}\int_0^\infty \frac{u^2 e^{-is(1+u^2)}}{1+u^2}\,du = \frac{\sqrt{i}e^{-is}}{\sqrt{\pi}\sqrt{s}} - i\,\mathrm{erfc}\left(\sqrt{is}\right)$

The Laplace transform of φ, $\Phi(p) := \mathcal{L}\varphi(p) = \displaystyle\int_0^\infty \varphi(s)e^{-ps}ds$

is analytic in the right half plane and satisfies the functional equation

$$\Phi(p) = \frac{i\alpha}{2}\frac{\Phi(p-i\omega)}{i\sqrt{ip+\omega-1}+1} - \frac{i\alpha}{2}\frac{\Phi(p+i\omega)}{i\sqrt{ip-\omega-1}+1} + \frac{\alpha\omega}{\omega^2+p^2}$$

Why take $\mathcal{L}$: the p-plane is the Borel re-summation plane.

New results: 1. Singularity structure for general α, ω

Theorem 1. For all $\alpha > 0$ and $\omega > 0$,
(i) In the closed right half plane Φ is analytic except for an array of branch points on $i\mathbb{R}$ at

$$-i\beta_n, \quad \beta_n = 1 + n\omega, \qquad n \in \mathbb{Z}$$

$\Phi(p)$ is analytic in $\sqrt{p + i\beta_n}$. Also, $(1 + |p|)^2\Phi(p)$ is bounded.
(ii) In the open left half plane Φ is analytic except for an array of simple poles at

$$p_n := p_n(\alpha, \omega) = p_0(\alpha, \omega) - in\omega, \qquad n \in \mathbb{Z} \tag{5}$$

The residues $R_n = \mathrm{res}(\Phi, p_n)$ can be calculated using continued fractions, and satisfy $R_n = O(|n!|^{-1/2})$; $\quad |n| \to \infty$.
Also, $(1 + |p|)^2\Phi(p)$ is bounded (away from the poles).
p_n and R_n are analytic in $\alpha \in [0, \infty)$;
(iii) $\Re p_0(\alpha; \omega) < 0$; p_0 satisfies an equation of the form $A(p, \alpha; \omega) = B(p, \alpha; \omega)$ where A, B are meromorphic functions (given by convergent continued fraction representations).

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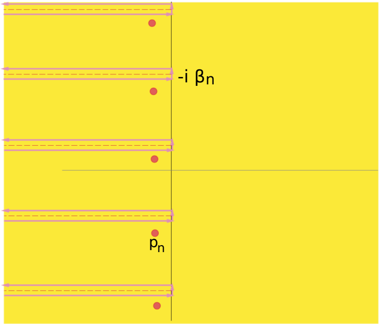
Singularity structure of $\Phi(p)$:



$$\varphi(t) = \mathcal{L}^{-1}\Phi = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} e^{pt}\Phi(p)\,dp$$

$|\Phi(p)| < C/(1+|p|)^{-2}$ $\rightsquigarrow$ can push the path of integration to the left

Branch points at $-i\beta_n = 1 + n\omega,\ n \in \mathbb{Z}$ $\rightsquigarrow$ path of int. hangs around them

Poles at $p_n = p_0 + n\omega$ where $\Re p_0 < 0,\ n \in \mathbb{Z}$ $\rightsquigarrow$ collect residues

$\rightsquigarrow$representation as a Borel summed transseries

Summed transseries representation of $\theta(t)$:

Form of the decay of the bound state, *non-perturbative* (arbitrary coupling)

Theorem 2.

(i) The function θ has a Borel summed **transseries** representation
(a **multi-instanton** expansion) *convergent for all* $t > 0$:

$$\theta(t) = -2 \sum_{n\in\mathbb{Z}} \frac{R_n}{p_n} e^{p_n t} + \sum_{n\in\mathbb{Z}} e^{-i\beta_n t} \int_0^\infty e^{-st} F_n(s;\alpha) ds \tag{6}$$

with $\beta_n \in \mathbb{R},\ p_n \in \mathbb{C},\ \Re p_n < 0,\ R_n \in \mathbb{C}$ as before:

$p_n = p_0 - in\omega$ are the poles, R_n are the residues of Φ

$-i\beta_n$ are the branch points of Φ

The F_n are analytic in α in a neighborhood of $[0, \infty)$, analytic in s if $\Re s > 0$ and in $\sqrt{s}$ for s near 0. For large $|s|$, $F_n = O(s^{-3})$.

The first sum converges factorially and the second at least as fast as $1/n^3$.

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$$\theta(t) = -2\sum_{n\in\mathbb{Z}} \frac{R_n}{p_n} e^{p_n t} + \sum_{n\in\mathbb{Z}} e^{-i\beta_n t} \int_0^\infty e^{-st} F_n(s;\alpha) ds \tag{6}$$

with $\beta_n \in \mathbb{R},\ p_n \in \mathbb{C},\ \Re p_n < 0,\ R_n \in \mathbb{C}$ as before:

$p_n = p_0 - in\omega$ are the poles, R_n are the residues of Φ

$-i\beta_n$ are the branch points of Φ

The F_n are analytic in α in a neighborhood of $[0, \infty)$, analytic in s if $\Re s > 0$ and in $\sqrt{s}$ for s near 0. For large $|s|$, $F_n = O(s^{-3})$.

The first sum converges factorially and the second at least as fast as $1/n^3$.

Summed transseries representation of $\Theta(k,t)$:

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(ii) Similarly, the function $\Theta(k,t)$ is a **Borel summed transseries** :

$$\Theta(k,t) = \sqrt{\frac{2}{\pi}} \frac{|k|}{1-i|k|} \left[\Phi(-i(1+k^2)) + i\sum_{n\in\mathbb{Z}} \frac{R_n e^{(p_n+i+ik^2)t}}{p_n + i(1+k^2)} \right. \\ \left. + \sum_{n\in\mathbb{Z}} e^{[-i\beta_n + i(1+k^2)]t} \int_0^\infty e^{-st} \frac{F_n(s,\alpha)}{-i\beta_n + i(1+k^2) - s} ds \right] \tag{8}$$

where the F_n are the same as above.

Ionization?

Corollary

For all $\alpha, \omega > 0$ we have

$$\lim_{t\to\infty} \theta(t) = 0, \quad \lim_{t\to\infty} \Theta(k,t) = \sqrt{\frac{2}{\pi}}\,\frac{|k|}{1 - i|k|}\,\Phi(-i(1+k^2)) \tag{9}$$

$|\Theta|^2$ calculated from a few leading orders, small t

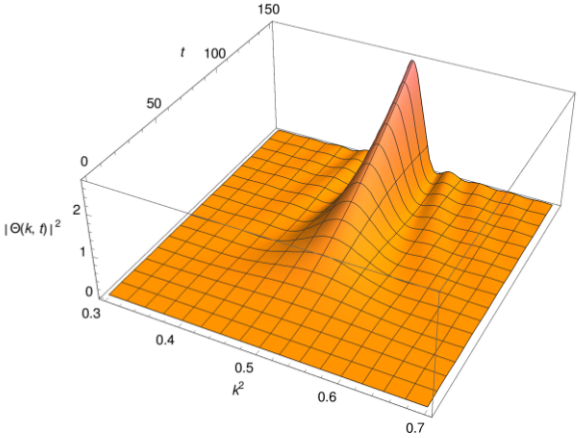

Figure: $|\Theta|^2$ function of (k^2, t) for $t \leq 150$ for $\alpha = 0.05$ and $\omega = 1.5$.

Strong peaks. Main peak centered at ω (energy corresp. to one photon).

$|\Theta|^2$ calculated from a few leading orders, larger t

Probability density of energies:

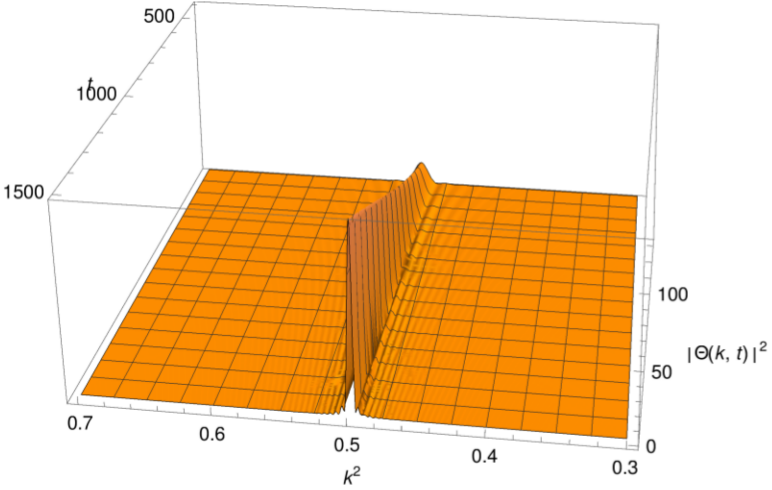

Figure: $|\Theta|^2$ function of (k^2, t) for $500 \leq t \leq 1500$ for $\alpha = 0.05$ and $\omega = 1.5$.

Perturbation theory: small α

Assume: $\omega \notin \mathbb{Z}$. Notation: $f = o_a$ means f an. at $\alpha = 0$ and $f(0) = 0$.

Recall: Φ *has an array of poles* at $p_n = p_0 - in\omega$ ($n \in \mathbb{Z}$), $p_0 = p_0(\alpha, \omega)$

Theorem 3.

(i) For $\omega > 1$: $\quad p_0 = \alpha^2 \dfrac{-\sqrt{\omega - 1} + i\sqrt{1+\omega}}{2\omega}(1 + o_a)$

For $\omega < 1$: let m be least integer s.t. $m\omega > 1$

$$\Re p_0 = -\frac{1}{m\omega} \frac{\sqrt{m\omega - 1}}{\prod_{k<m}(1 - \sqrt{1 - k\omega})^2} \frac{\alpha^{2m}}{2^{2m+1}}(1 + o_a)$$

(ii) The residues satisfy $R_0 = \frac{p_0}{2}$ for $\omega > 1$, and for $\omega < 1$

$$R_0 = \frac{im\alpha^{m-1}p_0}{2^m \prod_{k<m}(1 - \sqrt{1 - k\omega})}(1 + o_a) \qquad (10)$$

Furthermore, as $n \to \infty$, $R_n/R_0 = O(\alpha^{2|n|}/\Gamma(n/2))$ and $F_n = O(\alpha^{2n+2}/n^3)$.

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Furthermore, as $n \to \infty$, $R_n/R_0 = O(\alpha^{2|n|}/\Gamma(n/2))$ and $F_n = O(\alpha^{2n+2}/n^3)$.

(iii) As a function of α:
$\theta(t)$ is analytic for small $\alpha \in \mathbb{C}$ and real-analytic for $\alpha \in \mathbb{R}$.
With m as in (i), on the scale $t \in (0, o(\alpha^{-2m} \ln \alpha))$ we have

$$|\theta(t)|^2 = e^{-2\Re p_0 \, t}(1 + o(1))$$

This is the Fermi Golden Rule of exponential decay of the bound state valid for small amplitudes! ... and moderately large times...

As $t \to \infty$,

$$|\theta(t)|^2 = O(\alpha^4 t^{-3})$$

(iv) The distribution of energies satisfies

$$\Theta(k,t)=\sqrt{\frac{2}{\pi}}\,\frac{|k|}{1-i|k|}\,\frac{\alpha}{2}\,\left[\frac{1}{1+k^2+\omega}-\frac{1}{-ip_0+1+k^2-\omega}\right.$$
$$\left.+e^{(p_0+i+ik^2)t}\left(\frac{e^{i\omega t}}{-ip_0+1+k^2+\omega}-\frac{e^{-i\omega t}}{-ip_0+1+k^2-\omega}\right)\right](1+o_a) \quad (11)$$

Note: the order of Θ: it is $O(\alpha)$ *for most* k.
However, for k such that $1+k^2-\omega=O(\alpha^2)=O(p_0)$ we have
$\Theta(k,t)=O(\alpha^{-1})$ Sharp peaks!

Note

If for some $m\in\mathbb{N}$ we have $m\omega^{-1}=1+O(\alpha^{2m})$, which means that poles are close to branch points, there is a smooth transition region where $R_0,\&\Re p_0$ change from $O(\alpha^{2m+2})$ to $O(\alpha^{2m})$. We did not analyze this.

Corollary

The functions Θ and θ have fully convergent perturbation expansions in small α, in sup norm away from $t=0$, provided we keep the power series of p_n in the exponent in

Proofs

Recall: Φ satisfies

$$\Phi(p) = \frac{i\alpha}{2}\frac{\Phi(p-i\omega)}{i\sqrt{ip+\omega-1}+1} - \frac{i\alpha}{2}\frac{\Phi(p+i\omega)}{i\sqrt{ip-\omega-1}+1} + \frac{\alpha\omega}{\omega^2+p^2}$$

Discretize: let $p = -i(\sigma + n\omega)$, where $\Re\sigma \in [0,\omega),\ n \in \mathbb{Z}$
we obtain the difference equations with parameters σ, ω

$$g_n = \alpha h_{n+1} g_{n+1} - \alpha h_{n-1} g_{n-1} + f_n \tag{12}$$

or, in operator notation,

$$\mathbf{g} = K_0(\sigma,\alpha)\mathbf{g} + \mathbf{f} \tag{13}$$

Regularize the operator (h_n have poles):
Let $d_n = \frac{1}{4}(\sigma + n\omega - i\beta)^{-1}$ and $b_n = d_n/(h_{n+1}h_{n-1})$; $(\beta > 0)$
Then $g_n = (1-b_n)\, g_n + \frac{\alpha d_n}{h_{n-1}} g_{n+1} - \frac{\alpha d_n}{h_{n+1}} g_{n-1} + b_n f_n$ or,

$$\mathbf{g} = K(\sigma,\alpha)\mathbf{g} + B\mathbf{f} \tag{14}$$

$\mathbf{g} = K(\sigma, \alpha)\mathbf{g} + B\mathbf{f}$

Now K, $\mathbf{f}$ and B are pole-free in the closed lower half plane (analyticity of the solution in the upper half plane was proved in previous work).
Extension. Allow $\sigma \in \mathbb{C}$.
We prove that:

1. The operator $K(\sigma, \alpha)$ is compact in $\ell^2(\mathbb{Z})$. It is linear-affine in α, and analytic in σ except for a square root branch point at $1 - \lfloor \omega^{-1} \rfloor \omega$.

2. The homogeneous equation $\mathbf{g} = K(\sigma, \alpha)\mathbf{g}$ has no nontrivial ℓ^2 solution if $\Im\sigma \geqslant 0$.

$\rightsquigarrow$ By the Fredholm alternative $\exists!$ sol. w. same analyticity properties as K.

Calculate the poles in the lower half plane for small α:

We turn it into continued fraction representation.
Work with the continuous form of the homogeneous eq.:

$$g(q) = \alpha h(q+\omega) g(q+\omega) - \alpha h(q-\omega) g(q-\omega) \tag{15}$$

where

$$h(q) := \frac{1}{2} \frac{1}{\sqrt{q-1} - i}$$

For $q \to \infty$: look for small sol., define

$$\rho(q) := \rho(q;\alpha) = g(q)/g(q-\omega)$$

and obtain

$$\rho(q) = \mathcal{N}(\rho), \text{ where } \mathcal{N}(\rho)(q) = -\frac{\alpha h(q-\omega)}{1 - \alpha h(q+\omega)\rho(q+\omega)} \tag{16}$$

For $q \to -\infty$: look for small sol., define $\Omega(q) := \Omega(q;\alpha) = g(q-\omega)/g(q)$ satisfies

$$\Omega(q) = \mathcal{M}(\Omega), \text{ where } \mathcal{M}(\Omega)(q) = \frac{\alpha h(q)}{1 + \alpha h(q-2\omega)\Omega(q-\omega)} \tag{17}$$

Lots of technical details here... $\mathcal{N}$, $\mathcal{M}$ are contractive in suitable balls in a suitable Banach space (incorporating both the regularity and decay we aim to prove).
$\rightsquigarrow$ fixed point,$\exists!$ solutions w. regularity stated in parameters.

Corollary Iterating $\rho(q) = \mathcal{N}(\rho)$ yields a continued fraction which is convergent for $\Re(q) \geqslant N\omega$, $\Im q \in [0, \varepsilon]$ and $\alpha < 2/3$. For small α, the rate of convergence is $4^{-n}\alpha^{2n}$.
Similarly for $\Omega(q) = \mathcal{M}(\Omega)$.

From small α to general values

The structure of the resolvent $(I - K(\sigma, \alpha))^{-1}$ for any $\alpha \neq 0$ is established by

- we construct a periodic operator isospectral to the resolvent
- prove, and use, a general result on the constancy of number of zeros of analytic, periodic functions depending on a parameter

Thank you!