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Ionization in damped time-harmonic fields

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Abstract

We study the asymptotic behavior of the wavefunction in a simple onedimensional model of ionization by pulses, in which the time-dependent potential is of the form $V(x, t) = -2\delta(x)(1 - e^{-\lambda t} \cos \omega t)$, where δ is the Dirac distribution. We find the ionization probability in the limit $t \to \infty$ for all λ and ω . The long pulse limit is very singular and for $\omega = 0$, the survival probability is const $\lambda^{1/3}$, much larger than $O(\lambda)$, the one in the abrupt transition counterpart, $V(x, t) = \delta(x) \mathbf{1}_{\{t \ge 1/\lambda\}}$ where **1** is the Heaviside function.

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1. Introduction

Quantum systems subjected to external time-periodic fields which are not small have been studied in various settings.

In small enough oscillating fields with constant amplitude, perturbation theory typically applies and ionization is generic (the probability of finding the particle in any bounded region vanishes as time becomes large), see [7, 14] and references therein.

For larger time-periodic fields, a number of rigorous results have been recently obtained, see [3] and references therein, showing generic ionization. However, outside perturbation theory, the systems show a very complex and often nonintuitive behavior. The ionization fraction at a given time is not always monotonic with the field [1]. There even exist exceptional potentials of the form $\delta(x)(1+aF(t))$ with *F* periodic and of zero average, for which ionization occurs for all small *a*, while at larger fields the particle becomes confined once again [4]. Furthermore, if $\delta(x)$ is replaced with smooth potentials f_n such that $f_n \rightarrow \delta$ in distributions, then ionization occurs for all *a* if *n* is kept fixed. The relevance of a δ -potential model (also known as zero range potential, ZRP) is discussed in detail in many publications, see e.g. [12].

Numerical approaches are very delicate since one deals with the Schrödinger equation in $\mathbb{R}^n \times \mathbb{R}^+$, as $t \to \infty$ and artifacts such as reflections from the walls of a large box approximating the infinite domain are not easily suppressed. The mathematical study of systems in various limits is delicate and important.

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In physical experiments, one deals with forcing of finite effective duration, often with exponential damping. This is the setting we study in the present paper, in a simple model, a delta function in one dimension, interacting with a damped time-harmonic external forcing.

The equation is

$$i\frac{\partial\psi}{\partial t} = \left(-\frac{\partial^2}{\partial x^2} - 2\delta(x)\left(1 - A(t)\cos(\omega t)\right)\right)\psi,\tag{1}$$

where A(t) is the amplitude of the oscillation; we take

$$\psi_0 = \psi(0, x) \in C_0^{\infty}, \qquad A(t) = \alpha e^{-\lambda t}, \qquad \alpha = 1.$$
(2)

(The analysis for other values of α is very similar.) The quantity of interest is the large t behavior of ψ , and in particular the survival probability

$$P_B = \lim_{t \to \infty} P(t, B) = \lim_{t \to \infty} \int_B |\psi(t, x)|^2 \,\mathrm{d}x,\tag{3}$$

where *B* is a bounded subset of \mathbb{R} .

There is a vast literature on ionization by pulses, see e.g. [16, 17]. However, there is little in the way of mathematical work (with few exceptions, see [15] where rectangular pulses are discussed). Mathematical approaches are challenging in a number of ways. Purely time-periodic potentials can be dealt with using Floquet theory, especially in the perturbation regime. There is no known equivalent of that when A(t) is not a constant and the limit when A(t) goes to a constant is very singular, as the present results show. Even for the especially simple model (1), some aspects of the analysis are delicate.

Perturbation theory, Fermi golden rule. If α is small enough, *P* decreases exponentially on an intermediate timescale, long enough so that by the time the behavior is not exponential anymore, the survival probability is too low to be of physical interest. For all practical purposes, if α is small enough, the decay is exponential, following the Fermi golden rule, the derivation of which can be found in most quantum mechanics textbooks; the quantities of interest can be obtained by perturbation expansions in α . This setting is well understood; we mainly focus on the case where α is not too small, a toy model of an atom interacting with a field comparable to the binding potential.

No damping. The case $\lambda = 0$ is well understood for the model (1) in all ranges of α , see [2]. In that case, $P(t, A) \sim t^{-3}$ as $t \to \infty$.

However, since the limit $\lambda \to 0$ is singular, little information can be drawn from the $\lambda = 0$ case.

For instance, if $\omega = 0$, the limiting value of *P* is of order $\lambda^{1/3}$, while with an abrupt cutoff, $A(t) = \mathbf{1}_{\{t:t \leq 1/\lambda\}}$, the limiting *P* is $O(\lambda)$ (as usual, $\mathbf{1}_S$ is the characteristic function of the set *S*).

Thus, at least for fields which are not very small, the shape of the pulse cut-off is important. Even the simple system (1) exhibits a highly complex behavior.

We obtain a rapidly convergent expansion of the wavefunction and the ionization probability for any frequency and amplitude; this can be conveniently used to calculate the wavefunction with rigorous bounds on errors, when the exponential decay rate is not extremely large or small and the amplitude is not very large. For some relevant values of the parameters we plot the ionization fraction as a function of time.

We also show that for $\omega = 0$ the equation is solvable in the closed form, one of the few nontrivial integrable examples of the time-dependent Schrödinger equation. For other exactly solvable models, see [12, 13].

2. Main results

Theorem 1. Let $\psi(t, x)$ be the solution to (1) with initial condition $\psi_0 \in C_0^{\infty}$. Let

$$g_{m,n} = g_{m,n}(\sigma) = \frac{\mathrm{i}}{2} \int_{\mathbb{R}} e^{-\sqrt{\sigma + n\omega - \mathrm{i}m\lambda}|x'|} \psi_0(x') \,\mathrm{d}x'. \tag{4}$$

Then as $t \to \infty$ *we have*

$$\psi(t, x) = r(\lambda, \omega) e^{it} e^{-|x|} (1 + t^{-1/2} h(t, x)),$$
(5)

where $|h(t, x)| \leq C, \forall x \in \mathbb{R}, \forall t \in \mathbb{R}^+$, and where

$$r(\lambda,\omega) = [-A_{1,-1} - A_{1,1} + 2g_{0,0}]_{\sigma=1}.$$
(6)

Here $A_{m,n} = A_{m,n}(\sigma)$ solves

$$(\sqrt{\sigma + n\omega - \mathrm{i}m\lambda} - 1)A_{m,n} = -\frac{1}{2}A_{m+1,n+1} - \frac{1}{2}A_{m+1,n-1} + g_{m,n}.$$
 (7)

There is a unique solution of (7) satisfying

$$\sum_{m,n} (1+|n|)^{\frac{3}{2}} e^{-b\sqrt{1+|m|}} |A_{m,n}| < \infty,$$
(8)

where b > 1 is a constant. It is this solution that enters (6).

There is a rapidly convergent representation of $r(\lambda, \omega)$, see section 3.5.

Clearly, $|r(\lambda, \omega)|^2$ is the probability of survival, the projection onto the limiting bound state.

2.1. $\omega = 0$

Theorem 2. (*i*) For $\omega = 0$ we have

$$r(\lambda) = \int_0^\infty \frac{-\mathrm{e}^{-p}}{1 + \mathrm{e}^{-p}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} g(k) \exp\left(\frac{2\mathrm{i}\sqrt{-\mathrm{i}k}}{\sqrt{\lambda}}\right) \lambda^{\frac{1-k}{2}} \frac{1}{\sqrt{\Gamma(k)}}$$
$$\cdot \exp\left(-\int_0^\infty \mathrm{e}^{-kp} \frac{\sqrt{\mathrm{i}\lambda}\left(-2 + 2\,\mathrm{e}^{-p} - \mathrm{i}^{3/2}\sqrt{p\pi\lambda}\mathrm{erf}\left(\frac{-\mathrm{i}^{3/2}\sqrt{p}}{\sqrt{\lambda}}\right)\right)}{2(-1 + \mathrm{e}^{-p})\sqrt{\pi}(p\lambda)^{3/2}}\,\mathrm{d}p\right) \mathrm{d}k\,\mathrm{d}p \tag{9}$$

where $g(k) = g_{k,0}$ *.*

(ii) We look at the case when $\psi_0 = e^{-|x|}$, the bound state of the limiting time-independent system. Assuming the series of $r(\lambda)$ is Borel summable in λ for $\arg \lambda \in [0, \frac{\pi}{2}]$ (summability follows from (9), but the proof is cumbersome and we omit it), as $\lambda \to 0$ we have

$$r(\lambda) \sim 2^{-2/3} (-3i)^{1/6} \pi^{-1/2} \Gamma(2/3) e^{-\frac{3i}{2\lambda}} \lambda^{1/6}.$$
 (10)

We note that behavior (10) is confirmed numerically with high accuracy, with the constants included, see section 5.3.

We also discuss results in two limiting cases: the short pulse setting (see section 6) and the special case $\lambda = 0$ (see section 7).

3. Proofs and further results

3.1. The associated Laplace space equation

We study the analytic properties of the Laplace transform of ψ . This Laplace approach can be viewed as a mathematically rigorous way to study the Schrödinger equation in energy space, which has been used often in physics, see [8, 9, 12].

The existence of a strongly continuous unitary propagator for (1) (see [6] v.2, theorem X.71) implies that for $\psi_0 \in L^2(\mathbb{R}^d)$, the Laplace transform

$$\hat{\psi}(\cdot, p) := \int_0^\infty \psi(\cdot, t) \,\mathrm{e}^{-pt} \,\mathrm{d}t$$

exists for $\operatorname{Re}(p) > 0$ and the map $p \to \psi(\cdot, p)$ is L^2 valued analytic in the right half plane

$$p \in \mathbb{H} = \{z : \operatorname{Re}(z) > 0\}.$$

The Laplace transform of (1) is

$$\left(\frac{\partial^2}{\partial x^2} + ip\right)\hat{\psi}(x,p) = i\psi_0 - 2\delta(x)\hat{\psi}(x,p) + \delta(x)(\hat{\psi}(x,p-i\omega+\lambda) + \hat{\psi}(x,p+i\omega+\lambda)).$$
(11)

Let $p = i\sigma + m\lambda + in\omega$ and

$$y_{m,n}(x,\sigma) = \hat{\psi}(x, i\sigma + m\lambda + in\omega), \qquad (12)$$

where $i\sigma \in \{z : 0 \leq \operatorname{Im} z < \omega, 0 \leq \operatorname{Re} z < \lambda\}.$

Remark 3. Since the *p* plane equation only links values of *p* differing by $m\lambda + in\omega$, $m, n \in \mathbb{Z}$, it is useful to think functions of *p* as vectors with components *m* and *n*, parameterized by σ .

Thus we rewrite (1) as

$$\left(\frac{\partial^2}{\partial x^2} - \sigma - n\omega + \mathrm{i}m\lambda\right) y_{m,n} = \mathrm{i}\psi_0 - 2\delta(x)y_{m,n} + \delta(x)(y_{m+1,n+1} + y_{m+1,n-1}).$$
(13)

When $|n| + |m| \neq 0$, the resolvent of the operator

$$-\frac{\partial^2}{\partial x^2} + \sigma + n\omega - \mathrm{i}m\lambda$$

has the integral representation

$$(\mathfrak{g}_{m,n}f)(x) := \int_{\mathbb{R}} G(\kappa_{m,n}(x-x'))f(x')\,\mathrm{d}x' \tag{14}$$

with

$$\kappa_{m,n} = \sqrt{-\mathrm{i}p} = \sqrt{\sigma + n\omega - \mathrm{i}m\lambda},$$

where the choice of branch is so that if $p \in \mathbb{H}$, then $\kappa_{m,n}$ is in the fourth quadrant, and where the Green's function is given by

$$G(\kappa_{m,n}x) = \frac{1}{2}\kappa_{m,n}^{-1} e^{-\kappa_{m,n}|x|}.$$
(15)

Remark 4. If $f(x) \in C_0^{\infty}$, using integration by parts we have, as $p \to \infty$

$$\mathfrak{g}(f) \sim \frac{c(x)}{p} + o\left(\frac{1}{p}\right)$$

where we regard g as an operator with p as a parameter; see also remark 3. Furthermore, (14) implies $c(x) \in L^2$.

$$(\mathfrak{C}y)_{m,n} = \mathfrak{g}_{m,n}[2\delta(x)y_{m,n} - \delta(x)(y_{m+1,n+1} + y_{m+1,n-1})].$$
(16)

Then equation (13) can be written in the equivalent integral form

$$y = i\mathfrak{g}\psi_0 + \mathfrak{C}y,\tag{17}$$

where g is defined in (14).

Remark 5. Because of the factor $\kappa_{m,n}^{-1}$ in (15), we have, with the identification in remark 3,

$$\mathfrak{C}\phi(p) \sim \frac{c(x)}{\sqrt{p}}\phi(p)$$

as $p \to \infty$, for any function $\phi(p)$.

3.2. Further transformations, functional space

In this section, we assume $\psi_0 \in C_0^{\infty}$. As in remark 4, we obtain

$$ig\psi_0 = \frac{c_1(x)}{p} + O\left(\frac{1}{p^{3/2}}\right)$$
 (18)

for some $c_1(x) \in L^2$. Let

$$h_1(p) = h_1(x, p) = c_1(x)\mathcal{L}(\mathbf{1}_{[0,1]}(t))$$
(19)

For large *p* we have

$$h_1(p) = \frac{c_1(x)}{p} + O\left(\frac{1}{p^{3/2}}\right).$$
(20)

Remark 6. As a function of x, $h_1(p)$ is clearly in L^2 and

 $\mathcal{L}^{-1}(h_1(p)) = c_1(x)\mathbf{1}_{[0,1]}(t)$

thus for t > 1 we have

$$\mathcal{L}^{-1}(h_1(p)) = 0.$$

Substituting

$$y = y_1 + h_1 \tag{21}$$

into (17) we have

$$y_1 = i\mathfrak{g}\psi_0 - h_1 + \mathfrak{C}(h_1) + \mathfrak{C}y_1.$$
⁽²²⁾

Let $y_0 = i\mathfrak{g}\psi_0 - h_1 + \mathfrak{C}(h_1)$. Then remark 5 implies that for large p

$$y_0 = O\left(\frac{1}{p^{3/2}}\right) \tag{23}$$

and by construction $y_0 \in L^2$ as a function of *x*. We analyze (22) in the space $\mathscr{H}_b = L^2(\mathbb{Z}^2 \times \mathbb{R}, \|\cdot\|_b), b > 1$, where

$$\|y\|_{b} := \left(\sum_{m,n} (1+|n|)^{\frac{3}{2}} e^{-b\sqrt{1+|m|}} \|y_{m,n}\|_{L^{2}}^{2}\right)^{\frac{1}{2}}.$$
(24)

We denote by $\hat{\psi}_1$ the transformed wavefunction corresponding to y_1 . By writing y instead of y_1 , we obtain from (22)

$$y = y_0 + \mathfrak{C}y. \tag{25}$$

Lemma 7. \mathfrak{C} is a compact operator on \mathscr{H}_b , and it is analytic in $\sqrt{-ip}$.

Proof. Compactness is clear since \mathfrak{C} is a limit of bounded finite rank operators. Analyticity is manifest in the expression of \mathfrak{C} (see (14) and (16)).

Proposition 8. Equation (25) has a unique solution iff the associated homogeneous equation

$$y = \mathfrak{C}y \tag{26}$$

has no nontrivial solution. In the latter case, the solution is analytic in $\sqrt{\sigma}$.

Proof. This follows from lemma 7 and the Fredholm alternative.

When m = 0, n = 0 and $\sigma = 0$, \mathfrak{C} is singular, but the solution is not. Indeed, by adding $\mathbf{1}_{[-A,A]}$, A > 0, to both sides of (13) we get the equivalent equation

$$\left(\frac{\partial^2}{\partial x^2} - \sigma - n\omega + \mathrm{i}m\lambda + \mathbf{1}_{[-A,A]}\right) y_{m,n}$$

= $\mathrm{i}\psi_0 + (\mathbf{1}_{[-A,A]} - 2\delta(x)) y_{m,n} + \delta(x)(y_{m+1,n+1} + y_{m+1,n-1}).$ (27)

Arguments similar to those when $\mathbf{1}_{[-A,A]}$ is absent show that the operator \mathfrak{C} associated with (27) is analytic in $\sqrt{\sigma}$, thus $y_{m,n}$ is analytic in $\sqrt{\sigma}$.

3.3. Equation for A

Componentwise (17) reads

$$y_{m,n} = \int_{\mathbb{R}} \frac{1}{2} \kappa_{m,n}^{-1} e^{-\kappa_{m,n}|x-x'|} \psi_0(x') dx' + \frac{1}{2\kappa_{m,n}} e^{-\kappa_{m,n}|x|} [2y_{m,n}(0) - (y_{m+1,n+1}(0) + y_{m+1,n-1}(0))].$$
(28)

With $A_{m,n} = y_{m,n}(0)$, we have

$$(\sqrt{\sigma + n\omega - \mathrm{i}m\lambda} - 1)A_{m,n} = -\frac{1}{2}A_{m+1,n+1} - \frac{1}{2}A_{m+1,n-1} + g_{m,n}$$
(29)

where $g_{m,n}$ is defined in (4).

Proposition 9. The solution to (28) is determined by $A_{m,n}$ through

$$y_{m,n} = \int_{\mathbb{R}} \frac{1}{2} \kappa_{m,n}^{-1} e^{-\kappa_{m,n}|x-x'|} \psi_0(x') dx' + e^{-\kappa_{m,n}|x|} A_{m,n} - \frac{1}{\kappa_{m,n}} e^{-\kappa_{m,n}|x|} g_{m,n}.$$
(30)
It thus suffices to study (29).

Proof. Taking x = 0 in (28) we obtain (29); using now (29) in (28) we have

$$y_{m,n} = \int_{\mathbb{R}} \frac{1}{2} \kappa_{m,n}^{-1} e^{-\kappa_{m,n}|x-x'|} \psi_0(x') dx' + \frac{1}{2\kappa_{m,n}} e^{-\kappa_{m,n}|x|} [2A_{m,n} - (A_{m+1,+1} + A_{m+1,n-1})] = \int_{\mathbb{R}} \frac{1}{2} \kappa_{m,n}^{-1} e^{-\kappa_{m,n}|x-x'|} \psi_0(x') dx' + e^{-\kappa_{m,n}|x|} A_{m,n} - \frac{1}{\kappa_{m,n}} e^{-\kappa_{m,n}|x|} g_{m,n}.$$
(31)

Remark 10. If $y \in \mathscr{H}_b$, then $A_{m,n} = y_{m,n}(0)$ satisfies (8).

6

Let $A_{m,n}^0 = y_{m,n}^0(0)$ where $y_{m,n}^0$ is a solution to (26). The solution to (26) has the freedom of a multiplicative constant; we choose it by imposing

$$A_{0,0}^{0} = \lim_{\sigma \to 1} (\sigma - 1) A_{0,0}.$$
(32)

It is clear that $A_{m,n}^0$ satisfies the homogeneous equation associated with (29)

$$(\sqrt{\sigma + n\omega - \mathrm{i}m\lambda} - 1)A_{m,n}^0 = -\frac{1}{2}A_{m+1,n+1}^0 - \frac{1}{2}A_{m+1,n-1}^0.$$
(33)

3.4. Positions and residues of the poles

Define

$$\sigma_0 = 1 - \left\lfloor \frac{1}{\omega} \right\rfloor \omega \tag{34}$$

where $\lfloor x \rfloor$ is the integer part of x. To simplify notation we take $\omega > 1$ in which case $\sigma_0 = 1$. The general case is very similar.

Denote

$$\mathcal{B} := \{ in\omega + m\lambda + i : m \in \mathbb{Z}, n \in \mathbb{Z}, m \leqslant 0, |n| \leqslant |m| \}.$$
(35)

Proposition 11. The system (33) has nontrivial solutions in \mathcal{H}_b iff $\sigma = \sigma_0(=1 \text{ as discussed above})$. If $\sigma = 1$, then the solution is a constant multiple of the vector $A_{m,n}^0$ given by

$$\begin{cases}
A^{0}_{m,n} = 0 & m \ge 0 \quad and \quad (m,n) \ne (0,0) \\
A^{0}_{m,n} = 0 & m \le 0 \quad and \quad m \le n \le -m \\
A^{0}_{m,n} = 1 & (m,n) = (0,0)
\end{cases}$$
(36)

and obtained inductively from (33) for all other (m, n). (Note that $\sigma = 1$ is used crucially here since (33) allows for the nonzero value of $A_{0,0}^0$.)

Proof. Let $\sigma = 1$. By construction, A^0 defined in proposition 11 satisfies the recurrence and we only need to check (8). Since

$$A_{m,n}^{0} = -\frac{A_{m+1,n+1}^{0} + A_{m+1,n-1}^{0}}{2(\sqrt{\sigma + n\omega + im\lambda} - 1)}$$

and $\sqrt{\sigma + n\omega + im\lambda} - 1 \neq 0$, we have

$$\left|A_{m,n}^{0}\right| \leqslant C \frac{2^{m}}{\sqrt{(|n|+|m|)!}}$$

proving the claim.

Now, for any σ , if there exists a nontrivial solution, then for some n_0, m_0 we have $A^0_{n_0,m_0} \neq 0$. By (33), we have either

$$\left|A_{n_{0}-1,m_{0}+1}^{0}\right| \ge \frac{1}{2} \left|\left(\sqrt{\sigma + n_{0}\omega + \mathrm{i}m_{0}\lambda} - 1\right)\right| \cdot \left|A_{n_{0},m_{0}}^{0}\right|$$
(37)

or

$$\left|A_{n_{0}+1,m_{0}+1}^{0}\right| \ge \frac{1}{2} \left|\left(\sqrt{\sigma + n_{0}\omega + im_{0}\lambda} - 1\right)\right| \cdot \left|A_{n_{0},m_{0}}^{0}\right|.$$
(38)

It is easy to see that if $in_0\omega + m_0\lambda + i \in \mathcal{B}^c$ or $\sigma \neq 1$, the above inequalities lead to

$$\left|A_{n,m_0+m}^{0}\right| \geqslant c\sqrt{m!} \tag{39}$$

for large m > 0 (note that in these cases $\sqrt{\sigma + n\omega + im\lambda} - 1 \neq 0$), contradicting (8).

Finally, if $\sigma = 1$, then A^0 is determined by $A^0_{0,0}$ via the recurrence relation (33) (note that $A^0|_{\mathcal{B}^c} = 0$). This proves uniqueness (up to a constant multiple) of the solution.

Combining propositions 8 and 11 we obtain the following result.

Proposition 12. The solution $\hat{\psi}(p)$ to equation (11) is analytic with respect to $\sqrt{-ip}$, except for poles in \mathcal{B} .

Proof. Proposition 11 shows that (33) has a solution A^0 for $\sigma \in \mathcal{B}$; by proposition 8, *A* has singularities in \mathcal{B} , and the conclusion follows from proposition 9.

So far we showed that the solution has possible singularities in \mathcal{B} . To show that indeed $\hat{\psi}$ has poles for generic initial conditions, we need the following result:

Lemma 13. Let *H* be a Hilbert space. Let $K(\sigma) : H \to H$ be compact, analytic in σ and invertible in $B(0, r) \setminus \{0\}$ for some r > 0. Let $v_0(\sigma) \notin \text{Ran}(I - K(0))$ be analytic in σ . If $v(\sigma) \in H$ solves the equation $(I - K(\sigma))v(\sigma) = v_0(\sigma)$, then $v(\sigma)$ is analytic in σ in $B(0, r) \setminus \{0\}$ but singular at $\sigma = 0$.

Proof. By the Fredholm alternative, $v(\sigma)$ is analytic when $\sigma \neq 0$. If $v(\sigma)$ is analytic at $\sigma = 0$ then v_0 is analytic and $v_0(\sigma) \in \text{Ran}(I - K(0))$ which is a contradiction.

The operator \mathfrak{C} is compact by remark 7. The inhomogeneity y_0 in equation (26) is analytic in $\sqrt{\sigma}$. Furthermore, at $\sigma = 1$, Ran $(I - \mathfrak{C})$ is of codimension 1 (proposition 11). Combined with lemma 13 we have

Corollary 14. For a generic inhomogeneity y_0 , $y(\sigma)$ is singular at $\sigma = 1$. Equivalently, $\hat{\psi}(p)$ has a pole at p = i.

It can be shown that $\hat{\psi}(p)$ has a pole at p = i for generic ψ_0 . We prefer to show the following result which has a shorter proof.

Proposition 15. The residue $R_{0,0}$ of the pole for $\hat{\psi}$ at p = i is given by

$$R_{0,0} = \lim_{\sigma \to 1} (\sigma - 1) A_{0,0} = [-A_{1,-1} - A_{1,1} + 2g_{0,0}]_{\sigma = 1}$$
(40)

In particular, $R_{0,0} \neq 0$ for large λ and generic initial condition ψ_0 .

Proof. When m = 0 and n = 0, (29) gives

$$(\sqrt{\sigma} - 1)A_{0,0} = -\frac{1}{2}A_{1,-1} - \frac{1}{2}A_{1,1} + g_{0,0}.$$
(41)

Clearly $A_{0,0}$ is singular as $\sigma \to 1$, which implies that $\hat{\psi}$ has a pole at p = i with residue given in (40). Thus $R_{0,0}$ is not zero if the quantity $[-A_{1,-1} - A_{1,1} + 2g_{0,0}]_{\sigma=1}$ is not zero. First, $g_{0,0}|_{\sigma=1}$ is not zero by definition:

$$g_{0,0}|_{\sigma=1} = i \int_{\mathbb{R}} \frac{1}{2} e^{-|x'|} \psi_0(x') dx'$$

Next, taking m = 1, n = 1 and $\sigma = 1$ in (29) we obtain

$$(\sqrt{1+\omega-i\lambda}-1)A_{1,1} = \left[-\frac{1}{2}A_{2,2} - \frac{1}{2}A_{2,0} + g_{1,1}\right]_{\sigma=1}.$$

Thus for any c > 0 when λ is large enough we have

$$|A_{1,1}| \leq c^{-1}[|g_{1,1}| + \max\{|A_{2,2}|, |A_{2,0}|\}]_{\sigma=1}.$$

Estimating similarly $A_{2,2}$ and $A_{2,0}$ and so on, we see that $|A_{1,1}| = O(c^{-1})$. When c is large enough we have $|A_{1,1}| < |g_{0,0}|$. Analogous bounds hold for $A_{1,-1}$, showing that $[-A_{1,-1} - A_{1,1} + 2g_{0,0}]_{\sigma=1}$ is not zero.

Corollary 16. For generic initial condition $\hat{\psi}$ has simple poles in \mathcal{B} , and their residues are given by $R_{m,n} = A_{m,n}^0$.

Proof. We take a small loop around $\sigma = 0$ and integrate equation (28) along it. This gives a relation among $R_{m,n}$ which is identical to (33):

$$(\sqrt{\sigma + n\omega - \mathrm{i}m\lambda} - 1)R_{m,n} = -\frac{1}{2}R_{m+1,n+1} - \frac{1}{2}R_{m+1,n-1}.$$
 (42)

Proposition 15 and (32) imply that $R_{0,0} = A_{0,0}^0$. The rest of the proof follows from proposition 11.

Remark 17. It is easy to see that there exist initial conditions for which the solution has no poles. Indeed, if the solutions ψ_1 and ψ_2 have a simple pole at p = i with residue a_1 and a_2 respectively, then for the initial condition $\psi_{0,0} = a_2\psi_{1,0} - a_1\psi_{2,0}$, the corresponding solution ψ_0 has no pole at p = i.

3.5. Infinite sum representation of $A_{m,n}$

Taking $\sigma = 1$ in (29) we get

$$(\sqrt{1+n\omega-\mathrm{i}m\lambda}-1)A_{m,n} = -\frac{1}{2}A_{m+1,n-1} - \frac{1}{2}A_{m+1,n+1} + g_{m,n}.$$
(43)

For $\tau = (a_1, \dots, a_N) \in \{-1, 1\}^N$, we define $\tau_j^0 = (a_1, \dots, a_j, 0, \dots, 0)$. (Note that $\tau = \tau_N^0$.) We denote $\Sigma \tau_j^0 = \sum_{i=1}^j a_i$ and $\{-1, 1\}^0 = \{0\}$.

$$B_{m,n} = \frac{1}{\sqrt{1 + n\omega - \mathrm{i}m\lambda} - 1}$$

and for some $\tau \in \{-1, 1\}^N$ define

$$B_{mnN} = B_{mnN}(\tau) = \prod_{j=0}^{N-1} B_{m+j,n+\sum \tau_j^0}.$$

Equation (43) implies

$$A_{m,n} = (-1)^{N} \frac{1}{2^{N}} \sum_{\tau \in \{-1,1\}^{N}} B_{mnN-1} A_{m+N,n+\sum \tau} + \sum_{j=0}^{N-1} (-1)^{j} \frac{1}{2^{j}} \sum_{\tau \in \{-1,1\}^{j}} B_{mnj} g_{m+j,n+\sum \tau}.$$
(44)

As
$$N \to \infty$$
 we have

$$\prod_{j=0}^{N} B_{m+j,n} \sim \frac{1}{\sqrt{N!}}$$

and $A_{m,n}$ goes to zero as $m \to \infty$, and thus we have

$$\lim_{N \to \infty} (-1)^N \frac{1}{2^N} \sum_{\tau \in \{-1,1\}^N} B_{mnN-1} A_{m+N,n+\sum \tau} = 0$$

In the limit $N \to \infty$, we obtain

$$A_{m,n} = \sum_{j=0}^{\infty} (-1)^j \frac{1}{2^j} \sum_{\tau \in \{-1,1\}^i} B_{mnj} g_{m+j,n+\sum \tau}.$$
(45)

Remark 18. Truncating the infinite expansion to N, the error is bounded by

$$\left| \frac{1}{2^N} \sum_{\tau \in \{-1,1\}^N} \left(\prod_{j=0}^N B_{m+j,n+\sum \tau_j^0} A_{m+N,n+\sum \tau}^0 \right) \right|.$$
(46)

4. Proof of theorem 1

In section 3.4, it was shown that for a generic initial condition $\psi_0(x)$, the solution $\hat{\psi}(x, p)$ has simple poles in \mathcal{B} , with residues $R_{m,n} = A_{m,n}$.

Since $y \in \mathcal{H}_b$, the inverse Laplace transform can be expressed using the Bromwich contour formula. Recall that y differs from the original vector form of $\hat{\psi}$ by (21), we have

$$\psi(x,t) = \mathcal{L}^{-1}\hat{\psi}(x,p) = \mathcal{L}^{-1}(h_1) + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{pt} \hat{\psi}_1(x,p) \, dp.$$
(47)

The fact that $y \in \mathscr{H}_b$ also implies that $\hat{\psi}_1(x, p) \to 0$ fast enough as $p \to c \pm i\infty$. Thus, the contour of integration in the inverse Laplace transform can be pushed into the left half *p*-plane, after collecting the residues. As a result, for some small c < 0 the contour becomes one using the Bromwich contour formula coming from $c - i\infty$, joining $c - i\epsilon$, 0 and $c + i\epsilon$ (for arbitrarily small $\epsilon > 0$) in this order, then going toward $c + i\infty$.

Thus we have

$$\psi(t,x) = \mathcal{L}^{-1}(h_1) + \operatorname{Res}_{|p=i}(e^{pt}\hat{\psi}_1) + \frac{1}{2\pi i}e^{ct}\int_{\epsilon}^{\infty} e^{ist}(\hat{\psi}_1(x,c+is) + \hat{\psi}_1(x,c-is))\,ds + \frac{1}{2\pi i}\int_{0}^{c-i\epsilon} e^{pt}\hat{\psi}_1(x,p)\,dp + \frac{1}{2\pi i}\int_{0}^{c+i\epsilon} e^{pt}\hat{\psi}_1(x,p)\,dp.$$
(48)

By corollary 16 we have

 $\operatorname{Res}_{p=i}(e^{pt}\hat{\psi}_1) = R_{0,0} = A_{0,0}^0.$

The third term on the right-hand side of (48) decays exponentially for large t (note that c < 0 and the integral is bounded since $y \in \mathcal{H}_b$.), while the last two terms yield an asymptotic power series in $1/\sqrt{t}$, as easily seen from Watson's lemma.

Combining these results and the fact $\mathcal{L}^{-1}(h_1) = o(1/t)$ (remark 6), we obtain the first part of theorem 1, with $r(\lambda, \omega) = R_{0,0}$. The rest follows from proposition 15.

5. Proof of theorem 2

When $\omega = 0$, the equation

$$i\frac{\partial\psi}{\partial t} = \left(-\frac{\partial^2}{\partial x^2} - 2\delta(x) + 2\delta(x)e^{-\lambda t}\cos(\omega t)\right)\psi$$

becomes

$$i\frac{\partial\psi}{\partial t} = \left(-\frac{\partial^2}{\partial x^2} - 2\delta(x) + 2\delta(x)e^{-\lambda t}\right)\psi.$$

Rewriting $A_{m,n}$ and $g_{m,n}$ as A_n and g_n , (29) becomes

$$(\sqrt{\sigma - \mathrm{i}m\lambda} - 1)A_n = -A_{n+1} + g_n.$$

Since $\omega = 0$, (45) simplifies to

$$A_n = \sum_{l=0}^{\infty} (-1)^{l-1} \prod_{j=0}^{l} \frac{1}{\sqrt{1 - i(n+j)\lambda} - 1} g_{n+l}$$
(49)

5.1. Proof of theorem 2 (i)

When n = 1 equation (49) becomes

$$A_1 = \sum_{k=1}^{\infty} (-1)^k \prod_{j=1}^k \frac{1}{\sqrt{1 - ij\lambda} - 1} g_k.$$
(50)

With the notation

$$h_k = \prod_{j=1}^k (\sqrt{1 - ij\lambda} - 1)$$

equation (50) becomes

$$A_1 = \sum_{k=1}^{\infty} \frac{(-1)^k g_k}{h_k}.$$

Let

$$h_k = \mathrm{e}^{w_k} \sqrt{\lambda^{k-1}(k-1)!}.$$

We have

$$w_{k+1} - w_k = \log(\sqrt{1 - \mathrm{i}k\lambda} - 1) - \frac{1}{2}\log(\lambda k)$$

Differentiating in $\boldsymbol{\lambda}$ we obtain

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}(w_{k+1}-w_k)=\frac{1}{2\lambda\sqrt{1-\mathrm{i}k\lambda}}.$$

Let u_k be so that

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}u_k=\frac{\mathrm{d}}{\mathrm{d}\lambda}w_k-\frac{\mathrm{i}\sqrt{-\mathrm{i}k}}{\lambda^{3/2}}.$$

Then,

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}(u_{k+1}-u_k) = -\frac{\mathrm{i}\sqrt{-\mathrm{i}k-\mathrm{i}}}{\lambda^{3/2}} + \frac{\mathrm{i}\sqrt{-\mathrm{i}k}}{\lambda^{3/2}} + \frac{1}{2\lambda\sqrt{1-\mathrm{i}k\lambda}}.$$
(51)

By taking the inverse Laplace transform of (51) in k we get (we use p as the transformed variable here)

$$(e^{-p} - 1)\mathcal{L}^{-1}\frac{d}{d\lambda}u_k = \frac{\sqrt{i}(1 - e^{-p} + e^{-ip/\lambda}p)}{2\sqrt{\pi}(p\lambda)^{3/2}}.$$
(52)

Integrating (52) with respect to λ gives

$$\mathcal{L}^{-1}u_k = \frac{\sqrt{i}\lambda\left(-2 + 2\,\mathrm{e}^{-p} - \mathrm{i}^{3/2}\sqrt{p\pi\lambda}\mathrm{erf}\left(\frac{-\mathrm{i}^{3/2}\sqrt{p}}{\sqrt{\lambda}}\right)\right)}{2(-1 + \mathrm{e}^{-p})\sqrt{\pi}(p\lambda)^{3/2}}.$$

Thus

$$\frac{1}{h_k} = \frac{\mathrm{e}^{-w_k}}{\sqrt{\lambda^{k-1}(k-1)!}} = \exp\left(-\int_0^\infty \mathrm{e}^{-kp} \frac{\sqrt{\mathrm{i}\lambda}\left(-2+2\,\mathrm{e}^{-p}-\mathrm{i}^{3/2}\sqrt{p\pi\lambda}\mathrm{erf}\left(\frac{-\mathrm{i}^{3/2}\sqrt{p}}{\sqrt{\lambda}}\right)\right)}{2(-1+\mathrm{e}^{-p})\sqrt{\pi}(p\lambda)^{3/2}}\,\mathrm{d}p\right) \\ \times \exp\left(-\frac{2\mathrm{i}\sqrt{-\mathrm{i}k}}{\sqrt{\lambda}}\right)\lambda^{\frac{1-k}{2}}\frac{1}{\sqrt{\Gamma(k)}}.$$

Finally, we obtain

$$A_{1} = \sum_{k=1}^{\infty} \frac{(-1)^{k} g_{k}}{h_{k}} = \mathcal{L} \sum_{k=1}^{\infty} (-1)^{k} \mathcal{L}^{-1} \left(\frac{g_{k}}{h_{k}}\right)$$

$$= \int_{0}^{\infty} \sum_{k=1}^{\infty} (-1)^{k} e^{-kp} \mathcal{L}^{-1} \left(\frac{g_{k}}{h_{k}}\right) dp = \int_{0}^{\infty} \frac{-e^{-p}}{1 + e^{-p}} \mathcal{L}^{-1} \left(\frac{g_{k}}{h_{k}}\right) dp$$

$$= \int_{0}^{\infty} \frac{-e^{-p}}{1 + e^{-p}} \int_{c-i\infty}^{c+i\infty} g_{k} \exp\left(-\frac{2i\sqrt{-ik}}{\sqrt{\lambda}}\right) \lambda^{\frac{1-k}{2}} \frac{1}{\sqrt{\Gamma(k)}}$$

$$\cdot \exp\left(-\int_{0}^{\infty} e^{-kp} \frac{\sqrt{i}\lambda \left(-2 + 2e^{-p} - i^{3/2} \sqrt{p\pi\lambda} \operatorname{erf}\left(\frac{-i^{3/2} \sqrt{p}}{\sqrt{\lambda}}\right)\right)}{2(-1 + e^{-p}) \sqrt{\pi} (p\lambda)^{3/2}} dp\right) dk dp.$$

5.2. Proof of theorem 2 (ii)

Here we assume that the expansion of A_1 as $\lambda \to 0$ is invariant under a $\frac{\pi}{2}$ rotation; that is, there are no Stokes lines in the fourth quadrant; this would be ensured by Borel summability of the expansion in λ .

Let $\lambda = ir$ with r < 0, and for simplicity let $g \equiv 1$, then (50) implies

$$A_{1} = \sum_{n=1}^{\infty} \prod_{k=1}^{n} \frac{(-1)^{k}}{\sqrt{1+kr}-1} = \sum_{n=1}^{\infty} \frac{\prod_{k=1}^{n} (\sqrt{1+kr}+1)}{(-1)^{k} k! r^{k}}$$
$$= \sum_{n=1}^{\infty} \frac{\exp\left(\sum_{k=1}^{n} \log(\sqrt{1+kr}+1)\right)}{(-1)^{k} k! r^{k}}.$$
(53)

The Euler-Maclaurin summation formula gives

$$\sum_{k=1}^{n} \log(\sqrt{1+kr}+1) \sim \int_{0}^{n} \log(\sqrt{1+xr}+1) \, dx + C$$
$$= -\frac{1}{r} + k \log(\sqrt{1+kr}+1) - \frac{1}{2}k + \frac{\sqrt{1+kr}}{r} + C, \tag{54}$$

where

$$C \sim \sum_{k=1}^{1/r} \log(\sqrt{1+kr}+1) - \int_0^{1/r} \log(\sqrt{1+xr}+1) \, \mathrm{d}x \sim -\frac{\log(2)}{2}.$$

Therefore

$$A_1 \sim \sum_{k=1}^{\infty} \frac{\exp\left(-\frac{1}{r} + k\log(\sqrt{1+kr}+1) - \frac{1}{2}k + \frac{\sqrt{1+kr}}{r}\right)}{(-1)^k k! r^k}.$$
(55)

Since

$$\frac{\exp\left(-\frac{1}{r} + k\log(\sqrt{1+kr}+1) - \frac{1}{2}k + \frac{\sqrt{1+kr}}{r}\right)}{(-1)^k k! r^k} \sim \exp\left(-\frac{3}{2r} + \frac{2}{3}\sqrt{r}\left(k + \frac{1}{r}\right)^{(3/2)} - \frac{\log(2)}{2} - \frac{\log(\pi)}{2} + \frac{\log(-r)}{2}\right)$$

applying the Euler-Maclaurin summation formula again we get

$$A_1 \sim \frac{2^{1/3} 3^{1/6} \Gamma\left(\frac{2}{3}\right) e^{-\frac{3i}{2\lambda}} (-i\lambda)^{1/6}}{2\sqrt{\pi}}.$$
(56)



Figure 1. Log-log plot of $|R_0|$ as a function of λ for $\omega = 0$. $R_{0,0}$ is the residue of the pole of $\hat{\psi}(p, x)$ at p = i, see corollary 16.

5.3. Numerical results

Figure 1 shows $\log(|R_0|)$ as a function of $\log(\lambda)$, very nearly a straight line with slope 1/6 (corresponding to the $\lambda^{1/6}$ behavior), with good accuracy even for λ as large as 1.

6. Ionization rate under a short pulse

We now consider a short pulse, with fixed total energy and fixed total number of oscillations. The corresponding Schrödinger equation is

$$\frac{\partial \psi}{\partial t} = \left(-\frac{\partial^2}{\partial x^2} - 2\delta(x) + 2\lambda\delta(x) e^{-\lambda t} \cos(\omega t) \right) \psi, \tag{57}$$

where λ is now a large real parameter (note the factor λ in front of the exponential). We are interested in the ionization rate as $\lambda \to \infty$.

By similar arguments as in section 3.5 we have the convergent representation

$$A_{m,n} = \sum_{i=0}^{\infty} (-1)^{i} \left(\frac{\lambda}{2}\right)^{i} \sum_{\tau \in 2^{i}} \prod_{j=0}^{i} B_{n+j,m+|\tau_{j}^{0}|} g_{n+i,m+|\tau|}$$
(58)

Figures 2–4 give $|R_{0,0}|$ (see corollary 16) in terms of λ for different values of ω/λ .

7. Results for $\lambda = 0$ and $\omega \neq 0$

We briefly go over the case $\lambda = 0$, where ionization is complete; the full analysis is done in [5]. In this case, $\hat{\psi}$ does not have poles on the imaginary line; we give a summary of the argument in [5].

The homogeneous equation now reads

$$\sqrt{\sigma + m\omega}A_m = -\frac{1}{2}A_{m+1} - \frac{1}{2}A_{m-1} + A_m.$$
(59)



Figure 2. $|R_{0,0}|$ as a function of λ , with fixed ratio $\omega/\lambda = 5$. $R_{0,0}$ is the residue of the pole of $\hat{\psi}(p, x)$ at p = i, see corollary 16.



Figure 3. $|R_{0,0}|$ as a function of λ , with fixed ratio $\omega/\lambda = 15$.

Thus we have

$$\sum_{\mathbb{N}} \sqrt{\sigma + m\omega} A_m \overline{A_m} = -\frac{1}{2} \sum_{\mathbb{N}} A_{m+1} \overline{A_m} - \frac{1}{2} \sum_{\mathbb{N}} A_{m-1} \overline{A_m} + \sum_{\mathbb{N}} A_m \overline{A_m}.$$

The first and the second sums on the right-hand side are conjugate to each other, and each term in the third sum is real. So the right-hand side is real, thus the left-hand side is also real.

For $\text{Im}(\sigma) \neq 0$, $\text{Im}(\sqrt{\sigma + m\omega}A_m\overline{A_m})$ has the same sign as $\text{Im}\,\sigma$. Therefore, the sum cannot be real and the equation has no nontrivial solution. When $\text{Im}(\sigma) = 0$, for m < 0, all $\text{Im}(\sqrt{\sigma + m\omega}A_m\overline{A_m})$ have the same sign and for $m \ge 0$, $\sqrt{\sigma + m\omega}A_m\overline{A_m}$ is real. Since the final sum is purely real, this means $A_m = 0$ for m < 0. But then, recursively, all A_m should be 0.

Zero is thus the only solution to (59). By the Fredholm alternative the solution A is analytic in $\sqrt{\sigma}$ and thus the associated y is analytic in $\sqrt{\sigma}$. This entails complete ionization.



Figure 4. $|R_{0,0}|$ as a function of λ , with fixed ratio $\omega/\lambda = 30$.



Figure 5. $|R_{0,0}|$, at $\lambda = 0.01$, as a function of ω . $R_{0,0}$ is the residue of the pole of $\hat{\psi}(p, x)$ at p = i, see corollary 16.

7.1. Small λ behavior

We expect that the behavior of the system at $\lambda = 0$ is a limit of the one for small λ . However, this limit is very singular, as the density of the poles in the left half plane goes to infinity as $\lambda \rightarrow 0$, only to become finite for $\lambda = 0$. Nonetheless, given λ , formula (45) allows us to calculate the residue of $\hat{\psi}$.

Figure 5 shows the behavior of the residue versus ω , for $\lambda = 0.01$.

We show for comparison the corresponding result when $\lambda = 0$ in figure 6. The staircase shape in figure 6 corresponds to multi-photon ionization see, for example, [10, 11]. For qualitative and quantitative comparisons with experimental results on Rydberg atoms, see [2].



Figure 6. $\log_{10} \Gamma^{-1}$, at $\lambda = 0$, as a function of ω/ω_0 . Γ is the Fermi golden rule exponent for the probability decay and $\hbar\omega_0 = E_0$, the energy of the bound state of one delta function of amplitude *r* [2]. (We normalized so that $\omega_0 = 1$.)

8. Conclusions

We have shown rigorously that in the setting of a one-dimensional Schrödinger equation with a damped time-harmonic delta function potential, partial ionization occurs for generic initial wavefunctions (theorem 1). Unlike the case where there is no damping, there is generically a pole on the imaginary axis of the Laplace transform of the wavefunction. We have provided a formula that allows for the numerical calculation of the ionization rate (see (45)) with rigorous error bounds. The formula is especially useful when λ , the decay rate of the damping field, is not extremely small and when the amplitude of the time-dependent potential is not very large. We have provided numerical results for small λ (see figure 5) as well as the ionization rate under a short pulse (see figure 2-4). We note again that the limit $\lambda \rightarrow 0$ is mathematically very singular since the density of resonances goes to infinity only to become zero in the limit.

In addition, we obtain rigorously an explicit formula for the wavefunction with a timedependent damped delta function potential (without the periodic term—theorem 2). We provide a formula for calculating the ionization rate, and a simple and explicit formula (see part (ii) of theorem 2) describing the singular limit $\lambda \to 0$ in this case. Although we did not include a detailed proof for the $\lambda \to 0$ formula, the formula is numerically confirmed with very high accuracy (see figure 1).

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