TRANSITION TO THE CONTINUUM OF A PARTICLE IN TIME-PERIODIC POTENTIALS

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Abstract. We present new results for the transition to the continuum of an initially bound quantum particle subject to a harmonic forcing. Using rigorous exponential asymptotics methods we obtain explicit expressions, as generalized Borel summable transseries, for the probability of localization in a specified spatial region at time t. The transition to the continuum occurs for general compactly supported potentials in one dimension and our results extend easily to higher dimensional systems with spherical symmetry. This of course implies the absence of discrete spectrum of the corresponding Floquet operator.

1. Introduction

We investigate the delocalization (ionization) of an initially localized (bound) particle as a result of the action of a time periodic external potential. The time evolution of the particle wave function $\psi(x,t), x \in \mathbb{R}^d$ is described by the non-relativistic Schrödinger equation

$$i\,\frac{\partial\psi}{\partial t} = [H_0 + H_1(t)]\;\psi \tag{1.1}$$

Here H_0 is the time-independent reference (or intrinsic) Hamiltonian,

$$H_0 = -\Delta + V(x) \tag{1.2}$$

and H_1 is the external, not necessarily small, potential having the form

$$H_1 = \Omega(x)\,\eta(t) \tag{1.3}$$

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with $\eta(t) = \eta(t + 2\pi/\omega)$, $\omega > 0$. The potentials $V(x)$ and $\Omega(x)$ have compact support and $V(x)$ is such that H_0 has both bound and continuum (quasi-free) states. We are interested in the behavior of solutions ψ for large t, when $\psi(x, 0) \in L^2(\mathbb{R}^d)$, $\int_{\mathbb{R}^d} |\psi|^2 = 1$.

If the *survival probability* for the particle in the ball of radius B in $\mathbb{R}^d$, $\int_{|x|<B} |\psi|^2 dx := \mathcal{P}_B(t) \to 0$ as $t \to \infty$ for all B, we say that the particle escapes to infinity and *complete ionization* occurs.

The setting (1.1), (1.2), (1.3) with appropriate choices of V, Ω and η (not necessarily satisfying our conditions) is common for studying the ionization of atoms and the dissociation of molecules by electromagnetic fields [1, 2, 3, 4].

We apply techniques stemming from rigorous exponential asymptotics to obtain:

(1) Exact representation of the probability $\mathcal{P}_B(t)$ as generalized Borel summable transseries [5, 6, 7].
(2) Effective conditions for complete ionization. These imply ipso facto absence of discrete Floquet spectrum, see [8, 9].

Recently, Galtbayar, Jensen and K Yajima [17] obtained general results about the asymptotic behavior of the wave function in terms of the discrete spectrum of the Floquet operator. In our setting, the discrete spectrum of the Floquet operator is empty and furthermore the asymptotic expansion of the wave function is Borel summable providing a complete representation for $t > 0$.

2. Summary of previous results

In the first model that we studied the system was one-dimensional and both Ω and V where δ-functions centered at the origin. Equation (1.1) then takes the form

$$i\frac{\partial \psi}{\partial t} = \left(-\frac{\partial^2}{\partial x^2} - 2\delta(x)\right)\psi - \delta(x)\eta(t)\psi, \qquad x \in \mathbb{R} \tag{2.1}$$

For η we took a sine-function:

$$\eta(t) = 2\, r \, \sin \omega t \tag{2.2}$$

In this case the spectrum of the unperturbed system (equation (2.1) with $r = 0$) consists in one bound state $u_b(x) = e^{-|x|}$ with energy $E_b = -\omega_0 = -1$, and a continuous spectrum for energies $E = k^2 > 0$ with generalized eigenfunctions

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

The solution ψ of (2.1), (2.2) with initial condition $\psi(x,0) = u_b(x)$ can be written as $\psi(x;t) = \theta(t)u_b(x) + \psi_\perp$ (with $\psi_\perp$ orthogonal to the bound state); thus $|\theta(t)|^2$ is the survival probability *in the bound state.*

Theorem 1. *For the system (2.1), (2.2) we have*

$$\lim_{t\to\infty} |\theta(t)|^2 = 0$$

for all ω and $r \neq 0$.

As noted in §3 Remark 1 of [11] the result can be extended to show $\mathcal{P}_B(t) \to 0$ as $t \to \infty$.

The proof in [10] of Theorem 1 relies on showing that θ has a (unique) *rapidly convergent* representation of the form

$$\theta(t) = e^{-\gamma(r;\omega)t+it}F_\omega(t) + \sum_{m=-\infty}^{\infty} e^{(mi\omega-i)t}h_m(t) \tag{2.3}$$

where $\gamma(r;\omega) > 0$, F_ω is periodic of period $2\pi\omega^{-1}$, and

$$h_m(t) \sim \sum_{j=0}^{\infty} h_{m,j}t^{-3/2-j} \quad \text{as } t \to \infty,\ \arg(t) \in \Big(-\frac{\pi}{2}, \frac{\pi}{2}\Big) \tag{2.4}$$

One ingredient in the analysis which is worth stating in its own right is the absence of discrete spectrum of the Floquet operator associated to the problem.

Lemma 2. *The discrete spectrum of the Floquet operator for the model (2.1), (2.2) is empty.*

Proof. Let $\mathcal{L}\psi(x;p) = \int_0^\infty \psi(x;t)e^{-pt}dt$ be the Laplace transform of ψ with respect to t. Set $y_n(x) = \mathcal{L}\psi(x, i\sigma + in\omega)$ where $n \in \mathbb{Z}$ and $\Re(\sigma) \in [0,\omega)$ (for more details see §4.1 below). Then the y_n satisfy an infinite system of differential equations (closely related to eq. (14) of [11]) whose homogeneous part is:

$$-y_n''(x) + (-2\delta(x) + \sigma + n\omega)y_n(x) = ir\delta(x)(y_{n+1}(x) - y_{n-1}(x)) \tag{2.5}$$

An immediate calculation shows that the system (2.5) admits a nontrivial L^2 solution iff the Floquet operator has nontrivial discrete spectrum. On the other hand, it can be seen that any nonzero L^2 solution of (2.5) must be have $y_n = 0$ for $n < 0$. Then the two-step recurrence (2.5) implies that $y_n = 0$ for all n. □

A detailed description of the behavior of $\theta(t)$ is found in [10], [12].

2.1. **General periodic η.** The next step was to consider (2.1) for η a general periodic function

$$\eta(t) = \sum_{j=0}^{\infty} \left(C_j \, e^{i\omega j t} + \overline{C_j} \, e^{-i\omega j t} \right) \tag{2.6}$$

under the assumptions that

$$\eta \not\equiv 0, \ \eta \in L^{\infty}, \text{ and } C_0 = 0 \tag{2.7}$$

It turns out that the ionizing properties of the system (2.1), (2.6) depend nontrivially on special properties of the Fourier coefficients: ionization occurs for generic η, but there are exceptions.

Genericity condition (g). Consider the right shift operator T on $l_2(\mathbb{N})$ given by

$$T\,(C_1, C_2, ..., C_n, ...) \,=\, (C_2, C_3, ..., C_{n+1}, ...)$$

We say that $\mathbf{C} \in l_2(\mathbb{N})$ satisfies condition (g), if the Hilbert space generated by all the translates of $\mathbf{C}$ contains the kernel of T, i.e.,

$$e_1 \in \bigvee_{n=0}^{\infty} T^n \mathbf{C} \tag{2.8}$$

The right side of (2.8) denotes the closure of the space generated by the $T^n\mathbf{C}$ with $n \geq 0$. This condition, weaker than cyclicity, is generically satisfied. In particular it clearly holds for trigonometric polynomials.

Theorem 3 ([11])**.** *When condition (g) is satisfied then the system (2.1), (2.6) satisfies Theorem 1.*

A simple example for which (g) does not hold is $\mathbf{C}_\lambda = r(\lambda, \lambda^2, ..., \lambda^n, ...)$ (with $|\lambda| < 1$) since $\mathbf{C}_\lambda$ is an eigenvector of T. It corresponds to

$$\eta(t) = 2r\lambda \frac{\lambda - \cos(\omega t)}{1 + \lambda^2 - 2\lambda\cos(\omega t)} \tag{2.9}$$

Theorem 4 ([11])**.** *Consider the system (2.1) with $\eta(t)$ of the form (2.9). Then for any ω, r there exists λ for which*

$$\lim_{t\to\infty} |\theta(t)|^2 \,\neq\, 0$$

In this case $\theta(t)$ approaches a quasiperiodic function as $t \to +\infty$. The two periods correspond to ω and to the discrete eigenvalue of the Floquet operator. The proof of Theorem 4 gives a constructive way to find λ such that the Floquet operator has a discrete eigenvalue.

Theorem 4 is particularly striking in that an increase in the strength r of the forcing can lead to a suppression of ionization. We also found

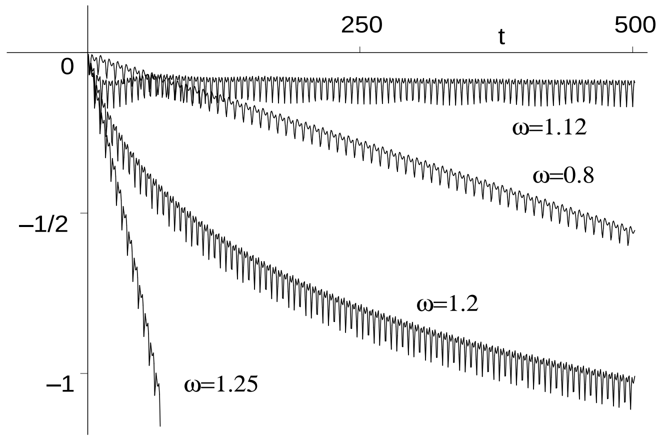

FIGURE 1. Plot of $\log_{10}|\theta(t)|^2$ for $a \approx 0.59,\ r = 1$.

other examples where one can adjust the parameters of the periodic forcing to prevent ionization. In particular, [13] studies the case where (1.1) takes the form

$$i\frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{\partial^2}{\partial x^2} - 2\delta(x) + \Omega_{1,2}(x) r \sin\omega t\right]\psi(x,t) \tag{2.10}$$

for $\Omega_1(x) = 2\delta(x-a)$ or $\Omega_2(x) = 2[\delta(x+a) - \delta(x-a)]$.

We showed in [13] that for this system there exists a two-dimensional manifold in the a, r, ω parameter space for which $\theta(t)$ is asymptotically a quasi-periodic function of t; this latter behavior occurs iff $a \geq 1/2$. Some representative curves are shown in Fig.1.

For Ω_2 we can have localization even when the term $-2\delta(x)$ is absent in (2.10) or $V(x) = 0$, i.e. the reference Hamiltonian H_0 is just that of a free particle.

We finally note that all cases where $\theta(t) \not\to 0$ are *nonperturbative*: $\eta(t)$ cannot be made arbitrarily small. This is consistent with perturbation theory, including the Fermi Golden Rule, proven under certain assumptions in [4, 14]. Note also that in Fig. 1 only the cases $\omega = 0.8$ and $\omega = 1.25$ correspond (aside from wiggles) to an exponential decay of $|\theta(t)|^2$, a form generally assumed on the basis of perturbation theory.

3. New results for general interactions

Consider now the general one-dimensional equation (1.1) with V and Ω compactly supported and continuous, and $\eta(t) = \sin\omega t$.

Theorem 5. *Assume $\Omega > 0$ throughout the support of V. Then*

$$\lim_{t\to\infty} \mathcal{P}_B(t) \;=\; 0 \tag{3.1}$$

Our techniques allow us in fact to find the full asymptotic expansion of $\psi(x,t)$, including the exponentially small corrections. More generally, if $\psi(0,x)$ is continuous and compactly supported then

Theorem 6. *For $t > 0$ there exist $N \in \mathbb{N}$ and $\{\Gamma_k\}_{k\le N}$, $\{F_{\omega;k}(t,x)\}_{k\le N}$, $2\pi/\omega$-periodic functions of t, such that*

$$\psi(t,x) = H_\omega(t,x) + \sum_{k=1}^{N} e^{-\Gamma_k t} F_{\omega;k}(t,x) \tag{3.2}$$

with $\Re\Gamma_k > 0$ for all $k \le N$, and

$$H_\omega(t,x) = \sum_{j\in\mathbb{Z}} e^{ij\omega t} h_j(t,x) \tag{3.3}$$

and $h_j(t,x)$ have Borel summable power series in t,

$$h_j(t,x) = \mathcal{LB}\sum_{k\ge 3} h_{kj}(x) t^{-k/2} \tag{3.4}$$

In particular, $H_\omega(t,x) = O(t^{-3/2})$, $t\to\infty$. The operator $\mathcal{LB}$ (Laplace-Borel) stands for generalized Borel summation [7]. The representation (3.2) generalizes (2.3).

Remark. In (3.2), Borel summability can be briefly stated as follows. We have

$$h_j(t,x) = \int_0^\infty F_j(\sqrt{p},x)\, e^{-pt}\, dp \sim \sum_{k\ge 3} h_{kj}(x)\, t^{-k/2},\ t\to+\infty$$

The functions $F_j(s,x)$ are analytic in s in a neighborhood of $\mathbb{R}^+$ and for any $B \in \mathbb{R}$ there exist constants K_1, K_2 such that for all j and $p \in \mathbb{R}^+$,

$$\sup_{p\ge 0;|x|<B} |F_j(\sqrt{p},x)e^{-K_2|p|}| \le (K_1)/(j!)^2$$

so the function series (3.3) is rapidly convergent.

Notes.

(1) It follows easily from (3.2)–(3.4) that $\mathcal{P}_B(t)$ also has a Borel summed transseries representation.
(2) Our present method does not provide a simple link between N and the parameters of the problem.
(3) Theorems 5 and 6 can be extended to $\eta(t)$ a trigonometric polynomial and to any compactly supported continuous $\Omega \not\equiv 0$.
(4) It is important for Theorem 5 that $\Omega(x)$ be a function (not a distribution) as *counter-examples* show (see (2.10)); see however §4.1.3 below.
(5) The form of $V(x)$ does not play an important role in the analysis.

3.1. **Higher dimensions.** Consider now equation (1.1) in 3 dimensions, with additional assumptions:

- $V(x) = V(|x|)$.
- $\Omega(x) = \Omega(|x|)$.
- Ω and V are compactly supported, and $\Omega > 0$ throughout the support of V.
- $\eta(t) = \sin\omega t$.

Theorem 7. *Under the above assumptions, (3.1) holds.*

4. Nature of proofs in the general case

The proof of Theorem 5 is constructive and can be used in more general settings to determine ionization conditions (for which all $\Re\Gamma_k$ are positive) [15].

The asymptotic expansion of $\mathcal{P}_B(t)$ is studied using Tauberian-type methods. The appropriate Tauberian duality for this problem is, as already indicated in §2, the *Laplace-Inverse Laplace* one (essential to modern exponential asymptotics and analyzability theory [6]).

Solutions of (1.1) are Laplace transformable, since the evolution is unitary, and $\mathcal{L}\psi(x,\cdot)$ is analytic in the open right half plane. Regularity of $\mathcal{L}\psi$ is then studied using *generalizations of the Fredholm alternative* to functions with singularities.

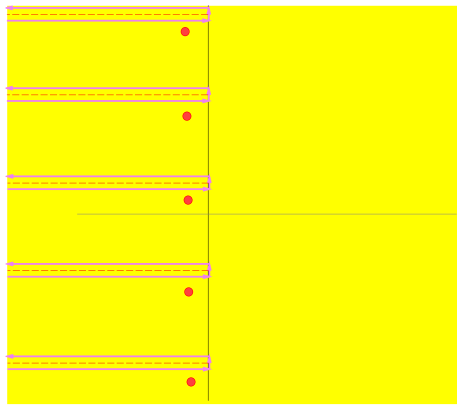

FIGURE 2

In Fig. 2 we illustrate the actual structure of singularities of $\mathcal{L}\psi$ for the model (2.1), (2.2). There are infinitely many square-root branch points on the imaginary line and infinitely many poles, equally spaced. These determine the transseries (2.3).

4.1. **Analytic properties of $\mathcal{L}\psi$.** Using the notation

$y_n(x) \equiv y_n(x;\sigma) = \mathcal{L}\psi\,(x,p)$, for $p = i\,(n\omega+\sigma)$, $n \in \mathbb{Z}$, $\Re\sigma \in [0,\omega)$ we get a coupled system of differential equations

$$-y_n'' + (V + n\omega + \sigma)y_n = -i\Omega\Big[y_{n+1} - y_{n-1}\Big] + \psi(x,0) \quad , \; n \in \mathbb{Z}$$

which can be written as a system of integral equations

$$y_n = \mathcal{K}_n(\sigma)\,[y_{n+1} - y_{n-1}] + f_{0;n} \quad , \; n \in \mathbb{Z} \tag{4.1}$$

where $\mathcal{K}_n(\sigma)$ is the the resolvent:

$$\mathcal{K}_n(\sigma)g = \frac{\phi_n^+(x)}{W_n}\int_{-\infty}^{x}\phi_n^-\,\Omega\,g\,ds + \frac{\phi_n^-(x)}{W_n}\int_{x}^{\infty}\phi_n^-\,\Omega\,g\,ds$$

The $\phi_n^\pm$ are the solutions of $-\psi'' + (V + n\omega + \sigma)\psi = 0$, which decay at $\pm\infty$ respectively and W_n is their Wronskian.

We write the system (4.1) as

$$Y = \mathcal{K}(\sigma)Y + F \tag{4.2}$$

and treat (4.2) as a fixed point problem in the Hilbert space

$$\mathcal{H} = L^2(\text{supp } \Omega) \otimes l^2(\mathbb{Z}, \langle n \rangle^{3/2})$$

(supp Ω is compact) where $l^2(\mathbb{Z}, \langle n \rangle^{3/2})$ denotes the Hilbert space of sequences $Y = \{y_n\}_{n \in \mathbb{Z}}$ with the norm

$$\|Y\|^2 = \sum_n (1 + |n|)^{3/2} |y_n|^2$$

(the weight $|n|)^{3/2}$ is natural for this problem, and at the same time ensures suitable decay). It is relatively easy to see that the operator $\mathcal{K}(\sigma)$ is compact (wherever well defined) and depends analytically on σ if $\Im(\sigma) < 0$.

We need to understand the singularities of $\mathcal{L}\psi(x,p)$ for $\Re p \le 0$, hence of $y_n(x;\sigma)$ for $\Im(\sigma) \ge 0$. Possible sources of singularities are:

(1) Discrete spectrum of the time-independent Hamiltonian H_0 (the values of σ for which $W_n = 0$). These give rise to poles of $\mathcal{K}(\sigma)$ and can only occur if σ is real. It turns out that at such points Y is analytic (unless $\Omega \equiv 0$).
(2) The bottom of the continuous spectrum at $\sigma = 0$ generates branch-points of Y.
(3) The noninvertibility of $I - \mathcal{K}(\sigma)$ gives rise to poles in Y.

The points of noninvertibility of $I - \mathcal{K}(\sigma)$ are crucial for the regularity of $Y = Y(x;\sigma)$ required for ionization.

For $\Im(\sigma) < 0$ it is not difficult to show, using the self-adjointness of the Hamiltonian, that $I - \mathcal{K}(\sigma)$ is invertible with an analytic inverse. The same clearly holds for small Ω, since then the norm of the operator $\mathcal{K}(\sigma)$ is also small. This in turns shows that ionization occurs whenever the forcing is small enough.

Our methods and results are however aimed at the case where the periodic forcing H_1 is not small. In this case it can happen that $I - \mathcal{K}(\sigma)$ does not have an analytic inverse at certain points with $\Im(\sigma) = 0$. This is exactly what happens in the examples in §2 when $\theta(t) \not\to 0$.

After some algebraic manipulations it can be shown that noninvertibility of $I - \mathcal{K}(\sigma)$ implies the existence of a nontrivial L^2 solution of the system

$$\begin{aligned} -y_n'' + (V + n\omega + \sigma) y_n &= -i\Omega(y_{n+1} - y_{n-1}) \qquad (n \in \mathbb{Z}^-) \\ |y_n| + |y_n'| &= 0 \text{ outside supp}(\Omega) \end{aligned} \tag{4.3}$$

(such a y would imply the existence of a Floquet eigenvalue). Intuitively it is clear that (4.3) should entail $y_n = 0$ as the system (4.3) is overdetermined.

We prove that indeed $y = 0$ under our assumptions. We assume, for definiteness and without loss of generality, that $\mathrm{supp}(\Omega) = [0, 1]$. We show that solutions of (4.3) which are zero for $x \le 0$ cannot be zero at $x = 1$.

The key result is the following Lemma.

Lemma 8. *Assume there exists a nonzero solution of (4.3) in the space* $L^2([0, 1]) \otimes l^2(\mathbb{Z}, \langle n\rangle^{3/2})$ *with* $|y_n(0)| + |y_n'(0)| = 0$ *for* $n < 0$. *Then there exist* n_0 *and* C *such that*

$$y_{n+n_0} = \frac{\left(\int_0^x \sqrt{\Omega(s)}ds\right)^{2|n|}}{(2|n|)!}\Omega^{-\frac{1}{4}}(1 + o(1)) \ (n \to -\infty) \tag{4.4}$$

uniformly on $[0, 1]$.

The proof of Lemma 8 is done by rigorous WKB (see also [16]).

Relation (4.4) precludes $y_n(1) = 0$ for large enough $-n$. This in turn shows that the operator $I - K(\sigma)$ is invertible and the solution of (4.2) is analytic away from the discrete spectrum of H_0.

*

Completion of the argument: Analysis of other singularities.

4.1.1. *Discrete spectrum of* V. Extended versions of Fredholm's alternative that we construct show that nonexistence of solutions of (4.6) implies regularity at the discrete spectrum of V, i.e. for values of σ at which $W_n = 0$.

4.1.2. *The bottom of the continuous spectrum of* V. For $\sigma = 0$ similar arguments and an appropriate version of the Fredholm alternative show that

$$y_n(x; is) = A_n(x; s)\sqrt{s - n\omega} + B_n(x; s)$$

with A_n, B_n analytic in s on $((n-1)\omega, (n+1)\omega)$. Deformation of contour provides now the proof of Borel summability of the transseries.

4.1.3. *Distributional* Ω. We proved that Theorem 5 also holds if Ω is a sum of delta functions:

$$\Omega(x) = \sum_{j=1}^{J} \Omega_j\, \delta(x - x_j), \quad 0 < x_1 < x_2 < ... < x_J < 1 \tag{4.5}$$

provided $\max_{j<J}\{x_{j+1} - x_j\}$ is *small enough* (note that this is not the case in the example (2.10)).

4.1.4. *More general approach to the problem of invertibility of $I - \mathcal{K}(\sigma)$.* This problem can be reformulated in terms of analytic properties an associated (generating function) $Y(x,z)$ satisfying the equation

$$-\frac{\partial^2 Y}{\partial x^2} + z\frac{\partial Y}{\partial z} + z\Omega(x)Y = 1 + \gamma(x,z;Y) \tag{4.6}$$
$$\text{with} \quad Y(0,z) = Y_x(0,z) = Y(1,z) = Y_x(1,z) = 0$$

where $\gamma(x,z;Y)$ is small in a precise sense.

In this setting, existence of some j with $\Gamma_j = 0$ (thus absence of ionization) implies that the problem (4.6), which is again overdetermined, has a solution Y which is entire in z. The solution Y can however be controlled by an extension of WKB methods in a more convenient way than the infinite system of ODEs (4.3).

4.2. **Higher-dimensional cases.** The proof follows the same lines as in the one-dimensional problem after using spherical symmetry to decouple the radial part of the Schrödinger equation. The differences with respect to one-dimension are the following. The form of the asymptotic expansion (4.4) is more complicated, since the radial equation is singular at $r = 0$ and in the WKB-like expansion Bessel functions are used to uniformize the asymptotics. Secondly, at $r = 0$ there is only one condition, boundedness of y; however the system remains overdetermined since, in addition, y has to vanish together with its radial derivative at the boundary of the support of Ω. The rest of the proof goes through without important changes.

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