Nonperturbative analysis of a model quantum system under time periodic forcing

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Abstract

We analyze the time evolution of a one-dimensional quantum system with an attractive delta function potential whose strength is subjected to a time periodic (zero mean) parametric variation $\eta(t)$. We show that for generic $\eta(t)$, which includes the sum of any finite number of harmonics, the system, started in a bound state will get fully ionized as $t \to \infty$ irrespective of the magnitude or frequency of $\eta(t)$. For the case $\eta(t) = r\sin(\omega t)$ we find an explicit representation of the probability of ionization. There are however exceptional, very non-generic $\eta(t)$, that do not lead to full ionization. These include rather simple explicit periodic $\eta(t)$ for which the system evolves to a nontrivial localized stationary state related to eigenfunctions of the Floquet operator.

Analyse non-perturbative d'un systeme quantique modèle avec force exterieure periodique

Résumé

Nous analysons l'évolution dans le temps d'un système unidimensionel avec un potentiel attractif de type fonction delta soumis a une variation périodique de moyenne nulle, $\eta(t)$. Nous démontrons que pour η générique (en particulier pour une somme finie d'oscillations harmoniques) le système qui est d'abord dans un état lié vat être complètement ionisé pour $t \to \infty$. Des fonctions $\eta(t)$ très nongénériques, toutefois explicites, existent pour lesquelles le système évolue vers un état localisé non-trivial, lié aux fonctions propres de l'opérateur de Floquet associé.

1 Version française abrégée

Nous étudions rigoureusement le comportement pour $t \to \infty$ d'un système quantique unidimensionnel simple, avec potentiel attractif de type delta, soumis à une variation paramétrique périodique. Dans des unités convenables, le Hamiltonien est de la forme

$$H(t) = H_0 - 2\,\eta(t)\delta(x) = \frac{\mathrm{d}^2}{\mathrm{d}x^2} - 2\,\delta(x) - 2\,\eta(t)\delta(x)$$

où H_0 a un seul état lié $u_b = e^{-|x|}$ d'énergie $\omega_0 = -1$ et un spectre continu sur l'axe réel positif, avec fonctions propres généralisées, voir eq. (3).

On peut développer la solution de l'équation de Schrödinger $\psi(x,t)$ par rapport aux fonctions propres de H_0 (5) avec conditions initielles $\theta(0) = \theta_0$, $\Theta(k,0) = \Theta_0(k)$ normalisées convenablement, eq. (6). Alors, la probabilité de survie de l'état lié est $P(t) = |\theta(t)|^2$, alors que $|\Theta(k,t)|^2 dk$ donne la "fraction de particules éjectées" avec (quasi-) impulsion dans l'intervalle dk. En prennant la fonction Y donnée par (7) on obtient les équations eq. (8) et Y satisfait une équation intégrale, (10). Notre méthode d'analyse utilise les propriétés analytiques de la transformation de Laplace $y(p)$ de $Y(t)$ pour déterminer les propriétés asymptotiques de $Y(t)$ par rapport à t.

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2 Cas où $\eta(t)$ est harmonique

Théorème 1 [9]. *Si $\eta(t) = r \sin \omega t$, la probabilité de survie $|\theta(t)|^2$ tend vers zéro quand $t \to \infty$, pour tous $\omega > 0$ et $r \neq 0$.*

Remarques. (**1**) On obtient une formule exacte (11) pour $\theta(t)$ où F_ω est périodique de période $2\pi\omega^{-1}$ et les fonctions h_m satisfont (12). Pas trop près des résonances, si $|\omega - n^{-1}| > O(r^{2-\delta})$ pour tout entier positif n, $|F_\omega(t)| = 1 \pm O(r^2)$ et les coefficients de Fourier de F décroissent plus vite que $r^{|2m|}|m|^{-|m|/2}$. Aussi, la somme en (11) est plus petite que $O(r^2 t^{-3/2})$ pour t grand, et les h_m décroissent avec m plus vite que $r^{|m|}$.

(**2**) On voit grâce à (11) que pour des temps d'ordre $1/\Gamma$ où $\Gamma = 2\Re(\gamma)$, la probabilité de survie pour ω pas trop près d'une résonance décroit comme $\exp(-\Gamma t)$, et que le comportement asymptotique en t est $|\theta(t)|^2 = O(t^{-3})$ avec beaucoup d'oscillations.

(**3**) Quand r est plus grand, le comportement polynomial-oscillatoire commence plus tôt et la probabilité de survie est plus *grande*. Ce phénomène est parfois appelé stabilisation atomique.

(**4**) En utilisant une fraction continue convergente, on peut calculer Γ pour ω and r arbitraires. Pour r petit, si n est la partie entière de $\omega^{-1} + 1$ et si $\omega^{-1} \notin \mathbb{N}$, alors, pour $T > 0$ ($t = r^{-2n}T$), Γ est donné par (13).

(**5**) Le comportement de Γ est différent aux résonances $\omega^{-1} \in \mathbb{N}$. Par exemple si $\omega - 1 = r^2/\sqrt{2}$ on trouve la formule (14).

2.1 Cas périodique général

On écrit η sous la forme (15) et nos hypothèses sur les C_j sont (a) $0 \not\equiv \eta \in L^\infty(\mathbb{T})$, (b) $C_0 = 0$ et (c) $C_{-j} = \overline{C_j}$. Considérons aussi l'hypothèse de généricité **(g)** suivante: on définit la translation a droite $T(C_1, C_2, ..., C_n, ...) = (C_2, C_3, ..., C_{n+1}, ...)$. Alors, $\mathbf{C} \in l_2(\mathbb{N})$ est *générique par rapport a T* si l'espace de Hilbert engendré par toutes les translations de $\mathbf{C}$ contient le vecteur $e_1 = (1, 0, 0...,)$, cf. (16). Un cas important est donné par les polynômes trigonométriques. Un exemple qui ne satisfait pas à l'hypothèse (g) est (17) pour $\lambda \in (0,1)$, pour lequel $C_n = -r\lambda^n$ for $n \geq 1$.

2.2 Resultats dans le càs périodique

Théorème 2 [10]. *Sous les hypothèses (a), (b), (c) et (g), la probabilité de survie $P(t)$ de l'état lié u_b, $|\theta(t)|^2$ tend vers zéro quand $t \to \infty$.*

Théorème 3 [10]. *Pour $\psi_0(x) = u_b(x)$ il existe des valeurs de λ, ω et r en (17), pour lesquelles $|\theta(t)| \not\to 0$ quand $t \to \infty$.*

Remarque. Le Théorème 3 peut être étendu pour démontrer que pour r et ω donnés en (17) il existe un ensemble infini de λ, avec un point d'accumulation en 1, pour lequel $\theta(t) \not\to 0$.

3 English version

3.1 The problem

We are interested in the nature of the solutions of the Schrödinger equation

$$i\hbar\partial_t\psi = [H_0 + H_1(t)]\psi \tag{1}$$

Here ψ is the wavefunction of the system, belonging to some Hilbert space $\mathcal{H}$, H_0 and H_1 are Hermitian operators and equation (1) is to be solved subject to some initial condition ψ_0. H_0 has both a discrete and a continuous spectrum corresponding respectively to spatially localized (bound) and scattering (free) states in $\mathbb{R}^d$. Starting at time zero with the system in a bound state and then "switching on" at $t = 0$ an external potential $H_1(t)$, we want to know the "probability of survival", $P(t)$, of the bound states, at times $t > 0$; $1 - P(t)$ is the probability of ionization [1]–[8].

When ω is sufficiently large for "one photon" ionization to take place, i.e., when $\hbar\omega > -E_0$, E_0 the energy of the bound (e.g. ground) state of H_0 and r is "small enough" for H_1 to be treated as a perturbation of H_0 then the long time behavior of $P(t)$ is asserted in the physics literature to be given by $P(t) \sim \exp[-\Gamma_F t]$. The rate constant Γ_F is computed from first order perturbation theory according to Fermi's golden rule. It is proportional to the square of the matrix element between the bound and free states, multiplied by the appropriate density of continuum states in the vicinity of the final state which will have energy $\hbar\omega + E_0$ [5, 7, 8].

The results described here show that the phenomenon of ionization by periodic fields is very complex indeed once one goes beyond the perturbative regime.

4 Our model

We consider a very simple quantum system where we can analyze rigorously many of the phenomena expected to occur in more realistic systems described by (1). This is a one dimensional system with an attractive delta function potential. The unperturbed Hamiltonian H_0 has, in suitable units, the form

$$H_0 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - 2\,\delta(x), \quad -\infty < x < \infty. \tag{2}$$

H_0 has a single bound state $u_b(x) = e^{-|x|}$ with energy $-\omega_0 = -1$. It also has continuous uniform spectrum on the positive real line, with generalized eigenfunctions

$$u(k,x) = \frac{1}{\sqrt{2\pi}}\left(e^{ikx} - \frac{1}{1+i|k|}e^{i|kx|}\right), \quad -\infty < k < \infty \tag{3}$$

and energies k^2.

Beginning at $t = 0$, we apply a parametric perturbing potential, i.e. for $t > 0$ we have

$$H(t) = H_0 - 2\,\eta(t)\delta(x) \tag{4}$$

and solve the time dependent Schrödinger equation (1) for $\psi(x,t)$, with $\psi(x,0) = \psi_0(x)$. Expanding ψ in eigenstates of H_0 we write

$$\psi(x,t) = \theta(t)u_b(x)e^{it} + \int_{-\infty}^{\infty} \Theta(k,t)u(k,x)e^{-ik^2t}dk \quad (t \geq 0) \tag{5}$$

with initial values $\theta(0) = \theta_0,\ \Theta(k,0) = \Theta_0(k)$ suitably normalized,

$$\langle\psi_0,\psi_0\rangle = |\theta_0|^2 + \int_{-\infty}^{\infty} |\Theta_0(k)|^2 dk = 1 \tag{6}$$

We then have that the survival probability of the bound state is $P(t) = |\theta(t)|^2$, while $|\Theta(k,t)|^2dk$ gives the "fraction of ejected particles" with (quasi-) momentum in the interval dk.

This problem can be reduced to the solution of an integral equation in a single variable [9]–[12]. Setting

$$Y(t) = \psi(x=0,t)\eta(t)e^{it} \tag{7}$$

we have

$$\theta(t) = \theta_0 + 2i\textstyle\int_0^t Y(s)ds\ , \tag{8}$$

$$\Theta(k,t) = \Theta_0(k) + 2|k|/\left[\sqrt{2\pi}(1-i|k|)\right]\textstyle\int_0^t Y(s)e^{i(1+k^2)s}ds\ . \tag{9}$$

$Y(t)$ satisfies the integral equation

$$Y(t) = \eta(t)\left\{I(t) + \int_0^t [2i + M(t-t')]Y(t')dt'\right\} = \eta(t)\Big(I(t) + (2i+M) * Y\Big) \tag{10}$$

where the inhomogeneous term is

$$I(t) = \theta_0 + \frac{i}{\sqrt{2\pi}}\int_0^\infty \frac{\Theta_0(k)+\Theta_0(-k)}{1+ik} e^{-i(k^2+1)t}dk,$$

and

$$M(s) = \frac{2i}{\pi}\int_0^\infty \frac{u^2 e^{-is(1+u^2)}}{1+u^2}du = \frac{1+i}{2\sqrt{2\pi}}\int_s^\infty \frac{e^{-iu}}{u^{3/2}}du$$

with

$$f * g = \int_0^t f(s)g(t-s)ds$$

Outline of the technical strategy. The method of analysis in [9, 10], relies on the properties of the Laplace transform of Y, $y(p) = \mathcal{L}Y(p) = \int_0^\infty e^{-pt}Y(t)dt$.

We show that (10) has a unique solution in suitable norms. This solution is Laplace transformable and the Laplace transform y satisfies a linear functional equation. The solution of the functional equation is unique in the right half plane provided it satisfies the additional property that $y(p_0+is)$ is square integrable in s for any $p_0>0$. We use the functional equation to determine the analytic properties of $y(p)$.

This is done using (appropriately refined versions of) the Fredholm alternative. After some transformations, the functional equation reduces to a linear inhomogeneous recurrence equation in l_2, involving a compact operator depending parametrically on p. The dependence is analytic except for a finite set of poles and square-root branch-points on the imaginary axis and we show that the associated homogeneous equation has no nontrivial solution. We then show that the poles in the coefficients do not create poles of y, while the branch points are inherited by y. The decay of $y(p)$ when $|\Im(p)|\to\infty$, and the degree of regularity on the imaginary axis give us the needed information about the decay of $Y(t)$ for large t.

4.1 Case when $\eta(t)$ is harmonic

Theorem 1 ([9]) *When $\eta(t) = r\sin\omega t$ the survival probability $|\theta(t)|^2$ tends to zero as $t\to\infty$, for all $\omega>0$ and $r\neq 0$.*

Remarks. (**1**) The detailed behavior of the system as a function of t, ω, and r is obtained from the singularities of $y(p)$ in the complex p-plane. We summarize them *for small* r; below $\delta>0$. For definiteness we assume in the following that $r>0$.

At $p = \{in\omega - i : n\in\mathbb{Z}\}$, y has square root branch points and y is analytic in the right half plane and also in an open neighborhood $\mathcal{N}$ of the imaginary axis with cuts through the branch points. As $|\Im(p)|\to\infty$ in $\mathcal{N}$ we have $|y(p)| = O(r\omega|p|^{-2})$. If $|\omega - \frac{1}{n}| > \text{const}_n O(r^{2-\delta})$, $n\in\mathbb{Z}^+$, then for small r the function y has a unique pole $p_m = p_0 + im\omega$ in each of the strips $-m\omega > \Im(p) + 1 \pm O(r^{2-\delta}) > -m\omega-\omega,\ m\in\mathbb{Z}$. $\Re(p_m)$ is strictly independent of m and gives the exponential decay of θ. Laplace transform techniques show that

$$\theta(t) = e^{-\gamma(r;\omega)t}F_\omega(t) + \sum_{m=-\infty}^{\infty} e^{(mi\omega-i)t}h_m(t) \tag{11}$$

where F_ω is periodic of period $2\pi\omega^{-1}$ and

$$h_m(t) \sim \sum_{j=0}^{\infty} c_{m,j}t^{-3/2-j} \quad \text{as } t\to\infty,\ \arg(t)\in\Big(-\frac{\pi}{2}-0, \frac{\pi}{2}+0\Big) \tag{12}$$

Not too close to resonances, i.e. when $|\omega - n^{-1}| > O(r^{2-\delta})$, $\delta > 0$, for all integer n, $|F_\omega(t)| = 1 \pm O(r^2)$ and its Fourier coefficients decay faster than $r^{|2m|}|m|^{-|m|/2}$. Also, the sum in (11) does not exceed $O(r^2 t^{-3/2})$ for large t, and the h_m decrease with m faster than $r^{|m|}$.

(**2**) By (11), for times of order $1/\Gamma$ where $\Gamma = 2\Re(\gamma)$, the survival probability for ω not close to a resonance decays as $\exp(-\Gamma t)$. It follows from our analysis that for small r the final asymptotic behavior for $t \to \infty$, is $|\theta(t)|^2 = O(t^{-3})$ with many oscillations as described by (11).

(**3**) When r is larger the polynomial-oscillatory behavior starts sooner. Since for small r the amplitude of the late asymptotic terms is $O(r^2)$, increased r yields higher late time survival probability. This phenomenon, sometimes referred to as atomic stabilization, can be associated with the perturbation-induced probability of back-transitions to the well.

(**4**) Using a continued fraction representation Γ can be calculated convergently for any ω and r. The limiting behavior for small r of the exponent Γ is described as follows. Let n be the integer part of $\omega^{-1} + 1$ and assume $\omega^{-1} \notin \mathbb{N}$. Then we have, for $T > 0$ ($t = r^{-2n}T$),

$$\hat{\Gamma} = -T^{-1} \lim_{r \to 0} \ln \left|\theta(r^{-2n}T)\right|^2 = \frac{2^{-2n+2}\sqrt{n\omega - 1}}{n\omega \prod_{m<n} (1 - \sqrt{1 - m\omega})^2} \tag{13}$$

(**5**) The behavior of Γ is different at the resonances $\omega^{-1} \in \mathbb{N}$. For instance, whereas if ω is not close to 1, the scaling of Γ implied by (13) is r^2 when $\omega > 1$ and r^4 when $\frac{1}{2} < \omega < 1$, by taking $\omega - 1 = r^2/\sqrt{2}$ we find

$$-T^{-1} \lim_{\substack{r \to 0 \\ \omega = 1 + r^2/\sqrt{2}}} \ln \left|\theta(r^{-3}T)\right|^2 = \frac{2^{1/4}}{8} - \frac{2^{3/4}}{16} \tag{14}$$

4.2 General periodic case

We write

$$\eta = \sum_{j=0}^{\infty} \left(C_j e^{i\omega j t} + C_{-j} e^{-i\omega j t} \right) \tag{15}$$

Our assumptions on the C_j are (a) $0 \not\equiv \eta \in L^\infty(\mathbb{T})$, (b) $C_0 = 0$ and (c) $C_{-j} = \overline{C_j}$.
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 $\mathbf{C} \in l_2(\mathbb{N})$ is *generic with respect to* T if the Hilbert space generated by all the translates of $\mathbf{C}$ contains the vector $e_1 = (1, 0, 0...,)$ (which is the kernel of T):

$$e_1 \in \bigvee_{n=0}^{\infty} T^n \mathbf{C} \tag{16}$$

(where the right side of (16) denotes the closure of the space generated by the $T^n\mathbf{C}$ with $n \geq 0$.) This condition is generically satisfied, and is obviously weaker than the "cyclicity" condition $l_2(\mathbb{N}) \ominus \bigvee_{n=0}^{\infty} T^n \mathbf{C} = \{\mathbf{0}\}$, which is also generic.

An important case, which satisfies (16), (but fails the cyclicity condition) corresponds to η being a trigonometric polynomial, namely $\mathbf{C} \not\equiv \mathbf{0}$ but $C_n = 0$ for all large enough n.

A simple example which fails (16) is

$$\eta(t) = 2r\lambda \frac{\lambda - \cos(\omega t)}{1 + \lambda^2 - 2\lambda \cos(\omega t)} \tag{17}$$

for some $\lambda \in (0,1)$, in which case $C_n = -r\lambda^n$ for $n \geq 1$. In this case the space generated by $T^n\mathbf{C}$ is one-dimensional. We prove that there are values of r and λ for which the ionization is incomplete, i.e. $\theta(t)$ does not go to zero for large t.

4.3 Results in the periodic case

Theorem 2 ([10]) *Under assumptions (a), (b), (c) and (g), the survival probability $P(t)$ of the bound state u_b, $|\theta(t)|^2$ tends to zero as $t \to \infty$.*

Theorem 3 ([10]) *For $\psi_0(x) = u_b(x)$ there exist values of λ, ω and r in (17), for which $|\theta(t)| \not\to 0$ as $t \to \infty$.*

Remarks.

1. Theorem 2 can be extended to show that $\int_D |\psi(x,t)|^2 dx \to 0$ for any compact interval $D \in \mathbb{R}$. This means that the initially localized particle wanders off to infinity since by unitarity of the evolution $\int_{\mathbb{R}} |\psi(x,t)|^2 dx = 1$. Theorem 3 can be extended to show that for some fixed r and ω in (17) there are infinitely many λ, accumulating at 1, for which $\theta(t) \not\to 0$. In these cases, it can also be shown that for large t, θ approaches a quasiperiodic function.

2. There is a direct connection between our results and Floquet theory where, for a time-periodic Hamiltonian $H(t)$ with period $T = 2\pi/\omega$, one constructs a quasienergy operator (QEO). Complete ionization thus corresponds to the absence of a discrete spectrum of the QEO and conversely stabilization implies the existence of such a discrete spectrum. In fact, an extension of Theorem 3 shows that for the initial condition $\psi_0 = u_b$, ψ_t approaches such a function with $\mu = -s_0$. More details about Floquet theory and stability can be found in [14, 15]

3. We are currently investigating extensions of our results to the case where $H_0 = -\nabla^2 + V_0(x)$, $x \in \mathbb{R}^d$, has a finite number of bound states and the perturbation is of the form $\eta(t)V_1(x)$ and both V_0 and V_1 have compact support. Preliminary results indicate that, with much labor, we shall be able to generalize Theorem 2, to generic $V_1(x)$. The definition of genericity will, however, depend strongly on V_0.

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