

Exact WKB and resurgence in Quantum Mechanics

Enric Solé Farré*

Facultat de Física, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain.

Advisor: Bartomeu Fiol Núñez

Abstract: A review of non-perturbative effects in Quantum Mechanics is presented. We pay special attention to the exact and uniform WKB methods. The double well potential is considered as a motivating example due to its physical modeling relevance. The first terms of the ground-state energy trans-series for this potential are calculated as a direct application of the uniform WKB method.

I. INTRODUCTION

Quantum mechanics is one of the cornerstones of modern physics. Despite its countless applications, very few cases can be solved exactly by means of ordinary functions. Instead, we need to turn to approximation techniques. A widely used method is perturbation theory, known as Rayleigh–Schrödinger theory when we consider time independent problems, on which we will focus.

However, some subtleties may arise in perturbation theory, such as non-convergence or undetectable effects.

Some illustrative examples of non-converging ground energy corrections, $E - E_0 = \sum_{n=1}^{\infty} a_n(g)^n$, for different systems would be:

- Zeeman effect: $a_n \sim (-1)^n (2n)!$
- Stark effect: $a_n \sim (2n)!$

where g denotes the coupling associated to the perturbation.

This divergence problem, among others, challenges the intuitive idea that the physics from *QM* should be captured by analytic functions of the couplings.

The issue becomes extremely relevant when we consider $g = \hbar$. This was studied in the early days of quantum mechanics, which led to the *WKB* (Wentzel, Kramers & Brillouin) approximation.

The WKB method consists of *approximately* solving the Schrödinger equation $-\frac{\hbar^2}{2m}\Delta\Psi + V(x)\Psi = E\Psi$ through an ansatz of the form

$$\Psi(x) = C(x)e^{\frac{i}{\hbar}\phi(x)} \quad (1)$$

Imposing some *reasonable* assumptions on $\phi(x)''$, we obtain the approximate solution

$$\Psi(x) \approx \frac{C}{\sqrt{p(x)}} \exp\left\{\pm \frac{i}{\hbar} \int^x p(\tilde{x})d\tilde{x}\right\} \quad (2)$$

where $p(x) = \sqrt{2m(E - V(x))}$ and C is the normalization constant. Notice that $\Psi(x)$ is not analytic in \hbar , and in fact presents an essential singularity for $\hbar = 0$.

The WKB ansatz has proven to be remarkably useful in countless problems, although it only provides us with an approximate solution to the problem and yields no further understanding on the topic.

A more insightful view was developed in the 70's by the physicists C. Bender, T. Wu, A. Voros and J. Zinn-Justin, known as *exact WKB*, which tries to unveil the geometric background behind the *WKB* approximation [1], [2]. An alternative approach to the problem is that of *uniform WKB*, which tries to approximate the solution by perturbing the solutions of the harmonic oscillator rather than plane waves, as the usual *WKB* approach does [3].

The mathematician J.Écalle provided a solid mathematical basis for such developments in the early 80's, referred as *resurgence theory* [4], [5], which relies heavily on complex analysis techniques.

In the next section, the need for this framework will be illustrated through a simple example, followed by a discussion of the main points of exact *WKB* and resurgence. To conclude, there will be a review of the example through this new perspective.

II. DOUBLE-WELL: NON-PERTURBATIVE CORRECTIONS

Let us first consider an introductory example, the double-well potential as in [8], §36:

$$H = -\frac{\hbar^2}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2(1 - \sqrt{g}x)^2 \quad (3)$$

where g is a small parameter. By performing a change of variable $x \mapsto \frac{x}{\sqrt{g}}$ and multiplying the Hamiltonian by g , we obtain

$$gH = -\frac{\hbar^2 g^2}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2(1 - x)^2 \quad (4)$$

Thus, identifying $g\hbar$ as a *redefined* Planck's constant, we get the Hamiltonian for $V(x) = \frac{1}{2}x^2(1 - x)^2$ times g .

The potential associated to (3) has two minima, one at the origin and one at $\frac{1}{\sqrt{g}}$, and admits a reflection symmetry R around the axis $x = \frac{1}{2\sqrt{g}}$.

*Electronic address: esolefar7@alumnes.ub.edu

We shall focus on studying the ground state of this problem. We might try to find the ground state by expanding from the unperturbed quantum harmonic oscillator ($g = 0$). However, such perturbative expansion fails for two separate reasons. First, the ground energy expansion is not convergent, as aforementioned. The first terms, up to fifth order in \sqrt{g} , are

$$E_0(\hbar, \sqrt{g}) = \frac{\hbar}{2} - \hbar^2 g - \frac{9}{2} \hbar^3 g^2 + \mathcal{O}(g^3) \quad (5)$$

Second, the expansion does not yield a splitting of the ground energy, as required for 1-D potentials in Quantum Mechanics (see [6] Prob. 2.42 for non-degeneracy in 1-D QM). Intuitively, any state of the unperturbed harmonic well should split into two different eigenfunctions with well defined parity and satisfying $E_- > E_+$, where the subscript denotes the parity with respect to R . Let us focus on the energy splitting, following the work of [7].

The cornerstone of this approach is the Herring's formula (see [7] Appendix A), which characterizes the energy splitting of an approximate solution of energy E_0

$$\Delta E = 2\hbar^2 \Psi\left(\frac{1}{2\sqrt{g}}\right) \Psi'\left(\frac{1}{2\sqrt{g}}\right) \quad (6)$$

where the formula holds for the wave function evaluated at the reflection point p which satisfies $\psi(p-x) = \psi(p+x)$. Similarly to the WKB ansatz of eq. (2), we can approximate our wave function as

$$\Psi(x) \approx \frac{C}{\sqrt{p(x)}} \exp\left\{\pm \frac{i}{g} \int^x p(t) dt\right\} \quad (7)$$

Fixing $\frac{1}{2\sqrt{g}}$ as the integral base point, we find that the energy splitting can be approximated as

$$\Delta E \approx \frac{2\hbar^2}{g} C^2 \quad (8)$$

So we are just left with calculating the normalization condition of Ψ . In order to estimate C we shall make use of the Hamiltonian in (4) and calculate the normalization constant of the ground state of the Hamiltonian

$$H = -\frac{\hbar^2}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 (1-x)^2 \quad (9)$$

by requiring that our wavefunction matches the ground state solution of the quantum oscillator in the overlapping region

$$\psi_0(x) = \frac{1}{\sqrt[4]{\pi\hbar}} e^{-x^2/2\hbar} \quad (10)$$

In the overlapping region we can approximate the momentum by $p(x) = \sqrt{x^2 - c^2}$ where c corresponds to the turning point $V(c) = E$ and can be neglected when substituting it in $\frac{1}{\sqrt{p}}$. Thus, we claim

$$\begin{aligned} \Psi(x) &= \frac{C}{\sqrt{p(x)}} \exp\left\{\frac{1}{\hbar} \int_x^{1/2} p(t) dt\right\} \\ &\approx \frac{C}{\sqrt{x}} \exp\left\{\frac{1}{\hbar} \int_c^{1/2} p(t) dt + \frac{1}{\hbar} \int_x^c \sqrt{t^2 - c^2} dt\right\} \end{aligned}$$

The second integral on the r.h.s can be solved exactly

$$\frac{1}{\hbar} \int_x^c \sqrt{t^2 - c^2} dt = -\frac{x\sqrt{x^2 - c^2}}{2\hbar} + \frac{c^2}{2\hbar} \ln\left(\frac{\sqrt{x^2 - c^2} + x}{c}\right) \quad (11)$$

Since the harmonic part dominates, it is reasonable to assume $c \approx \sqrt{\hbar}$ and that $c \ll x$ so that c/x is small. Taylor-expanding the r.h.s of eq. (11) we get

$$\frac{1}{\hbar} \int_x^c \sqrt{t^2 - c^2} dt \approx -\frac{x^2}{2\hbar} + \frac{1}{4} + \frac{1}{2} \ln\left(\frac{2x}{\hbar}\right) + \mathcal{O}\left(\frac{1}{x^2}\right) \quad (12)$$

Thus, we are left with

$$\Psi(x) \approx C \left(\frac{4e}{\hbar}\right)^{1/4} e^{-x^2/2} \exp\left\{\frac{1}{\hbar} \int_c^{1/2} p(t) dt\right\} \quad (13)$$

Comparing equations (13) and (10), we deduce that

$$C \approx \frac{1}{\sqrt[4]{4\pi e}} \exp\left\{\frac{-1}{\hbar} \int_c^{1/2} p(t) dt\right\} \quad (14)$$

Substituting in eq. (8), and using the fact that the potential is symmetric around $1/2$, we get

$$\Delta E \approx \frac{\hbar^2}{g} \frac{1}{\sqrt{e\pi}} \exp\left\{\frac{-1}{g} \int_c^{1-c} p(t) dt\right\} \quad (15)$$

where the integral of $p(t)$ is the one associated to the Hamiltonian (4). Notice that eq.(15) depends on c , which is also unknown to us. An elaborate computation allows us to evaluate this instanton correction [7].

Removing the extra factor g on eq.(4) and restoring natural units, the final result takes the form

$$\Delta E \sim \frac{2}{\sqrt{\pi g}} e^{-\frac{1}{6g}} \quad (16)$$

This result can be derived in a completely different framework, that of instanton mechanics (see [8] §36), which is how it was originally obtained.

It is important to note that this is not in any case the full answer. However, it should suffice to convince the reader that there is an energy splitting, and that it is of non-perturbative nature.

III. EXACT WKB AND RESURGENCE

The reader should now feel confident that non perturbative terms can be essential in capturing the physics in QM problems. However, the question of what type of non-perturbative effects should be considered arises.

There is mathematical foundation (see [5]) that ensures us that considering perturbations in the form of trans-series should be enough. Trans-series are the main object of study in resurgence, which illustrates that our dependence on the coupling should be of the form

$$f(g) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \sum_{k=0}^{j-1} c_{i,j,k} g^i \left(e^{-\frac{c}{g}}\right)^j \ln^k\left(\pm \frac{1}{g}\right) \quad (17)$$

rather than just analytic functions (power series) of g , where $c_{i,j,k}, c$ are *smooth* functions of the generalized coordinates.

The first standard approach to obtain such trans-series, which correspond to a more careful treatment of the WKB approach, is known as exact WKB. The basic idea, which we will just sketch, is that exact results for observables can be obtained from suitable continued expressions for the periods of an auxiliary Riemann surface.

In what follows, we shall consider complex variables and functions instead of real-valued ones, since all considered functions can be extended reasonably in a unique way. In fact, the mathematical foundations of resurgence makes extensive use of the notion of holomorphicity, intrinsic to complex analysis.

A. Exact WKB

In the complex setting, the ansatz (1) is rewritten as

$$\Psi(z) = \exp \left\{ \frac{i}{\hbar} \int^z \psi(\tilde{z}, \hbar) d\tilde{z} \right\} \quad (18)$$

which, when plugged into the Schrödinger equation, leads to the Riccati equation

$$\frac{\hbar}{i} \frac{d\psi}{dz} + \psi^2 = E - V(z) \quad (19)$$

This equation does not admit a solution in terms of usual functions, but can be written down as a formal power series in \hbar .

$$\psi(z) = \sum_{n=0}^{\infty} p_n(z) \hbar^n \quad (20)$$

It can be proven that the odd terms of such a solution will not contribute to the integral in eq. (18). Thus, and by imposing normalizing conditions, we obtain an exact solution to the Schrödinger equation in terms of formal power series

$$\Psi(z) = \frac{1}{\sqrt{P(z)}} \exp \left\{ \frac{i}{\hbar} \int^z P(\tilde{z}, \hbar) d\tilde{z} \right\} \quad (21)$$

$$P(z) = \sum_{n=0}^{\infty} p_{2n}(z) \hbar^{2n} = \sum_{n=0}^{\infty} q_n(z) \hbar^n \quad (22)$$

Notice that $p_0(z) = p(z) = \sqrt{2m(E - V(z))}$.

In virtue of equation (19), the meromorphic differential $P(z)dz$ defined in equation (22) can be regarded as a curve in the two dimensional Riemann surface Σ_{WKB}

$$w^2 = 2m(E - V(z)) \quad (23)$$

seen as a section of $T^*\Sigma$, where Σ is the coordinate manifold. We will assume $\Sigma = \mathbb{P}_{\mathbb{C}}^1$. Because of this, the

natural objects to study are the periods of $P(z)dz$ along the cycles $\gamma \in H_1(\Sigma_{\text{WKB}})$:

$$\Pi_{\gamma}(\hbar) := \int_{\gamma} P(z) dz \quad (24)$$

Similarly to $P(z)dz$, Π_{γ} is defined as a formal power series in \hbar :

$$\Pi_{\gamma}^{(n)} := \int_{\gamma} q_n(z) dz \quad \Pi_{\gamma}(\hbar) = \sum_{n=0}^{\infty} \Pi_{\gamma}^{(n)} \hbar^n \quad (25)$$

We would expect $\Pi_{\gamma}(\hbar)$ to be an analytical function of \hbar , thus making sense of Ψ as a wave function, which would be a solution to the Schrödinger problem. However it can be proven that the formal power series in eq. (25) has a zero radius of convergence, with growth $\Pi_{\gamma}^{(n)} \sim n!$.

In order to make sense of the WKB periods, we introduce the Borel and Laplace transforms, which are what will give rise to the instanton ($e^{-1/x}$) and quasi-zero mode ($\ln(1/x)$) corrections.

B. Borel and Laplace transforms

The Borel and Laplace transforms will only be presented, without much further comment. Further discussion can be found in [5].

The Borel transform acts on formal power series as follows. Given a formal power series $S = \sum_{n \geq 0} a_n g^n$, we define its Borel transform by

$$\mathcal{B}(S)(\xi) = \sum_{n=0}^{\infty} \frac{a_n}{n!} \xi^n \quad (26)$$

A remarkable aspect of the Borel transform is that it guarantees us that the Borel transform of our WKB periods will define a holomorphic function in a neighborhood of 0, as long as the growth condition $\Pi_{\gamma}^{(n)} \sim n!$ holds. By means of analytic continuation, we can extend $\mathcal{B}(\Pi_{\gamma})$ to a larger open set.

The Laplace transform is a widely used tool in analysis and admits several definitions. We shall use a particular case that suits us due to our index choices and the complex setting we are working with. Let $f(z)$ be an a.e. integrable function whose growth is dominated by e^{Az} at infinity. Then, the Laplace transform of f is defined as

$$\mathcal{L}_{\varphi}(f)(\xi) = \frac{1}{\xi} \lim_{t \rightarrow \infty} \int_0^{te^{i\varphi}} f(z) e^{-z/\xi} dz \quad (27)$$

The Laplace and Borel can be viewed as inverse of each other, due to the fact that any holomorphic function f on \mathbb{C} , whose growth is dominated by e^{Az} at infinity, satisfies

$$\mathcal{B}(\mathcal{L}_0(f))(z) = \mathcal{L}_0(\mathcal{B}(f))(z) = f(z) \quad (28)$$

Remarkably, this procedure can provide us with some interesting new results to *sum* divergent series whenever

the previous growth condition is not met. In the context of exact WKB, we define the Borel sum of a period as

$$s_\varphi(\Pi_\gamma)(\hbar) = \mathcal{L}_\varphi(\mathcal{B}(f))(\hbar) \quad (29)$$

and say Π_γ is summable if $s_\varphi(\Pi_\gamma)$ is well-defined for a small enough \hbar .

The instanton corrections appear whenever $s_\varphi(\Pi_\gamma)$ is ill-defined and one needs to take lateral re-summations. In that case, they are related to the quantity

$$\text{disc}_\varphi(\Pi) = \lim_{\delta \rightarrow 0} s_{\varphi+\delta}(\Pi_\gamma) - s_{\varphi-\delta}(\Pi_\gamma) \quad (30)$$

IV. DOUBLE-WELL: REVISITED

Let us reconsider the example of §2 from an exact perspective. Whilst exact *WKB* provides the conceptual framework to understand the *WKB* in order to actually carry out computations, we will resort to uniform WKB, detailed in [3]. The uniform WKB studies the problem of the double-well by making use of the parabolic cylinder functions

$$-\frac{d^2}{dz^2}D_\nu(z) + \frac{z^2}{4}D_\nu(z) = \nu + 1/2 \quad (31)$$

rather than perturbing a plane wave, like the usual WKB method. Notice that parabolic cylinder functions when $\nu \in \mathbb{N}$ are related to the solution of the n^{th} energy state of the harmonic oscillator by

$$\psi_n(x) = \frac{1}{\sqrt{n!}} \sqrt{\frac{m\omega}{\pi\hbar}} D_n\left(\sqrt{\frac{2m\omega}{\hbar}}x\right) \quad (32)$$

In the case of the double well, by performing the transformation $y = \sqrt{g}z$, our ansatz for the wave function is

$$\Psi(y) = \frac{1}{\sqrt{u'(y)}} D_\nu\left(\frac{u(y)}{\sqrt{g}}\right) \quad (33)$$

where ν is given by some global conditions which we will discuss in the next subsection. Plugging Ψ in the Schrödinger equation and making use of eq. (31) we obtain the differential equation

$$g\left(\nu + \frac{1}{2}\right) + \frac{g^2}{2}\sqrt{u'}\left(\frac{u''}{(u')^{3/2}}\right)' - \frac{u^2(u')^2}{4} = 2gE - y^2(1-y)^2 \quad (34)$$

which can be solved recursively in terms of g , in the same way we did with eq.(19). Although this expansion might seem more complicated to work with than (19), uniform WKB offers some advantages in front of exact WKB. If we set $n = \nu + 1/2$, the first terms of the energy expansions are

$$E(g) = n - g\left(3n^2 + \frac{1}{4}\right) - g^2n\left(17n^2 + \frac{19}{4}\right) + \dots \quad (35)$$

Notice that if we take $\nu = 0$, the quantization condition of the unperturbed oscillator, we obtain the same expansion (5) which had been calculated through Rayleigh-Schrödinger perturbation theory.

A. Quantization condition

When first studying the double potential it was argued that there should be a splitting of the energy and that the corresponding wave eigenfunctions should have well defined parity, the even wavefunction having lower energy.

The uniform WKB method allows us to derive a quantization condition for our problem. But in order to fully capture the essence of this, it is necessary to use the resurgent expansion of the parabolic cylinder functions, which can be calculated for the different regions of the complex plane as explained in §III.B. and becomes relevant whenever $\nu \notin \mathbb{N}$. According to the NIST function database [9],

$$D_\nu(z) \sim z^\nu e^{-z^2/4} F_1(z^2) + e^{\pm i\pi\nu} \frac{\sqrt{2\pi}}{\Gamma(-\nu)} z^{-1-n} e^{z^2/4} F_2(z^2) \quad (36)$$

with

$$F_1(z^2) = \sum_{k=0}^{\infty} \frac{\Gamma(k - \frac{\nu}{2})\Gamma(k - \frac{\nu-1}{2})}{\Gamma(\frac{\nu}{2})\Gamma(\frac{1-\nu}{2})k!} \left(\frac{-2}{z^2}\right)^k$$

$$F_2(z^2) = \sum_{k=0}^{\infty} \frac{\Gamma(k + \frac{\nu+1}{2})\Gamma(k + \frac{\nu+2}{2})}{\Gamma(\frac{\nu+1}{2})\Gamma(\frac{\nu+2}{2})k!} \left(\frac{2}{z^2}\right)^k$$

which can be related to the hypergeometric function of the first kind through the reflection formula of the Gamma function: $\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi z)}$.

The parity condition can be translated in terms of the value of the wavefunction or its derivative at the critical point. Thus, an even function will fulfill $\Psi'(\frac{1}{2}) = 0$ whilst an odd function will be characterized by $\Psi(\frac{1}{2}) = 0$.

Using the expansion (36), and performing some calculations, we arrive at

$$\frac{1}{\Gamma(-\nu)} \left(\frac{2e^{\pm i\pi}}{g}\right)^{-\nu} = (-1)^{(1+P_\Psi)/2} \xi H(\nu, g) \quad (37)$$

where P_Ψ is the parity eigenvalue of Ψ , and

$$\xi = \frac{1}{\sqrt{\pi g}} \exp\left\{-\frac{u_0^2(1/2)}{2g}\right\} \quad (38)$$

$$H = \left(\frac{u^2(1/2)}{2}\right)^{\nu+1/2} \frac{F_1\left(\frac{u^2(1/2)}{g}\right)}{F_2\left(\frac{u^2(1/2)}{g}\right)} \times \exp\left\{-\frac{1}{2g}(u^2(1/2) - u_0^2(1/2))\right\} \quad (39)$$

with u_0 the zeroth order term of eq.(34), which is given by

$$u_0^2(u_0')^2 = 4V \implies u_0^2(y) = 4 \int_0^y \sqrt{2V} dy \quad (40)$$

with $V(y) = y^2(1 - y)^2$. Evaluating for the double well, we get

$$u_0^2\left(\frac{1}{2}\right) = \frac{1}{3} \implies \xi = \frac{1}{\sqrt{\pi g}} e^{\frac{-1}{6g}} \quad (41)$$

The reader will immediately realize that $2\xi = \Delta E$ from §II. This follows from the parity dependence of (37).

B. Energy trans-series

Let us end this dissertation by giving the first terms of the trans-series of what has been our main topic of discussion: the ground state energy of the double well potential.

First, recall the Taylor expansion [9]

$$\frac{1}{\Gamma(-x)} \approx -x + \gamma x^2 + \frac{1}{12}(\pi^2 + 6\gamma^2)x^3 + \mathcal{O}(x^4) \quad (42)$$

where γ is the Euler-Mascheroni constant.

The strategy will be to approximate the quantization condition (37) around zero in terms of the instanton factor ξ by taking $\delta\nu = \sum_k a_k \xi^k$. Take $\sigma_{\pm} = \ln\left(\frac{2}{g}\right) \pm i\pi$ and $H_0 = H(0, g)$, $H_0^{(i)} = \frac{d^i}{d\nu^i} H(0, g)$. By (42), we get

$$\sum_i P_i(\sigma_{\pm}) \delta\nu^{i+1} = (-1)^{(1+P_{\Psi})/2} \xi \sum_i \frac{1}{i!} H_0^{(i)} \delta\nu^i \quad (43)$$

where the P_i are polynomials in σ_{\pm} , the first three being

$$\begin{aligned} P_0(\sigma_{\pm}) &= -1 \\ P_1(\sigma_{\pm}) &= \gamma + \sigma_{\pm} \\ P_2(\sigma_{\pm}) &= \frac{\pi^2}{12} - \frac{1}{2}(\gamma + \sigma_{\pm})^2 \end{aligned}$$

Solving for $\delta\nu$, we get

$$\delta\nu = \beta \xi H_0 + \xi^2 \left(H_0 H_0^{(1)} + (\gamma + \sigma_{\pm}) H_0^2 \right) + \dots \quad (44)$$

where $\beta = -(-1)^{(1+P_{\Psi})/2}$. All that remains is to replace $n = \frac{1}{2} + \delta\nu$ into the expansion (35) with $\delta\nu$ as previously

stated. Thus, the first terms of the energy trans-series of the ground state are

$$\begin{aligned} E(g) &= \frac{1}{2} - \xi H_0 + \xi^2 \left(H_0 H_0^{(1)} + (\gamma + \sigma_{\pm}) H_0^2 \right) \\ &- g \left(1 + 3\xi H_0 \left[1 - \xi H_0 (1 + \gamma + \sigma_{\pm}) + \xi H_0^{(1)} \right] \right) \quad (45) \end{aligned}$$

since $\beta = -1$ as the ground state is even. The provided tools would allow us to continue expansions (44) and (45) algorithmically to any order, yielding an expansion of the form of (17), in agreement to the previous statements.

V. CONCLUSIONS

The Schrödinger equation gives rise to non classical phenomena which can not be captured by standard means of perturbation theory, but their physical significance can be captured through instanton and quasi-zero mode corrections in the form of (17).

Our study has led us to two different approaches on how to calculate such generalized corrections. Exact *WKB* presents itself as the more geometric approach to the problem and allows us to investigate the conceptual nature behind such phenomena. The paper [2] points out how this more conceptual understanding has allowed to relate trans-series with problems in the theory of integrable systems.

In contrast, uniform *WKB* can easily be used to derive the precise coefficients of the trans-series expansion algorithmically for a given potential, as it has been done for the double well potential. Geometrical and topological information can also be obtained through this method, as explained in [3].

Acknowledgments

I would like to thank Dr. Bartomeu Fiol, without whom this work would have not been possible and Dr. Joan Carles Naranjo, for the mathematical perspective he shed on this work.

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