The Schrödinger equation with time-periodic forcing: beyond perturbation theory

Ovidiu Costin (OSU), collaboration with R. D. Costin, M. Huang, I. Jauslin, J L Lebowitz, A. Rokhlenko, S. Tanveer

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CMP (2023, 2018, 2010, 2001), J. Stat. Phys (2019, 2011, 2004, 2002), TAMS (2015)

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- **Setting**: The Schrödinger equation for one particle:

$$i\partial_t\psi = \Big[\underbrace{-\Delta_x + V_0(x)}_{H_0} + \underbrace{V_1(x)F(e^{i\omega t})}_{\text{external field}}\Big]\psi,\ x\in\mathbb{R}^d, t>0;\ \psi(x,0)=\psi_0$$

  where $H_0 = -\Delta_x + V_0$ is the time-independent part of the Hamiltonian.
- E.g., for a Coulomb system, $V_0(x) = a/|x|, x \in \mathbb{R}^3$ $V_1(x)F(e^{i\omega t}) = A(x)\cos\omega t$ describes a monochromatic laser field, $A(x)$ is the laser amplitude in space (say $E\cdot x$ in a common approximation, where E is the electric field).
- ψ is the wave function; $|\psi|^2$ is the probability density of find the particle at x, at time t.
- **Question**: behavior of ψ for large t in **nonperturbative** settings, i.e., when V_1 is not necessarily small or large,
- Particularly important problem: **ionization** defined by the condition $\int_K |\psi|^2 \to 0$ as $t\to\infty$ for any compact set $K\in\mathbb{R}^3$.

- With the advent of lasers, going beyond perturbation theory into fields which are moderate to large is theoretically and experimentally very important,
- and also mathematically very difficult. There is a vast theoretical and experimental literature. Significant rigorous results in such settings were obtained starting in the 80s, among others, by B. Simon, K. Yajima, Soffer, Weinstein using the limit absorption principle and related methods.
- These results are typically conditional. I.e., they consist of decay estimates contingent on a condition left open, that of absence of discrete spectrum of an associated quasi-energy (Floquet) operator.
- We use techniques based on resurgence theory (Borel plane analysis), the analytic Fredholm alternative and asymptotics of systems of PDEs to verify the above condition and,
- In a number of models, we furthermore provide a convergent representation of the wave function as a transseries, Borel summed series plus typically infinitely many exponential corrections (encoding the generalized Fermi Golden Rule in a nonperturbative setting).

The Schrödinger equation

$$i\partial_t\psi = \Big[\underbrace{-\Delta_x + V_0(x)}_{H_0} + \underbrace{V_1(x)F(e^{i\omega t})}_{\text{external field}}\Big]\psi,\ \ x \in \mathbb{R}^d, t > 0;\ \ \psi(x,0) = \psi_0$$

- Starting around 2000 analyzed a variety of one particle nonrelativistic models of **ionization** with various types of potentials, including 3d Coulomb, with a parametric spherically symmetric forcing and a model of **photoionization** common in physics

$$i\partial_t\psi(x,t) = -\frac{1}{2}\Delta\psi(x,t) + \Theta(x)(U - Ex\cos(\omega t))\psi(x,t) \tag{1}$$

where $\Theta(x)$ is the Heaviside function. The last two are especially challenging due to slow decay of the potential (Coulomb) and unboundedness in both physical and Fourier space in the case of (1).

Bibliography at the end of the slides.

Advantages of a Laplace-Borel approach

- Asymptotic questions in t become, in Borel plane, analyticity ones which are easier to address.

Transformed problem

- The periodic potential in Laplace space: Multiplication by $e^{i\omega t}$ becomes shift by $i\omega$ and the Schrödinger equation becomes an infinite nonhomogeneous system of elliptic PDEs, coupled by this shift.
- Absence of quasi-energy discrete spectrum is (proved using the analytic Fredholm alternative), equivalent to the absence of nonzero solutions to the homogeneous system subjected to both Dirichlet and Neumann conditions. Typically solutions of such systems develop caustics.
- We effectively decide whether this happens by rigorous WKB analysis of the system.

Beyond perturbation theory, new phenomena. A simple example (from CMP 2018, [18a])

- Our the simplest model [2000], revisited in [18a], is

$$i\psi_t = -\Delta\psi - 2(1 + \alpha \cos \omega t)\delta(x)\psi; \quad \psi(0, x) = \psi_0(x) \ \ (*)$$

  α is the amplitude of the parametric perturbation, and $\psi_0 = \psi_b = e^{-|x|}$ is the unique bound state of $H_0 = -\Delta - 2\delta$.

- Due an underlying universality, this simple model is "generic", illustrating many of the phenomena of realistic models, sometimes numerically quite accurately.

The survival probabilities and energies of particles

$$i\psi_t = -\Delta\psi - 2(1 + \alpha\cos\omega t)\delta(x)\psi; \quad \psi(0,x) = \psi_0(x) \ \ (*)$$

- At $\alpha = 0$ there is a unique bound state of energy 1, $e^{-|x|}$ and quasi-free states,

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

- To calculate the ionization probability, and energies of the "ejected particles", we decompose $\psi(x,t)$ as

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

$|\Theta(k,t)|^2 dk$ is the fraction of ejected particles with (quasi-) momentum in the interval $(k, k+dk)$ and $|\theta(t)|^2$, is the survival probability of the particle in the bound state. Both θ and Θ are given by rapidly convergent Borel summed transseries [1]

[1] Rapidly converging expansions in exponentials and Borel summed series.

The formula for the survival amplitude

- θ, is given by a **transseries representation** is

$$\theta(t) = 2i \sum_{n\in\mathbb{Z}} \frac{R_n e^{-\gamma t + in\omega t}}{-\gamma + in\omega} + \sum_{n\in\mathbb{Z}} e^{-i(1+n\omega)t}\theta_n(t) \quad (*)$$

- – convergent for $t > 0, \ \alpha, \ \omega$, rapidly so after just a few oscillations.
- – Here $\gamma = \gamma(\alpha, \omega)$, $\operatorname{Re}\gamma > 0$ is a Fermi Golden Rule (FGR) exponent, $R_n = O(|n|!^{-1/2})$[2], and $\theta_n(t) = O(|n|!^{-1/2})$ have pure power[3] series decay, $O(t^{-3/2})$.
- – If $\alpha \ll 1$, we have $\operatorname{Re}\gamma = O(\alpha^2)$, $R_n = O(\alpha^{2|n|})$ and $\theta_n = O(\alpha^{2+|n|})$.
- – Hence, for $t \lesssim O(\alpha^{-5})$, FGR is valid to leading order in α.
- An exponential behavior is still visible initially, even when $\alpha = O(1)$.
- The coefficients in the expansion have explicit continued fraction expressions. $\Theta(k, t)$ has a similar formula.
- Next: pictures.

[2] In the complex energy plane they are residues at poles at $n\omega - i\gamma$.

[3] In a precise sense. They are $O(t^{-3/2})$ Borel summed series

Fermi Golden Rule, α ranging from $o(1)$ to $O(1)$

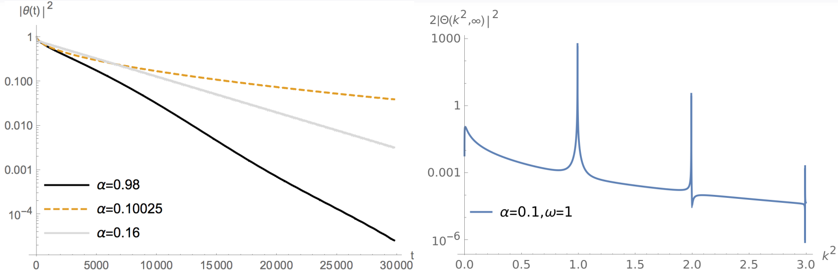


Figure: FGR: Log-plots of survival probability $|\theta(t)|^2$ (left) at $\omega = 1.007071...$. Energy spectrum at $\omega = 1$; α is the forcing amplitude.

We see nearly near perfect exponential decay for all amplitudes, and an outlier for some (very!) special amplitude, $0.10025...$ (the yellow curve has power law behavior at all times).

FGR for some $\alpha = O(1)$

$$\theta(t) = 2i \sum_{n\in\mathbb{Z}} \frac{R_n e^{-\gamma t + in\omega t}}{-\gamma + in\omega} + \sum_{n\in\mathbb{Z}} e^{-i(1+n\omega)t}\theta_n(t)$$

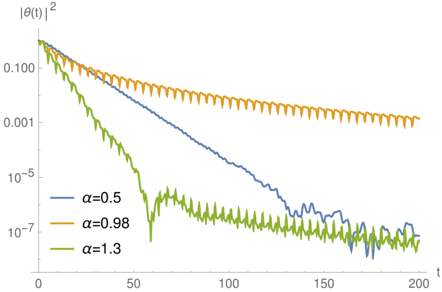
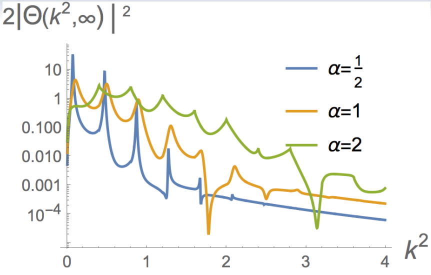
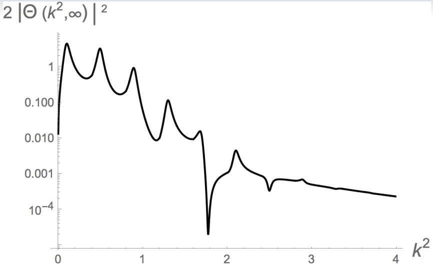


Figure: Log-plot of survival probability $|\theta(t)|^2$, at $\omega = 1.51$, $\alpha = O(1)$.

- Note: **(1)** the initial FGR-like decay (for $\alpha \neq 0.98$) **(2)** the $t^{-3/2}$ behavior, with oscillations, later; **(3)** non-FGR behavior and slower ionization at $\alpha = 0.98$.
- The "wild behavior" before the breakdown of FGR is due to interferences between exponential and non-exponential terms. This shape is quite universal.

Energy spectrum of emitted particles





- Log plots: Energy spectrum of emitted particles, for $\omega = 0.4$ and $\alpha = 1/2, 1, 2$ (left) and $\alpha = 1$ and $\omega = 0.51$ (right). We see:
  - multiphoton effects;
  - the "spectral lines" are very sharp for small α;
  - they become weaker and flatter at larger α;
  - non-monotonicity in α; dips and noise at higher α. (These, too, originate in interferences between exponential and power-law terms.)

The spectral lines growing with time

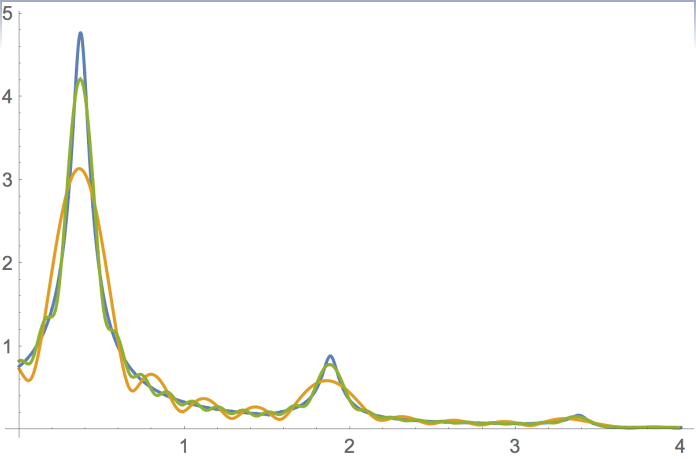
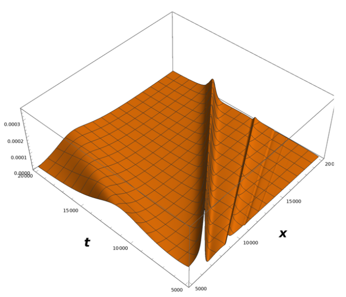
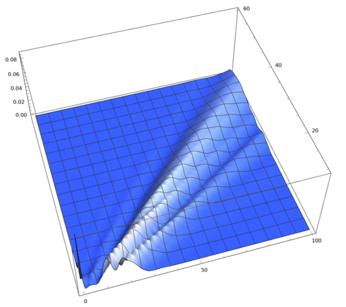


Figure: Time evolution of (momentum, k) spectrum, from short time until onset of asymptotics. (In k^2, it would be energy spectrum.) Plot of $|\Theta(k,t)|^2$ at $\omega = 1.51$, $\alpha = 0.5$ and $t = 5T$ (yellow) $10T$ (green), ∞ (blue), $T := \frac{2\pi}{\omega}$.

The probability density $|\psi(x,t)|^2$





- After a short time we see creases forming, the semiclassical trajectories. (Due to multiphoton interactions, there are several, with different velocities.)
- Let $v = x/t$ As $t \to \infty$, with $v = O(1)$,

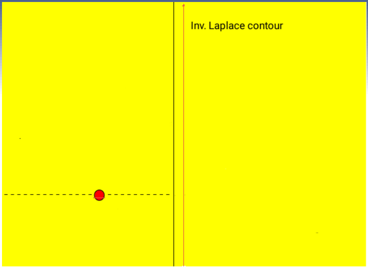
$$\psi(x,t) \sim \frac{e^{i\frac{x^2}{4t}}}{2\sqrt{i\pi}} \frac{|v|}{\sqrt{t}} \left(\hat{\psi}\left(0, v^2/4\right) - \frac{i}{1+v^2/4} \right) \tag{3}$$

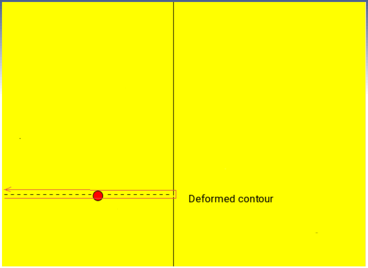
where $\hat{\psi}(x,E) = \mathcal{L}\psi(x,t) = \int_0^\infty e^{iEt}\psi(x,t)dt$.

Borel-Laplace vs. Laplace-Borel

- Mathematically we are relying on a Borel plane analysis (inverse-Laplace space analysis). Counterintuitively perhaps, in linear problems we are free to interchange the order Laplace-inverse-Laplace.
- Let me illustrate this on Borel summing the prototypical series $\sum_{k=0}^{\infty} \frac{k!}{x^{k+1}}$, a formal solution of $xy' + xy = 1$ which we Laplace transform. The result is the equation

$$(1+p)Y' + Y = -p^{-1} \ \text{ with solution } \ Y(p) = -\frac{\ln p}{1+p} + \frac{C}{1+p}$$





$$Y(p) = -\frac{\ln p}{1+p} + \frac{C}{1+p}$$

- Take now the inverse Laplace transform, $y(x) = (2\pi i)^{-1} \int_{-i\infty}^{i\infty} Y(p) e^{px} dp$.
- Bending the contour into the left half plane we collect the residue Ce^{-x} and the branch jump across the cut of the log. The change of variable $p = -q$ leads to

$$y(x) = \underbrace{PV \int_0^{\infty} (1-q)^{-1} e^{-qx} dq + Ce^{-x}}_{\textit{Borel summed transseries}}$$

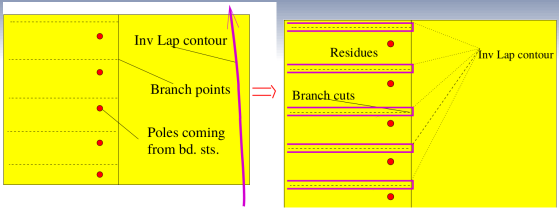


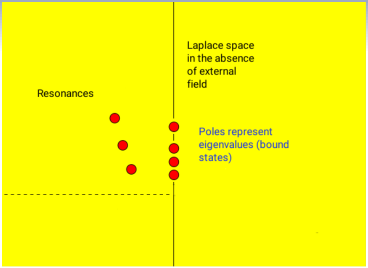
Figure: Laplace plane of $\theta = \langle\psi, \psi_b\rangle$.

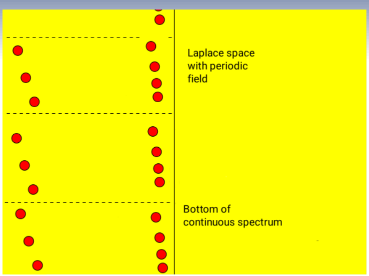
- $i\psi_t = -\Delta\psi - 2(1 + \alpha\cos\omega t)\delta(x)\psi; \quad \psi(0, x) = \psi_0(x) \ \ (*)$

  Once we have obtained the analytic structure of $\mathcal{L}\theta$, plots above, a similar contour deformation gives

$$\theta(t) = 2i \sum_{n\in\mathbb{Z}} \frac{R_n e^{-\gamma t + in\omega t}}{-\gamma + in\omega} + \sum_{n\in\mathbb{Z}} e^{-i(1+n\omega)t}\theta_n(t) \tag{4}$$

  Here $\theta_n(t)$ are Borel summed series and R_n are residues.





- For a more general Hamiltonian, the picture is similar, except that typically there are **resonances (a.k.a. Gamow vectors, dressed states)**, poles in in the LHP. All poles move left when the external field is turned on, and we show the imaginary line is pole-free by showing that the spectrum of the quasi-energy operator has no discrete component, usually the more difficult part of the proof. (There are exceptions, see [01], when the quasienergy operator does have bound states.)

Mathematical underpinnings

- The Schrödinger equation with time-periodic potential has the form

$$i\frac{\partial\psi}{\partial t} = -\Delta\psi + (V(x) + \Omega(x,t))\psi; \quad x \in \mathbb{R}^3$$

  where $\Omega(x, t+T) = \Omega(x,t)$.

  Existence of a strongly differentiable unitary propagator implies that for $\psi_0 \in H^2(\mathbb{R}^d)$, the Laplace transform

$$i\frac{\partial\psi}{\partial t} = -\Delta\psi + (V(x) + \Omega(x,t))\psi \qquad \hat{\psi}(\cdot,p) := \int_0^\infty \psi(\cdot,t)e^{-pt}dt$$

  exists for $\mathrm{Re}\,(p) > 0$. It satisfies the equation ($\partial_t \mapsto -p$; $e^{i\omega t}\psi \mapsto \psi(p-i\omega)$).

$$-\Delta\psi + (V(x) - ip)\hat{\psi}(x,p) = -i\psi_0 - \sum_{j\in\mathbb{Z}} \Omega_j(x)\hat{\psi}(x, p - ij\omega) \tag{5}$$

- Set $-ip = n\omega + \sigma$ with $\mathrm{Im}\ \sigma \in [0,\omega)$ $\psi(x,p) = y_n(x;\sigma)$;

$$(-\Delta + V(x) + \sigma + n\omega)y_n = -i\psi_0 - \sum_{j\in\mathbb{Z}} \Omega_j(x)y_{n-j}(*) \tag{6}$$

  Question: find the analytic structure of $\hat{\psi}$ w.r.t. p, poles and branch points.

- We are now dealing with an infinite system of elliptic PDEs:

$$(-\Delta + V(x) + \sigma + n\omega)y_n = -i\psi_0 - \sum_{j\in\mathbb{Z}} \Omega_j(x) y_{n-j} (*) \tag{7}$$

- The transformed problem looks more involved and harder to tackle. This is not a serious issue, since solving the original problem in any closed form is not hopeful anyway. On the other hand the transformed **question**, analyticity, is simpler. As in one-d problems, Borel-Laplace transforms questions of asymptotics into questions of analyticity.

- In questions of regularity, it is natural to rewrite the system in integral form (which needs care: the differential operators on left side are not invertible as such, in general) as

$$y_n = -i\mathfrak{g}_n\psi_0 - \mathfrak{g}_n \sum_{j\in\mathbb{Z}} \Omega_j(x) y_{n-j}$$

or with $Y = (y_n)_n$, $C_\sigma = (\mathfrak{g}_n)_n$, $\boxed{Y = Y_0 + C_\sigma Y}$

- $\boxed{Y = Y_0 + C_\sigma Y}$
- Crucially, C_σ is (can be arranged to be, by suitable choices of spaces) a **compact operator**, ramified-analytic in p. By the **Fredholm alternative**, Y exists and is ramified-analytic in p iff $Y = C_\sigma Y$ has no **nonzero** solution (the kernel is empty). $\mathcal{L}^{-1}Y$ is then deformable into the LHP, collecting the transseries. The resurgent singularities are the aforementioned branch points and poles.
- Generically, the kernel is trivial, since the infinite system of PDEs cannot have a solution. Indeed, it can be verified that each equation is an elliptic PDE with **both** Dirichlet and Neumann conditions– and generically caustics form.
- Proving that the infinite system of PDEs cannot have a solution in a concrete case is much more difficult. We have by now developed techniques for that, and proved that the kernel is empty in all models we analyzed, except for one deliberately built to show that with finely tuned parameters the kernel can be nonempty.

Photoionization, w. RD Costin, I Jauslin, JL Lebowitz CMP 2023, [23])

- In the quasi-free model of photoemission, electrons in solids move freely. The solid surface is described by a step potential. Placing the surface of a metal in the yz plane, the Schrödinger equation in the **electric gauge** reads

$$i\frac{\partial\varphi}{\partial t} = -\Delta\varphi - \Theta(x)(V - E(t)x)\varphi \tag{8}$$

if we ignore the field inside the metal. V is the sum of the Fermi energy [4] and the work needed to remove an electron from the metal.

[4] The energy difference between the highest and lowest occupied states by the fermions at $T = 0$.

- A non-L^2 initial condition s.a. the plane wave $\psi(x,0)=e^{ik_0x}$ simulates continuous injection of energy in the system.
- In spite of its apparent simplicity, this model poses substantial mathematical problems: the potential is an unbounded operator, with a discontinuity at $x=0$, the metal interface, making it unbounded in Fourier space too.
- Beyond perturbation theory, there was only a conjectural theoretical physics proposal for the steady state (Faisal & al, 2005). Numerical integration based on typical Crank-Nicolson approach does not work (but fails subtly!).
- Even the existence of the unitary propagator, and of classical solutions, do not follow from the literature and needed a proof.

- Existence of classical solutions and unitarity are proved using one-sided Fourier transforms in x resulting in a singular integral equation for the matching condition, which is then regularized and solved by contractive mapping arguments.
- The time Laplace transform $\int_0^\infty \psi(x,t)e^{-pt}dt = \Psi_p(x)$ is replaced with a discrete one, sampled at the periods of the forcing. The fractional part of t is the parameter relevant for regularity and evolution to the steady state conjectured by Faisal &al, 2005. In appropriate spaces it is compact establishing the equivalence of the latter condition and absence of eigenvalues of the QE operator.
- A discrete Laplace transform should streamline the analysis of most time-periodic models.

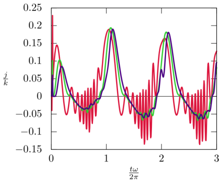


Figure 4. The normalized current $\frac{j}{k}$ as a function of $\frac{t\omega}{2\pi}$ at positive x. The parameters here are $E = 30$ V nm^{-1} and $\omega = 1.55$ eV, and the values of x are 0.12 nm (red), 0.24 nm (green) and 0.37 nm (purple). The fast oscillations die down as x gets larger.

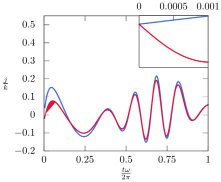


Figure 5. The current computed with our method (blue), compared with the Crank–Nicolson algorithm (red), for $\omega = 1.55$ eV and $E = 15$ V nm^{-1}. The maxima and minima seem to occur at the same time, and the agreement is pretty good for $t > \frac{\pi}{\omega}$. The inset focuses on short times, for $\frac{t\omega}{2\pi} < 0.0005$, for which the Crank–Nicolson algorithm produces a different, and unphysical result: the current initially shoots down to negative values before rising back up.

Absence of discrete quasi-energy spectrum

- Since the potential is periodic in t, with period $T = 2\pi/\omega$, the propagator is periodic, with the same period. We look for eigenvalues of the quasi-energy operator corresponding to eigenfunctions in $L^2(\mathbb{T}, L^2(\mathbb{R}))$ where $\mathbb{T}$ is the torus $\mathbb{R}/T\mathbb{Z}$. Since the Hamiltonian $(i\nabla - \Theta(x)A_t)^2 + \Theta(x)V$ is self-adjoint, the spectrum is real, and we look for $\lambda \in \mathbb{R}$ for which

$$i\partial_t\psi - (-\Delta + \Theta(x)(V - E_t x))\psi = \lambda\psi \tag{9}$$

A nonzero solution, a **quasi-energy eigenfunction** would correspond to L^2 time-periodic solutions of the problem. For $x < 0$ periodic solutions must be given by a Fourier series,

$$\psi = \sum_{k\in\mathbb{Z}, k>\lambda/\omega} C_k \, e^{\sqrt{k\omega-\lambda}\, x} \, e^{ik\omega t} \tag{10}$$

Absence of discrete quasi-energy spectrum

- For $x > 0$ we find that the quasi-energy equation is completely integrable. Using the Lax pairs we get, with $\kappa_n = \sqrt{n\omega + V + 2C^2 - \lambda}$,

$$\psi = \sum_{n\in\mathbb{Z}, n>n_0} D_n f_n(t)\, e^{-\kappa_n x}\, e^{in\omega t} \tag{11}$$

$$f_n(t) = e^{\frac{iC^2}{\omega}\sin(2\omega t) - \kappa_n \frac{4C}{\omega}(2+\cos(\omega t))}; \quad n_0 = (\lambda - V - 2C^2)/\omega; \tag{12}$$

- Continuity of $\psi(x,t)$ and $\psi_x(x,t)$ at $x = 0$ imply

$$\sum_{k\in\mathbb{Z}, k>\lambda/\omega} C_k\, e^{ik\omega t} = \sum_{n\in\mathbb{Z}, n>n_0} D_n\, e^{in\omega t} f_n(t) := \Phi(t)$$

$$\sum_{k\in\mathbb{Z}, k>\lambda/\omega} C_k \sqrt{k\omega - \lambda}\, e^{ik\omega t} = \sum_{n\in\mathbb{Z}, n>n_0} D_n\, e^{in\omega t} f_n(t)\, (2iC\sin(\omega t) - \kappa_n)$$

Absence of discrete quasi-energy spectrum

- Equivalently, in the variable $z = e^{i\omega t}$, half of the Laurent coefficients of Φ vanish, which means Φ extends as a meromorphic function in the open unit disk. From its definition however, in the unit disk Φ has a convergent transseries expansion

$$\Phi = e^{\frac{C^2}{2\omega}(z^2 - \frac{1}{z^2})} \sum_{n\in\mathbb{Z}, n>n_0} D_n z^n e^{-\kappa_n \frac{4C}{\omega}(2+\frac{z}{2}+\frac{1}{2z})} = e^{-\frac{C^2}{2\omega}\frac{1}{z^2}} \sum_{n>n_0} e^{-\kappa_n \frac{2C}{\omega}\frac{1}{2z}} g_n(z) \tag{13}$$

with g_n meromorphic and κ_n strictly increasing in n.

- When transseries representations exist, they are unique. Since Φ is also given by a convergent one-sided Laurent expansion, we must have $g_n = 0\, \forall n \in \mathbb{N}$ therefore $\Phi \equiv 0$.

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