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A Class of Higher Landau-Zener -Type Problems

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Abstract: We present a new class of time-dependent Hamiltonians for the Schrödinger equation :

$$H_p(t) = \begin{pmatrix} \mathrm{Re}(t+iz)^p & \mathrm{Im}(t+iz)^p \\ \mathrm{Im}(t+iz)^p & -\mathrm{Re}(t+iz)^p \end{pmatrix}$$

where $p \in \mathbb{N}^*$, and $z \geqslant 0$ is a scalar coupling parameter. The purpose of this short paper is to overview some common properties to all H_p.

Keywords: Coupled Schrödinger equations, avoided level crossings, 2-state transition probabilities, asymptotic solutions

1 Introduction

Let $p \in \mathbb{N}^*$. We shall consider the vector-valued Schrödinger equation :

$$\frac{\hbar}{i}\frac{\partial \psi(t,z)}{\partial t} = H_p(t,z)\psi(t,z) \ , \tag{1}$$

where H_p is the matrix-valued Hamiltonian :

$$H_p(t,z) = \begin{pmatrix} \mathrm{Re}(t+iz)^p & \mathrm{Im}(t+iz)^p \\ \mathrm{Im}(t+iz)^p & -\mathrm{Re}(t+iz)^p \end{pmatrix} \tag{2}$$

and $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$ is a spinor of $\mathscr{F} = \{\psi_1, \psi_2 \in \mathbb{C} \,|\, t \in \mathbb{R},\, z \in \mathbb{R}_+\}$. Equation (1) falls into the class of nonautonomous linear first-order ordinary differential equations.

By Cauchy-Kovalevskaya, the analyticity of H_p in both variables implies the existence and uniqueness of the evolution operator for the Cauchy problem. Moreover, a Liouville theorem states that the evolution of (1) is volume-preserving since $\mathrm{tr}\, H_p = 0$. Without loss of generality, we can restrict ourselves to elements in $S\mathscr{F} = \{|\psi_1|^2 + |\psi_2|^2 = 1\}$.

*Remark.*The case $p = 1$ gives birth to the renowned Landau-Zener problem.

The 2 by 2 real symmetric and traceless Hamiltonian H_p has two real eigenvalues $\lambda_p^{\pm} = \pm(t^2+z^2)^{p/2}$. The difference of these eigenvalues $\Delta E = \dfrac{\lambda_p^+ - \lambda_p^-}{\hbar}$ is strictly positive. In the vicinity of the crossing, the energy gap is equal to $\Delta E \simeq \dfrac{2z^p}{\hbar}$.

From the physical viewpoint, λ_p^+ and λ_p^- do not cross (avoided level crossing). But the transition between eigenstates $|-\rangle$ and $|+\rangle$ occurs through the quantum tunnelling effect. The quantum effect decreases in the adiabatic limit.

*Remark.*The case $z = 0$ is trivial, and the corresponding S-matrix is simply the identity matrix 1_2.

2 General features of the asymptotic solutions of (1)

2.1 Invariants

Observe that the Hamiltonian H_p is a real-valued matrix. By using shorter notations $r_p = \mathrm{Re}(t+iz)^p$ and

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$i_p = \mathrm{Im}(t+iz)^p$, Equation (1) reads as :

$$\frac{\hbar}{i}\frac{d\psi_1}{dt} = r_p\psi_1 + i_p\psi_2 \quad (3)$$

and

$$\frac{\hbar}{i}\frac{d\psi_2}{dt} = i_p\psi_1 - r_p\psi_2 \; . \quad (4)$$

Consider the linear combination $\psi_1^*(3)+\psi_2^*(4)$:

$$\frac{\hbar}{i}\left(\psi_1^*\frac{d\psi_1}{dt}+\psi_2^*\frac{d\psi_2}{dt}\right) = r_p\left(|\psi_1|^2-|\psi_2|^2\right)+i_p\left(\psi_1^*\psi_2+\psi_1\psi_2^*\right) \; .$$

The RHS is real-valued. Hence :

$$\mathrm{Re}\left(\psi_1^*\frac{d\psi_1}{dt}+\psi_2^*\frac{d\psi_2}{dt}\right) = 0 \; .$$

The derivation $\frac{d}{dt}$ commutes with complex conjugation, as well as with Re and Im, then the identity :

$$\left(\psi_1^*\frac{d\psi_1}{dt}+\psi_1\frac{d\psi_1^*}{dt}\right)+\left(\psi_2^*\frac{d\psi_2}{dt}+\psi_2\frac{d\psi_2^*}{dt}\right) = \frac{d}{dt}\left(|\psi_1|^2+|\psi_2|^2\right) = 0 \quad (5)$$

establishes the conservation of the probability density $\psi^*\psi = 1$.

Now consider the linear combination $\psi_2^*(3)-\psi_1^*(4)$:

$$\frac{\hbar}{i}\left(\psi_2^*\frac{d\psi_1}{dt}-\psi_1^*\frac{d\psi_2}{dt}\right) = r_p\left(\psi_1\psi_2^*+\psi_1^*\psi_2\right)+i_p\left(|\psi_2|^2-|\psi_1|^2\right) \; .$$

Again, the RHS is real-valued. So we have :

$$\mathrm{Re}\left(\psi_2^*\frac{d\psi_1}{dt}-\psi_1^*\frac{d\psi_2}{dt}\right) = \left(\psi_2^*\frac{d\psi_1}{dt}-\psi_1\frac{d\psi_2^*}{dt}\right)+\left(\psi_2\frac{d\psi_1^*}{dt}-\psi_1^*\frac{d\psi_2}{dt}\right) = 0 \; , \quad (6)$$

which implies the conservation of the Poynting flux.

2.2 Local analysis at $\pm\infty$

Let $\Lambda_p(t,z) = \int^t \lambda_p(s,z)ds$. Insert the following Ansatz into (1) :

$$\begin{cases} \psi_1(t,z) = a_1(t)\exp\left[\frac{i\Lambda_p(t,z)}{\hbar}\right] - b_1(t)\exp\left[-\frac{i\Lambda_p(t,z)}{\hbar}\right] \\ \psi_2(t,z) = b_2(t)\exp\left[\frac{i\Lambda_p(t,z)}{\hbar}\right] + a_2(t)\exp\left[-\frac{i\Lambda_p(t,z)}{\hbar}\right] \end{cases} . \quad (7)$$

Differentiate with respect to t, we find that the functions $a_i(t)$ and $b_i(t)$ must satisfy two independent sets of ODEs :

$$(\Sigma') : \begin{cases} i\hbar\frac{da_1}{dt} - \lambda_p a_1 + r_p a_1 + i_p b_2 = 0 \\ i\hbar\frac{db_2}{dt} - \lambda_p b_2 - r_p b_2 + i_p a_1 = 0 \end{cases} ,$$

$$(\Sigma'') : \begin{cases} i\hbar\frac{da_2}{dt} + \lambda_p a_2 - r_p a_2 - i_p b_1 = 0 \\ i\hbar\frac{db_1}{dt} + \lambda_p b_1 + r_p b_1 - i_p a_2 = 0 \end{cases} .$$

At $t\to+\infty$, let us solve first (Σ'). Take a_1 to be t-independent (i.e. a constant $\omega_+\in\mathbb{C}$). The first equation in (Σ') yields readily :

$$b_2 = \frac{\lambda_p - r_p}{i_p}\omega_+ = \mathcal{O}\left(\frac{1}{t}\right) \; .$$

Then in the second equation, the term $\frac{db_2}{dt}$ is a $\mathcal{O}\left(\frac{1}{t^2}\right)$ while the 3 last terms are of magnitude $\mathcal{O}(t^{p-1})$. By neglecting the former, we obtain that :

$$b_2 = \frac{i_p}{\lambda_p + r_p}\omega_+ \; ,$$

and thanks to the relation $\lambda_p^2 = r_p^2 + i_p^2$, this is fully compatible. By doing the same trick for (Σ''), we get :

$$a_2 = \omega_- \quad , \quad b_1 = \frac{\lambda_p - r_p}{i_p}\omega_- \; .$$

Finally, up to a $\mathcal{O}\left(\frac{1}{t^2}\right)$ error term in (1), we find that the linear combinations :

$$\begin{cases} \widetilde{\psi}_1 = \omega_+\exp\left(\frac{i\Lambda_p}{\hbar}\right) - \frac{\lambda_p - r_p}{i_p}\omega_-\exp\left(-\frac{i\Lambda_p}{\hbar}\right) \\ \widetilde{\psi}_2 = \frac{\lambda_p - r_p}{i_p}\omega_+\exp\left(\frac{i\Lambda_p}{\hbar}\right) + \omega_-\exp\left(-\frac{i\Lambda_p}{\hbar}\right) \end{cases} ,$$

with constants ω_-, $\omega_+\in\mathbb{C}$ (that may depend only on z and the initial conditions), are approximate asymptotic solutions of (1) when $t\to+\infty$. Similar computations can be performed at $t\to-\infty$ to obtain :

$$\begin{cases} \widetilde{\psi}_1 = \alpha_+\exp\left(\frac{i\Lambda_p}{\hbar}\right) - \frac{\lambda_p - r_p}{i_p}\alpha_-\exp\left(-\frac{i\Lambda_p}{\hbar}\right) \\ \widetilde{\psi}_2 = \frac{\lambda_p - r_p}{i_p}\alpha_+\exp\left(\frac{i\Lambda_p}{\hbar}\right) + \alpha_-\exp\left(-\frac{i\Lambda_p}{\hbar}\right) \end{cases}$$

with constants α_-, $\alpha_+\in\mathbb{C}$. Observe that for large values of t :

$$\forall p\geqslant 1, \; \frac{\lambda_p - r_p}{i_p} = \frac{(t^2+z^2)^{p/2} - \mathrm{Re}(t+iz)^p}{\mathrm{Im}(t+iz)^p} \sim_{\pm\infty} \frac{pz}{2}\frac{1}{t} \; . \quad (8)$$

2.3 Scattering matrix

Definition 1. *The scattering matrix S (or the S-matrix for short) of the coupled Schrödinger equations (1) is the element of SU_2 such that :*

$$\begin{pmatrix} \omega_+ \\ \omega_- \end{pmatrix} = S \begin{pmatrix} \alpha_+ \\ \alpha_- \end{pmatrix} \tag{9}$$

in a suitable basis of eigenstates.

The S-matrix carries all the scattering data and the tunnelling effect occurring at the avoided level crossing. We also introduce the two transition probabilities $a(z)$ and $b(z)$ (as they depend on the coupling parameter z) by :

$$S(z) = \begin{pmatrix} a(z) & b(z)^* \\ -b(z) & a(z)^* \end{pmatrix} .$$

For reasons that will be made clear in a moment, we have :

$$\begin{cases} \alpha_+ = a(z)^* \omega_+ - b(z)^* \omega_- \\ \alpha_- = b(z)\omega_+ + a(z)\omega_- \end{cases} .$$

Let us explain our current framework. Per se, we might consider a single normalized state $|+\rangle$ in the limit $t \to +\infty$. Put it in another way : $\psi(+\infty) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. But to achieve such a final state, it is required to start at $t \to -\infty$ with a mixed initial state, such that $\psi(-\infty) = \begin{pmatrix} \alpha_+ \\ \alpha_- \end{pmatrix}$. Going backwards, then $\psi(-\infty) = \begin{pmatrix} a(z)^* \\ b(z) \end{pmatrix}$.

2.4 Stability discussion

Let ψ be the exact solution of (1), and denote by $\widetilde{\psi}$ an approximate solution satisfying :

$$\frac{\hbar}{i} \frac{\partial \widetilde{\psi}(t,z)}{\partial t} = H_p(t,z)\widetilde{\psi}(t,z) + \mathscr{O}\left(\frac{1}{t^2}\right) .$$

Set $\varepsilon_\psi = \psi - \widetilde{\psi}$. Then the quantity ε_ψ satisfies :

$$\frac{\hbar}{i} \frac{\partial \varepsilon_\psi(t,z)}{\partial t} = H_p(t,z)\varepsilon_\psi(t,z) + \eta(t) , \tag{10}$$

where $\eta(t)$ stands for the $\mathscr{O}\left(\frac{1}{t^2}\right)$ function in the RHS of (10). Introduce the evolution operator $U(t,t_0,\cdot) : \mathbb{C}^2 \to \mathbb{C}^2$ of the linear homogeneous equation (1), enabling us to write any solution in the form :

$$\psi(t,\cdot) = U(t,t_0,\cdot)\psi(t_0,\cdot) .$$

This operator $U(t,t_0,\cdot)$ is a linear 1-parameter operator of transformation, propagating the solution over time from t_0 to t. Using the constant variation method, the solution of the inhomogeneous equation (10) with the initial condition $\varepsilon_\psi(t_0,z)$ at some, say, positive t_0 is given by :

$$\forall t \geqslant t_0,\ \varepsilon_\psi(t,z) = U(t,t_0,z)\left\{\varepsilon_\psi(t_0,z) + \int_{t_0}^{t} U(s,t_0,z)^{-1}\eta(s)ds\right\} .$$

Therefore :

$$|\varepsilon_\psi(t,z)|^2 = \|U(t,t_0,z)\|^2_{\mathscr{F}\to\mathscr{F}}$$
$$\left\{|\varepsilon_\psi(t_0,z)|^2 + 2\,\mathrm{Re}\left\langle \varepsilon_\psi(t_0,z), \int_{t_0}^{t} U(s,t_0,z)^{-1}\eta(s)ds\right\rangle + \left|\int_{t_0}^{t} U(s,t_0,z)^{-1}\eta(s)ds\right|^2\right\} ,$$

with $\langle\cdot,\cdot\rangle$ denoting the usual sesquilinear product of $\mathbb{C}^2$. Since $U(t,t_0,z)$ is a measure-preserving isometry and $\eta(t) = \mathscr{O}\left(\frac{1}{t^2}\right)$, we get the estimate :

$$|\varepsilon_\psi(t,z)| = |\varepsilon_\psi(t_0,z)| + \mathscr{O}\left(\frac{1}{t_0}\right) ,$$

implying the relevancy of the Ansatz. Stated differently, the stability is not actually an issue : as any physicist knows, solutions of (1) feature pseudo-oscillations, without exponential growth.

2.5 How to separate the coupled system

Sometimes, the theory of second-order linear differential equations can be used to find the solutions of 2 simultaneous first-order equations as in (1). The key idea is to eliminate one of the unknown functions, say ψ_2, and then find ψ_1 as the solution of a second-order linear differential equation. From the first equation :

$$\psi_2 = \frac{1}{i_p}\left(\frac{\hbar}{i}\frac{d\psi_1}{dt} - r_p\psi_1\right)$$
$$\Longrightarrow \frac{d\psi_2}{dt} = \frac{1}{i_p}\left(\frac{\hbar}{i}\frac{d^2\psi_1}{dt^2} - r_p\frac{d\psi_1}{dt} - \frac{dr_p}{dt}\psi_1\right) - \frac{1}{i_p^2}\frac{di_p}{dt}\left(\frac{\hbar}{i}\frac{d\psi_1}{dt} - r_p\psi_1\right) .$$

Insert these 2 relations into the second equation of (1). Eliminate thus ψ_2 :

$$-\frac{\hbar^2}{i_p}\frac{d^2\psi_1}{dt^2} + \left(\frac{\hbar^2}{i_p^2}\frac{di_p}{dt} - \frac{r_p}{i_p}\frac{\hbar}{i}\right)\frac{d\psi_1}{dt} + \frac{\hbar}{i}\frac{1}{i_p^2}\left(r_p\frac{di_p}{dt} - i_p\frac{dr_p}{dt}\right)\psi_1$$
$$= i_p\psi_1 - \frac{r_p}{i_p}\left(\frac{\hbar}{i}\frac{d\psi_1}{dt} - r_p\psi_1\right)$$
$$\Leftrightarrow -\hbar^2\frac{d^2\psi_1}{dt^2} + \frac{\hbar^2}{i_p}\frac{di_p}{dt}\frac{d\psi_1}{dt} + \frac{\hbar}{i}\frac{1}{i_p}\left(r_p\frac{di_p}{dt} - i_p\frac{dr_p}{dt}\right)\psi_1 = \left(i_p^2 + r_p^2\right)\psi_1 .$$

Let us evaluate the quantity :

$$r_p\frac{di_p}{dt} - i_p\frac{dr_p}{dt}$$
$$= \mathrm{Re}(t+iz)^p\frac{d\,\mathrm{Im}(t+iz)^p}{dt} - \mathrm{Im}(t+iz)^p\frac{d\,\mathrm{Re}(t+iz)^p}{dt}$$
$$= p\left[\mathrm{Re}(t+iz)^p\,\mathrm{Im}(t+iz)^{p-1} - \mathrm{Re}(t+iz)^{p-1}\,\mathrm{Im}(t+iz)^p\right]$$

by using the fact that $\frac{d}{dt}$ commutes with Re and Im. Note that for any $\zeta \in \mathbb{C}$, the identity :

$$\begin{aligned}
&\operatorname{Re}\zeta^p \operatorname{Im}\zeta^{p-1} - \operatorname{Re}\zeta^{p-1}\operatorname{Im}\zeta^p \\
&= \frac{\zeta^p+\zeta^{*p}}{2}\frac{\zeta^{p-1}-\zeta^{*p-1}}{2i} - \frac{\zeta^{p-1}+\zeta^{*p-1}}{2}\frac{\zeta^p-\zeta^{*p}}{2i} \\
&= \frac{\zeta^{p-1}\zeta^{*p}-\zeta^p\zeta^{*p-1}}{2i} = -|\zeta|^{2(p-1)}\operatorname{Im}\zeta
\end{aligned}$$

holds. Hence :

$$\hbar^2\frac{d^2\psi_1}{dt^2} - \frac{\hbar^2}{i_p}\frac{di_p}{dt}\frac{d\psi_1}{dt} - i\hbar\frac{pz}{i_p}(t^2+z^2)^{p-1}\psi_1 = -(t^2+z^2)^p\psi_1 ,$$

and we finally obtain the general form of the separated ODEs for both ψ_1 and ψ_2 :

$$\hbar^2\frac{d^2\psi_1}{dt^2} - \frac{\hbar^2}{i_p}\frac{di_p}{dt}\frac{d\psi_1}{dt} + \left[(t^2+z^2) - i\hbar\frac{pz}{i_p}\right](t^2+z^2)^{p-1}\psi_1 = 0 \tag{11}$$

and

$$\hbar^2\frac{d^2\psi_2}{dt^2} - \frac{\hbar^2}{i_p}\frac{di_p}{dt}\frac{d\psi_2}{dt} + \left[(t^2+z^2) + i\hbar\frac{pz}{i_p}\right](t^2+z^2)^{p-1}\psi_2 = 0 . \tag{12}$$

Note that the latter equation (12) is merely the complex conjugate of (11). The system (1) is now solvable in terms of second-order linear differential equations, whose Wronskian has a simple expression, to wit :

$$\operatorname{Wr}[\psi_1,\psi_2](t) = \psi_1\frac{d\psi_2}{dt} - \psi_2\frac{d\psi_1}{dt} \propto i_p .$$

3 WKB approximations of the Schrödinger equation (11)

While the exact solutions to the differential equation may be analytic and thus valid everywhere in $\mathbb{C}$, the WKB solutions $\psi_{1\pm}$ are not and have very different properties from the exact solutions (namely discontinuities, existence of Riemann cuts). Yet they are valid within the Stokes sectors, far from the singularities.

3.1 Computing the action S

A convergent series solution at an essential singular point is impossible. In general, one finds that either the series does not exist, or it is divergent for all $t \in \mathbb{C}$. We follow the idea of Poincaré and attempt a solution of (11) of the form $\psi_1(t) = \exp\frac{S(t)}{\hbar}$. Substitute and find :

$$\begin{aligned}
&\hbar^2\left[\frac{S''}{\hbar} + \left(\frac{S'}{\hbar}\right)^2\right] - \frac{\hbar^2}{i_p}\frac{di_p}{dt}\frac{S'}{\hbar} + \left[(t^2+z^2) - i\hbar\frac{pz}{i_p}\right](t^2+z^2)^{p-1} = 0 \\
\Longleftrightarrow\quad &\hbar S'' + (S')^2 - \hbar\frac{1}{i_p}\frac{di_p}{dt}S' + (t^2+z^2)^p - i\hbar\frac{pz}{i_p}(t^2+z^2)^{p-1} = 0 .
\end{aligned}$$

By expanding the action $S = \sum_{k=0}^{+\infty}\hbar^k S_k$ as a perturbation series :

$$S' = \sum_{k=0}^{+\infty}\hbar^k S'_k \quad , \quad (S')^2 = \sum_{k=0}^{+\infty}\hbar^{2k}(S'_k)^2 + 2\sum_{k=1}^{+\infty}\sum_{0\leqslant\ell<\lfloor k/2\rfloor}\hbar^k S'_\ell S'_{k-\ell} .$$

The LHS :

$$\begin{aligned}
&\sum_{k=1}^{+\infty}\hbar^k S''_{k-1} + \left[\sum_{k=0}^{+\infty}\hbar^{2k}(S'_k)^2 + 2\sum_{k=1}^{+\infty}\sum_{0\leqslant\ell<\lfloor k/2\rfloor}\hbar^k S'_\ell S'_{k-\ell}\right] \\
&- \frac{1}{i_p}\frac{di_p}{dt}\sum_{k=1}^{+\infty}\hbar^k S'_{k-1} + (t^2+z^2)^p - i\hbar\frac{pz}{i_p}(t^2+z^2)^{p-1}
\end{aligned}$$

yields the necessary conditions :

- order 0 : $(S'_0)^2 + (t^2+z^2)^p = 0$ (13)
- order 1 :
$$S''_0 + 2S'_0S'_1 - \frac{1}{i_p}\frac{di_p}{dt}S'_0 - i\frac{pz}{i_p}(t^2+z^2)^{p-1} = 0 \tag{14}$$
- order 2 : $S''_1 + (S'_1)^2 + 2S'_0S'_2 - \frac{1}{i_p}\frac{di_p}{dt}S'_1 = 0$

For the next odd powers in $\hbar$:

$$S''_{2k} + 2\sum_{\substack{\ell+m=2k+1\\0\leqslant\ell<k+1}} S'_\ell S'_m - \frac{1}{i_p}\frac{di_p}{dt}S'_{2k} = 0$$

$$\Longrightarrow S'_{2k+1} = -\frac{1}{S'_0}\left[\sum_{\substack{\ell+m=2k+1\\1\leqslant\ell<k+1}} S'_\ell S'_m + \frac{1}{2}\left(S''_{2k} - \frac{1}{i_p}\frac{di_p}{dt}S'_{2k}\right)\right] .$$

For the even powers in $\hbar$:

$$S''_{2k-1} + (S'_k)^2 + 2\sum_{\substack{\ell+m=2k\\0\leqslant\ell<k}} S'_\ell S'_m - \frac{1}{i_p}\frac{di_p}{dt}S'_{2k-1} = 0$$

$$\Longrightarrow S'_{2k} = -\frac{1}{S'_0}\left[\sum_{\substack{\ell+m=2k\\1\leqslant\ell<k}} S'_\ell S'_m + \frac{1}{2}\left(S''_{2k-1} + (S'_k)^2 - \frac{1}{i_p}\frac{di_p}{dt}S'_{2k-1}\right)\right] .$$

3.2 Correction factor $\exp S_1$

By integration of (13), it is immediate that :

$$S_0^\pm = \pm i\int (t^2+z^2)^{p/2}dt = \pm i\Lambda_p .$$

Let us improve this estimate. From (14), we deduce :

$$S_1^{\pm\prime} = -\frac{1}{2}\left[\frac{S_0^{\pm\prime\prime}}{S_0^{\pm\prime}} - \frac{1}{i_p}\frac{di_p}{dt} - i\frac{pz}{i_p}\frac{(t^2+z^2)^{p-1}}{S_0^{\pm\prime}}\right]$$

$$= -\frac{1}{2}\left[\frac{pt}{t^2+z^2} - \frac{p\operatorname{Im}(t+iz)^{p-1}}{\operatorname{Im}(t+iz)^p} \mp \frac{pz}{\operatorname{Im}(t+iz)^p}(t^2+z^2)^{p/2-1}\right] .$$

As $t \to \pm\infty$:

$$S_1^{\pm\prime} = -\frac{1}{2}\left[\frac{p}{t} - \frac{p-1}{t} \mp \frac{\operatorname{sgn} t}{t} + \mathscr{O}\left(\frac{1}{t^3}\right)\right] = -\frac{1 \mp \operatorname{sgn} t}{2t} + \mathscr{O}\left(\frac{1}{t^3}\right) , \quad (15)$$

yielding a 0-order correction (in $\hbar$) factor : $\exp S_1^{\pm} \simeq \left\{ \begin{array}{c} 1 \\ \text{or } \frac{1}{t} \end{array} \right\}$ according to the selected combination of sign / endpoint, that happens to be independent of p. Finally, the WKB forms associated to ψ_1 are defined as :

$$\psi_{1\pm} = \exp\left(\pm\frac{i\Lambda_p}{\hbar}\right) \exp S_1^{\pm} \prod_{k=2}^{+\infty} \exp\left(\hbar^{k-1} S_k^{\pm}\right) , \quad (16)$$

and the Ansatz of Subsection 2.2 is somehow recovered.

4 WKB approximations of the SDE

In [1], we have already encountered the SDE associated to the Landau-Zener model ($p = 1$). In the same vein, the second-order differential equation :

$$\hbar^2 \frac{d^2\phi}{dt^2} + (t^2 + z^2)^p \phi = 0 \quad (17)$$

is called the SDE associated to (1). The pulsation is actually λ_p^2. From the WKB perspective, it is immediate to see that the functions :

$$\phi_{\pm} = \frac{1}{t^{p/2}} \exp\left(\pm\frac{i}{\hbar}\Lambda_p\right) \quad (18)$$

are the approximate asymptotic solutions of the SDE. Observe that expressions of $\phi_{\pm}$ are now symmetric at the leading order in $\hbar$ - without the presence of a multiform $\exp S_1$.

5 Transition probabilities in the Hamiltonian H_p case

In the cases we are interested in, the action $\Lambda_p(t,z) = \int^t (s^2 + z^2)^{p/2} ds$ always has a polynomial part (whose degree is greater than 2) in the variable t. Then the continuation through the complex plane of the exponentials $\exp\left(\pm\frac{i}{\hbar}\Lambda_p\right)$ gives rise to Stokes and anti-Stokes lines, attached to singularities. For a generic point in $\mathbb{C}$, crossing a Stokes line implies a rapid jump in the multiplier of the subdominant exponential, whilst hidden behind the dominant one. The correction in the vicinity of a Stokes line is provided by the Stokes constant. Crossing an anti-Stokes line swaps their subdominancy / dominancy character.

Our previous work [2] shed a new perspective on how to determine the transfer probabilities in a 2-state system, whose eigenstates can be represented by $|\pm\rangle = \exp\left(\pm\frac{i}{\hbar}\Lambda_1\right)$ on the real line, and the Stokes phenomenon which affects the exponentials when joining $+\infty$ to $+\infty e^{i\pi^+}$. Given a differential equation involving such exponentials, there exists an intrinsic link between the transition probabilities and the underlying Stokes geometry.

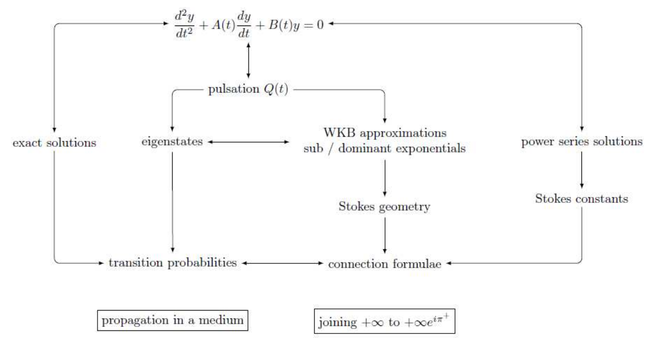

Fig. 1 Diagrammatic correspondence between the transition probabilities and the connection formulae derived from the Stokes phenomenon.

The partial Schrödinger equation (11) has two independent solutions which are ψ_1 and a twisted ψ_2 (in the sense that it is multiplied by an other function). In Subsection 2.2, we showed how to get the coefficients of the scattering matrix from $\psi_1(-t)$.

Assume now (for the sake of simplicity) that $f \in \mathbb{C}(t)$. Then f is non sensitive to the Stokes phenomenon : when joining $+\infty$ to $+\infty e^{i\pi^+}$, there is ”no change in the coefficients” of f. It follows that the connection formulae are identical for $\exp\left(\frac{i}{\hbar}\Lambda_p\right)$ and any $f(t)\exp\left(\frac{i}{\hbar}\Lambda_p\right)$ - with the trivial modifications $f(t) \rightsquigarrow f(-t)$. Try for an moment a slight change of paradigm : we have two subdominant / dominant exponentials, and we seek a second-order linear differential equation admitting them as solutions. Them, or a product by a function that is unaffected by the Stokes phenomenon. The SDE is thus a perfect candidate.

Under these considerations, we can prescribe a set of rules :

Rule 1 (Schrödinger)*Starting with a single eigenstate* $\psi_{1+}(+\infty) = |+\rangle$ *of (11). In order to determine the transition probabilities in the S-matrix :*

- $a(z)^*$ *is read as the factor before* $\exp\left(\frac{i\Lambda_p}{\hbar}\right)$
- $b(z)$ *is equal to* $\left(-\frac{2}{pz}\right)$ *times the factor before* $\frac{1}{t}\exp\left(-\frac{i\Lambda_p}{\hbar}\right)$

in the asymptotic expression of $\psi_1(t)$ *when* $t \to -\infty$.

Rule 2 (SDE)*Starting with a single eigenstate* $\phi_+(+\infty) = \frac{1}{t^{p/2}}|+\rangle$ *of the SDE (17). In order to determine the transition probabilities :*

- $a(z)^*$ *is the factor before* $\exp\left(\frac{i\Lambda_p}{\hbar}\right)$
- $b(z)$ *is the factor before* $\exp\left(-\frac{i\Lambda_p}{\hbar}\right)$

in the asymptotic expression of $\phi(t)$ *when* $t \to -\infty$.

The relevancy of the phase-integral methods has been tested in [2]. We did retrieve perfectly the Landau-Zener effect, i.e. its description in terms of transition probabilities in a conical intersection.

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References

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