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ADIABATIC PERTURBATION THEORY
Semiclassical Limit of the Reflection Coefficient on a Potential Barrier

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Abstract

Using methods of Adiabatic Perturbation Theory, the asymptotic behaviour in the semiclassical limit of the reflection coefficient for one dimensional collisions in quantum mechanics is studied rigorously. In this limit we give a recursive method for an exact calculation to all orders. In contrast to other methods (which fail), our method still works when the energy is near or equal to the top of the potential. First we derive the coefficient for a specific potential. Then we give the coefficient to first three orders for an arbitrary potential depending only on the potential's behaviour around its maximum. We point out that each term needs to be analysed to "all orders".

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1 Introduction

As a starting point of the problem's references we consider Landau and Lifschitz's [7], chapter 7, paragraphs 50 and 52, where an expression for the semiclassical limit of the reflection coefficient on a potential barrier is given. The justification for this expression is valid under the usual constraints of the W.K.B. approximation. In general the problem has different approaches according to whether the energy is above or below the maximum of the barrier potential. For the case of the energy being below the top of the barrier the proof from [7] for the result to order $\hbar^{-1}$ is valid if the potential barrier is large. This is equivalent to the fact that the energy is far away from the top of the barrier. We shall give in this article a rigorous proof valid everywhere, including when energy is in the neighbourhood of the barrier's top (or even at the top). In [7] the generalization to complex values of time is made, which is needed for the case of the energy being above the barrier.

This idea is used too in the article [13], which gives a derivation up to order $\hbar^{-1}$ for the reflection coefficient above the barrier using an interesting approach of the Adiabatic Theorem in the complex plane. We shall briefly present it.

Accurate and relatively recent results for these subjects can be found in the bibliography of [24] .

For the neighbourhood of the barrier's top we refer to the articles [10, 11] where, using Lange's method for comparison, the first term (in $\hbar^{-1}$) is obtained (with many technicalities).

Recently, there have been rigorous approaches to the problem proceeding from the methods of "microlocal analysis" developed by Helffer and Sjostrand. For these we point out the paper of Th.Ramon

[12]. It is a powerful method (it can be applied in other situations as well) but it is complicated. For the considered case we shall develop a simple method which obtains the whole series in $\hbar$.

This method transforms the formulation in terms of scattering theory in the semiclassical limit into one of temporal evolution in the adiabatic limit. After this transformation the subject becomes a problem of perturbation theory.

Some of the main difficulties are avoided by allowing complex values for time. Results of Adiabatic Perturbation Theory are used.

2 Formulation of the problem and results

The one-dimensional movement of a particle is described by the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\psi''(x)+V(x)\psi(x)=E\psi(x), x\in\mathcal{R} \tag{1}$$

m and E being the mass and the energy of the particle.

We restrict ourselves to potentials which obey:

- $V(x)=V^*(x)$ for $x\in\mathcal{R}$
- $\sup_{x\in\mathcal{R}}\|V(x)\|=V_0<\infty$ (uniformly bounded)
- $(\exists)$ asymptotic limits $\lim_{x\to\pm\infty}V(x)=V_{r,l}$ and $V(x)$ approaches them fast enough:
- sometimes we will consider $V(x)=V_{\pm}+o(\frac{1}{x^{1+\alpha}})$ when $x\to\infty,\alpha>0$ but the following is sufficient:

  $$\mid V(x)-V_l\mid\leq b(x) \text{ for } x<\beta$$

  $$\mid V(x)-V_r\mid\leq b(x) \text{ for } x<\gamma$$

  with β and γ real, $\beta\leq\gamma$,

  $$b(x)\in\mathcal{L}^1((-\infty,\beta)\cup(\gamma,+\infty))$$

  and $\lim_{x\to\pm\infty}b(x)=0$
- when we extend the equation to the complex plane we will need that $V(z)$, whose restriction to real arguments is $V(x)$, is an analytical function in a strip S around the real axis with width σ. ($V(z)$ is analytic $(\forall)$ z with $\mid \mathrm{Im}\ z\mid<\sigma/2$.)

The semiclassical limit means $\hbar\to 0$. Denoting $\varepsilon^2=\hbar^2/2m$, we see that the limit can also be obtained when m is increased, a situation which may concern chemistry where molecules with big mass often appear.

It is known that the behaviour of a differential equation's solutions for a limit with the small parameter appearing in the front of the derivative is essentially different from the usual case in physics (and perturbation theory) when the small parameter appears in the potential. In the first case the behaviour of the equation is strongly singular.

For this behaviour classical analysis of a differential equation predicts that the reflection and the transmission coefficients R and T are uniquely determined by ε. For ε small, $R(\varepsilon)$ and $T(\varepsilon)$ are asymptotic series in ε.

It is known [10], [11] that R has 0-expansions

$$R=0+0\ \varepsilon+0\ \varepsilon^2+\dots$$

("the problem of the reflection coefficient"). This expansion is valid in the case with the energy above the barrier. For the case where the energy is below the barrier's top the first 0 is replaced with 1. Nontrivial behaviour of R needs an analysis up to all orders. We will give a simple method which supplies these results.

Firstly, we do a calculation for the potential $V(x)=\frac{1}{1+bx^2}$ and obtain for the reflection and transmission coefficients:

$$R=\frac{u(\varepsilon,\Delta)}{1+u(\varepsilon,\Delta)} \quad , \quad T=\frac{1}{1+u(\varepsilon,\Delta)},$$

with

$$u(\varepsilon,\Delta)=\exp\left\{-\frac{\pi\Delta}{\varepsilon\sqrt{b}}[1+o(\Delta)]-\frac{3}{8}\pi\varepsilon\sqrt{b}\left[1+\frac{5}{8}\Delta+o(\Delta^2)\right]+o(\varepsilon^2)\right\},$$

where

$$\varepsilon^2=\frac{\hbar^2}{2m}\quad,\quad E=1+\Delta.$$

The coefficients of terms of order ε^{-1}, 1 and ε in the exponent are calculated exactly. For example the term of order ε^{-1} has the Taylor expansion:

$$\exp\left\{-\frac{\Delta\pi}{\varepsilon\sqrt{b}}\left[\sum_{n=1}^{\infty}\left[\frac{(2n-1)!!}{(2n)!!}\right]^2(-1)^n\Delta^n\frac{2n}{2n-1}\right]\right\}.$$

For a general potential with a maximum at the origin which has a Taylor expansion about the origin:

$$V(x)=1-bx^2+cx^3+dx^4+ex^5+fx^6+\ldots$$

(this can be obtained with a change of scale and a removal of argument) we obtain the result:

$$u(\varepsilon,\Delta)=\exp\left\{-\frac{\Delta\pi}{\varepsilon\sqrt{b}}[1+o(\Delta)]-\frac{\pi\varepsilon}{4\sqrt{b}}\left\{\left[-\left(\frac{c}{b}\right)^2+\frac{3}{2}\frac{d}{b}\right]-\right.\right.$$

$$\left.\left.-\Delta\frac{5}{48b}\left[51\left(\frac{d}{b}\right)^2+60\frac{f}{b}\right]+o(\Delta^2)\right\}+o(\varepsilon^2)\right\}$$

(the term of order $\varepsilon\Delta$ is valid for a symmetrical potential only). We give an algorithm which supplies the next orders in ε.

In the semiclassical limit we obtain the known results of R, which are 1 for energy below the top of the barrier, and 0 for the energy above the barrier, but the results supply its behaviour before the limit.

3 The transformation of the problem into one obeying a first order differential equation

The small parameter of the limit appearing in the front of the derivative is also needed when we study "the adiabatic limit" of the evolution for a quantum system with a time-dependent Hamiltonian. If the rate of variation of the Hamiltonian is described with a supplementary parameter $H(t,\lambda)=H(\lambda t)$; this limit means $\lambda\rightarrow 0$. After a time rescale $s=\lambda t$ the temporal Schrödinger equation becomes

$$\mathrm{i}\hbar\lambda\frac{\partial\psi(s)}{\partial s}(s)=H(s)\psi(s) \tag{2}$$

Here the adiabatic and semiclassical limits are identical and mean that the coefficient of the derivative goes to 0. At this point we recall the "Adiabatic Theorem" (see Messiah chap. 17.2) which gives a property for the spectrum's states of H, namely the fact that in the adiabatic limit the subspace associated with an eigenvalue (or an isolated part of the spectrum) is kept invariant in the evolution generated by the Schrödinger equation. We are interested in the asymptoticbehavior of this invariance.

It can be observed that because the method is formulated for a general Hamiltonian system of differential equations it is valid for any kind of problem with this formalism. If we formulate it in the framework of the perturbation theory we obtain nonanalytic perturbations or the theory of singular or asymptotic perturbations respectively.

3.1 The transformation of the scattering theory problem in the semiclassical limit into a temporal evolution problem in the adiabatic limit

To put our problem in the framework of the adiabatic theory we first transform equation (1) into a first order equation in the usual way:

$$\varepsilon^2\frac{d^2}{dx^2}\psi(x)+w(x)\psi(x)=0 \tag{3}$$

with

$$w(x) = E - V(x) \tag{4}$$

is equivalent with the system

$$\mathrm{i}\varepsilon \frac{d}{dx}\Psi(x) = K(x)\Psi(x) \tag{5}$$

where

$$\Psi = \begin{pmatrix} \psi(x) \\ \varepsilon \frac{d}{dx}\psi(x) \end{pmatrix} \in \mathcal{C}^2 \quad \text{and} \quad K(x) = \mathrm{i}\begin{pmatrix} 0 & 1 \\ -w(x) & 0 \end{pmatrix}. \tag{6}$$

We can apply the theory of first order differential equations. For any t_0 in S and any Ψ_0 in $\mathcal{C}^2$ there is a unique solution $\Psi(x)$ of (5) analytical in S so that $\Psi(t_0) = \Psi_0$. Equation (5) is equivalent to the equation for the associated propagator $U(x, x_0)$, which is an operator analytic in S being defined by $\Psi(x) = U(x, x_0)\Psi(x_0)$ and obeying the differential equation

$$\mathrm{i}\varepsilon \frac{d}{dx}U(x, x_0) = K(x)U(x, x_0) \tag{7}$$

with initial condition

$$U(x_0, x_0) = \mathbf{1}. \tag{8}$$

The difference from the usual case is the nonself-adjointness of K, but this difficulty can be overcome and results like those given by the theory of adiabatic perturbation can be proven to be valid in cases like this.

The connection between the two functions of physical interest :

- the S-matrix for the scattering problem
- the transitions probabilities for the temporal problem

needs usual properties of hermiticity and unitarity which can be restored by changing the scalar product. In the usual way we define

$$< \Phi, \Psi >_I = < \Phi, I\Psi > \tag{9}$$

for any Φ, Ψ in $\mathcal{C}^2$. If we denote by $A^\natural$ the adjoint of a matrix A for the new scalar product (I-adjoint) we have from the scalar product's properties :

$$< \Phi, \Psi >_I^* = < \Psi, \Phi >_I \Rightarrow I^* = I$$

$$(AB)^\natural = B^\natural A^\natural \text{ with } A, B \text{ matrices } \Rightarrow II^* = \mathbf{1}$$

This restrictions impose for I the form

$$\begin{pmatrix} a & c + \mathrm{i}d \\ c - \mathrm{i}d & \pm a \end{pmatrix}$$

with $a, b, c \in \Re$. If we impose K 's I-hermiticity we obtain

$$I = \begin{pmatrix} 0 & \mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix}.$$

We define I-adjoint $A^\natural = IA^*I^*$ and name A I-selfadjoint if $A^\natural = A$ and I-unitary if $A^\natural = A^{-1}$. Moreover $\|A^\natural\| = \|A\|$ is obtained.

At this point we make the analogue of a change of the representation between two Hilbert spaces with different scalar products which also block-diagonalizes K (we use this name because this step works for dimension greater than 1). We do this change in two steps using an intermediate Hilbert space. This has the advantage that in one step we work with adjunction and scalar product of the first space and in the other step with those of the second space. The intermediate space is defined by the fact that the Hamiltonian in this space is self-adjoint for both scalar products and therefore between the two steps we do a canonical immersion. Self-adjoint matrices for both scalar products have the form

$$\begin{pmatrix} a & \mathrm{i}c \\ -\mathrm{i}c & a \end{pmatrix}$$

with a and c real. At the end we want a diagonal matrix, thus the second step is done by

$$F = \frac{1}{\sqrt{2}} \begin{pmatrix} I & -\mathrm{i} \\ \mathrm{i} & I \end{pmatrix}$$

because it diagonalizes the previous matrix:

$$F^* \begin{pmatrix} a & \mathrm{i}c \\ -\mathrm{i}c & a \end{pmatrix} F = \begin{pmatrix} a+c & 0 \\ 0 & a-c \end{pmatrix}$$

The first transformation matrix is quickly obtained:

$$G = \begin{pmatrix} w^{-1/4}(x) & 0 \\ 0 & -w^{-1/4}(x) \end{pmatrix}$$

Thus, doing the total transformation we obtain:

Lemma 1

$$R^{-1}(x)K(x)R(x) = W^{1/2}(x) \tag{10}$$

where $R(x) = G(x)F$ *and* $W^{1/2}(x) = \begin{pmatrix} w^{1/2} & 0 \\ 0 & -w^{1/2} \end{pmatrix}$ *is a self-adjoint matrix.*

Also, we have obviously:

Lemma 2

$$K_{l,r} = \lim_{x \to \pm\infty} K(x) = i \begin{pmatrix} 0 & 1 \\ -w_{l,r} & 0 \end{pmatrix}$$

with

$$\|K(x) - K_l\| \leq 2b(x) \ , \ x \leq \alpha \ , \ \|K(x) - K_R\| \leq 2b(x) \ , \ x \geq \beta \ , \ \alpha, \beta \in \Re.$$

A self-adjoint and I-self-adjoint matrix is of course matrix I. With transformation (10) we obtain the block-diagonal matrix

$$\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \tag{11}$$

which is the difference of the two projectors

$$\Pi_+ = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \Pi_- = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}$$

If we transform back the matrix (11) in the first step we obtain the expression $I = Q_+ - Q_-$ with the projectors:

$$Q_\pm = \frac{1}{2} \begin{pmatrix} I & \pm\mathrm{i} \\ \mp & I \end{pmatrix} \quad , \quad \Pi_\pm = F^* Q_\pm F \tag{12}$$

and with total transformation we obtain the projectors:

$$R^{-1}(x)P_\pm(x)R(x) = \Pi_\pm \quad , \quad P_\pm(x) = \frac{1}{2} \begin{pmatrix} 1 & \pm\mathrm{i}w^{-1/2}(x) \\ \mp\mathrm{i}w^{1/2}(x) & 1 \end{pmatrix} \tag{13}$$

which obey the relation $P_+(x) + P_-(x) = I$. Thus for our case with a space of dimension 1 (for the equation 3) $P_\pm$ are the projectors for the two eigenvalues. Also we obtain for the spectrum $\sigma(K(x)) = \sigma(w^{1/2}(x)) \cup \sigma(-w^{1/2}(x))$ and where w(x) is strictly positive,

$$\mathrm{dist}[\sigma(w^{1/2}(x)), \sigma(-w^{1/2}(x))] \geq 2 \inf(w^{1/2}(x)). \tag{14}$$

At complex values (we will see the sign for powers) $w(x)$ will have the property $|w(x)| \geq d > 0$.

3.2 The connection between the S-matrix and the operator of temporal evolution

Equation (7) has a unique solution.The limits of the evolution operator exist, a fact which is proved in the interaction picture using the Dyson series (obtained from the integral equation). This needs the separation of free evolution from the evolution operator.

$$K(x) = K^{\natural}(x) \quad \Rightarrow \quad \frac{d}{dx} < \Psi(x), \Phi(x) >_I = 0$$

(a form of the Wronskian theorem for this differential system). This also involves the fact that $U(x, x_0)$ is I-selfadjoint and

$$U(x, x_1)U(x_1, x_0) = U(x, x_0).$$

Asymptotic propagators are:

$$\exp(-\frac{\mathrm{i}}{\varepsilon}K_l x) = R_l \exp(-\frac{\mathrm{i}}{\varepsilon}w_l^{1/2}x)R_l^{-1}$$

$$\exp(-\frac{\mathrm{i}}{\varepsilon}K_r x) = R_r \exp(-\frac{\mathrm{i}}{\varepsilon}w_r^{1/2}x)R_r^{-1}$$

with $R_l, R_r, w_l^{1/2}, w_r^{1/2}$ obviously defined.

¿From $w_l^{1/2}, w_r^{1/2}$ self-adjoint $\Rightarrow$ free propagators are uniformly bounded as function of x. The evolution operator in the interaction picture as usual is:

$$U_{l,r}^I(x) = \exp(\frac{\mathrm{i}}{\varepsilon}K_{l,r}x)U(x, 0)$$

with equation

$$\mathrm{i}\varepsilon\frac{d}{dx}U_{l,r}^I(x) = K_{l,r}^I(x)U_{l,r}^I(x) \tag{15}$$

where

$$U_{l,r}^I(0) = I \quad \text{and} \quad K_{l,r}^I(x) = \exp(\frac{\mathrm{i}}{\varepsilon}K_{l,r}x)(K(x) - K_{l,r})\exp(-\frac{\mathrm{i}}{\varepsilon}K_{l,r}x)$$

Lemma 3 *The limits* $\lim_{x\to\pm\infty} U_{l,r}^I(x) = U_{l,r}^I$ *exist and are I-unitary.*

Proof: $\|K_{l,r}^I(x)\| < \ c\, b(x)$ (with $b(x) \in \mathcal{L}^1(\Re)$ and c a constant independent of x) $\Rightarrow$ (from Dyson series of (15)) $U_r^I(x)$ is uniformly bounded as a function of x:

$$\|U_r^I(x)\| \ < \ \exp(\frac{c}{\varepsilon}\|b\|_1)$$

¿From the integral equation associated with (15) $\Rightarrow$

$$\|U_r^I(x_2) - U_r^I(x_1)\| \leq \frac{1}{\varepsilon}\int_{x_1}^{x_2} \|K_r^I(x)U_R^I(x)\|\, dx \ \leq \ \frac{c}{\varepsilon}\exp(\frac{c}{\varepsilon}\|b\|_1)\int_{x_1}^{x_2} b(x)\ dx$$

$\Rightarrow$ $U(x)$ is a Cauchy sequence in the limit $x \rightarrow +\infty \Rightarrow$ the limit exists.

$$U_r^I \text{ is I} - \text{unitary } \Rightarrow \text{ the limit is I} - \text{unitary.}\square$$

This lemma involves the existence of the global limit:

$$U_I = \lim_{x_0\to-\infty, x\to+\infty} \exp(\frac{\mathrm{i}}{\varepsilon}K_r x)U(x, x_0)\exp(-\frac{\mathrm{i}}{\varepsilon}K_l x_0) =$$

$$\lim_{x_0\to-\infty, x\to+\infty} U_r^I(x)[Ul^I(x_0)]^{\natural} = U_r^I(U_l^I)^{\natural}$$

¿From this point we obtain the relation with the initial S-matrix. This needs asymptotic behaviour of the solutions of (5). Some steps of our paper are valid if the initial dimension of the equation is greater than 1. For this reason we use in a few places the notation 1(n).

In the following for the 1(n)-dimensional problem we use the following shorthand

- "a" and "b" for the coefficients of the exponentials in the limit $x \to -\infty$ and $x \to +\infty$ respectively
- "in" and "out" for the coefficients of the exponentials which go towards and from the origin respectively.

For the 2(2n)-dimensional problem the existence of the limits:

$$\lim_{x \to \pm\infty} \exp(\frac{\mathrm{i}}{\varepsilon} K_{r,l}(x) U(x,0)) = U^I_{r,l}$$

imply $(\forall)\Psi(0) \in \mathcal{C}^2$ we obtain the asymptotic expansion

$$\Psi(x) = \exp(\frac{\mathrm{i}}{\varepsilon} K_{l,r} x) U^I_{l,r} \Psi(0) + o(1) \quad \text{in} \quad x \to \pm\infty.$$

¿From the behaviour at $x \to -\infty$ we can obtain the behaviour at $x \to +\infty$.

Further we denote:

$$\Phi_{in} \stackrel{\text{def}}{=} U^I_l \Psi(0) \quad \text{and} \quad \Phi_{out} \stackrel{\text{def}}{=} U^I_r \Psi(0)$$

which obey

$$\Phi_{out} = U_I \Phi_{in}. \tag{16}$$

In connection with the 1(n)-dimensional problem we can see the need for diagonalization of K (and thus of the exp matrices) where the two eigenvalues (diagonal block) correspond to the two directions of propagation.

If we consider:

$$\Phi_{in} = R_l \begin{pmatrix} a_{out} \\ a_{in} \end{pmatrix} \quad \text{and} \quad \Phi_{out} = R_l \begin{pmatrix} b_{in} \\ b_{out} \end{pmatrix}$$

We obtain the asymptotic behaviours:

$$\Psi(x) = R_l \begin{pmatrix} \exp(-\frac{\mathrm{i}}{\varepsilon} w_l^{1/2}(x)) & a_{out} \\ \exp(\frac{\mathrm{i}}{\varepsilon} w_l^{1/2}(x)) & a_{in} \end{pmatrix} \quad \text{at} \quad x \to -\infty$$

and

$$\Psi(x) = R_r \begin{pmatrix} \exp(-\frac{\mathrm{i}}{\varepsilon} w_r^{1/2}(x)) & b_{in} \\ \exp(\frac{\mathrm{i}}{\varepsilon} w_l^{1/2}(x)) & b_{out} \end{pmatrix} \quad \text{at} \quad x \to +\infty.$$

$$R(x) = G(x)F = \begin{pmatrix} w^{-1/4}(x) & 0 \\ 0 & w^{1/4}(x) \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -\mathrm{i} \\ \mathrm{i} & 1 \end{pmatrix} =$$

$$\frac{1}{\sqrt{2}} \begin{pmatrix} w^{-1/4}(x) & \mathrm{i}w^{-1/4}(x) \\ -\mathrm{i}w^{1/4}(x) & w^{1/4}(x) \end{pmatrix}$$

¿From (6) we obtain the asymptotic behaviours:

$$\psi(x) \simeq \frac{1}{\sqrt{2}} w_l^{-1/4} (a_{out}\, e^{-\frac{\mathrm{i}}{\varepsilon} w_l^{1/2} x} - \mathrm{i} a_{in}\, e^{\frac{\mathrm{i}}{\varepsilon} w_l^{1/2} x}) \quad \text{at} \quad x \to -\infty$$

and

$$\psi(x) \simeq \frac{1}{\sqrt{2}} w_r^{-1/4} (b_{in}\, e^{-\frac{\mathrm{i}}{\varepsilon} w_r^{1/2} x} - \mathrm{i} b_{out}\, e^{\frac{\mathrm{i}}{\varepsilon} w_r^{1/2} x}) \quad \text{at} \quad x \to +\infty.$$

We have $U_I R_l \begin{pmatrix} a_{out} \\ a_{in} \end{pmatrix} = R_r \begin{pmatrix} b_{in} \\ b_{out} \end{pmatrix}$. Here we make a change of notation: $-\mathrm{i}a_{in} \to a_{in}$ and $-\mathrm{i}b_{out} \to b_{out}$ thus S is defined clearly:

$$S \begin{pmatrix} a_{in} \\ b_{in} \end{pmatrix} = \begin{pmatrix} b_{out} \\ a_{out} \end{pmatrix} \tag{17}$$

and (16) becomes

$$U_I R_l \begin{pmatrix} 1 & 0 \\ 0 & \mathrm{i} \end{pmatrix} \begin{pmatrix} a_{out} \\ a_{in} \end{pmatrix} = R_r \begin{pmatrix} 1 & 0 \\ 0 & \mathrm{i} \end{pmatrix} \begin{pmatrix} b_{in} \\ b_{out} \end{pmatrix}$$

We denote

$$\mathcal{U} = R_r^{-1} U_I R_l \stackrel{\text{def}}{=} \begin{pmatrix} U_{++} & U_{+-} \\ U_{-+} & U_{--} \end{pmatrix} \text{ and}$$

$$\begin{pmatrix} 1 & 0 \\ 0 & -\mathrm{i} \end{pmatrix} \begin{pmatrix} U_{++} & U_{+-} \\ U_{-+} & U_{--} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \mathrm{i} \end{pmatrix} \stackrel{\text{def}}{=} \hat{U}$$

$$\text{Thus } \hat{U} \begin{pmatrix} a_{in} \\ b_{in} \end{pmatrix} = \begin{pmatrix} b_{out} \\ a_{out} \end{pmatrix} \text{ with } \hat{U} = \begin{pmatrix} U_{++} & \mathrm{i}U_{+-} \\ -\mathrm{i}U_{-+} & U_{--} \end{pmatrix}. \tag{18}$$

If we use the notation $\Phi = R \begin{pmatrix} a \\ \mathrm{i}b \end{pmatrix}$ and use (12) we obtain for any two vectors in the space the I-scalar product:

$$< \Phi, \Phi' >_I = < R \begin{pmatrix} a \\ \mathrm{i}b \end{pmatrix}, IR \begin{pmatrix} a' \\ \mathrm{i}b' \end{pmatrix} >,$$

which, using

$$R^* IR = F^* G^* IGF = F^* I^2 G * IGF = F^* IGGF =$$

$$F^* IF = F^*(Q_+ - Q_-)F = \Pi_+ - \Pi_-,$$

implies

$$< \Phi, \Phi' >_I = < a.a' > - < b, b' > .$$

Also in this case we have the usual property:

Lemma 4 *S-matrix is unitary.*

Proof: This fact is easily proved using I-unitarity for U_I:

$$< \Phi, \Phi' >_I = < U_I \Phi, U_I \Phi' >_I \Rightarrow < b_{in}, b'_{in} > + < a_{in}, a'_{in} > =$$

$$= < a_{out}, a'_{out} > + < b_{out}, b'_{out} >$$

which is the relation for the unitarity of the matrix:

$$S = \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix} \square$$

Now the connection between the S-matrix and the evolution operator can be easily obtained.
For the $\mathcal{U}$-matrix we have obviously from the block-diagonalization of K and the definition of U_I:

$$\mathcal{U} = \lim_{\substack{x_0 \to -\infty \\ x \to +\infty}} \exp(\frac{\mathrm{i}}{\varepsilon} W_r^{\frac{1}{2}} x) R_r^{-1} U(x, x_0) R_1 \exp(-\frac{\mathrm{i}}{\varepsilon} W_I \frac{1}{2} x) \tag{19}$$

¿From (18) we have:

$$\begin{pmatrix} I & 0 \\ \mathrm{i}U_{+-} & U_{++} \end{pmatrix} \begin{pmatrix} a_{in} \\ a_{out} \end{pmatrix} = \begin{pmatrix} a_{in} \\ a_{in} \end{pmatrix} \text{ and}$$

$$\begin{pmatrix} U_{--} & -\mathrm{i}U_{-+} \\ 0 & I \end{pmatrix} \begin{pmatrix} a_{in} \\ a_{out} \end{pmatrix} = \begin{pmatrix} b_{out} \\ a_{out} \end{pmatrix} \Rightarrow$$

$$\Rightarrow S = \begin{pmatrix} U_{--} & -\mathrm{i}U_{-+} \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ \mathrm{i}U_{+-} & U_{++} \end{pmatrix}^{-1} \text{ and}$$

$$S^* = \begin{pmatrix} I & 0 \\ \mathrm{i}U_{+-} & U_{++} \end{pmatrix} \begin{pmatrix} U_{--} & -\mathrm{i}U_{-+} \\ 0 & I \end{pmatrix}^{-1}$$

$$\text{with } \begin{pmatrix} I & 0 \\ \mathrm{i}U_{+-} & U_{++} \end{pmatrix}^{-1} = \begin{pmatrix} I & 0 \\ -\mathrm{i}U_{++}^{-1} U_{+-} & U_{++}^{-1} \end{pmatrix}$$

Thus, for the elements of S we obtain:

$$S_{++} = U_{--} - U_{-+} U{+ +}^{-1} U_{+-} = (U_{--}^*)^{-1} \ ,$$

$$S_{+-} = -\mathrm{i}U_{-+}U_{++}^{-1} = -\mathrm{i}(U_{--}^{*})^{-1}U_{+-}^{*} \quad ,$$
$$S_{-+} = -\mathrm{i}U_{++}^{-1}U_{+-} = -\mathrm{i}U_{-+}^{*}(U_{--}^{*})^{-1} \quad ,$$
$$S_{--} = U_{++}^{-1} = U_{++}^{*} - U_{-+}^{*}(U_{--}^{*})^{-1}U_{+-}^{*} \quad .$$

We will study the transmission coefficient denoted by T and defined by:

$$T = \frac{w_r^{\frac{1}{2}}}{w_l^{\frac{1}{2}}}|\frac{w_r^{-\frac{1}{4}}}{w_l^{-\frac{1}{4}}}|^2|S_{++}|^2 = |S_{++}|^2.$$

The reflection coefficient is $R = |S_{-+}|^2$. T and R are defined for the propagation from left to right. For the inverse propagation we have $T' = |S_{--}|^2$ and $R' = |S_{+-}|^2$.

The unitarity of S can be written as:

$$|S_{++}|^2 + |S_{-+}|^2 = 1 \text{ and } |S_{--}|^2 + |S_{+-}|^2 = 1$$

Also,

$$S_{+-} = S_{-+} \quad , \quad U_{++} = U_{--}^{*}$$

are valid.

¿From $R = \frac{|U_{+-}|^2}{|U_{++}|^2}$, $|S_{++}|^2 = \frac{1}{|U_{++}|^2}$ and $|S_{++}|^2 + |S_{-+}|^2 = 1$ we obtain:

$$|U_{++}|^2 = 1 + |U_{+-}|^2 \Rightarrow T = \frac{1}{|U_{+-}|^2 + 1} \text{ and } R = \frac{|U_{+-}|^2}{1 + |U_{+-}|^2}$$

This is the relation which we will use in the following. In the one-dimensional case, because K is completely diagonalized, the cartesian elements of matrix for S (and thus for $\mathcal{U}$) are directly connected with the transition probabilities of the evolution operator (the cartesian vectors through transformation become eigenvectors of K). Thus from (10) we obtain that $R_l \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |e_l^- >$ is eigenvector of K_l with the eigenvalue $-w_l^{1/2}$ and $R_r \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |e_r^+ >$ is eigenvector of K_r with the eigenvalue $w_r^{1/2}$. We need:

$$U_{+-} = \lim_{\substack{x_0 \to -\infty \\ x \to +\infty}} < \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} e^{\frac{\mathrm{i}}{\varepsilon}W_r^{\frac{1}{2}}x} & 0 \\ 0 & e^{-\frac{\mathrm{i}}{\varepsilon}W_r^{\frac{1}{2}}x} \end{pmatrix} R_r^{-1}U(x,x_0)R_l$$

$$\begin{pmatrix} e^{-\frac{\mathrm{i}}{\varepsilon}W_l^{\frac{1}{2}}x} & 0 \\ 0 & e^{\frac{\mathrm{i}}{\varepsilon}W_l^{\frac{1}{2}}x} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} >_I =$$

$$= \lim_{\substack{x_0 \to -\infty \\ x \to +\infty}} e^{\frac{\mathrm{i}}{\varepsilon}W_r^{\frac{1}{2}}x + \frac{\mathrm{i}}{\varepsilon}W_l^{\frac{1}{2}}x} < e_r^+|U(x,x_0)|e_l^- >_I \ . \tag{20}$$

¿From this point on the problem is completely analogous to a problem of temporal evolution except for the fact that the hamiltonian K(x) is not self-adjoint.

4 Linear adiabatic theory

4.1 The adiabatic theorem

In the last years important progress has been made in the rigorous study of the adiabatic regime of the Schrödinger equation. The adiabatic regime is characterized by the singular limit $\varepsilon \to 0$ of the equation:

$$\mathrm{i}\varepsilon\frac{\partial}{\partial t}U_\varepsilon(t,s) = H(t)U_\varepsilon(t,s) \text{ with } U_\varepsilon(s,s) = 0 \tag{21}$$

where $H(t)$, $t \in \Re$ is a smooth enough family of self-adjoint operators (for the initial formulation) on a separable Hilbert space (although some parts of the theory are valid in a more general case).Thus the framework is unitary evolutions in Hilbert spaces.

The study of the problem is closely connected with the spectral decomposition of the evolution operator.

Papers about Adiabatic Theorem have been appearing since 1928 (M. Born, V. Fock, "Zeit.f.Phys."). We briefly outline its enunciation (see the proof in [15] chapter 17).If the Hamiltonian is continuously changing from an initial value H_0 at the moment t_0 to the final value H_1 at t_1 and if we define $t_1 - t_0 = T$, $s = \frac{t-t_0}{T}$ and $H(s)$ the Hamiltonian at $t_0 + sT$ then T determines the transition rate. We denote $U(t, t_0) = U_T(s)$. The theorem asserts that in the limit $T \to \infty$ the system passes from an eigenstate of H_0 to an eigenstate of H_1 determined through continuity from the first one.

So, let ε_1 , ... , ε_j , ... be eigenvalues of H and $P_1, \ldots, P_j, \ldots$ be the projectors on the respective subspaces. If $\varepsilon_j(s) \neq \varepsilon_k(s) \quad (\forall) j, k$ and $\frac{d\,P_j}{d\,s}$, $\frac{d^2 P_j}{d\,s^2}$ are well defined while $0 \leq s \leq 1$ and the discontinuity points are at most of the first kind[1] the theorem asserts:

$$\lim_{T\to\infty} U_T(s)P_j(0) = P_j(s) \lim_{T\to\infty} U_T(s).$$

Let A(s) be the operator which satisfies the relation $P_j(s) = A(s)P_j(0)A^*(s)$ $(\forall) j$. This relation is equivalent to the equation $\mathrm{i}\hbar\frac{dA}{ds} = k(s)A(s)$ with $A(0) = 1$ where $k(s)$ obeys the necessary and sufficient condition $[k(s), P_j(s)] = \mathrm{i}\hbar\frac{dP_j}{ds}$. If we impose the constraints $P_j(s)k(s)P_j(s) = 0$, $(\forall) j$ we obtain unique

$$k(s) = \mathrm{i}\hbar \sum_j \frac{dP_j}{ds} P_j(s) \quad .$$

Also, let

$$\Phi_T(s) = \sum_j \exp(-\mathrm{i}\frac{T}{\hbar}\int_0^s \varepsilon_j(\sigma)\, d\sigma) P_j(0).$$

More accurately the Adiabatic Theorem asserts :

$$U_T(s) \underset{T\to\infty}{\sim} A(s)\Phi_T(s)(1 + o(\frac{1}{T}))$$

with

$$A(s)\Phi_T(s)P_j(0) = P_j(s)A(s)\Phi_T(s) \ .$$

Since a few years ago (1984) a number of papers have appeared about the so called Berry's phase, geometric phase or quantum phase.These have as a starting point the adiabatic theorem. Thus, the two operators which give $U_T(s)$ in first order in $\frac{1}{T}$ have an action which can be written explicitly. For $\Phi_T(s)$ it is as above and for $A(s)$ it can be easily obtained. So, if we fix a differentiable family of normed vectors $n(s)$ in the subspaces of $P(s)$ (the spectral projectors) and write the action of $A(s)$ with a phase factor, it can be easily obtained from its differential equation (we will see this below in a general context). Thus:

$$U_T(s, s_0)n(s_0) = \exp\left[-\mathrm{i}T\int_{s_0}^s < n(\sigma), H\, n(\sigma) > \, d\sigma\right]$$

$$\exp\left[\int_{s_0}^s < n(\sigma), \frac{d\, n(\sigma)}{d\sigma} > \, d\sigma\right] \, n(s) + o(\frac{1}{T})$$

The first exponential is the dynamical phase and the second is the Berry phase. Thus, this is the factor of Berry's papers but he obtained it in a different manner, namely from anholonomy of the parallel transport. So, the fact that $A(s, s_0)$ is a parallel transport therefore

$$< A(s, s_0)n(s_0), \frac{d\, A(s, s_0)}{ds} n(s_0) >= 0$$

is a starting point in these papers for the deduction of Berry phase and this fact is obtained from other considerations.

The adiabatic theorem can be approached without this factor changing the scalar product like in [13] where results without this factor's effect (like Dykhne's formula) are obtained.

[1] It is not necessary that the whole spectrum be discrete but it is required to check this condition of continuity and to be crossing free.

4.2 Higher order results

We point out a few important progresses in the approach to the Adiabatic Theory. It is now understood that the higher orders of the asymptotic expansion of the transition probabilities are determined by the order of differentiability of $H(s)$. Thus if $H(s)$ is differentiable to order k the transition probability is a power of ε^k and this can be proven by the technique of integration by parts (we will see a rigorous proof which can be easy generalized). When $H(s)$ is indefinitely differentiable and all its derivatives vanish at the ends of the real axis, the transition probabilities are exponentially small in ε, and for their study the analytical structure of the $H(s)$'s spectrum in the complex plane must be known accurately .

The theory appears in [1], [3]. Let us now turn to equation (21). The important fact is that information about U_ε can be obtained without the integration of (21).

For H we assume (supplementary conditions will be at the extension in the complex plane) that ($\forall$) s it has an isolated and bounded part of the spectrum $\sigma_0(s)$ with the spectral projector $P_0(s)$. The results of Adiabatic Theorem are valid in higher orders.

A first idea for higher orders was to take off the restriction that the subspaces which are invariant under the evolution are associated through spectral projectors (like P_0) to a part of the spectrum (which are invariant to first order in ε), and to construct subspaces which are are invariant to higher order, but which (in the case when H tends quickly enough to its limits at the ends of the axis) tend to P_0 at the ends of the real axis. The evolution equation is integrated on these subspaces (for examples this is trivial when the dimension of the subspace is 1).

We denote this subspace by $K(s,\varepsilon)$:

$$U_\varepsilon(s,s_0)K(s_0,\varepsilon) \simeq K(s,\varepsilon)$$

or

$$P_\varepsilon(s)U_\varepsilon(s,s_0) \simeq U_\varepsilon(s,s_0)P_\varepsilon(s_0) \tag{22}$$

This step is important because, as it is known, the temporal evolution operator does not have an expansion in ε while $P_\varepsilon(s)$ can have an expansion in ε. This is explained by the fact that the singular behaviour for $U_\varepsilon(s,s_0)\Psi(s_0)$ is concentrated in a phase factor.

Therefore, we start with the equation obtained by the derivation of (22) (Heisenberg equation):

$$\mathrm{i}\varepsilon\frac{d\,P_\varepsilon(s)}{ds} \simeq [H(s),P_\varepsilon(s)] \tag{23}$$

For the solving of this problem there are different approaches. One way is the recurrent approach. The starting point in this approach is the generalization of the Krein-Kato lemma (from [1]) which for a differentiable family of bounded

projectors

$$Q(s)\ ,\ s\in(a,b)\subset\Re$$

constructs a wide class of bounded operators with bounded inverse $V(s,s_0)$ under the evolution of which $Q(s)$ is invariant:

$$Q(s) = V(s,s_0)Q(s_0)V^{-1}(s,s_0)$$

where $V(s,s_0)$ is supplied by a tip Schrödinger equation:

$$\mathrm{i}\frac{d}{ds}V(s,s_0) = K(s)V(s,s_0)\ \ ;\ \ V(s,s_0)=1$$

with a suitable $K(s)$. If $K(s)$ is unbounded supplementary conditions are needed for the solutions' existence. For orthogonal projectors in a Hilbert space the generalization mentioned above makes this construction starting from a family of evolutions with the Hamiltonians $N(s)$ (self-adjoint operators) which do not conserve $Q(s)$. For $N(s)$ general conditions are required like:

- the domain $D(N(s)) = D$ is s-independent and
- $N(s)[N(s_0)-\mathrm{i}]^{-1}$ is strong differentiable at $s\in(a,b)$

which supply for their Schrödinger equations unique and strong continuous solutions.

A recursive solution for the adiabatic theory problem can be obtained from this generalization ([3],[2]) via the Riesz formula, which supplies the spectral projectors as an integral of the resolvent on a suitable path:

$$P = -\frac{1}{2\pi \mathrm{i}} \oint_{\Gamma} [H - z]^{-1} \, dz.$$

Thus, given $H(s)$ the Riesz formula supplies $P_0(s)$, which is not invariant under the H's evolution. Using the above generalization of the Krein-Kato lemma we obtain a Hamiltonian $H_1 = H - B_1$ under the evolution of which $P_0(s)$ is invariant. Thus, heuristically for invariance under evolution B_1 is missing in the Hamiltonian. At the next step we start with a projector obtained with the Riesz formula from the Hamiltonian $H + B_1$. The result is that at each step a projector is obtained which is invariant under the evolution of H with a precision which is an increasing power of ε .

The theory (and the later improvements) is local in s (it involves only finite order derivatives in s).

Recent results ([1]) show that the previous precision is in fact exponentially small in ε.If in the above method we try to apply the usual approach for the asymptotic series and we do the induction in an ε-dependent order for the improvement of the evaluation we face difficulties because the frequent utilization of the Riesz formula makes the estimation of the above precision impossible. For this reason the theory is reconsidered keeping only the essential facts in the proof. Thus a projector is constructed which obeys better equation (23) (in the sense that for the norm of the difference

$$\|\mathrm{i}\varepsilon \frac{dP_\varepsilon(s)}{ds} - [H(s), P_\varepsilon(s)]\|$$

a higher order in asymptotic series is obtained).

For H the gap condition and smoothness conditions are assumed. The construction of the series is moved from the hamiltonian to the projectors and it looks directly for the factorized form:

$$P_\varepsilon(s) = \sum_{j=0}^{\infty} E_j(s) \, \varepsilon^j \tag{24}$$

If we insert (24) in

$$P_\varepsilon(s) = P_\varepsilon(s)^2 \ \text{ and } \ \mathrm{i}\varepsilon \frac{d}{ds} P_\varepsilon(s) \simeq [H(s), P_\varepsilon(s)],$$

we obtain

$$E_j(s) = \sum_{m=0}^{j} E_m(s) E_{j-m}(s) \ \text{ and}$$

$$[H(s), E_0(s)] = 0 \ , \ \ \mathrm{i}\frac{d}{ds} E_j(s) = [H(s), E_{j+1}(s)]$$

A first result is an explicit (local in s) solving of these equation. The explicit formulas obtained give also a control of the norms $\|E_j^{(k)}(s)\|$. The series for $P_\varepsilon(s)$ is generally not convergent. It is used however through truncation using this norm control. Following the usual approach of the asymptotic series (24) is truncated in an ε-dependent order. The result is an operator T_ε which is not idempotent and also does not obey the Heisenberg equation accurately, but these goals are better achieved if the series is truncated at a higher order. The Riesz formula associates P_ε to T_ε. It is proven that

> if T_ε is a bounded operator with
>
> $$\|T_\varepsilon^2 - T_\varepsilon\| \leq f(\varepsilon)$$
>
> where $f(\varepsilon) \to 0$ at $\varepsilon \to 0$ and if $\lim_{\varepsilon \to 0} \|T_\varepsilon - P\| = 0$ with P bounded projector $\Rightarrow (\exists) k > 0$ so that $\|T_\varepsilon - P_\varepsilon\| \leq k f(\varepsilon)$ for ε small enough.

Thus, by checking the conditions:

- higher order truncation for an accurate checking of the Heisenberg equation and the idempotent condition by T_ε (and also by P_ε)
- lower order truncation for keeping $\lim_{\varepsilon \to 0} \|T_\varepsilon(s) - P_0(s)\| = 0$ (and also for P_ε)

an optimal truncation is done which gives for $\|T_\varepsilon^2(s) - T_\varepsilon(s)\|$ and also for

$$\|\mathrm{i}\varepsilon\frac{dP_\varepsilon(s)}{ds} - [H(s), P_\varepsilon(s)]\|$$

an exponentially small estimation. This includes the better results obtained for the adiabatic theorem.

The case with holomorphic resolvent and the case with the resolvent in Geverey class (which interpolate between holomorphic and $\mathcal{C}^\infty$ cases) are separately considered. Moreover, the results are valid for any rescaled time.

The exponentially small approximations for the adiabatic approximation can be obtained using also the adiabatic theorem in the complex plane (as in [13]). It is proven that the adiabatic theorem is valid on a path which obeys the "dissipativity" conditions (we will use it). If the theorem is proven for the subspace of the eigenvalue e_i this condition is:

$$\mathrm{Im}\ \Delta_{ji}(t) \geq \mathrm{Im}\ \Delta_{ji}(t')\ \ (\forall) j$$

where t and t' are on the path at parameters $s < s'$. We have used:

$$\Delta_{ji}(t) = \int_0^{(t)} d\tau (e_j - e_i)(\tau).$$

Although the Hamiltonian and the evolution operator are analytical, their expansion in terms of eigenvectors and eigenvalues is not analytic, because the eigenvalues (and thus the eigenvectors) are not analytic. For example, at a point where two eigenvalues are equal they have a branch point in general with a square tip. This fact can be taken advantage of by following a dissipative path which is separated from the real axis by such a point. Because of the nonanalyticity for eigenvalues, starting with one of the eigenvalues at $-\infty$ and following it on the two paths: real and complex we reach $+\infty$ with two different eigenvalues. This fact can be used for obtaining exponentially small probabilities for nonadiabatic transitions on the real axis from the adiabatic theorem on the complex path.

4.3 The adiabatic theorem for nonself-adjoint Hamiltonians and the lowest orders of the evolution operator

If the Hamiltonian is not self-adjoint, then in general (when at least one eigenvalue has the imaginary part greater in absolute value than ε) the adiabatic theorem-like results are still valid for the evolution of the subspace which corresponds to the least dissipative eigenvalue (the greatest imaginary part)([2]). Because there is no restriction on the sign of the imaginary part, the theory is also valid for pumping systems.

We show briefly the justifications of this fact and we obtain the Landau-Zener-Friedrichs formula. We take for simplicity the 2-dimensional case. We consider a nonself-adjoint Hamiltonian:

$$H(s) = \sum_{j=1}^{2} e^{(j)}(s)|n^{(j)}><m^{(j)}(s)|$$

where $|n^{(j)}>$ are eigenvectors for H and $|m^{(j)}>$ for H^* which obey

$$<\ m^{(j)}(s)|n^{(k)}(s)>=\delta_{jk}$$

while $e^{(j)}(s)$ is eigenvalue for $H(s)$.

A solution of the Schrödinger equation

$$\mathrm{i}\varepsilon\frac{d}{ds}|\Psi(s)>=H(s)|\Psi(s)>$$

can be written as

$$|\Psi(s)>=\sum_{j=1}^{2} c^{(j)}(s)\exp(-\frac{\mathrm{i}}{\varepsilon}w^{(j)}(s))|n^{(j)}(s)>\quad \text{with}$$

$$w^{(j)}(s) = \int_{s_0}^{s} e^{(j)}(u)\,du$$

Thus, we assume

$$|e^{(2)}(s) - e^{(1)}(s)| \geq d > 0 \text{ and } \mathrm{Im}\,(e^{(2)}(s) - e^{(1)}(s)) \leq 0.$$

We consider $e^{(1)}(s) = 0$ because the general case is easily obtained with $H(s) + e^{(1)}(s)\mathbf{1}$ which changes the evolution operator by the numerical factor

$$\exp(-\frac{\mathrm{i}}{\varepsilon}\int_{s_0}^{s} e^{(1)}(u)\, du)$$

.

So, we have the gap condition and if we assume enough smoothness for the Hamiltonian we can apply the iterative method recalled in the previous section. This method provides the projectors $P_k^{(j)}$ which tend to the ends of the axis at $P_0^{(j)}$ (if the Hamiltonian tends quickly enough to its limit) and which are invariant under the evolution to order ε^k :

$$P_k^{(j)}(s;\varepsilon)U_k(s,s_0;\varepsilon) = U_k(s,s_0;\varepsilon)P_k^{(j)}(s_0;\varepsilon)$$

$$\mathrm{i}\varepsilon\frac{d}{ds}U_k(s,s_0;\varepsilon) = H_k(s;\varepsilon)U_k(s,s_0;\varepsilon)$$

$$H_k(s;\varepsilon) = H(s) - B_k(s;\varepsilon) \text{ with } \|B_k(s;\varepsilon)\| \leq \varepsilon^{k+1}b_k(s)$$

If we write

$$\Omega_k(s,s_0;\varepsilon) = U_k^{-1}(s,s_0;\varepsilon)U(s,s_0;\varepsilon)$$

we need to prove that the norm of the operator:

$$\Omega_k(s,s_0;\varepsilon) - \mathbf{1} = \frac{1}{\mathrm{i}\varepsilon}\int_{s_0}^{s} U_k^{-1}(u,s_0;\varepsilon)B_k(u;\varepsilon)U_k(u,s_0;\varepsilon)\Omega(u,s_0;\varepsilon)\, du$$

is small compared to ε^k. In contrast to the self-adjoint case, in the nonself-adjoint case the norm of this operator must be carefully evaluated. Because we want to prove the adiabatic expansion for the evolution restricted at $P^{(1)}$ we write

$$P_k^{(1)}(s;\varepsilon)U(s,s_0;\varepsilon)P_k^{(1)}(s_0;\varepsilon) =$$

$$= P_k^{(1)}(s;\varepsilon)U_k(s,s_0;\varepsilon)P_k^{(1)}(s_0;\varepsilon)\{\mathbf{1} + P_k^{(1)}(s_0;\varepsilon)[\Omega_k(s,s_0;\varepsilon) - \mathbf{1}]P_k^{(1)}(s_0;\varepsilon)\}$$

If we prove

$$\|P_k^{(1)}(s_0;\varepsilon)[\Omega_k(s,s_0;\varepsilon) - \mathbf{1}]P_k^{(1)}(s_0;\varepsilon)\| \ < \ \varepsilon^k$$

we obtain the fact that up to the order ε^k, U has the same expansion in ε as U_k. For the estimation of this norm the Dyson series is used which needs the expression of $U_k(s,s_0;\varepsilon)$ restricted to the subspace of $P_k^{(j)}$. From the invariance condition this contains only a numerical factor:

$$U_k(s,s_0;\varepsilon)n_k^{(j)}(s_0;\varepsilon) = \exp[-\mathrm{i}\phi_k^{(j)}(s,s_0;\varepsilon)]n_k^{(j)}(s;\varepsilon)$$

where

- $n_k^{(j)}(s;\varepsilon) = P_k^{(j)}(s;\varepsilon)n^j(s)$
- $m_k^{(j)}(s;\varepsilon) = P_k^{(j)*}(s;\varepsilon)m^j(s)$

We obtain this factor for the general case. We do not use the Hamiltonian's shift and we change notation from $P_k^{(j)}$ to $P_\varepsilon^{(j)}$. We consider $\phi_\varepsilon^{(1)}$ ($\phi_\varepsilon^{(2)}$ is obtained analogously) and we denote it by $\phi(s,s_0)$. If we replace the expression of $U_k(s,s_0;\varepsilon)$ (which we denote by $U_\varepsilon(s,s_0)$) in the Schrödinger equation we obtain

$$\phi(s,s_0) = \varepsilon^{-1}\int_{s_0}^{s}\frac{< m_{1,\varepsilon}(u); Hn_{1,\varepsilon}(u) >}{< m_{1,\varepsilon}(u); n_{1,\varepsilon}(u)}\,du - \mathrm{i}\int_{s_0}^{s}\frac{< m_{1,\varepsilon}(u); \dot{n}_{1,\varepsilon}(u) >}{< m_{1,\varepsilon}(u); n_{1,\varepsilon}(u)}\,du$$

We replaced H_k with H because we calculated up to the order ε^k. From now on we shall restrict ourselves to the order ε^2. We use:

$$P_{1,\varepsilon} = P_{1,0} + \varepsilon E_1 + \varepsilon^2 E_2 + \dots$$

(with the notation $P_k^{(1)}$ we use the fact that for $n \le k$ in the expansion of $P_k^{(1)}$ the factors up to the order ε^n do not depend by k).

¿From the fact that the projector is idempotent:

$$P_{1,0}E_1P_{1,0} = 0 \ , \ P_{1,0}E_2P_{1,0} = -P_{1,0}E_1^2P_{1,0} \Rightarrow$$

$$< m_{1,\varepsilon}; n_{1,\varepsilon} >= 1 - < m_1 \ , \ P_{1,0}E_1^2P_{1,0}n_1 > \varepsilon^2 + \dots$$

Also

$$< m_{1,\varepsilon}; Hn_{1,\varepsilon} >= e_1 + \varepsilon^2(< m_1; P_{1,0}E_1(H - e_1)E_1P_{1,0}n_1 > -$$
$$-e_1 < m_1; P_{1,0}E_1^2P_{1,0}n_1 >)$$

Thus

$$\frac{< m_{1,\varepsilon}; Hn_{1,\varepsilon} >}{< m_{1,\varepsilon}; n_{1,\varepsilon} >} = e_1 + \varepsilon^2 < m_1; P_{1,0}E_1(H - e_1)E_1P_{1,0}n_1 > + o(\varepsilon^3)$$

Also we keep $< m_{1,\varepsilon}; n_{1,\varepsilon} >= 1 + o(\varepsilon^2)$. Up to the order ε^2 we have:

$$< m_{1,\varepsilon}, \dot{n}_{1,\varepsilon} >=< P_{1,\varepsilon}^* m_1; \dot{P}_{1,\varepsilon}n_1 + P_{1,\varepsilon}\dot{n}_1 >=$$

$$=< m_1; [P_{1,0}\dot{P}_{1,0} + \varepsilon(E_1\dot{P}_{1,0} + P_{1,0}\dot{E}_1)]P_{1,0}n_1 > + < m_1; \dot{n}_1 > +$$
$$+\varepsilon < m_1; E_1\dot{n}_1 > + o(\varepsilon^2) =$$
$$= \alpha + \beta\varepsilon + o(\varepsilon^2)$$

¿From $P_{1,0}\dot{P}_{1,0}P_{1,0} = 0 \ \Rightarrow \ \alpha =< m_1; \dot{n}_1 >$. Using $P_{1,0}\dot{E}_1P_{1,0} = -\dot{P}_{1,0}E_1P_{1,0} - P_{1,0}E_1\dot{P}_{1,0}$

$$\mathrm{i}\dot{P}_{1,0} = [H, E_1] \ , \ \dot{n}_1 = \dot{P}_{1,0}n_1 + P_{1,0}\dot{n}_1.$$

and $< m_1; E_1\dot{n}_1 >=< m_1; P_{1,0}\dot{E}_1\dot{P}_{1,0}P_{1,0}n_1 >$, we obtain for β

$$\beta =< m_1; (P_{1,0}E_1\dot{P}_{1,0}P_{1,0} - P_{1,0}\dot{P}_{1,0}E_1P_{1,0})n_1 >=$$

$$=< m_1;(-\mathrm{i}P_{1,0}E_1[H-e_1E_1]P_{1,0}+\mathrm{i}P_{1,0}[H-e_1E_1]E_1P_{1,0})n_1 >=$$
$$=-2\mathrm{i}< m_1;P_{1,0}E_1(H-e_1)E_1P_{1,0}n_1 >$$

We also obtain

$$< m_{1,\varepsilon};\dot{n}_{1,\varepsilon} >=< m_1;\dot{n}_1 > -2\mathrm{i}\varepsilon < m_1;P_{1,0}E_1(H-e_1)E_1P_{1,0}n_1 > .$$

If we add all the results:

$$\phi(s,s_0)=\int_{s_0}^{s}[\varepsilon^{-1}e_1-\mathrm{i}< m_1;\dot{n}_1 >$$
$$-\varepsilon < m_1;P_{1,0}E_1(H-e_1)E_1P_{1,0}n_1 >]\,du \quad +o(\varepsilon^2)$$

For the final expression we need E_1 which can be calculated from [1].

$$P_1^{(1)}=-\frac{1}{2\pi\mathrm{i}}\oint_\Gamma(H_1-z)^{-1}\,dz=$$

$$=-\frac{1}{2\pi\mathrm{i}}\oint_\Gamma[(H-z)^{-1}-(H-z)^{-1}\mathrm{i}\varepsilon\sum_{j=1}^{2}P^{(j)}\dot{P}^{(j)}(H-z)^{-1}]\,dz \quad +o(\varepsilon^2)=$$
$$P^{(1)}+\varepsilon E_1+o(\varepsilon^2)\Rightarrow$$
$$E_1=\mathrm{i}(1-P_{1,0})(H-e_1)^{-1}\dot{P}_{1,0}P_{1,0}-\imath P_{1,0}\dot{P}_{1,0}(H-e_1)(1-P_{1,0})=$$
$$=\frac{\mathrm{i}}{e_2-e_1}[(1-P_{1,0})\dot{P}_{1,0}P_{1,0}-P_{1,0}\dot{P}_{1,0}(1-P_{1,0})]$$

Using also $\dot{P}_{1,0}n_1+P_{1,0}\dot{n}_1=\dot{n}_1$, $\dot{P}^*_{1,0}m_1+P^*_{1,0}\dot{m}_1=\dot{m}_1$ $\Rightarrow$

$$< m_1;P_{1,0}E_1(H-e_1)E_1P_{1,0}n_1 >=$$
$$\frac{1}{e_2-e_1}< m_1;P_{1,0}\dot{P}_{1,0}(1-P_{1,0})\dot{P}_{1,0}P_{1,0}n_1 >=< \dot{m}_1;(1-P_{1,0})\dot{n}_1 >$$

So, at the end we obtain the Landau-Zener-Friedrichs formula used in the following chapters:

$$\phi(s,s_0)=\int_{s_0}^{s}[\varepsilon^{-1}e_1-\mathrm{i}< m_1;\dot{n}_1 > -\varepsilon\frac{1}{e_2-e_1}< \dot{m}_1;(1-P_{1,0})\dot{n}_1 >]\,du \quad +o(\varepsilon^2)$$

In [2] starting from this point it is proven that in the case of nonself-adjoint Hamiltonians, adiabatic-theorem-like results are valid for the subspace of the least dissipative eigenvalue. For the estimation of the norm using the Dyson series and (4.3) the result is obtained from considerations of the eigenvalue's sign.

5 The reflection coefficient for the potential $V(x) = \frac{1}{1+bx^2}$

5.1 The transition to a complex path

For this potential and with the notation $E = 1 + \Delta$ the K-matrix becomes:

$$K(x) = \mathrm{i}\begin{pmatrix} 0 & 1 \\ -[E - V(x)] & 0 \end{pmatrix} = \mathrm{i}\begin{pmatrix} 0 & 1 \\ -[(1+\Delta) - \frac{1}{1+bX^2}] & 0 \end{pmatrix}$$

The idea will be to move the calculation of

$$\lim_{\substack{t \to +\infty \\ t_0 \to -\infty}} P_1(t) U_\varepsilon(t, t_0) P_1(t_0)$$

to a complex path which avoids the cut which we will do in the complex plane and the crossing points for the eigenvalues. If the eigenvalues cross on the real axis the adiabatic theorem faces difficulties even for the enunciation. Thus, even in a self-adjoint case we do not know which subspace is kept invariant after the crossing point. While in the self-adjoint case we can chose the one which is analytically connected with the subspace before the crossing point, in our case, when the Hamiltonian is nonself-adjoint, the Rellich theorem is not valid, which can be seen by the divergence of the projectors at $\Delta = 0$ and $x = 0$. At $\Delta \neq 0$ the difficulties proceed from the cuts done in the complex plane and the choices of the arguments for the complex numbers (if the path of evolution crosses a cut done in the complex plane).

The enunciation's difficulties are overcome as follows. If we start with the projector $P_1(t)$ at $-\infty$ the problem is, which projector we have to consider at $x \to +\infty$. After having done this the enunciation can be written with

$$\lim_{\substack{t \to +\infty \\ t_0 \to -\infty}} P(t) U_\varepsilon(t, t_0) P_1(t_0) \tag{25}$$

In this form the nonanalyticity of eigenvectors and eigenvalues can not be seen because $U_\varepsilon(t, t_0)$ is global, without references to a path of evolution or a expansion in eigenvalues and eigenvectors and is an analytic operator in the strip where the Hamiltonian is analytic. However, for the proof of the adiabatic theorem we must consider a particular path because in general the theorem is proven by iterative solving of a Volterra equation with integral kernel.Thus, for obtaining the projector from enunciation at $+\infty$ and for proving the Adiabatic Theorem we use the form (25) and we move the problem to a complex path:

$$\lim_{\substack{t \to +\infty \\ t_0 \to -\infty}} P(t) U_\varepsilon(t, t_0) P_1(t_0) = \lim_{\substack{t \to +\infty \\ t_0 \to -\infty}} P(t + \mathrm{i}a) U_\varepsilon(t + \mathrm{i}a, t_0 + \mathrm{i}a) P_1(t_0 + \mathrm{i}a)$$

We will show that the paths from t_0 to $t_0 + \mathrm{i}a$ and from t to $t + \mathrm{i}a$ have zero contribution.

The problem is that on the complex path we have a nonself-adjoint Hamiltonian but we can apply the theory showed above.The eigenvalues of K are:

$$e_{1,2} = \pm\sqrt{(1+\Delta)}\frac{\sqrt{(z + \mathrm{i}\sqrt{\frac{\Delta}{(1+\Delta)b}})(z - \mathrm{i}\sqrt{\frac{\Delta}{(1+\Delta)b}})}}{\sqrt{(z - \frac{\mathrm{i}}{\sqrt{b}})(z + \frac{\mathrm{i}}{\sqrt{b}})}}$$

with poles at $\pm\frac{1}{\sqrt{b}}$ and zeros at $\pm\sqrt{\frac{1}{b}(1 - \frac{1}{1+\Delta})}$. In the Appendix we prove that the horizontal path $x + \mathrm{i}a$ with

- $\frac{1}{\sqrt{b}} > a > \mathrm{Im}\sqrt{\frac{1}{b}(1 - \frac{1}{1+\Delta})}$ for $\Delta > 0$
- $\frac{1}{\sqrt{b}} > a > 0$ for $\Delta < 0$

keeps the sign of the difference of the imaginary parts of the $K(z)$'s eigenvalues.

For the eigenvalues we choose the signs as follows:

- for $\sqrt{1+bz^2}$ doing cuts in the complex plane from $\pm\frac{\mathrm{i}}{\sqrt{b}}$ to $+\infty$ we choose the sign which for $x \in \Re$ makes this square root positive.
- for $\sqrt{(1+\Delta)(1+bz^2))-1}$ doing cuts in the complex plane between its zeros we choose the sign which in the left side of the real axis for real x makes the square root positive.

With this choice, taking the eigenvalue with the greatest imaginary part, we must start with the negative solution at $x \rightarrow -\infty$ and end with the positive solution at $x \rightarrow +\infty$. This fact can be seen in the same manner in the Appendix. The eigenvalue is antisymmetric under $z \rightarrow -z$.

Thus, with the above theory we calculate (20). When we pass from x_0 to $x_0 + \mathrm{i}a$ and from x to $x + \mathrm{i}a$, the eigenvectors do not change too much because in this asymptotic zone the Hamiltonian does not depend greatly on the imaginary part of the argument. But for U we have:

$$U(x, x_0) = U(x, x + \mathrm{i}a)U(x + \mathrm{i}a, x_0 + \mathrm{i}a)U(x_0 + \mathrm{i}a, x_0)$$

¿From the asymptotic behaviour of the evolution operator we obtain:

$$U(x, y) = U(x, 0)U^{\natural}(y, 0) \underset{x, y \rightarrow \pm\infty}{\sim} \exp(-\frac{\mathrm{i}}{\varepsilon}K_{l,r}(x - y))$$

Thus, we must calculate the square of the absolute value of:

$$\lim_{\substack{x_0 \rightarrow -\infty \\ x \rightarrow +\infty}} \exp(\frac{\mathrm{i}}{\varepsilon}w_r^{1/2}(x + \mathrm{i}a) + \frac{\mathrm{i}}{\varepsilon}w_l^{1/2}(x_0 + \mathrm{i}a)) < e_r^+ |U(x + \mathrm{i}a, x_0 + \mathrm{i}a)| e_l^- >_I \tag{26}$$

5.2 The expression of the matrix element for the temporal evolution operator

The general assumptions from [2] are checked. At the ends of the axis

$$P_{j,\varepsilon}(z) \rightarrow P_j(z). \tag{27}$$

We use the adjunction properties of K and work with the I-scalar product. On the real axis K is I-self adjoint. We work with

$$e_1(z) \stackrel{def}{=} -\sqrt{\frac{(1+\Delta)(1+bz^2)-1}{1+bz^2}}$$

Thus, $K(z) = \mathrm{i}\begin{pmatrix} 0 & 1 \\ -e_j^2(z) & 0 \end{pmatrix}$ has the eigenvectors $n_j(z) = \begin{pmatrix} 1 \\ -\mathrm{i}e_j(z) \end{pmatrix}$ with the projectors $P_j(z) = \frac{1}{2}\begin{pmatrix} 1 & \frac{\mathrm{i}}{e_j(z)} \\ -\mathrm{i}e_j(z) & 1 \end{pmatrix}$. The I-norm for $|e_l^- >= R_l \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ is 1 and for $|e_r^+ >$ is -1. Also, $m_j(z) = \frac{1}{2}\begin{pmatrix} e_j^{-2}(\bar{z}) \\ -\mathrm{i} \end{pmatrix}$ is the eigenvector of $K^{\natural}(z)$ for the eigenvalue $e_j^*(z) = e_j(\bar{z})$. They obey $< m_j(z), n_k(z) >=$

$\delta_{j,k}$. If we do not use $e_j^*(z) = e_j(\bar{z})$ we will use the fact that analyticity of $e_j(z)$ involves the analyticity of $\overline{e_j(\bar{z})}$ (we need the analyticity when we will deform the path of integration). $n_j(-\infty)$ is identical with $|e_l^- >$ up to a constant. The same is true for $m_j(+\infty)$ and $|e_r^+ >$. We used $K^\dagger(z) = K(\bar{z})$.

In (26) $w_r^{1/2}$ and $w_r^{1/2}$ are taken to be positive. Using (27), $\mathbf{1} = |n_1(z) >_I < m_1(z)| + |n_2(z) >_I < m_2(z)|$ and the same for z_0, (26) becomes:

$$U_{+-} = \lim_{\substack{x_0 \to -\infty \\ x \to +\infty \\ z_0 = x_0 + \mathrm{i}a \\ z = x + \mathrm{i}a}} \exp(\frac{\mathrm{i}}{\varepsilon} e_1(+\infty)z - \frac{\mathrm{i}}{\varepsilon} e_1(-\infty)z_0)$$

$$< m_{1,\varepsilon}(z)|U(z,z_0)|n_{1,\varepsilon}(z_0) >_I$$

Using the theory recalled above:

$$< m_{1,\varepsilon}(z)|U(z,z_0)|n_{1,\varepsilon}(z_0) >_I = e^{-\mathrm{i}\phi(z,z_0)}$$

with ϕ obtained from

$$\phi(z,z_0) = \int_{z_0}^{z} [\varepsilon^{-1} e_1 - \mathrm{i} < m_1, \dot{n}_1 >_I -$$

$$-\varepsilon \frac{1}{e_2 - e_1} < \dot{m}_1; (1 - P_{1,0})\dot{n}_1 >] \, du + o(\varepsilon^2).$$

Using the expressions of $|n_1(z) >$ and $|m_1(z) >$ we obtain

$$< m_1, \dot{n}_1 >_I = \frac{1}{2} < (e_1^{-1}(z), \mathrm{i}), \mathrm{i} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ -\mathrm{i}\dot{e}_1(z) \end{pmatrix} >= \frac{\dot{e}_1(z)}{2e_1(z)}$$

$$< m_1, n_2 >_I = 0 \;\; \Rightarrow \;\; < \dot{m}_1, n_2 >_I = - < m_1, \dot{n}_2 >_I$$

$$< m_2, \dot{n}_1 >_I = \frac{1}{2} < (e_2^{-1}(z), \mathrm{i})\mathrm{i} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ -\mathrm{i}\dot{e}_1(z) \end{pmatrix} >= \frac{-\dot{e}_1(z)}{2e_1(z)}$$

$$< \dot{m}_1, n_2 >_I = - < m_1, \dot{n}_2 >_I =$$

$$= -\frac{1}{2} < (e_1^{-1}(z), \mathrm{i})\mathrm{i} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ \mathrm{i}\dot{e}_1(z) \end{pmatrix} >= \frac{\dot{e}_1(z)}{2e_1(z)}$$

We replace in the integral:

$$\phi(z,z_0) = \int_{z_0}^{z} \varepsilon^{-1} e_1(u) - \frac{\mathrm{i}}{2} \frac{\dot{e}_1(u)}{e_1(u)} - \varepsilon \frac{\dot{e}_1(u)^2}{8e_1(u)^3} \, du \;\; + o(\varepsilon^2) \stackrel{def}{=}$$

$$\stackrel{not}{=} \int_{z_0}^{z} \alpha(u) \, du \;\; + o(\varepsilon^2) \tag{28}$$

$e_1(z)$ is analytic in the complex plane without the poles, zeros and cuts which appear.

5.3 The calculation of the reflection coefficient.

5.3.1 The case where the energy equals the top of the barrier.

For the calculation of the previous integral using the analyticity of the terms in the integrand we deform the path of integration on the real axis avoiding the cuts, zeroes and poles. We obtain contributions for

the square of the absolute value of U_{+-} only from the imaginary part of ϕ. We deform the path in the manner:

Let Γ be the lower path from x_0 to x:

$$\int_{z_0}^{z} \alpha(u)du = \int_{z_0}^{x} \alpha(u)du + \int_{\Gamma} \alpha(u)du + \int_{x}^{z} \alpha(u)du.$$

We obtain a compensation between the first exp in

$$U_{+-} = \lim_{\substack{x_0 \to -\infty \\ x \to +\infty}} \exp(\frac{\mathrm{i}}{\varepsilon} e_1(+\infty)z - \frac{\mathrm{i}}{\varepsilon} e_1(-\infty)z_0) e^{\mathrm{i}\phi(z,z_0)}$$

and the above first and third integral in the limit ($e_1(u)$ tend to a constant $\neq 0$ and $\dot{e}_1(u) \to 0$) . This is also true in the case $\Delta \neq 0$ with the paths of integration chosen as we will see in the next subsections.

Thus

$$|U_{+-}|^2 = \lim_{\substack{x_0 \to -\infty \\ x \to +\infty}} \exp(2\ \mathrm{Im}\phi)$$

where

$$\phi(x, x_0) = \int_{\Gamma} \alpha(u)\ du$$

For the real part of Γ we obtain contributions for $\mathrm{Im}(\phi)$ only from the term with i in the integrand of (28). Because $e_1(u)$ is antisymmetric under $u \to -u$ this contribution is zero. From this point on we calculate separately the case $\Delta = 0$. Thus, only the calculation on the semicircle $\stackrel{def}{=} \Gamma_r$ remains. After the calculation we do the limit $r \to 0$. In this limit the first term in the integrand of (28) gives zero contribution and the second term gives a real contribution. For the third term, we do an integration by parts for the reduction of the divergence order. Using also $z \ln z \to 0$ for $z \to 0 \Rightarrow$

$$\lim_{r \to 0}\ \mathrm{Im} \int_{\Gamma_r} -\frac{\varepsilon}{8} \frac{\dot{e_1}^2}{e_1^3} = -\frac{3\varepsilon\sqrt{b}\pi}{16} \ \Rightarrow\ |U_{+-}|^2 = e^{-\frac{3\pi\sqrt{b}}{8}\varepsilon}$$

5.3.2 The energy above the barrier

We do the calculation of the integrals for $\Delta \neq 0$. In the case $\Delta > 0$ we choose the next path of integration :

(after deformation the lower path) We denote the path from $-r$ to r with Γ_2. So, we calculate Imϕ in (28) with the integration done on Γ_2 and replace it in $|U_{+-}|^2 = \exp(2\text{Im}\phi)$. We take the cuts and the choices of the signs as mentioned above.

The first term in the integrand of (28) has zero contribution on the path BC in the limit $r \to 0$. For the AB and CD sections we use the real elliptic integrals in the Legendre's standard form of the first and second kind

$$F(\Phi, k^2) = \int_0^{\Phi} \frac{d\theta}{\sqrt{1 - k^2 \sin^2\theta}} \quad , \quad E(\Phi, k) = \int_0^{\Phi} \sqrt{1 - k^2 \sin^2\theta}\, d\theta$$

with $|k| < 1$. For $\Phi = \pi/2$ we obtain the complete integrals:

$$F(k) = F(\pi/2, k) \text{ and } E(k) = E(\pi/2, k)$$

with the expansions:

$$F(k) = \frac{\pi}{2}\{1 + (\frac{1}{2})^2 k^2 + \ldots + [\frac{(2n-1)!!}{(2n)!!}]^2 k^{2n} + \ldots\}$$

$$E(k) = \frac{\pi}{2}\{1 - (\frac{1}{2})^2 k^2 - \ldots - [\frac{(2n-1)!!}{(2n)!!}]\frac{k^{2n}}{2n-1} + \ldots\}$$

which converge for $|k| < 1$.

The result is:

$$\int_{\Gamma_2} \varepsilon^{-1} e_1(u)\, du \xrightarrow{r \to 0} -\text{i}2\sqrt{1+\Delta}\varepsilon^{-1}\beta^2\sqrt{b}\left[\left(1 - \frac{1}{b\beta^2}\right) F(b\beta^2) + \frac{1}{b\beta 2} E(b\beta^2)\right]$$

with $\beta = \sqrt{\frac{\Delta}{(1+\Delta)b}}$

For small Δ (which implies small β) the result can be developed in Δ. We will obtain the same series for $\Delta > 0$ and $\Delta < 0$. This fact can be justified if we do this expansion and the calculation of the integral before the path's deformation and next we do these operations for each term of the expansion. The first term of the expansion is $\exp(-\frac{\pi\Delta}{\varepsilon\sqrt{b}})$ (Δ contains its sign).

The second term in the integrand of (28) has zero contribution, with the same proof as for $\Delta = 0$ and for the third term we follow the next steps.

We do a few integrals by parts firstly to obtain an integrand which has zero contribution in the limit $r \to 0$ on the semicircle CD. The rest of path is separated as follows:

$$\int_A^C + \int_D^F = (\int_A^B + \int_E^F) + (\int_B^C + \int_D^E)$$

with B and E at the middle of the segments.

We do this separation because we apply the integration by parts in two distinct ways for the reduction of order at the divergences from the ends of the segments.

The final expression is:

$$|U_{+-}|^2 = \exp\left\{\frac{\varepsilon}{4\sqrt{1+\Delta}}\left(\frac{1}{b}-\beta\right)^2\left[\frac{2}{3}\int_0^{\frac{\beta}{2}}\frac{2x^2+1/b}{(\beta^2-x^2)^{3/2}(\sqrt{\frac{1}{b}-x^2})^5}dx+\right.\right.$$

$$\left.\left.+\frac{-8}{3\sqrt{3}\beta^2}\left(\frac{\beta^2}{2}+\frac{1}{b}\right)\left(\frac{1}{b}-\frac{\beta^2}{4}\right)^{-5/2}+\frac{2}{3}\int_{\beta/2}^{\beta}\frac{1}{(\beta^2-x^2)^{1/2}}\frac{8x^4+\frac{8x^2}{b}-\frac{1}{b^2}}{-x^2(\frac{1}{b}-x^2)^{7/2}}dx\right]\right\}$$

This is an intermediate results for $\Delta > 0$. The integrals can be expressed as elliptic integrals but the expansion for small Δ (and so small β) is more interesting. We do this expansion in the expressions from the integrals after the change of the variable $x/\beta = \sin\theta$. We obtain the 0-order in Δ (which is the same as that above calculated for $\Delta = 0$) and the 1-order term is:

$$\exp(-\frac{15}{64}\pi\varepsilon\sqrt{b}\Delta)$$

5.3.3 The energy below the top of the barrier.

For $\Delta < 0$ we take the path of integration:

(after deformation the lower path) with $\beta = \sqrt{\frac{|\Delta|}{(1+\Delta)b}} > 0$. We take the cuts and deformation mentioned above. In the same manner as in the previous sections for the imaginary part of the integrals we obtain contributions only from the path from $-\beta - r$ to $\beta + r$ (we note it with Γ_2). Analogously, the first term in the integrand of (28) has zero contribution in the limit $r \to 0$ on the parts of the path A'A and DD'. From AD this term gives:

$$|U_{+-}|^2 = \exp\left[\frac{4\varepsilon^{-2}\sqrt{1+\Delta}\sqrt{1+b\beta^2}}{\sqrt{b}}\left(F\left(\frac{b\beta^2}{1+b\beta^2}\right)-E\left(\frac{b\beta^2}{1+b\beta^2}\right)\right)\right]$$

In the same manner as above the second term of (28) has zero contribution to the imaginary part. For the third term we follow analogous steps. Firstly, with integrations by parts we obtain an integral which

is zero on A'A and DD' in the limit $r \to 0$. Then we separate the path:

$$\int_A^D = (\int_A^B + \int_C^D) + \int_B^C$$

and we treat in different manners the parts of the path.

We treat distinctly the divergences from the ends of the segments, and so we do in different ways the integrations by parts. The result (for $\Delta < 0$) can be written:

$$|U_{+-}|^2 = \exp\left\{\frac{\varepsilon}{4}\frac{1}{\sqrt{1+\Delta}}\left(\frac{1}{b}+\beta^2\right)^2\left[\frac{8}{3\sqrt{3}\beta^2}\frac{(\frac{1}{b}-\frac{\beta^2}{2})}{(\frac{1}{b}+\frac{\beta^2}{4})^{5/2}}-\right.\right.$$

$$\left.\left.-\frac{2}{3}\int_0^{\frac{\beta}{2}}\frac{-2x^2+\frac{1}{b}}{(\beta^2-x^2)^{3/2}(x^2+\frac{1}{b})^{5/2}}dx+\frac{2}{3}\int_{\frac{\beta}{2}}^{\beta}\frac{1}{(\beta^2-x^2)^{1/2}}\frac{8x^4-\frac{8x^2}{b}-\frac{1}{b^2}}{x^2(x^2+\frac{1}{b})^{7/2}}dx\right]\right\}$$

If we expand for small Δ we obtain the same series as for $\Delta > 0$ (the same justifications as in previous sections).

6 The reflection coefficient for a general potential

6.1 The existence of a dissipative path for the case where the energy equals the top of the barrier

In the case of a general potential we take a potential which tends quickly enough to its limit at the ends of the axis (for simplicity we take these limits equal and so equal to 0), and with a maximum at the origin equal to 1 (this can be done with a rescaling and a removal of the argument). We take the energy in a neighbourhood of the maximum $E = 1 + \Delta$ with Δ small. We also require that the potential is the restriction to the real argument of an analytic function in a strip around the real axis. In the general case, the problem is the existence of a dissipative path in the analyticity strip which does not undulate too much at the ends of the axis (for the convergence of the integrals from [2]), and which avoids the zeroes, the cuts and the poles of $\sqrt{1-V}$ (of $\sqrt{E-V}$ for $\Delta \neq 0$) (hence obeys the gap conditions $|e^{(2)}(s) - e^{(1)}(s)| \geq d > 0$ on it). Also, the previous method of calculation is valid if no other zeroes, cuts and poles for $\sqrt{1-V}$ (distinct by the zero from the origin) exist between this path and the real axis. We assume the existence of such a path for $\Delta \neq 0$, and give a justification at $\Delta \neq 0$ for the existence of such a path almost horizontal:

V is analytic and thus $\sqrt{1-V}$ is analytic in a strip around the real axis (which can be smaller than the strip of V because of the zeros for $\sqrt{1-V}$), so the Cauchy-Riemann conditions are satisfied:

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \text{ and } \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}$$

where u and v are the real and imaginary parts of $\sqrt{1-V}$. The argument is valid for $V(x)$ (at x real) monotonic between the ends of the axis and origin:

$$\frac{\partial u}{\partial x} = \frac{\partial}{\partial x}\sqrt{1-V} = \frac{1}{2}\frac{(-1)\frac{\partial V}{\partial x}}{\sqrt{1-V}}$$

$\frac{\partial V}{\partial x}$ has opposite signs from one side of the origin to the other. If $V(x)$ has the Taylor expansion:

$$V(x) = 1 - bx^2 + cx^3 + dx^4 + \ldots \text{ with } b > 0 \Rightarrow$$

$$\sqrt{1-V} = \sqrt{bx^2(1 - \frac{c}{b}x - \frac{d}{b}x^2 - \ldots)}.$$

Thus near the origin, $\sqrt{1-V}$ for real x has opposite signs from one side of the origin to the other. Because $\sqrt{1-V}$ does not have another zero on the real axis and it is a continuous function, $\frac{\partial}{\partial x}\sqrt{1-V}$ has constant sign on all the real axis, so $\frac{\partial}{\partial y}\mathrm{Im}\sqrt{1-V}$ has the same property. So if we take a horizontal path in the upper semiplane, this is dissipative on a larger part if we take it closer to the real axis. For example, we take it at the distance δ from the real axis, we denote it by d_δ and we study the behaviour in the limit $\delta \to 0$. Far from the real axis, the points with $\mathrm{Im}\sqrt{1-V} = 0$ can appear on this path.

For the theory of [2] we need $\mathrm{Im}\sqrt{1-V} > 0$. From the Cauchy-Riemann conditions we obtain the fact that we must take for $\sqrt{1-V}$ the sign which makes it negative on the left side of the origin, where $\frac{dV}{dx}$ is positive.

The points with $\mathrm{Im}\sqrt{1-V} = 0$ on d_δ go away from the origin in the limit $\delta \to 0$. More accurately $(\forall)D > 0(\exists)\delta' > 0$ so that those points with $\delta < \delta'$ are situated on d_δ at argument greater in absolute value than D. If this were not true, an accumulation point (noted Ω) would exist for these arguments in the segment $[-D, D]$. On the real axis, in any case, $\mathrm{Im}\sqrt{1-V} = 0$, and so this fact would involve the annulation of $\frac{\partial}{\partial y}\mathrm{Im}\sqrt{1-V}$ in the accumulation point. But $\frac{\partial}{\partial y}\mathrm{Im}\sqrt{1-V} \neq 0$ from the Cauchy-Riemann conditions. Thus, the points with $\mathrm{Im}\sqrt{1-V} = 0$ are going away from the origin when $\delta \to 0$.

We take δ small enough for these points to be in the asymptotic zone where

$$\|H(x) - H_{\text{limit}}\| < \frac{1}{|x|^{1+\alpha}}, \text{ with } \alpha > 0.$$

¿From the point where $\mathrm{Im}\sqrt{1-V} = 0$ on d_δ, we must deform the path to keep a dissipative path. Because in the asymptotic zone $\sqrt{1-V}$ is close to its limits and $\mathrm{Im}\sqrt{1-V}$ tends to 0 more quickly than $\frac{1}{x^{1+\alpha}}$, we obtain that paths like

$$-\frac{1}{|x|^\alpha} + \text{const}$$

obey the dissipativity conditions in this zone.

With these paths and d_δ we can construct a dissipative path in the strip of analyticity which obeys the conditions requested.

6.2 The lowest orders for the reflection coefficient

If a path with the conditions requested exists, we can apply the theory from the previous sections. We follow the same steps with the Landau-Zener-Friedrichs formula and then with the deformation of the path at the real axis. Only e_1 is different. We obtain again (28) with the integral on the path:

with the semicircle close enough to the origin.

$$|U_{+-}|^2 = e^{2\mathrm{Im}\phi(-\infty,+\infty)}$$

The case with $\Delta = 0$. We have $e_1 = -\sqrt{1-V}$ where for the square root we have the sign which on the negative part of the real axis makes it positive. In a neighbourhood of the origin, $V(z) = 1 - bz^2 + cz^3 + dz^4 + \ldots$ and

$$-\sqrt{1-v(z)} = \sqrt{b}z \ sqrt1 - \sqrt{c}bz - \sqrt{d}bz^2 - \ldots$$

where the last square root has no zeros or cuts in the neighbourhood considered. We apply the same considerations as in the previous sections for the contributions to the imaginary part of (28) and obtain contributions only from the third term of its integrand.

Using the expansion:

$$\frac{\dot{e_1^2}}{e_1^3} = \frac{1}{\sqrt{b}}\frac{1}{z^3}\left(1 - \frac{c}{2b}z - \frac{1}{2}\left(-2\left(\frac{c}{b}\right)^2 + 3\frac{d}{b}\right)z^2 + \ldots\right)$$

all terms but $\frac{1}{z}$ give real contributions when integrated on the semicircle.

The result obtained is:

$$|U_{+-}|^2 = \exp\left[-\pi\frac{\varepsilon}{4\sqrt{b}}\left(-\left(\frac{c}{b}\right)^2 + \frac{3}{2}\frac{d}{b}\right)\right].$$

The case with $\Delta \neq 0$. In this case we assume that we have a path with the conditions requested. Before the path's deformation we do the expansion in Δ for all terms in the integrand of (28) where $e_1 = -\sqrt{1+\Delta-V}$. For this square root we choose the sign which for $\Delta \to 0$ on the negative real semiaxes makes it positive. We prove in the same manner the fact that the first (only the 0-order in Δ) and the second term in the integrand of (28) have zero contributions for the imaginary part. For the 1-order of the expansion in Δ at the first and the third term of this integrand, we calculated the imaginary contributions in the same manner as above for $\Delta = 0$, doing the expansion in z of the integrand and observing that only the term in z^{-1} gives a contribution. For the term in $\varepsilon\Delta$ we take a symmetric potential for the simplification of the expansion.

We obtained

- for the term in $\varepsilon^{-1}\Delta$ the result $|U_{+-}|^2 = \exp(\frac{-\Delta\pi}{\varepsilon\sqrt{b}})$
- for the term in $\varepsilon\Delta$ the result

$$\exp\left[\Delta\frac{\varepsilon}{8}\frac{5}{4!}\frac{\pi}{b\sqrt{b}}\left(51\frac{d^2}{b^2} + 60\frac{f}{b}\right)\right].$$

The comparison with an accurate result. We compare the previous results with the accurate solution for the potential

$$V(x) = \frac{\hbar^2}{2m}\frac{k^2+\frac{1}{4}}{\cosh^2 x}$$

In this paragraph we use the notation $E = \frac{p^2\hbar^2}{2m}$.

¿From the Schrödinger equation, after the change of variable $z = \tanh x$, the equation of associated Legendre functions is obtained with the linearly independent solutions P_ν^μ and Q_ν^μ (in our case $\mu = \mathrm{i}p$, $\nu = \mathrm{i}k - \frac{1}{2}$. We take the normalized solutions

$$\psi_{p,k}(x) = \sqrt{\frac{p\sinh(\pi p)}{2(\cosh^2(\pi k)+\sinh^2(\pi p))}}P^{\mathrm{i}p}_{\mathrm{i}k-\frac{1}{2}}(\tanh x)$$

For the asymptotic behaviour we consider

$$P_\nu^\mu(z) \simeq \frac{1}{\Gamma(1-\mu)}(\frac{2}{1-z})^{\mu/2} \text{ at } z \to +1;$$

$$P_\nu^\mu(z) \simeq \frac{\Gamma(-\mu)}{\Gamma(1+\nu-\mu)\Gamma(-\nu-\mu)}(\frac{1+z}{2})^{\mu/2} \text{ at } z \to -1$$

and

$$(\frac{1+\tanh x}{2})^{\pm \mathrm{i}p/2} = \frac{e^{\pm \mathrm{i}px}}{(1+e^{2x})^{\pm \mathrm{i}p/2}}.$$

For the reflection coefficient ($\mu = \mathrm{i}p$, $\nu = \mathrm{i}k - \frac{1}{2}$), using

$$|\Gamma(\mathrm{i}y)|^2 = \frac{\pi}{y\sinh \pi y} \text{ and } |\Gamma(\frac{1}{2}+\mathrm{i}y)|^2 = \frac{\pi}{\cosh \pi y}$$

with y real (I.S. Gradshteyn,I.M. Ryzhik Table of integrals, series and products page 937), we obtain

$$R = \frac{\cosh^2 \pi k}{\cosh \pi(k-p)\ \cosh \pi(-k-p)}$$

The correspondence with the above notation is $\frac{1}{k^2+\frac{1}{4}} = \varepsilon^2$ and $\frac{p^2}{k^2+\frac{1}{4}} = E = 1+\Delta$. Thus $k = \sqrt{\frac{1}{\varepsilon^2} - \sqrt{1}4}$, $p = \frac{\sqrt{1+\Delta}}{\varepsilon}$ and we study R in the limit $\varepsilon \to 0$, $\Delta \to 0$. If we write R in the form of the previous results:

$$R = \frac{u'(\varepsilon,\Delta)}{1+u'(\varepsilon,\Delta)}$$

where u' is an exp function with the argument developed in series of ε and Δ we obtain:

$$u'(\varepsilon,\Delta) = \frac{\cosh^2 \pi k}{\sinh^2 \pi p} = e^{2\pi(k-p)}\frac{1+e^{-4\pi k}+2e^{-2\pi k}}{1+e^{-4\pi p}+2e^{-2\pi p}}.$$

We firstly do the development of $\ln u'(\varepsilon,\Delta)$ in ε-powers and then each term in Δ-powers. From

$$\ln \frac{1+e^{-4\pi k}+2e^{-2\pi k}}{1+e^{-4\pi p}+2e^{-2\pi p}}$$

we obtain only exponentially little terms. Thus, the first terms of the development are:

$$\ln u'(\varepsilon,\Delta) = -\frac{\pi\Delta}{\varepsilon}[1+o(\Delta)] - \frac{\pi\varepsilon}{4} + o(\varepsilon^3)$$

For the comparison with the previous results we write:

$$V(x) = \mathrm{sech}^2 x = 1 - z^2 + \frac{2}{3}z^4 - \frac{17}{45}z^6 + \ldots =$$

$$= 1 - bx^2 + cx^3 + dx^4 + ex^5 + fx^6 + \ldots \Rightarrow b = 1, c = 0, d = \frac{2}{3}, e = 0, f = -\frac{17}{45}$$

Thus

$$u(\varepsilon, \Delta) = \exp\{-\frac{\pi\Delta}{\varepsilon\sqrt{b}}[1 + o(\Delta)] - \frac{\pi\varepsilon}{4\sqrt{b}}[[-(\frac{c}{b})^2 + \frac{3}{2}\frac{d}{b}]-$$

$$-\Delta\frac{5}{48b}[51(\frac{d}{b})^2 + 60\frac{f}{b}] + o(\Delta^2)] + o(\varepsilon^2]\} =$$

$$= \exp\{-\frac{\pi\Delta}{\varepsilon}[1 + o(\Delta)] - \frac{\pi\varepsilon}{4}[1 + o(\Delta^2)] + o(\varepsilon^2)\}.$$

So we obtained the same result.

A Appendix

Lemma. The horizontal path $z(x) = x + \mathrm{i}a$ ($x \in \Re$, $a \in \Re$) is a dissipative path for the Hamiltonian

$$K(z) = \mathrm{i}\begin{pmatrix} 0 & 1 \\ -[(1+\Delta) - \frac{1}{1+bz^2}] & 0 \end{pmatrix}$$

with $\Delta \in \Re$, for

- $\frac{1}{\sqrt{b}} > a > 0$ at $\Delta < 0$
- $\frac{1}{\sqrt{b}} > a > |\mathrm{Im}\sqrt{\frac{1}{b}(\frac{1}{1+\Delta} - 1)}|$ at $\Delta > 0$.

Proof. Because the path is horizontal, the dissipativity request means that on the path, the sign of the difference of the imaginary parts of the $K(z)$'s eigenvalues is the same:

$$e_{1,2} = \pm\sqrt{(1+\Delta) - \frac{1}{1+bz^2}}.$$

We do the same cuts and choices of the signs as in the previous chapters. Because the eigenvalues have opposite signs, it is sufficient to prove that the sign of imaginary part (in fact the phase) of:

$$\frac{\sqrt{x + \mathrm{i}\sqrt{\frac{\Delta}{(1+\Delta)b}}}\sqrt{x - \mathrm{i}\sqrt{\frac{\Delta}{(1+\Delta)b}}}}{\sqrt{x - \frac{\mathrm{i}}{\sqrt{b}}}\sqrt{x + \frac{\mathrm{i}}{\sqrt{b}}}}$$

is unchanged on the path (where for $\sqrt{b}$ and $\sqrt{(1+\Delta)b}$ we take the signs which make them positive).

The case $\Delta > 0$. We take $\sqrt{\Delta} > 0$. For z in the zone with x negative:

The phase of the square root in the numerator is:

$$\frac{\widehat{D'ZB} + \widehat{C'ZB}}{2} - \pi = -(\pi - \widehat{D'ZB} - \widehat{DZB}) = -\widehat{BZG}$$

The π produces the above choice of the sign. The symbol $\widehat{\ }$ means the small angle with the positive sign. Also, the phase of the square root in the denominator is:

$$\frac{(2\pi - \widehat{BZA'}) + \widehat{BZE'}}{2} - \pi = -(\pi - \widehat{BZE'} - \widehat{EZF}) = -\widehat{BZF}$$

The phase of the whole expression is:

$$\widehat{BZF} - \widehat{BZG} = -\widehat{FZG}$$

which is everywhere negative, i.e. it has a constant sign (the circles have everywhere this relative position because they cross only at the two points $x + \mathrm{i}a$ and $x - \mathrm{i}a$).

For z in the zone with x positive:

The phase of the square root in the numerator is:

$$\frac{\widehat{D'ZB'} + \widehat{C'ZB'}}{2} - \pi = \widehat{BZG} - \pi$$

and that in the denominator is:

$$\frac{\widehat{E'ZB'} + (2\pi - \widehat{B'ZA'})}{2} - \pi = \widehat{BZF}$$

The phase of the whole expression is:

$$\widehat{FZG} - \pi$$

which is negative everywhere.

The case with $\Delta < 0$ We take $\sqrt{\frac{|\Delta|}{(1+\Delta)b}} > 0$. For z in the zone of the path with x negative, we have the phase of the square root in the denominator. It is, in the previous notation,

$$-\widehat{BZF} > -\widehat{BZO}.$$

For the phase of the square root in the numerator we have:

$$\frac{\widehat{ZCX} + \widehat{ZDX}}{2} - \pi = -\widehat{BZR} < -\widehat{BZO}$$

Thus, the phase of the whole expression is $-\widehat{BZR} + \widehat{BZF} < -\widehat{BZO} + \widehat{BZO} = 0$, i.e. everywhere negative. For z in the zone of the path with x positive, the phase of the square root in the denominator is (in the previous notation):

$$0 < \widehat{BZF} < \widehat{BZO}.$$

For the phase of the square root in the numerator we have:

$$\frac{\widehat{ZCX} + \widehat{ZDX}}{2} - \pi = \widehat{BZR} < \pi$$

with $\pi > \widehat{BZR} > \widehat{BZO}$. Thus, the phase of the whole expression is $\widehat{BZR} - \pi - \widehat{BZF}$ with $0 > \widehat{BZR} - \pi - \widehat{BZF} > -\pi$, so it is everywhere negative.

Thus, on the whole path the sign of the imaginary part of the difference of the Hamiltonian's eigenvalues is unchanging. So the path is dissipative.□

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