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# A formal computation of the splitting for the Klein–Gordon operator

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## Abstract

We study the semi-classical Klein–Gordon operator in the one dimensional case, for a double-well potential. We obtain a formal computation of the splitting in cases that were not yet studied. *To cite this article: E. Servat, C. R. Acad. Sci. Paris, Ser. I 338 (2004).*

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## Résumé

**Un calcul formel du splitting pour l'opérateur de Klein–Gordon.** On étudie l'opérateur de Klein–Gordon dans le cas de la dimension un, pour un potentiel présentant un double puits symétrique. On obtient une expression formelle du splitting dans des cas qui n'étaient pas envisagés auparavant. *Pour citer cet article : E. Servat, C. R. Acad. Sci. Paris, Ser. I 338 (2004).*

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## 1. Introduction and results

We are interested in the semi-classical Klein–Gordon operator  $P = \sqrt{1 - h^2 \Delta} + V$ , in the one-dimensional case. For  $(x, \xi) \in \mathbb{R}^2$ , we write  $p(x, \xi) = \sqrt{1 + \xi^2} + V(x)$  the symbol of  $P$ . We make the following assumptions on  $V$ :

(H1)  $V$  is smooth, even, has a finite minimum denoted  $E_0 - 1$ , and  $\lim_{|x| \rightarrow \infty} V = E_1 - 1 > E_0 - 1$ .

(H2) The minimum of  $V$  is attained at only two points  $\pm x_0$ , called potential wells, and  $V'(\pm x_0) \neq 0$ .

Therefore, we know that  $P$  has a self-adjoint extension [4] – still denoted  $P$  – and that its spectrum is discrete in  $[E_0, E_1[$  [1]. Thanks to WKB constructions in a neighbourhood of  $\pm x_0$  [3], we can calculate the first eigenvalues of  $P$ . The symmetry of the potential ensures that the two first eigenvalues are very close to each other, and we call splitting their difference.

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Many papers deal with the calculation of the splitting for Schrödinger operators. In particular in [3], Helffer and Sjöstrand define a matrix, that expresses the interaction between the potential wells of the problem. This interaction matrix can be defined for the Klein–Gordon operator. In the case of a double well and assuming that:

(H) There is a unique minimal geodesic for the Agmon distance  $d = (1 - (V - E_0)_+^2)_+ dx^2$  between  $\pm x_0$ , and it lies in the region  $\{x \in \mathbb{R}^n, V(x) < E_0\}$ .

Helffer and Parisse obtain the following limit which gives an estimate for the splitting  $s(h)$  [2]:

$$\lim_{h \rightarrow 0} \frac{s(h) e^{S/h}}{\sqrt{h}} = C_n(V), \quad \text{with } S = d(-x_0, x_0), \quad (1)$$

where  $C_n(V)$  can be calculated. Let us give an idea of their proof: define the operator with one well  $P + \beta_j$ , where for  $\varepsilon_0 > 0$ ,  $\beta_1 \in C_0^\infty(]x_0 - \varepsilon_0, x_0 + \varepsilon_0[)$ ,  $\beta_1 \geq 0$ ,  $\beta_1(x_0) > 0$ , and  $\beta_2(x) = \beta_1(-x)$ . Let  $u^j$ ,  $j = 1, 2$ , be the normalised eigenfunctions of  $P + \beta_j$  associated to the first eigenvalue. Starting from the interaction matrix, the authors obtain an estimate for the splitting that involves the  $u^j$ 's only in a neighbourhood of the minimal geodesic. Thanks to hypothesis (H), WKB solutions can be constructed in this region – exactly as for the Schrödinger operator – and lead to (1).

The aim of this work is to calculate a splitting in the one dimensional case, when the hypothesis (H) is no more satisfied. We then have to deal with the region  $\{V > E_0\}$ , where analogies with the Schrödinger operator cannot be made anymore. Actually, the problem comes from the fact that the function  $\xi \mapsto p(x, \xi)$  is not holomorphic at  $\pm i$  and thus prevents deformations of paths integral in a strip larger than  $\{z \in \mathbb{C}, |\Im z| < 1\}$ . For later use, we denote  $\Delta = i[1, +\infty[ \cup i] - \infty, -1]$ , so that  $\mathbb{C} \setminus \Delta$  is a simply connected domain where  $\xi \mapsto p(x, \xi)$  is holomorphic.

Our strategy is the following: we start with the formula of the splitting in term of the  $u^j$ 's, using the interaction matrix. We prove that the main contribution is given by an integral involving the Fourier transforms of the  $u^j$  in a neighbourhood of  $\pm i$  in  $\mathbb{C} \setminus \Delta$ . We then have to replace these Fourier transforms by explicit approximations. Such approximations can be calculated in the vicinity of  $\{z \in \mathbb{C}, \Re z = 0, 1 - 2\varepsilon_0 \leq |\Im z| \leq 1 - \varepsilon_0\}$ . Moreover, we can extend them holomorphically near  $\pm i$  in  $\mathbb{C} \setminus \Delta$ , if we make the assumption:

(H3) The set of point  $V^{-1}(0) \cap [-x_0, x_0]$  is given by  $\pm b \in \pm]0, x_0[$ , and  $V'(b) \neq 0$ .

We use these extensions to compute what we call a formal splitting:

**Theorem 1.1.** *The formal splitting  $s(h)$  of a Klein–Gordon operator  $P$  satisfying (H1), (H2) and (H3) is given by*

$$\lim_{h \rightarrow 0} \frac{s(h) e^{S/h}}{h} = C_1(V) = \frac{4}{|V'(b)|(2\pi b)^{3/2} V''(x_0)^{1/4}} \Gamma\left(\frac{1}{2}\right) \Gamma(-1), \quad (2)$$

where  $S$  is the Agmon distance between the two wells,  $S = d(-x_0, x_0)$ , and  $\Gamma(s) = \int_{\mathbb{R}^+} e^{-u} u^s du$  for  $s > -1$  and can be extended.

Remark that the power of  $h$  in the splitting (2) is different from the one obtained in [2] when the assumption (H) is made, see (1).

To obtain the splitting from (2), one should prove that the Fourier transforms of the eigenfunctions  $u^j$ ,  $j = 1, 2$ , is well approximated by the extensions we have constructed. The lack of holomorphy of  $\xi \mapsto p(x, \xi)$  arises again.

In the following, we first study the Fourier transforms of the  $u^j$ 's, and then rewrite the splitting to prove Theorem 1.1. Without loss of generality, we take from now on  $E_0 = 0$ .

## 2. Fourier Transforms of the $u^j$

In this section, we concentrate on the Fourier transform of the first eigenfunction  $u^1$  associated to the potential well  $-x_0$ . The symmetry of the problem will give similar results for  $u^2$ .

**Theorem 2.1.** *There exists  $W_i$  a neighbourhood of  $i$  in  $\mathbb{C} \setminus \Delta$ , there exists holomorphic functions  $\psi_1$  and  $b_n^1$ ,  $n \geq 0$ , defined in  $W_i$ , such that the Fourier transform of  $u^1$  can be written:*

$$\forall N \in \mathbb{N}, \quad \widehat{u}^1(\xi, h) = h^{1/4} e^{i\psi_1(\xi)/h} \left( \sum_{n \geq 0}^N h^n b_n^1(\xi) + O(h^{N+1}) \right), \tag{3}$$

for  $\xi \in W \subset W_i$  a neighbourhood in  $\mathbb{C}$  of the segment  $i[1 - 2\varepsilon_0, 1 - \varepsilon_0]$ ,  $\varepsilon_0 > 0$  small.

**Proof.** Let us recall a result from [2] concerning the exponential decreasing of the eigenfunction  $u^1$ :

$$\forall K \Subset \mathbb{R}, \exists N \in \mathbb{N}, \exists C > 0, \quad \|e^{d_1/h} u^1\|_{L^2(K)} \leq Ch^{-N}, \quad h < h_0, \tag{4}$$

where  $d_1$  is the Agmon distance to the well  $-x_0$  for the operator  $P + \beta_1$ . Moreover, if  $K$  is a compact, that belongs to the connected component of  $\{V < 0\}$  which contains  $-x_0$ , we can construct a WKB solution  $v^1$  such that

$$\|e^{d_1/h} (u^1 - v^1)\|_{L^2(K)} = O(h^\infty), \quad \text{i.e., } \forall N \in \mathbb{N}, \exists C_N, \quad \|e^{d_1/h} (u^1 - v^1)\|_{L^2(K)} \leq C_N h^N. \tag{5}$$

Let  $\xi \in W$  a neighbourhood of  $i[1 - 2\varepsilon_0, 1 - \varepsilon_0]$ . The estimate (4) implies that modulo  $O(h^\infty)$ , we can replace  $u^1$  by  $\chi u^1$  in the computation of  $\widehat{u}^1$ , for a cut off  $\chi \in C_0^\infty([-b - 2\varepsilon, -b - \varepsilon])$ ,  $\varepsilon = \varepsilon(\varepsilon_0)$ . Then, (5) allows to replace  $\chi u^1$  by its WKB approximation  $v^1$ . Since  $v^1$  is known explicitly, the method of the stationary phase [1] gives functions  $\psi_1$  and  $b_n^1$  in  $W$  as in (3). Furthermore, we can prove that  $\psi_1$  satisfies the so called eiconal equation:

$$p(-\psi_1'(\xi), \xi) = 0, \tag{6}$$

and the  $b_n^1$ 's satisfy some first order differential equations, called transport equations. The assumption (H3) permits us to extend holomorphically these functions in  $W_i$ , by means of (6) and the transport equations.  $\square$

As  $\xi$  tends to  $i$ , the transport equations give the singularity of the  $b_n^1$ 's at  $i$ :

**Proposition 2.2.** (i) *We have  $b_0^1(i) = \frac{2(2\pi)^{1/4}}{|V'(-b)|^{1/2}|V''(-x_0)|^{1/8}} \neq 0$ .*

(ii) *For  $n \geq 0$  there exists holomorphic functions in  $W_i$   $c_n^1$ , continuous at  $i$ , such that*

$$b_0^1(\xi) - b_0^1(i) = c_0^1(\xi) \sqrt{\xi - i}, \tag{7}$$

$$\forall n \geq 1, \quad b_n^1(\xi) = \frac{c_n^1(\xi)}{(\xi - i)^{n-1/2}}. \tag{8}$$

We have similar results for  $u^2$  near  $-i$ . We now come to the splitting and Theorem 1.1.

### 3. Computation of the splitting

In this section, we first prove that the splitting can be written with an expression involving the  $\widehat{u}^j$ 's near  $\pm i$ , then we replace these functions by the extensions given by (3). Let  $\tilde{\chi} \in C_0^\infty([-3\varepsilon_0, 3\varepsilon_0])$ ,  $\tilde{\chi} \equiv 1$  in  $[-2\varepsilon_0, 2\varepsilon_0]$ , then:

**Theorem 3.1.** *The splitting  $s(h)$  is given by  $s(h) = 2w(h) + O(e^{-(S+\varepsilon_0)/h})$ , where for any  $x \in [-x_0 + \varepsilon_0, x_0 - \varepsilon_0]$ ,*

$$w(h) = -\frac{h}{i} \frac{1}{(2\pi h)^2} \int_{\Gamma^1 \times \Gamma^2} e^{ix(\xi+\eta)/h} \frac{q(\xi) - q(\eta)}{\xi + \eta} \widehat{u}^1(\xi, h) \widehat{u}^2(\eta, h) d\xi d\eta (1 + O(h^\infty)). \tag{9}$$

We have denoted  $\Gamma^1 = i - i\beta h + [-\varepsilon_0, \varepsilon_0]$  and  $\Gamma^2 = -i + i\beta h + [-\varepsilon_0, \varepsilon_0]$ , for any  $\beta > 0$ .

**Proof.** On the one hand, we remark that the definition of the  $u^j$ 's implies:

$$(P + \beta_j)u^j = \lambda(h)u^j \implies (P - \lambda(h))u^j = -\beta_j u^j = 0 \text{ for } x \in [-x_0 + \varepsilon_0, x_0 - \varepsilon_0]. \tag{10}$$

Here  $\lambda(h)$  is the first eigenvalue of both  $P + \beta_1(x)$  and  $P + \beta_2(x) = P + \beta_1(-x)$ , because of the symmetry of  $V$ .

On the other hand, the splitting is given by  $s(h) = 2w(h) + O(e^{-(S+\varepsilon_0)/h})$ , where  $w(h) = ((P - \lambda(h))u^2, u^1)$  is the interaction coefficient [3]. If  $q(\xi) = \sqrt{1 + \xi^2}$ , (10) entails that for any  $x \in [-x_0 + \varepsilon_0, x_0 - \varepsilon_0]$ ,

$$w(h) = -\frac{h}{i} \frac{1}{(2\pi h)^2} \int_{\mathbb{R}_\xi \times \mathbb{R}_\eta} e^{ix(\xi+\eta)/h} \frac{q(\xi) - q(\eta)}{\xi + \eta} \widehat{u}^1(\xi, h) \widehat{u}^2(\eta, h) d\xi d\eta. \tag{11}$$

We deform the integral path  $\mathbb{R}_\xi$  of (11) in the complex plan  $\mathbb{C}$  and prove that we can replace it by  $(\mathbb{R} + i - i\beta h)_\xi$  for any  $\beta > 0$ . Indeed, this set is homotopic to  $\mathbb{R}_\xi$  in  $\mathbb{C} \setminus \Delta$ . Similarly, we replace  $\mathbb{R}_\eta$  by  $(\mathbb{R} - i + i\beta h)_\eta$ . We finally write  $\widehat{u}^j$  in term of  $u^j$ , and use the exponential decreasing of the eigenfunctions (4) to find the  $\Gamma^j$ 's in (9).  $\square$

**Remark 1.** In higher dimensions, the function  $(\xi, \eta) \mapsto \frac{q(\xi) - q(\eta)}{\xi + \eta}$  is no longer smooth and formula (9) does not hold. B. Helffer and B. Parisse solve this problem in [2].

We now replace in (9) the Fourier transforms of  $u^j$ ,  $j = 1, 2$ , by the explicit formulas (3). Since (9) is independent of  $x \in [-x_0 + \varepsilon_0, x_0 - \varepsilon_0]$  and  $\beta > 0$ , we calculate it for  $x = 0$  and  $\beta = \frac{1}{2b}$ . We have to estimate the integrals:

$$I_{p,q} = h^{p+q} \int_{\Gamma^1 \times \Gamma^2} e^{i\psi_1(\xi)/h} e^{i\psi_2(\eta)/h} \frac{q(\xi) - q(\eta)}{\xi + \eta} b_p^1(\xi) b_q^2(\eta) d\xi d\eta. \tag{12}$$

Because of the holomorphy of the functions in the integral  $I_{p,q}$ , we can deform  $\Gamma^j$  in  $\mathbb{C} \setminus \Delta$ . To calculate  $I_{0,0}$  we prove that we only have to consider the paths:

$$\Gamma_1: \xi = i - i\frac{h}{2b}(1 + iu - u^2), \quad |u| \leq \varepsilon/\sqrt{h}, \tag{13}$$

$$\Gamma_2: \eta = -i - i\frac{h}{2b}v_\pm, \quad 0 \leq v_\pm \leq \frac{\varepsilon}{h}, \text{ where } v_\pm = \lim_{\delta \rightarrow 0^+} v \pm i\delta \in \mathbb{C} \setminus \Delta. \tag{14}$$

Then  $I_{0,0} = (i/2)(h/b)^{3/2} e^{-S/h} b_0^1(i) b_0^2(-i) \int_{\mathbb{R}_u \times \mathbb{R}_v^+} \frac{e^{(1+iu-u^2)/2} (1+2iu) e^{-v/2} \sqrt{v}}{1+iu-u^2+v} du dv (1 + O(h^{1/2}))$ .

We can compute the integral in the expression of  $I_{0,0}$  in term of the  $\Gamma$  function.

Similarly, we can calculate the  $I_{p,q}$  using the expression of the  $b_n^j$  in Proposition 2.2, and obtain the Theorem 1.1.  $\square$

**Remark 2.** Let us mention that the  $I_{p,q}$ 's have the same order of magnitude for all  $(p, q) \in (\mathbb{N}^*)^2$ , as  $h$  goes to 0. The scaling in power of  $h$  is thus broken when integrating along the  $\Gamma^j$ 's.

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