

Trace formulas and Dirichlet-Neumann problems with variable boundary : the scalar case

Autor(en): **Robert, D. / Sordoni, V.**

Objektyp: **Article**

Zeitschrift: **Helvetica Physica Acta**

Band (Jahr): **69 (1996)**

Heft 2

PDF erstellt am: **28.04.2024**

Persistenter Link: <https://doi.org/10.5169/seals-116914>

Nutzungsbedingungen

Die ETH-Bibliothek ist Anbieterin der digitalisierten Zeitschriften. Sie besitzt keine Urheberrechte an den Inhalten der Zeitschriften. Die Rechte liegen in der Regel bei den Herausgebern.

Die auf der Plattform e-periodica veröffentlichten Dokumente stehen für nicht-kommerzielle Zwecke in Lehre und Forschung sowie für die private Nutzung frei zur Verfügung. Einzelne Dateien oder Ausdrucke aus diesem Angebot können zusammen mit diesen Nutzungsbedingungen und den korrekten Herkunftsbezeichnungen weitergegeben werden.

Das Veröffentlichen von Bildern in Print- und Online-Publikationen ist nur mit vorheriger Genehmigung der Rechteinhaber erlaubt. Die systematische Speicherung von Teilen des elektronischen Angebots auf anderen Servern bedarf ebenfalls des schriftlichen Einverständnisses der Rechteinhaber.

Haftungsausschluss

Alle Angaben erfolgen ohne Gewähr für Vollständigkeit oder Richtigkeit. Es wird keine Haftung übernommen für Schäden durch die Verwendung von Informationen aus diesem Online-Angebot oder durch das Fehlen von Informationen. Dies gilt auch für Inhalte Dritter, die über dieses Angebot zugänglich sind.

Trace Formulas and Dirichlet-Neumann Problems With Variable Boundary: the Scalar Case

By D. Robert

URA CNRS No 758
Département de Mathématiques, Université de Nantes
2, rue de la Houssinière 44072 Nantes Cédex 03 (France)
email:robert@math.univ-nantes.fr

and V. Sordoni

Dipartimento di Matematica, Università di Bologna
Piazza di Porta S.Donato,5 40127 Bologna (Italy)
email:sordoni@dm.unibo.it

(20.III.1996, revised 27.V.1996)

Abstract. The main motivation for this work comes from a formula giving the splitting between the first two eigenvalues for a Schrödinger operator with a symmetric double wells potential, in the semi-classical limit. To give a natural spectral interpretation for this result, we prove some trace formulas for Dirichlet and Neumann problems on large boxes, as the size of the boxes increases to infinity. This gives a natural definition of some relative determinants.

1 Introduction

Let $Q : \mathbb{R}^n \rightarrow \mathbb{R}$, be a smooth function converging sufficiently fast to some real number ω as $|x| \rightarrow \infty$. More precisely, let us suppose that:

$$|Q(x) - \omega| \leq C \langle x \rangle^{-\delta} \quad \text{for some } \delta > n \quad (1.1)$$

Here $\langle x \rangle = (1 + |x|)$.

Associated to Q and ω , we consider the Hamiltonians

$$H_Q = -\Delta_x + Q(x) \quad (1.2)$$

$$H_\omega = -\Delta_x + \omega. \quad (1.3)$$

and we denote by

$$H_{Q,T}^D \quad \text{and} \quad H_{\omega,T}^D \quad (1.4)$$

their Dirichlet realizations in the box $I_T^n =: I_T \times I_T \times \dots \times I_T$, where $I_T =]-T/2, T/2[$. In the same way, we denote by

$$H_{Q,T}^N \quad \text{and} \quad H_{\omega,T}^N \quad (1.5)$$

the operators $H_{Q,T}$ and $H_{\omega,T}$ respectively, with Neumann boundary conditions in I_T^n .

It is well known (see, for example, [18]) that the spectrum of H_Q is consisting of a finite number of eigenvalues

$$\lambda_1 < \lambda_2 \leq \dots \leq \lambda_p < \omega$$

counted with their multiplicity and of a continuous spectrum part in $[\omega, +\infty)$.

On the other hand, for any fixed T , $H_{Q,T}^X$ (resp: $H_{\omega,T}^X$) ($X = D, N$) has an orthonormal base of eigenfunctions $g_{j,T}^X$ (resp: $\tilde{g}_{j,T}^X$) associated to an increasing sequences of eigenvalues $(\lambda_{j,T}^X)_{j \in \mathbf{N}}$ (resp: $(\mu_{j,T}^X)_{j \in \mathbf{N}}$).

Let $a < \lambda_1$ (λ_1 is the bottom of the spectrum of H_Q) and let f be an analytic function defined on the sector

$$A_\varepsilon = \{z \in \mathbf{C} ; |\operatorname{Im} z| < \varepsilon(\operatorname{Re} z - a)\} \quad (1.6)$$

satisfying the following estimate : there exist $\eta > 0$, $c > 0$ such that

$$|f(z)| \leq c \langle z \rangle^{1-\frac{n}{2}-\eta}, \quad \forall z \in A_\varepsilon. \quad (1.7)$$

The purpose of this paper is to prove the following formula:

$$\begin{aligned} \lim_{T \rightarrow +\infty} \operatorname{tr}(f(H_{Q,T}^X) - f(H_{\omega,T}^X)) &= \operatorname{tr}(f(H_Q) - f(H_\omega)) \\ &= \sum_{j=1}^p f(\lambda_j) + \int_\omega^{+\infty} s(\lambda) f'(\lambda) d\lambda, \end{aligned} \quad (1.8)$$

where $s(\lambda)$ is the spectral shift function associated to the pair (H_Q, H_ω) . In the particular case when $n = 1$, $a > 0$ and $f(z) = \ln(z)$, (1.8) gives the following formula for the generalized determinant:

$$\lim_{T \rightarrow +\infty} \left(\frac{\det(H_{Q,T}^X)}{\det(H_{\omega,T}^X)} \right) = \frac{\det(H_Q)}{\det(H_\omega)} = \left(\prod_{j=1}^p \lambda_j \right) \exp\left(\int_\omega^{+\infty} \frac{s(\lambda)}{\lambda} d\lambda \right). \quad (1.9)$$

This formula was suggested to one of the authors (V.S.) by Y. Colin de Verdière. Formulas involving the limit, as $T \rightarrow +\infty$, of the quotient $\frac{\det(H_Q^X)}{\det(H_\omega^X)}$ often appears in physics literature and came out applying a kind of stationary phase theorem to path integrals (see, for example: [3], [13], [15], [16]). In particular, in [23], one of the authors (V.S.) has shown that the Helffer-Sjöstrand's formula ([12]) for the splitting of the two low-lying eigenvalues of a semiclassical one-dimensional Schrödinger operator

$$P(h) = -\frac{h^2}{2} \frac{d^2}{dx^2} + V(x)$$

with symmetric non-degenerate double wells at $\pm a$, can be rewritten as:

$$\lambda_1(h) - \lambda_0(h) = h^{1/2}(G_0 + \mathcal{O}(h))e^{-\frac{S_0}{h}}, \quad (1.10)$$

where

$$G_0 = 2\left(\frac{S_0}{2\pi}\right)^{\frac{1}{2}} \sqrt{\omega} \lim_{T \rightarrow +\infty} \left(\prod_{j \geq 2} \frac{\mu_j^T(\omega)}{\mu_j^T(V''(y))} \right)^{\frac{1}{2}}. \quad (1.11)$$

Here $\omega = V''(\pm a) > 0$, $y(t)$ is an instanton joining the wells $\{-a\}$ and $\{a\}$ i.e. the solution of the Newton equation $y''(t) = V'(y(t))$ with $y(0) = 0$ and $\lim_{t \rightarrow \pm\infty} y(t) = \pm a$, S_0 is the square of the L^2 -norm of the instanton. Moreover $\mu_j^T(V''(y))$ (resp: $\mu_j^T(\omega)$) are the eigenvalues of the Dirichlet realization $H_{Q,T}$ of $H_Q =: -\frac{d^2}{dt^2} + V''(y(t))$ (resp: $H_{\omega,T}$ of $H_\omega =: -\frac{d^2}{dt^2} + \omega$) in the interval $I_T =]-T/2, T/2[$. We remark that this result agrees with the heuristic formula contained in [3].

The results of the present paper allow to rewrite (1.11) as follows :

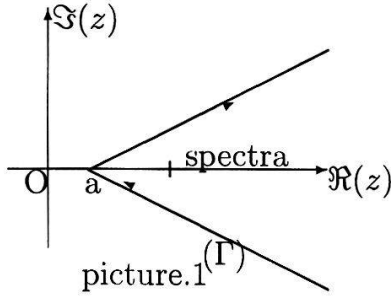
$$G_0 = 2\left(\frac{S_0}{2\pi}\right)^{\frac{1}{2}} \left(\prod_{j=2}^p \lambda_j \right)^{-\frac{1}{2}} \exp \left(-\frac{1}{2} \int_\omega^{+\infty} \frac{s(\lambda)}{\lambda} d\lambda \right). \quad (1.12)$$

Let us remark here that $\lambda_1 = 0$ is a simple eigenvalue. We shall see in Section 3 that (1.12) follows from (1.9). Moreover, in [23] it is shown that a formula similar to (1.12) holds even for the splitting of the two low-lying eigenvalues of a semiclassical Schrödinger operator in arbitrary dimension n . Such a formula involves the eigenvalues of a system of Schrödinger operators with Dirichlet boundary conditions. We shall consider this case in a forthcoming paper.

2 Trace class operators

In this section we prove some relative trace formulas for slow increasing functions in the one dimensional case and also for $n = 2, 3$. (arbitrary n -dimensional case will be considered in Appendix)

Let us consider the curve Γ in picture.1



Since $\text{Sp}(H_{Q,T}^X) \cup \text{Sp}(H_Q) \cup \text{Sp}(H_{\omega,T}^X) \cup \text{Sp}(H_\omega) \subset (a, +\infty)$ the curve Γ in the picture does not intersect $\text{Sp}(H_{Q,T}^X) \cup \text{Sp}(H_Q) \cup \text{Sp}(H_{\omega,T}^X) \cup \text{Sp}(H_\omega)$ for $X = D$ or $X = N$.

If $z \notin (a, +\infty)$, we will denote by $\mathcal{R}(z)$ (resp: $\mathcal{R}_0(z), \mathcal{R}_T^X(z), \mathcal{R}_{0,T}^X(z)$) the resolvent of H_Q (resp: $H_\omega, H_{Q,T}^X, H_{\omega,T}^X$)

Let us start by proving that, if (A, B) is one of the pair $(H_{Q,T}^X, H_{\omega,T}^X)$ or (H_Q, H_ω) then a formula like

$$\text{tr}(f(A) - f(B)) = \frac{i}{2\pi} \int_{\Gamma} \text{tr}((A - z)^{-1} - (B - z)^{-1}) f(z) dz. \quad (2.1)$$

is true. More precisely we prove the following proposition:

Proposition 2.1 *Let us assume that $1 \leq n \leq 3$ and f is an analytic function satisfying (1.7). Then we have:*

1. $f(H_Q) - f(H_\omega)$ is a trace class operator in $L^2(\mathbb{R}^n)$ and

$$\text{tr}(f(H_Q) - f(H_\omega)) = \frac{i}{2\pi} \int_{\Gamma} \text{tr}(\mathcal{R}(z) - \mathcal{R}_0(z)) f(z) dz. \quad (2.2)$$

2. For any positive $T > 0$, $f(H_{Q,T}^X) - f(H_{\omega,T}^X)$ is a trace class operator in $L^2(I_T^n)$ and

$$\begin{aligned} \text{tr}(f(H_{Q,T}^X) - f(H_{\omega,T}^X)) &= \frac{i}{2\pi} \int_{\Gamma} \text{tr}(\mathcal{R}_T^X(z) - \mathcal{R}_{0,T}^X(z)) f(z) dz \\ &= \sum_{j=1}^{\infty} (f(\lambda_{j,T}^X) - f(\mu_{j,T}^X)). \end{aligned} \quad (2.3)$$

Proof :

1) Let us begin by proving that the integral on the RHS of (2.2) converges. We are going to prove that there exists $C > 0$ such that

$$\|\mathcal{R}(z) - \mathcal{R}_0(z)\|_{\text{tr}} \leq C(1 + |z|)^{\frac{n}{2}-2}, \quad \forall z \in \Gamma.$$

Here and in the following $\|\cdot\|_{\text{tr}}$ denotes the trace norm, $\|\cdot\|_{HS}$ the Hilbert-Schmidt norm, and $\|\cdot\|$ the operator norm in $\mathcal{L}(L^2, L^2)$.

We can write, for $z \in \Gamma$, $|z|$ large enough,

$$\mathcal{R}_0(z) - \mathcal{R}(z) = \mathcal{R}_0(z)(Q - \omega)\mathcal{R}(z) = \mathcal{R}_0(z)(Q - \omega)\mathcal{R}_0(z)(I + (Q - \omega)\mathcal{R}_0(z))^{-1}$$

Hence

$$\begin{aligned} \|\mathcal{R}_0(z) - \mathcal{R}(z)\|_{\text{tr}} &\leq \|\mathcal{R}_0(z)(Q - \omega)^{1/2}\|_{HS} \| |Q - \omega|^{1/2} \mathcal{R}_0(z) \|_{HS} \cdot \\ &\quad \cdot \|(I + (Q - \omega)\mathcal{R}_0(z))^{-1}\| \end{aligned}$$

(Here $(Q - \omega)^{1/2} = \text{sgn}(Q - \omega)|Q - \omega|^{1/2}$).

The Hilbert-Schmidt kernel of $\mathcal{R}_0(z)$ in the case $n = 1$ is explicitly given by the Green function

$$G(s, t; z) = \frac{\exp(i\sqrt{z - \omega}|s - t|)}{2i\sqrt{z - \omega}}, \quad (2.4)$$

and it is easy to check that:

$$\begin{aligned} \|\mathcal{R}_0(z)(Q - \omega)^{1/2}\|_{HS}^2 &= \|\mathcal{R}_0(z)|Q - \omega|^{1/2}\|_{HS}^2 \\ &= \int |G(s, t; z)|^2 |Q(t) - \omega| ds dt \leq \frac{C'}{(1 + |z|)^{3/2}}, \end{aligned}$$

for some constant $C' > 0$ independent of $z \in \Gamma$.

For $n = 2, 3$ using Lemma B.1 with $p = 2$, $k = 1$, $\rho = \delta/2$ we get

$$\|\mathcal{R}_0(z)(Q - \omega)^{1/2}\|_{HS}^2 \leq C''(1 + |z|)^{\frac{n}{2}-2}$$

for some constant $C'' > 0$ independent of $z \in \Gamma$.

Here and in the following we choose the determination of $\sqrt{z - \omega}$ with positive imaginary part.

If f is rapidly decreasing, the identity between $\text{tr}(f(H_Q) - f(H_\omega))$ and the integral on the RHS of (2.2) is an easy consequence of the Cauchy formula and of the spectral theorem. On the other hand, for a general function f satisfying (1.7) we have, for any $\varepsilon > 0$,

$$\text{tr}(f_\varepsilon(A) - f_\varepsilon(B)) = \frac{i}{2\pi} \int_\Gamma \text{tr}((A - z)^{-1} - (B - z)^{-1}) f_\varepsilon(z) dz, \quad (2.5)$$

with $f_\varepsilon(z) = e^{-\varepsilon z} f(z)$. Taking the limit for $\varepsilon \rightarrow 0$ and applying the dominate convergence theorem we obtain (2.2).

The proof of the part 2 of the proposition is analogous to 1. Actually, the Hilbert-Schmidt kernel of $\mathcal{R}_{0,T}^X$ is given in the case $n = 1$ by the Green function:

$$G_T^X(s, t; z) = -\frac{\cosh(i(\sqrt{(z - \omega)}(T - |s - t|)) + S^X \cosh(i(\sqrt{(z - \omega)}(s + t)))}{2i\sqrt{(z - \omega)} \sinh(Ti\sqrt{(z - \omega)})}, \quad (2.6)$$

where $S^X = -1$ for $X = D$ and $S^X = 1$ for $X = N$.

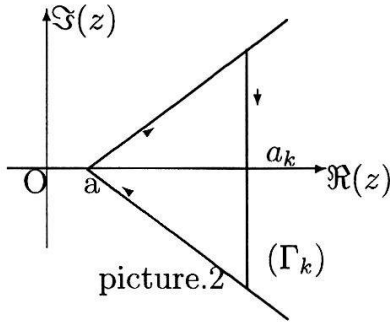
Hence, arguing as before

$$\begin{aligned}
 \|\mathcal{R}_{0,T}^X(z) - \mathcal{R}_T^X(z)\|_{\text{tr}} &\leq \|\mathcal{R}_{0,T}^X(z)|Q - \omega|^{1/2}\|_{HS}^2 \|(I + (Q - \omega)\mathcal{R}_0(z))^{-1}\| \\
 &\leq C_1 \|\mathcal{R}_{0,T}^X(z)|Q - \omega|^{1/2}\|_{HS}^2 \\
 &= \int |G_T^X(s, t; z)|^2 |Q(t) - \omega| dt ds \\
 &\leq \frac{C_2}{(1 + |z|)^{3/2}},
 \end{aligned}$$

for some constant $C_1, C_2 > 0$ independent of $z \in \Gamma$. This gives easily the first part of (2.3). For $n = 2, 3$, using estimate (B.3) in Appendix B, with $k = 1$, $p = 2$, we get easily

$$\|\mathcal{R}_{0,T}^X(z) - \mathcal{R}_T^X(z)\|_{\text{tr}} \leq C \langle z \rangle^{\frac{n}{2}-2}.$$

On the other hand, for fixed T , let Γ_k be the curve in picture 2 with $a_k \notin \text{Sp}(H_{Q,T}^X) \cup \text{Sp}(H_{\omega,T}^X)$ and $a_k \rightarrow +\infty$.



Using the residue theorem we obtain:

$$\begin{aligned}
 \text{tr}(f(H_{Q,T}) - f(H_{\omega,T})) &= \lim_{k \rightarrow +\infty} \frac{i}{2\pi} \int_{\Gamma_k} \text{tr}(\mathcal{R}_T(z) - \mathcal{R}_{0,T}(z)) f(z) dz \\
 &= \lim_{k \rightarrow +\infty} \sum_{\lambda_{j,T}^X < a_k} f(\lambda_{j,T}^X) - \sum_{\mu_{j,T}^X < a_k} f(\mu_{j,T}^X) = \sum_{j=1}^{\infty} (f(\lambda_{j,T}^X) - f(\mu_{j,T}^X)),
 \end{aligned}$$

and this ends the proof of Proposition 2.1. ■

The main result of this section will be the following:

Proposition 2.2 *Let us assume $1 \leq n \leq 3$ (see appendix for $n \geq 4$). Then for every analytic function f satisfying (1.7), we have*

$$\lim_{T \rightarrow +\infty} \text{tr}(f(H_{Q,T}) - f(H_{\omega,T})) = \text{tr}(f(H_Q) - f(H_{\omega})) \quad (2.7)$$

Proof :

We have to prove that:

$$\begin{aligned} \lim_{T \rightarrow +\infty} \frac{i}{2\pi} \int_{\Gamma} \text{tr}(\mathcal{R}_T(z) - \mathcal{R}_{0,T}(z)) f(z) dz \\ = \frac{i}{2\pi} \int_{\Gamma} \text{tr}(\mathcal{R}(z) - \mathcal{R}_0(z)) f(z) dz. \end{aligned} \quad (2.8)$$

Let us consider

$$\rho_T : L^2(\mathbb{R}) \rightarrow L^2(I_T), \quad \rho_T(u) = u|_{I_T}$$

and

$$\pi_T : L^2(I_T) \rightarrow L^2(\mathbb{R}), \quad (\pi_T u)(t) = \begin{cases} u(x) & \text{for } x \in I_T \\ 0 & \text{for } x \in (I_T)^c \end{cases}$$

Since $\rho_T \pi_T = \mathbb{1}_{L^2(I_T)}$ we have, for $z \in \Gamma$,

$$\text{tr}(\pi_T(\mathcal{R}_T^X(z) - \mathcal{R}_{0,T}^X(z))\rho_T) = \text{tr}(\mathcal{R}_T^X(z) - \mathcal{R}_{0,T}^X(z)).$$

Hence:

$$\begin{aligned} \frac{i}{2\pi} \int_{\Gamma} \text{tr}((\mathcal{R}_T^X(z) - \mathcal{R}_{0,T}^X(z)) - \text{tr}(\mathcal{R}(z) - \mathcal{R}_0(z))) f(z) dz \\ = \frac{i}{2\pi} \int_{\Gamma} \text{tr}(\pi_T(\mathcal{R}_T^X(z) - \mathcal{R}_{0,T}^X(z))\rho_T - (\mathcal{R}(z) - \mathcal{R}_0(z))) f(z) dz. \end{aligned}$$

Lemma 2.3 *Let us assume that $1 \leq n \leq 3$.*

Then, for $z \in \Gamma$, $\mathcal{R}_0(z)\langle x \rangle^{-\delta/2}$ and $\pi_T \mathcal{R}_{0,T}^X(z)\langle x \rangle^{-\delta/2} \rho_T$, with $X = D$ or $X = N$, are Hilbert-Schmidt operators and, in particular,

$$\|\mathcal{R}_0(z)\langle x \rangle^{-\delta/2}\|_{HS} + \|\pi_T \mathcal{R}_{0,T}^X(z)\rho_T \langle x \rangle^{-\delta/2}\|_{HS} \leq C(1 + |z|)^{\frac{n}{4}-1}. \quad (2.9)$$

Moreover there exists $\varepsilon \in]0, 1[$ and a constant $C > 0$, independent of z and T , such that, for T large enough and $z \in \Gamma$, we have

$$\|\pi_T \mathcal{R}_{0,T}^X(z)\langle x \rangle^{-\delta/2} \rho_T - \mathcal{R}_0(z)\langle x \rangle^{-\delta/2}\|_{HS} \leq CT^{-\varepsilon/2}(1 + |z|)^{\frac{n}{4}-1}. \quad (2.10)$$

Proof : See Appendix A for an elementary proof for $n = 1$ and Lemma B.2 for $n = 2, 3$. ■

Using Lemma 2.3 we can obtain :

Lemma 2.4 *For $1 \leq n \leq 3$, there exist $C > 0$, $T_0 > 0$, $\varepsilon > 0$ such that*

$$\|\pi_T(\mathcal{R}_T^X(z) - \mathcal{R}_{0,T}^X(z))\rho_T - (\mathcal{R}(z) - \mathcal{R}_0(z))\|_{\text{tr}} \leq CT^{-\varepsilon}(1 + |z|)^{\frac{n}{2}-2}, \quad (2.11)$$

for any $z \in \Gamma$ and $T \geq T_0$.

Proof :

Using the resolvent identity, we can estimate

$\|\pi_T(\mathcal{R}_T^X(z) - \mathcal{R}_{0,T}^X(z))\rho_T - (\mathcal{R}(z) - \mathcal{R}_0(z))\|_{\text{tr}}$ as:

$$\begin{aligned} & \|\pi_T(\mathcal{R}_T^X(z) - \mathcal{R}_{0,T}^X(z))\rho_T - (\mathcal{R}(z) - \mathcal{R}_0(z))\|_{\text{tr}} \\ &= \|\pi_T\mathcal{R}_T^X(z)(Q - \omega)\mathcal{R}_{0,T}^X(z)\rho_T - \mathcal{R}(z)(Q - \omega)\mathcal{R}_0(z)\|_{\text{tr}} \\ &\leq \|\pi_T\mathcal{R}_{0,T}^X(z)(Q - \omega)\mathcal{R}_{0,T}^X(z)\rho_T - \mathcal{R}_0(z)(Q - \omega)\mathcal{R}_0(z)\|_{\text{tr}} \\ &+ \|\pi_T\mathcal{R}_T^X(z)(Q - \omega)\mathcal{R}_{0,T}^X(z)(Q - \omega)\mathcal{R}_{0,T}^X(z)\rho_T \\ &- \mathcal{R}(z)(Q - \omega)\mathcal{R}_0(z)(Q - \omega)\mathcal{R}_0(z)\|_{\text{tr}} = I + II. \end{aligned}$$

We have:

$$\begin{aligned} I &= \|\pi_T\mathcal{R}_{0,T}^X(z)(Q - \omega)^{1/2}\rho_T \left(\pi_T|Q - \omega|^{1/2}\mathcal{R}_{0,T}^X(z)\rho_T - |Q - \omega|^{1/2}\mathcal{R}_0(z) \right)\|_{\text{tr}} \\ &+ \left\| \left(\pi_T\mathcal{R}_{0,T}^X(z)|Q - \omega|^{1/2}\rho_T - \mathcal{R}_0(z)|Q - \omega|^{1/2} \right) (Q - \omega)^{1/2}\mathcal{R}_0(z) \right\|_{\text{tr}} \\ &\leq \left(\|\pi_T\mathcal{R}_{0,T}^X(z)|Q - \omega|^{1/2}\rho_T\|_{HS} + \||Q - \omega|^{1/2}\mathcal{R}_0(z)\|_{HS} \right) \\ &\times \left\| \left(\pi_T\mathcal{R}_{0,T}^X(z)|Q - \omega|^{1/2}\rho_T - \mathcal{R}_0(z)|Q - \omega|^{1/2} \right) \right\|_{HS}, \end{aligned}$$

where $(Q - \omega)^{1/2} = (\text{sign}(Q - \omega))|Q - \omega|^{1/2}$. Since $|Q - \omega|^{1/2} \leq c\langle x \rangle^{-\delta/2}$, using (2.9) and (2.10), we obtain

$$I \leq \frac{C}{T^{\epsilon/2}}(1 + |z|)^{\frac{n}{2}-2}.$$

On the other hand,

$$\begin{aligned} II &\leq \|\pi_T\mathcal{R}_T^X(z)(Q - \omega)\mathcal{R}_{0,T}^X(z)\rho_T \left(\pi_T(Q - \omega)\mathcal{R}_{0,T}^X(z)\rho_T - (Q - \omega)\mathcal{R}_0(z) \right)\|_{\text{tr}} \\ &+ \left\| \left(\pi_T\mathcal{R}_T^X(z)(Q - \omega)\mathcal{R}_{0,T}^X(z)\rho_T - \mathcal{R}(z)(Q - \omega)\mathcal{R}_0(z) \right) (Q - \omega)\mathcal{R}_0(z) \right\|_{\text{tr}} \\ &= III + IV. \end{aligned}$$

We have:

$$\begin{aligned} III &\leq \|\pi_T\mathcal{R}_T^X(z)\rho_T\| \|\pi_T(Q - \omega)\mathcal{R}_{0,T}^X(z)\rho_T\|_{HS} \times \\ &\|\pi_T(Q - \omega)\mathcal{R}_{0,T}^X(z)\rho_T - (Q - \omega)\mathcal{R}_0(z)\|_{HS}. \end{aligned}$$

The spectral theorem gives, on Γ ,

$$\|\pi_T\mathcal{R}_T^X(z)\rho_T\| \leq C(|z| + 1)^{-1}$$

Using (2.9) and (2.10), we obtain

$$III \leq \frac{C}{T^{\epsilon/2}}(1 + |z|)^{\frac{n}{2}-2}.$$

On the other hand

$$\begin{aligned} IV &\leq \|\pi_T \mathcal{R}_T^X(z) \rho_T (\pi_T(Q - \omega) \mathcal{R}_T^X \rho_T - (Q - \omega) \mathcal{R}_0(z)) (Q - \omega) \mathcal{R}_0(z)\|_{\text{tr}} \\ &\quad + \|\left(\pi_T \mathcal{R}_T^X(z) \rho_T - \mathcal{R}(z)\right) (Q - \omega) \mathcal{R}_0(z) (Q - \omega) \mathcal{R}_0(z)\|_{\text{tr}} = V + VI. \end{aligned}$$

As before, we have

$$\begin{aligned} V &\leq \|\pi_T \mathcal{R}_T^X(z) \rho_T\| \|\pi_T(Q - \omega) \mathcal{R}_T^X \rho_T - (Q - \omega) \mathcal{R}_0(z)\|_{HS} \|(Q - \omega) \mathcal{R}_0(z)\|_{HS} \\ &\leq \frac{C}{T^{\varepsilon/2}} (1 + |z|)^{\frac{n}{2}-2} \end{aligned}$$

Let us consider two cutoff function $\chi, \tilde{\chi}$ such that

$$\begin{aligned} \text{supp}(\chi) &\subset [-1/4, 1/4], & \chi &= 1 \quad \text{on } [-1/8, 1/8] \\ \text{supp}(\tilde{\chi}) &\subset [-3/8, 3/8], & \tilde{\chi} &= 1 \quad \text{on } [-1/4, 1/4] \end{aligned}$$

and

$$\chi_T(x) = \chi(x/T), \quad \tilde{\chi}_T(x) = \tilde{\chi}(x/T)$$

We have $\chi \tilde{\chi} = \chi$. Let us write now

$$\begin{aligned} VI &\leq \|(\pi_T \mathcal{R}_T^X(z) \rho_T - \mathcal{R}(z)) (1 - \chi_T) (Q - \omega) \mathcal{R}_0(z) (Q - \omega) \mathcal{R}_0(z)\|_{\text{tr}} \\ &\quad + \|(1 - \tilde{\chi}_T) \pi_T \mathcal{R}_T^X(z) \rho_T \chi_T (Q - \omega) \mathcal{R}_0(z) (Q - \omega) \mathcal{R}_0(z)\|_{\text{tr}} \\ &\quad + \|(\tilde{\chi}_T \pi_T \mathcal{R}_T^X(z) \rho_T - \mathcal{R}(z)) \chi_T (Q - \omega) \mathcal{R}_0(z) (Q - \omega) \mathcal{R}_0(z)\|_{\text{tr}} \\ &= VII + VIII + IX. \end{aligned}$$

Using (2.4) and Lemma 2.3, it is easy to prove that

$$\begin{aligned} VII + VIII &\leq (\|(\pi_T \mathcal{R}_T^X(z) \rho_T - \mathcal{R}(z))\| \times \\ &\quad \times \|(1 - \chi_T) (Q - \omega) \mathcal{R}_0(z)\|_{HS} \|(Q - \omega) \mathcal{R}_0(z)\|_{HS} \\ &\quad + \|\pi_T \mathcal{R}_T^X(z) \rho_T\| \|\chi_T (Q - \omega) \mathcal{R}_0(z)\|_{HS} \|(Q - \omega) \mathcal{R}_0(z) (1 - \tilde{\chi}_T)\|_{HS} \\ &\leq \frac{C}{T^{\varepsilon/2}} (1 + |z|)^{\frac{n}{2}-2}. \end{aligned}$$

On the other hand

$$\begin{aligned} IX &\leq \|(\tilde{\chi}_T \pi_T \mathcal{R}_T^X(z) \rho_T - \mathcal{R}(z)) \chi_T\| \|(Q - \omega) \mathcal{R}_0(z)\|_{HS} \|(Q - \omega) \mathcal{R}_0(z)\|_{HS} \\ &\leq C(1 + |z|)^{\frac{n}{2}-2} \|(\tilde{\chi}_T \pi_T \mathcal{R}_T^X(z) \rho_T - \mathcal{R}(z)) \chi_T\|. \end{aligned}$$

Observe now that

$$\begin{aligned} (\tilde{\chi}_T \pi_T \mathcal{R}_T^X(z) \rho_T - \mathcal{R}(z)) \chi_T &= \tilde{\chi}_T \pi_T \mathcal{R}_T(z) \rho_T \chi_T - \mathcal{R}(z) \chi_T \\ &= \mathcal{R}(z) (H_Q - z) \tilde{\chi}_T \pi_T \mathcal{R}_T(z) \rho_T \chi_T - \mathcal{R}(z) \chi_T \\ &= \mathcal{R}(z) [\Delta, \tilde{\chi}_T] \pi_T \mathcal{R}_T(z) \rho_T \chi_T \\ &= \mathcal{R}(z) \left(-\frac{(\Delta \tilde{\chi})(x/T)}{T^2} - \frac{2(\nabla \tilde{\chi})(x/T)}{T} \nabla \right) \pi_T \mathcal{R}_T(z) \rho_T \chi_T. \end{aligned}$$

Hence

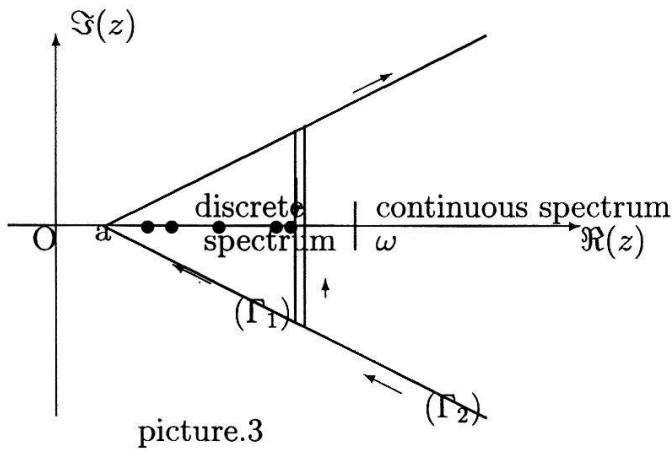
$$\|(\tilde{\chi}_T \pi_T \mathcal{R}_T^X(z) \rho_T - \mathcal{R}(z)) \chi_T\| \leq \frac{C}{T}$$

for some constant C . This ends the proof of Lemma 2.4. ■

End of the proof of Proposition 2.2:

Proposition 2.2 follows easily from Lemma 2.3, and Lemma 2.4. ■

Now we want to separate, in the above trace formula, the discrete spectrum and the continuous spectrum. For that purpose let us consider the curve Γ_1 and Γ_2 in picture 3.



We have:

Corollary 2.5 For $1 \leq n \leq 3$, we have :

$$\begin{aligned} & \lim_{T \rightarrow +\infty} \frac{i}{2\pi} \int_{\Gamma} \text{tr}(\mathcal{R}_T(z) - \mathcal{R}_{0,T}(z)) f(z) dz \\ &= \sum_{j=1}^p f(\lambda_j) + \frac{i}{2\pi} \int_{\Gamma_2} \text{tr}(\mathcal{R}(z) - \mathcal{R}_0(z)) f(z) dz. \end{aligned} \quad (2.12)$$

Proof :

We can write

$$\frac{i}{2\pi} \int_{\Gamma} \text{tr}(\mathcal{R}(z) - \mathcal{R}_0(z)) f(z) dz = \left(\int_{\Gamma_1} + \int_{\Gamma_2} \right) \text{tr}(\mathcal{R}(z) - \mathcal{R}_0(z)) f(z) dz.$$

An application of the residue theorem gives

$$\frac{i}{2\pi} \int_{\Gamma_1} \text{tr}(\mathcal{R}(z) - \mathcal{R}_0(z)) f(z) dz = \sum_{j=1}^p f(\lambda_j). \quad (2.13)$$

Proposition 2.2 and (2.13) gives (2.12). ■

Remark 2.6 Using the arguments of [6] (see also [23]) it is possible to prove that, in the case $n = 1$,

$$\lambda_{j,T}^X = \lambda_j + \tilde{\mathcal{O}}(e^{-T\sqrt{\omega-\lambda_j}})$$

as $T \rightarrow +\infty$, for $j = 1, \dots, p$.

Here $f = \tilde{\mathcal{O}}(e^{-at})$ means that, for any $\delta > 0$, $f = \mathcal{O}_\delta(e^{-(a-\delta)t})$ as $t \rightarrow +\infty$

In particular:

$$\lim_{T \rightarrow +\infty} \lambda_{j,T}^X = \lambda_j$$

for $j = 1, \dots, p$. ■

3 The Birman-Krein formula

Using the Birman-Krein formula [1], it is possible to write $\text{tr}(f(H_Q) - f(H_\omega))$ in terms of the discrete eigenvalue of H_Q and of the spectral shift function $s(\lambda)$ of the scattering matrix $S(\lambda)$ associate to the pair (H_Q, H_ω) (i.e. $\det S(\lambda) = e^{-2\pi i s(\lambda)}$, for $\lambda > \omega$).

Theorem 3.1 For f satisfying (1.7), we have:

$$\lim_{T \rightarrow +\infty} \text{tr}(f(H_{Q,T}^X) - f(H_{\omega,T}^X)) = \sum_{j=1}^p f(\lambda_j) + \int_{\omega}^{+\infty} s(\lambda) f'(\lambda) d\lambda \quad (3.1)$$

where $s(\lambda)$ is the spectral shift function of the scattering matrix associate to the pair (H_Q, H_ω) .

Proof :

As above we assume here $1 \leq n \leq 3$ (For $n \geq 4$ the proof is done in Appendix B). Using Corollary 2.5 we get

$$\lim_{T \rightarrow +\infty} \text{tr}(f(H_{Q,T}^X) - f(H_{\omega,T}^X)) = \sum_{j=1}^p f(\lambda_j) + \frac{i}{2\pi} \int_{\Gamma_2} \text{tr}(\mathcal{R}(z) - \mathcal{R}_0(z)) f(z) dz \quad (3.2)$$

The Birman-Krein formula (see [1]) gives, for $z \in \Gamma$

$$\text{tr}(\mathcal{R}(z) - \mathcal{R}_0(z)) = - \int_a^\infty \frac{s(\lambda)}{(\lambda - z)^2} d\lambda. \quad (3.3)$$

Let us recall that, for $\lambda < \omega$, $s(\lambda)$ is defined as the number of eigenvalues of H_Q smaller than λ . So we have

$$\text{tr}(\mathcal{R}(z) - \mathcal{R}_0(z)) = \sum_{1 \leq j \leq p} \frac{1}{\lambda_j - z} - \int_{\omega}^{\infty} \frac{s(\lambda)}{(\lambda - z)^2} d\lambda \quad (3.4)$$

Hence

$$\frac{i}{2\pi} \int_{\Gamma_2} \text{tr}(\mathcal{R}(z) - \mathcal{R}_0(z)) f(z) dz = -\frac{i}{2\pi} \int_{\Gamma_2} \int_{\omega}^{\infty} \frac{s(\lambda)}{(\lambda - z)^2} d\lambda f(z) dz. \quad (3.5)$$

Since $s(\lambda) = O(\lambda^{n/2-1})$ as $\lambda \rightarrow +\infty$ (see, for example, [4], [5], [9], [10], [19]) and $s(\lambda) = 0$ for $\lambda < a$, we can change the order of integration in (3.5) to get finally

$$\begin{aligned} \frac{i}{2\pi} \int_{\Gamma_2} \text{tr}(\mathcal{R}(z) - \mathcal{R}_0(z)) f(z) dz &= -\frac{i}{2\pi} \int_{\omega}^{\infty} \int_{\Gamma_2} \frac{f(z)}{(\lambda - z)^2} dz s(\lambda) d\lambda \\ &= \int_{\omega}^{\infty} s(\lambda) f'(\lambda) d\lambda, \end{aligned}$$

and this ends the proof of Theorem 3.1. ■

Remarks:

- i) Trace formulas for $\text{tr}(f(H_Q) - f(H_w))$ with the spectral shift function $s(\lambda)$ and suitable functions f are well known (see [2, 22, 24]). Here we want to put emphasis on the limit for large intervals and the transition between the discrete spectrum in the box $] - T, T[$ and the continuous spectrum in the whole space $\mathbb{R}$. We do not know other reference for a rigorous proof concerning this limit.
- ii) The contour integration approach used in Sections 2 and 3 is well known (see for example [8], ch.IV). We could use the more general results on the spectral shift function ([24]). Here we have chosen a more direct and more explicit approach.
- iii) For the interpretation of the spectral shift function as the average of the quantum process, see [14].

Now we come back to our main application, the computation of the splitting in the double well problem.

Corollary 3.2 *Let G_0 the number defined in the introduction by (1.10) and (1.11). Then we have*

$$G_0 = 2 \left(\frac{S_0}{2\pi} \right)^{\frac{1}{2}} \left(\prod_{j=2}^p \lambda_j \right)^{-\frac{1}{2}} \exp \left(-\frac{1}{2} \int_{\omega}^{+\infty} \frac{s(\lambda)}{\lambda} d\lambda \right).$$

Proof :

For $b > 0$, let us consider the pair of Hamiltonians $(H_{\omega+b}, H_{Q+b})$ with $Q(t) = V''(y(t))$. Let us recall that $\lambda_1 = 0$ is a simple eigenvalue; so we can clearly apply the above results with $0 < a < b$ and $f(z) = \log(z)$ and we get

$$\lim_{T \nearrow +\infty} \sum_{j \geq 1} \log \left(\frac{\mu_j^T(Q+b)}{\mu_j^T(\omega+b)} \right) = \sum_{1 \leq j \leq p} \log(\lambda_j + b) + \int_{\omega+b}^{\infty} \frac{s_b(\lambda)}{\lambda} d\lambda$$

where s_b is the scattering phase for $(H_{\omega+b}, H_{Q+b})$. Then using

$\lim_{T \nearrow +\infty} \mu_1^T(Q) = \lambda_1$, we get

$$\lim_{T \nearrow +\infty} \sum_{j \geq 2} \log \left(\frac{\mu_j^T(Q+b)}{\mu_j^T(\omega+b)} \right) = \sum_{2 \leq j \leq p} \log(\lambda_j + b) + \int_{\omega+b}^{\infty} \frac{s_b(\lambda)}{\lambda} d\lambda \quad (3.6)$$

Now in (3.6) we can go to the limit $b \searrow 0$ and taking the exponential we get the corollary using the formula (1.11) for G_0 ■

A APPENDIX: Proof of Lemma 2.3 for $n=1$

Since (2.9) and (2.10) are proved along the same lines, let us prove only (2.10). Notice that, we can rewrite $G_{0,T}^X(t, s; z)$, $(t, s) \in (I_T)^2$ as

$$\begin{aligned} G_T^X(t, s; z) &= -\frac{\exp(-\mu|t-s|)}{2\mu} \\ &+ \frac{\exp(-\mu T')}{2\mu} \left(\frac{\cosh(\mu t) \cosh(\mu s)}{\cosh(\mu T')} + \frac{\sinh(\mu t) \sinh(\mu s)}{\sinh(\mu T')} \right) \end{aligned}$$

if $X = D$, and

$$\begin{aligned} G_T^X(t, s; z) &= -\frac{\exp(-\mu|t-s|)}{2\mu} \\ &- \frac{\exp(-\mu T')}{2\mu} \left(\frac{\cosh(\mu t) \cosh(\mu s)}{\sinh(\mu T')} + \frac{\sinh(\mu t) \sinh(\mu s)}{\cosh(\mu T')} \right) \end{aligned}$$

if $X = N$, with $T' = T/2$ and $\mu = -i\sqrt{z-\omega}$. Hence, we need to estimate the following two integrals :

$$I_1 = \int \int_{\mathbb{R}^2 \setminus I_T^2} \frac{\exp(-2\mu|s-t|)}{4\mu^2} \langle t \rangle^{-(1+\varepsilon)} ds dt \quad (\text{A.1})$$

$$I_2 = \int \int_{I_T^2} \left| G_T^X(t, s; z) + \frac{\exp(-\mu|s-t|)}{2\mu} \right|^2 \langle t \rangle^{-(1+\varepsilon)} dt ds \quad (\text{A.2})$$

It is sufficient to consider $|z|$ large enough and $z \in \Gamma$. Let us recall that $\sqrt{z-\omega}$ is the determination such that $0 < \arg(z-\omega) < 2\pi$. So we see easily that it exists $c \in]0, 1]$ such that

$$c|\mu| \leq \operatorname{Re} \mu, \quad \text{for } z \in \Gamma, |z| \text{ large enough}$$

Let us denote $\operatorname{Re} \mu = r$ and $|\mu| = d$. We have :

$$I_1 \leq I'_1 + I''_1$$

where

$$\begin{aligned} I'_1 &= \frac{1}{4d^2} \int_{|t| \geq T'} \int_{\mathbb{R}} \exp(-2cd|s-t|) \langle t \rangle^{-(1+\varepsilon)} ds dt \\ I''_1 &= \frac{1}{4d^2} \int_{|s| \geq T'} \int_{\mathbb{R}} \exp(-2cd|s-t|) \langle t \rangle^{-(1+\varepsilon)} dt ds. \end{aligned}$$

Then

$$I'_1 = \frac{1}{4d^2} \left(\int_{\mathbb{R}} \exp(-2cd|r|) dr \right) \left(\int_{|t| \geq T'} \langle t \rangle^{-(1+\varepsilon)} dt \right) \leq \frac{C}{T^\varepsilon d^3}.$$

Using Peetre inequality $\langle t \rangle^{-(1+\varepsilon)} \leq 2^{(1+\varepsilon)/2} \langle s \rangle^{-(1+\varepsilon)} \langle s - t \rangle^{(1+\varepsilon)}$ for I_1'' , we obtain

$$I_1'' \leq \frac{2^{(1+\varepsilon)/2}}{4d^2} \int_{|s| \geq T'} \int_{\mathbb{R}} \exp(-2cd|s - t|) \langle s - t \rangle^{(1+\varepsilon)} \langle s \rangle^{-(1+\varepsilon)} dt ds$$

and I_1'' can be estimated in the same way as I_1' .

For I_2 we have clearly:

$$\begin{aligned} I_2 &\leq 8 \frac{\exp(-4rT')}{d^2} \int_{[0, T']^2} \exp(2r(t + s)) \langle t \rangle^{-(1+\varepsilon)} dt ds \\ &\leq 4 \frac{\exp(-2rT')}{c d^3} \int_0^{T'} \exp(2rt) \langle t \rangle^{-(1+\varepsilon)} dt \end{aligned}$$

for T sufficiently large.

Splitting the integral $\int_0^{T'} = \int_0^{T'/2} + \int_{T'/2}^{T'}$, we get easily

$$I_2 \leq I_2' + I_2''$$

with

$$I_2' \leq 4 \frac{T'}{c d^3} \exp(-rT'), \quad I_2'' \leq \frac{C}{T^\varepsilon d^3}.$$

This proves (2.10) in the case $n = 1$. ■

B APPENDIX: The n -dimensional case

Let us remark that for $n \geq 4$, $\mathcal{R}_0(z) \langle x \rangle^{-\rho}$ is not in the Hilbert-Schmidt class but in the more general Schatten class $\mathcal{S}_p$ on the Hilbert space $L^2(\mathbb{R}^n)$, $1 \leq p \leq +\infty$. (See [8] for the definitions and properties of these classes of operators). For $p = 2$, it coincides with the Hilbert-Schmidt class. The usual operator norm for $T \in \mathcal{S}_p$ is denoted by $\|T\|_p$. We need in particular the following lemmas

Lemma B.1 *Let us consider a pseudodifferential operator in the Weyl quantization, $a^w(x, D)$, defined for $u \in \mathcal{S}(\mathbb{R}^n)$ by*

$$a(x, D)u(x) = (2\pi)^{-n} \int_{\mathbb{R}^{2n}} e^{i(x-y) \cdot \xi} a((x+y)/2, \xi) u(y) dy d\xi$$

For every p , $1 \leq p < +\infty$ it exists a real $\gamma(n, p)$ and an integer $N(n, p)$ such that if $\partial^\gamma a \in L^p(\mathbb{R}^{2n})$ for $|\gamma| \leq N(n, p)$ then $a^w(x, D)$ is in $\mathcal{S}_p$ and the following estimate holds

$$\|a^w(x, D)\|_p^p \leq \gamma(n, p) \sum_{|\gamma| \leq N(n, p)} \int_{\mathbb{R}^{2n}} |\partial^\gamma a(z)|^p dz$$

sketch of proof :

For $p = +\infty$ the result is the Calderon-Vaillancourt theorem. For $p = 1$ the estimate is proved in several places, for example in [20]. The general case comes easily by complex interpolation [8]. ■

Lemma B.2 *Let $k \in \mathbb{N}$, $k \geq 1$, $n \in \mathbb{N}$, $n \geq 1$ and real numbers p, ρ such that $p > \frac{n}{2k}$, $\rho p > n$. Then there exists $C > 0$ such that, for $z \in \Gamma$, we have*

$$\|\mathcal{R}_0^k(z)\langle x \rangle^{-\rho}\|_p \leq C\langle z \rangle^{\frac{n}{2p}-k}. \quad (\text{B.1})$$

Proof :

We get easily (B.1) by computing the Weyl symbol of $\mathcal{R}_0^k(z)\langle x \rangle^{-\rho}$ ■

Concerning the resolvent estimates in boxes, using the spectral decomposition, we have

$$\|(\mathcal{R}_{0,T}^X)^k(z)\|_p \leq \left(\sum_{\alpha \in \mathbb{N}^n} \frac{|\alpha|^2}{T^2} \pi^2 + \omega - z \right)^{-kp} \frac{1}{p}. \quad (\text{B.2})$$

Hence, for $kp > \frac{n}{2}$, there exists C such that for $z \in \Gamma$, we have

$$\|(\mathcal{R}_{0,T}^X(z))^k\|_p \leq C(1 + |z|)^{\frac{n}{2p}-k}. \quad (\text{B.3})$$

For $n > 3$, $\mathcal{R}_{0,T}(z) - \mathcal{R}_0(z)$ is not in the trace class but we shall see that $(\mathcal{R}_{0,T}(z))^N - (\mathcal{R}_0(z))^N$ is in the trace class, for N large enough.

Lemma B.3 *Let us assume that $n \geq 1$ and $\rho > \frac{n}{p}$. Then for $z \in \Gamma$, $\mathcal{R}_0^k(z)\langle x \rangle^{-\rho}$ and $\pi_T(\mathcal{R}_{0,T}^X)^k(z)\langle x \rangle^{-\rho}\rho_T$, with $X = D$ or $X = N$, are in the Schatten class $\mathcal{S}_p$, for $kp > \frac{n}{2}$. In particular, there exists C such that for $z \in \Gamma$ we have*

$$\|(\mathcal{R}_0(z))^k\langle x \rangle^{-\rho}\|_p + \|\pi_T(\mathcal{R}_{0,T}^X(z))^k\rho_T\langle x \rangle^{-\rho}\|_p \leq C(1 + |z|)^{\frac{n}{2p}-k}. \quad (\text{B.4})$$

Moreover there exists $\varepsilon \in]0, 1[$ and a constant $C > 0$ independent of z and T such that for T large enough and $z \in \Gamma$ we have

$$\|\pi_T(\mathcal{R}_{0,T}^X(z))^k\langle x \rangle^{-\rho}\rho_T - (\mathcal{R}_0(z))^k\langle x \rangle^{-\rho}\|_p \leq CT^{-\varepsilon}(1 + |z|)^{\frac{n}{2p}-k}. \quad (\text{B.5})$$

Proof : The first inequality comes from (B.1) and (B.3).

Let us introduce the cut-off functions $\chi \in C_0^\infty(I_1^n)$ such that $\chi(x) = 1$ for $x \in I_{1/2}^n$ and $\chi_T(x) = \chi(\frac{x}{T})$.

Using (B.4) we have, with $\delta > n$, $0 < \varepsilon < \rho - \frac{n}{p}$,

$$\|\pi_T(\mathcal{R}_{0,T}^X)^k(z)(1 - \chi_T(x))\langle x \rangle^{-\delta/2}\rho_T - (\mathcal{R}_0)^k(z)(1 - \chi_T(x))\langle x \rangle^{-\delta/2}\|_p \leq C T^{-\varepsilon}(1 + |z|)^{\frac{n}{2p}-k}. \quad (\text{B.6})$$

By a standard computation on resolvents, we have

$$\pi_T \mathcal{R}_{0,T}^X(z) \chi_T \rho_T - \mathcal{R}_0(z) \chi_T = (\mathcal{R}_0(z) - \pi_T \mathcal{R}_{0,T}^X(z) \rho_T) [\chi_T, \Delta] \mathcal{R}_0(z). \quad (\text{B.7})$$

But we have $[\chi_T, \Delta] = -\frac{1}{T^2} \Delta \chi(\frac{x}{T}) - \frac{2}{T} \nabla \chi(\frac{x}{T}) \nabla$. So the estimate follows for $k = 1$. For $k > 1$ we use the same argument. Taking $(k-1)$ derivatives in z , we get

$$\begin{aligned} & \pi_T (\mathcal{R}_{0,T}^X(z))^k \chi_T \rho_T - (\mathcal{R}_0(z))^k \chi_T = \\ & \sum_{j+\ell=k} c_{j,\ell} ((\mathcal{R}_0(z))^j - \pi_T (\mathcal{R}_{0,T}^X)^j(z) \rho_T) [\chi_T, \Delta] (\mathcal{R}_0(z))^\ell \end{aligned} \quad (\text{B.8})$$

where the $c_{j,\ell}$ are numerical constants. The estimate follows. ■

Proof of Theorem 3.1 for $n \geq 4$:

We have to modify the statement of the Proposition (2.1). Let us start with the functional calculus formula, for f satisfying (1.7),

$$f(H_Q) - f(H_\omega) = \frac{i}{2\pi} \int_{\Gamma} (\mathcal{R}(z) - \mathcal{R}_0(z)) f(z) dz$$

and integrate $N-1$ times in z , with $N > \frac{n}{2} - 1$,

$$f(H_Q) - f(H_\omega) = (-1)^{N-1} (N-1)! \frac{i}{2\pi} \int_{\Gamma} (\mathcal{R}(z)^N - \mathcal{R}_0(z)^N) f^{(1-N)}(z) dz \quad (\text{B.9})$$

where $f^{(-k)}(z)$ is such that $\frac{d^k}{dz^k} f^{(-k)}(z) = f(z)$ and $f^{(-k)}(z) = O(\langle z \rangle^{k+1-\frac{n}{2}-\eta})$

Proposition B.4 *Let us assume that $n \geq 4$ and f be an analytic function satisfying (1.7). Then we have:*

1. $f(H_Q) - f(H_\omega)$ is a trace class operator in $L^2(\mathbb{R}^n)$ and for $N > \frac{n}{2} - 1$ we have

$$\begin{aligned} & \text{tr}(f(H_Q) - f(H_\omega)) = \\ & (-1)^{N-1} (N-1)! \frac{i}{2\pi} \int_{\Gamma} \text{tr}(\mathcal{R}(z)^N - \mathcal{R}_0(z)^N) f^{(1-N)}(z) dz \end{aligned}$$

2. For any positive $T > 0$, $f(H_{Q,T}^X) - f(H_{\omega,T}^X)$ is a trace class operator in $L^2(I_T^n)$ and

$$\begin{aligned} & \text{tr}(f(H_{Q,T}^X) - f(H_{\omega,T}^X)) \\ & = (-1)^{N-1} (N-1)! \frac{i}{2\pi} \int_{\Gamma} \text{tr}(\mathcal{R}_T^X(z)^N - \mathcal{R}_{0,T}^X(z)^N) f^{(1-N)}(z) dz \\ & = \sum_{j=1}^{\infty} (f(\lambda_{j,T}^X) - f(\mu_{j,T}^X)). \end{aligned} \quad (\text{B.10})$$

Proof :

1) Let us begin by proving that the integral on the RHS of (B.10) converges by proving that

$$\|\mathcal{R}(z)^N - \mathcal{R}_0^N(z)\|_{\text{tr}} \leq C(1 + |z|)^{-N-1+\frac{n}{2}}.$$

We can write, for $z \in \Gamma$, $|z|$ large enough,

$$\mathcal{R}_0(z) - \mathcal{R}(z) = \mathcal{R}_0(z)(Q - \omega)\mathcal{R}(z).$$

Taking $N - 1$ derivatives in z , we get

$$\mathcal{R}_0^N(z) - \mathcal{R}^N(z) = \sum_{k+j=N+1} c_{j,k} \mathcal{R}_0^j(z)(Q - \omega)\mathcal{R}^k(z).$$

But we have $(Q - \omega) = \langle x \rangle^{-\delta/p} a(x) \langle x \rangle^{-\delta/q}$, where $a(x)$ is uniformly bounded. The Hölder inequality in $\mathcal{S}_p$ gives

$$\|\mathcal{R}_0^j(z)(Q - \omega)\mathcal{R}^k(z)\|_1 \leq \|\mathcal{R}_0^j(z)\langle x \rangle^{-\delta/p}\|_p \cdot \|\mathcal{R}(z)^k \langle x \rangle^{-\delta/q}\|_q$$

Let us write down $\mathcal{R}(z)^k = \mathcal{R}_0(z)^k (H_\omega - z)^k \mathcal{R}(z)^k$ hence, using uniform ellipticity of $H_Q - z$, we can see that it exists $C_k > 0$ such that

$$\|(H_\omega - z)^k \mathcal{R}(z)^k\| \leq C_k, \quad \forall z \in \Gamma$$

Choosing $p > 1, q > 1$ such that $\frac{1}{p} + \frac{1}{q} = 1$, $jp > \frac{n}{2}$, $kq > \frac{n}{2}$, using (B.4) and $j + k = N + 1$, we get easily

$$\|\mathcal{R}(z)^N - \mathcal{R}_0^N(z)\|_{\text{tr}} \leq C(1 + |z|)^{-N-1+\frac{n}{2}}$$

This finishes the proof of the first part of the proposition. The proof of the second part is analogous to the case $n = 1$ so we omit the details. $\blacksquare$

Let us state now the extension of Lemma 2.4 for $n \geq 3$

Lemma B.5 *There exist $C > 0$, $\varepsilon > 0$, $T_0 > 0$ such that for $z \in \Gamma$, $T \geq T_0$ and $N > \frac{n}{2} - 1$ we have*

$$\|\pi_T(\mathcal{R}_T^X(z))^N - (\mathcal{R}_{0,T}^X(z))^N \rho_T - ((\mathcal{R}(z))^N - (\mathcal{R}_0(z))^N)\|_{\text{tr}} \leq \frac{C}{T^\varepsilon} (1 + |z|)^{\frac{n}{2}-N-1} \quad (\text{B.11})$$

Proof :

The proof is similar to the proof of Lemma 2.4 using the resolvent identity, taking derivatives in z and using the above estimates in $\mathcal{S}_p$ -norms. $\blacksquare$

Now we can finish the proof of Theorem 3.1. By applying Proposition B.4, Lemma B.5 and Lemma B.3 we get a proof of Proposition 2.2 for $n \geq 4$ and hence a proof of Theorem 3.1 for $n \geq 4$. $\blacksquare$

References

- [1] M.S. Birman, M.G. Krein, *On the theory of wave operators and scattering operators*, Dokl.Akad.Nauk.SSSR 144 (1962), pp. 475-478.
- [2] M.S. Birman, D. Yafaev, *The Spectral Shift Function. The work of M. G. Krein and its further development*, St. Petersburg Math. J., Vol.4, pp.833-870 No.5 (1993).
- [3] S. Coleman, *The use of instantons*, Proc. Internat. School of Physics, Erice (1977).
- [4] Y. Colin de Verdière, *La matrice de scattering pour l'opérateur de Schrödinger sur la droite réelle*, Séminaire Bourbaki (1979/80), pp.246-257.
- [5] Y. Colin de Verdière, *Une formule de traces pour l'opérateur de Schrödinger dans $\mathbb{R}^3$* , Ann. Scient. E.N.S. 14 (1981) pp.27-39.
- [6] M. Dauge, B. Helffer, *Eigenvalues variation I. Neumann problem for Sturm-Liouville operators*, J. of Diff. Equations 104 (2) (1993), pp.243-262.
- [7] S.Yu.Dobrokhotov, V.N. Kolokol'tsov, V.P. Maslov, *Splitting of the lowest energy levels of the Schrödinger equation and asymptotic behavior of the fundamental solution of the equation $hu_t = h^2\Delta u/2 - V(x)u$* , (translated from Teor.Math.Phys. 87(3) (1991)).
- [8] I.C. Gohberg, M.G. Krein, *Opérateurs linéaires non autoadjoints dans un espace hilbertien*, Dunod, Paris (1971).
- [9] L. Guillopé, *Asymptotique de la phase de diffusion pour l'opérateur de Schrödinger dans $\mathbb{R}^n$* , Séminaire Bony-Sjöstrand-Meyer (exposé n.V) (1984/85).
- [10] L. Guillopé, *Asymptotique de la phase de diffusion pour l'opérateur de Schrödinger avec potentiel*, C.R.Acad.Sc.Paris (293) (1981), pp.601-603.
- [11] B. Helffer, *Semiclassical analysis for the Schrödinger operator and applications*, Lecture Notes in Math. 1336, Springer Verlag (1988).
- [12] B. Helffer, J. Sjöstrand, *Multiple wells in semiclassical limit I*, Comm. in PDE, 9(4) (1984), pp.337-408.
- [13] M. Kac, *Integration in function spaces and some of its applications*, Lezioni Fermiane, Acc.Naz.Lincei (1980).
- [14] Ph. Martin, *Time-delay of quantum scattering process*, Acta Phys. Austriaca, Suppl. XXIII (1981), pp. 157-208.
- [15] G. Parisi, *Statistical fields theory*, Frontiers in Physics, Addison Wesley Inc. (1988).
- [16] R. Rajaraman, *Solitons and instantons*, North-Holland, Amsterdam (1984).

- [17] S. Levit, U. Smilansky, *A theorem on infinite products of eigenvalues of Sturm-Liouville type operators*, Proc. of the AMS, 65(2) (1977), pp.299-302.
- [18] M. Reed, B. Simon, *Methods of modern mathematical physics*, Academic Press (1979).
- [19] D. Robert, *Asymptotique à grande energie de la phase de diffusion pour un potentiel*, Asymptotic Analysis (3), IV, (1991), pp.301-320.
- [20] D. Robert, *Autour de l'approximation semi-Classique*, Birkhäuser, Progress in Mathematics, Vol. 68 (1987)
- [21] B. Simon, *Trace Ideals and their Applications*, Cambridge (1979).
- [22] A.V. Sobolev, *Efficient bounds for the spectral shift function*, Ann. Inst. H. Poincaré, 58A, pp. 55-83 (1993).
- [23] V. Sordoni, *Instantons and splitting* (preprint, University of Bologna) (1995)?
- [24] D. Yafaev, *Mathematical Scattering Theory*, AMS, (1992).