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

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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

$$H_Q = -\Delta_x + Q(x) \tag{1.2}$$

$$H_\omega = -\Delta_x + \omega. \tag{1.3}$$

and we denote by

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

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

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

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

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

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

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

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

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

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:

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

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

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

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

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

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 :

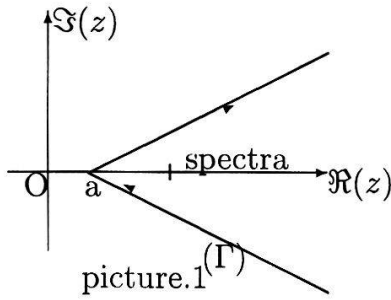
$$G_0 = 2\left(\frac{S_0}{2\pi}\right)^{\frac{1}{2}} \left(\prod_{j=2}^p \lambda_j \right)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} \int_\omega^{+\infty} \frac{s(\lambda)}{\lambda} d\lambda\right). \quad (1.12)$$

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 $X = N$.

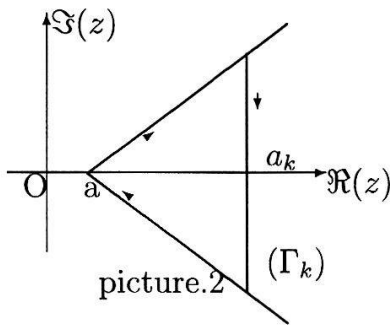
Hence, arguing as before

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

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*

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

Proof :

We have to prove that:

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

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 $z \in \Gamma$,

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

Hence:

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

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*

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

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:

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

We have:

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

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

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

On the other hand,

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

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

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

On the other hand

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

As before, we have

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

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

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

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

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

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

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

On the other hand

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

Observe now that

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

Hence

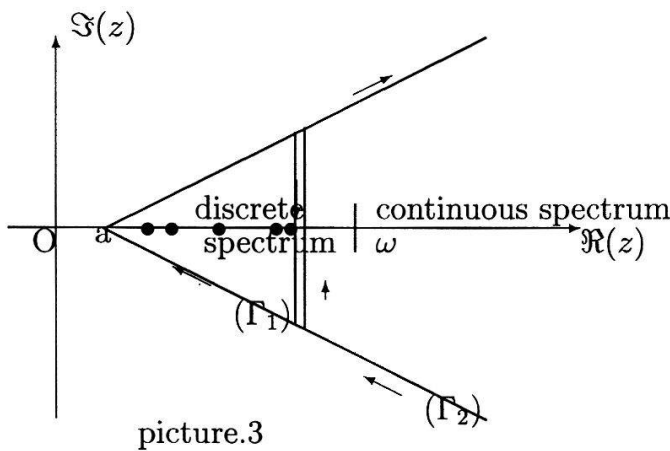
$$\|(\tilde{\chi}_T \pi_T \mathcal{R}_T^X(z) \rho_T - \mathcal{R}(z)) \chi_T\| \leq \frac{C}{T}$$

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.



picture.3

We have:

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

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

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

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

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:*

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

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

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

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

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

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

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

Hence

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

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

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

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

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

if $X = D$, and

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

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

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

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

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*

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

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

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

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*

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

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

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

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

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

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

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