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

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

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

$$H^D_{Q,T} \quad \text{and} \quad H^D_{\omega,T} \tag{1.4}$$

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

$$H^N_{Q,T} \quad \text{and} \quad H^N_{\omega,T} \tag{1.5}$$

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

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

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

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

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

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

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

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

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

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

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

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:

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

This formula was suggested to one of the authors (V.S.) by Y. Colin de Verdière. Formulas involving the limit, as $T \to +\infty$, of the quotient $\dfrac{\det(H_Q^X)}{\det(H_\omega^X)}$ 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:

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

where

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

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 $\lim_{t\to\pm\infty} y(t) = \pm a$, 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 :

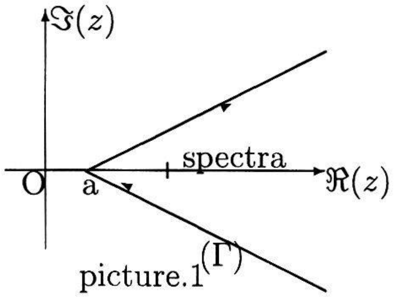
$$G_0 = 2(\frac{S_0}{2\pi})^{\frac{1}{2}}\left(\prod_{j=2}^{p}\lambda_j\right)^{-\frac{1}{2}}\exp\left(-\frac{1}{2}\int_\omega^{+\infty}\frac{s(\lambda)}{\lambda}d\lambda\right). \tag{1.12}$$

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



picture.1

Since $\mathrm{Sp}(H_{Q,T}^X) \cup \mathrm{Sp}(H_Q) \cup \mathrm{Sp}(H_{\omega,T}^X) \cup \mathrm{Sp}(H_\omega) \subset (a, +\infty)$ the curve Γ in the picture does not intersect $\mathrm{Sp}(H_{Q,T}^X) \cup \mathrm{Sp}(H_Q) \cup \mathrm{Sp}(H_{\omega,T}^X) \cup \mathrm{Sp}(H_\omega)$ 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

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

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*

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

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*

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

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

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

Here and in the following $\|.\|_{\mathrm{tr}}$ denotes the trace norm, $\|.\|_{HS}$ the Hilbert-Schmidt norm, and $\|.\|$ 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

$$\|\mathcal{R}_0(z) - \mathcal{R}(z)\|_{\mathrm{tr}} \le \|\mathcal{R}_0(z)(Q-\omega)^{1/2}\|_{HS}\||Q-\omega|^{1/2}\mathcal{R}_0(z)\|_{HS} \cdot \\ \cdot\|(I + (Q-\omega)\mathcal{R}_0(z))^{-1}\|$$

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

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

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

and it is easy to check that:

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

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

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

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 $\mathrm{tr}(f(H_Q) - f(H_\omega))$ 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 $\varepsilon > 0$,

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

with $f_\varepsilon(z) = e^{-\varepsilon z}f(z)$. Taking the limit for $\varepsilon \to 0$ 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 $\mathcal{R}^X_{0,T}$ is given in the case $n = 1$ by the Green function:

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

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

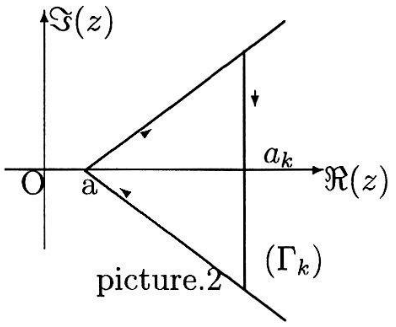
Hence, arguing as before

$$\begin{aligned} \|\mathcal{R}^X_{0,T}(z) - \mathcal{R}^X_T(z)\|_{\rm tr} &\leq \|\mathcal{R}^X_{0,T}(z)|Q-\omega|^{1/2}\|^2_{HS}\|(I+(Q-\omega)\mathcal{R}_0(z))^{-1}\| \\ &\leq C_1\|\mathcal{R}^X_{0,T}(z)|Q-\omega|^{1/2}\|^2_{HS} \\ &= \int \left|G^X_T(s,t;z)\right|^2 |Q(t)-\omega| dtds \\ &\leq \frac{C_2}{(1+|z|)^{3/2}}, \end{aligned}$$

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

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

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



picture.2

Using the residue theorem we obtain:

$$\mathrm{tr}(f(H_{Q,T}) - f(H_{\omega,T})) = \lim_{k\to+\infty} \frac{i}{2\pi}\int_{\Gamma_k} \mathrm{tr}(\mathcal{R}_T(z) - \mathcal{R}_{0,T}(z))f(z)dz$$

$$= \lim_{k\to+\infty} \sum_{\lambda^X_{j,T}<a_k} f(\lambda^X_{j,T}) - \sum_{\mu^X_{j,T}<a_k} f(\mu^X_{j,T}) = \sum_{j=1}^{\infty}(f(\lambda^X_{j,T}) - f(\mu^X_{j,T})),$$

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*

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

Proof :
We have to prove that:

$$\lim_{T\to+\infty}\frac{i}{2\pi}\int_\Gamma \mathrm{tr}(\mathcal{R}_T(z)-\mathcal{R}_{0,T}(z))f(z)dz$$
$$=\frac{i}{2\pi}\int_\Gamma \mathrm{tr}(\mathcal{R}(z)-\mathcal{R}_0(z))f(z)dz. \tag{2.8}$$

Let us consider

$$\rho_T : L^2(\mathbb{R}) \to L^2(I_T), \qquad \rho_T(u) = u_{|I_T}$$

and

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

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

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

Hence:

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

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

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

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*

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

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* $1 \le n \le 3$, *there exist* $C > 0$, $T_0 > 0$, $\varepsilon > 0$ *such that*

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

for any $z \in \Gamma$ *and* $T \ge T_0$.

Proof :
Using the resolvent identity, we can estimate
$\|\pi_T(\mathcal{R}_T^X(z) - \mathcal{R}_{0,T}^X(z))\rho_T - (\mathcal{R}(z) - \mathcal{R}_0(z))\|_{\mathrm{tr}}$ as:

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

We have:

$$\begin{aligned}
I &= \|\pi_T\mathcal{R}_{0,T}^X(z)(Q-\omega)^{1/2}\rho_T\left(\pi_T|Q-\omega|^{1/2}\mathcal{R}_{0,T}^X(z)\rho_T - |Q-\omega|^{1/2}\mathcal{R}_0(z)\right)\|_{\mathrm{tr}} \\
&+ \|\left(\pi_T\mathcal{R}_{0,T}^X(z)|Q-\omega|^{1/2}\rho_T - \mathcal{R}_0(z)|Q-\omega|^{1/2}\right)(Q-\omega)^{1/2}R_0(z)\|_{\mathrm{tr}} \\
&\le \left(\|\pi_T\mathcal{R}_{0,T}^X(z)|Q-\omega|^{1/2}\rho_T\|_{HS} + \||Q-\omega|^{1/2}R_0(z)\|_{HS}\right) \\
&\times \|\left(\pi_T\mathcal{R}_{0,T}^X(z)|Q-\omega|^{1/2}\rho_T - \mathcal{R}_0(z)|Q-\omega|^{1/2}\right)\|_{HS},
\end{aligned}$$

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

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

On the other hand,

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

We have:

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

The spectral theorem gives, on Γ,

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

Using (2.9) and (2.10), we obtain

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

On the other hand

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

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 χ, $\tilde{\chi}$ such that

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

and

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

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

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

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

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

On the other hand

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

Observe now that

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

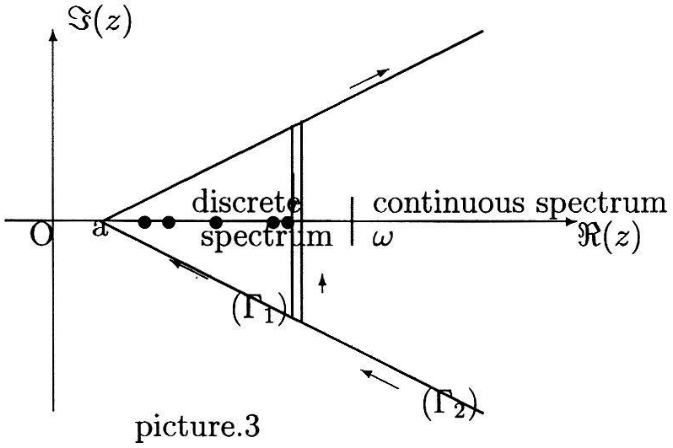
Hence

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

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 :*

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

Proof :

We can write

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

An application of the residue theorem gives

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

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 $T \to +\infty$, for $j = 1, .., p$.

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

In particular:

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

for $j = 1, .., p$. ∎

3 The Birman-Krein formula

Using the Birman-Krein formula [1], it is possible to write $\mathrm{tr}(f(H_Q) - f(H_\omega))$ 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:*

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

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

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

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

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

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

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

Hence

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

Since $s(\lambda) = O(\lambda^{n/2-1})$ as $\lambda \to +\infty$ (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

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

and this ends the proof of Theorem 3.1. ∎

Remarks:

i) Trace formulas for $\mathrm{tr}(f(H_Q)-f(H_w))$ 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*

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

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 $G^X_{0,T}(t,s;z)$, $(t,s) \in (I_T)^2$ as

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

if $X = D$, and

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

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

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

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

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

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

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

$$I_1 \le I_1' + I_1''$$

where

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

Then

$$I_1' = \frac{1}{4d^2}\left(\int_{\mathbb{R}} \exp(-2cd|r|)dr\right)\left(\int_{|t|\ge T'} \langle t\rangle^{-(1-\varepsilon)} dt\right) \le \frac{C}{T^\varepsilon d^3}.$$

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

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

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*

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

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*

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

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

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

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

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

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*

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

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

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

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 $\delta > n$, $0 < \varepsilon < \rho - \frac{n}{p}$,

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

By a standard computation on resolvents, we have

$$\pi_T\mathcal{R}^X_{0,T}(z)\chi_T\rho_T - \mathcal{R}_0(z)\chi_T = (\mathcal{R}_0(z) - \pi_T\mathcal{R}^X_{0,T}(z)\rho_T)[\chi_T,\triangle]\mathcal{R}_0(z). \tag{B.7}$$

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

$$\begin{gathered}\pi_T(\mathcal{R}^X_{0,T}(z))^k\chi_T\rho_T - (\mathcal{R}_0(z))^k\chi_T = \\ \sum\nolimits_{j+\ell=k} c_{j,\ell}((\mathcal{R}_0(z))^j - \pi_T(\mathcal{R}^X_{0,T})^j(z)\rho_T)[\chi_T,\triangle](\mathcal{R}_0(z))^\ell\end{gathered} \tag{B.8}$$

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 $N > \frac{n}{2}-1$,

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

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*

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

2. *For any positive $T>0$, $f(H^X_{Q,T}) - f(H^X_{\omega,T})$ is a trace class operator in $L^2(I^n_T)$ and*

$$\begin{aligned}&\operatorname{tr}(f(H^X_{Q,T}) - f(H^X_{\omega,T})) \\ &= (-1)^{N-1}(N-1)!\frac{i}{2\pi}\int_\Gamma \operatorname{tr}(\mathcal{R}^X_T(z)^N - \mathcal{R}^X_{0,T}(z)^N)f^{(1-N)}(z)dz \\ &= \sum_{j=1}^{\infty}(f(\lambda^X_{j,T}) - f(\mu^X_{j,T})).\end{aligned} \tag{B.10}$$

Proof :

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

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

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

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

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

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

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

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

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. ∎

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

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

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

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. ∎

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 $n \ge 4$ and hence a proof of Theorem 3.1 for $n \ge 4$. ∎

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