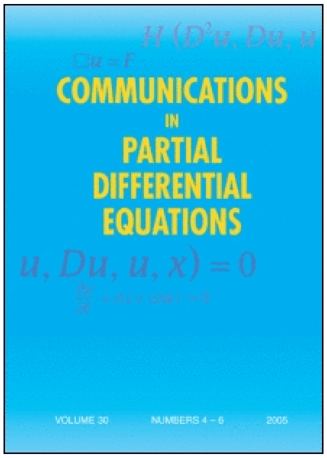

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Helffer Bernard; Knauf Andreas [a]; Siedentop Heinz [a]; Rudi Weikard [a]
[a] Fachbereich Mathematik, Berlin 12

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ON THE ABSENCE OF A FIRST ORDER CORRECTION FOR THE NUMBER OF BOUND STATES OF A SCHRÖDINGER OPERATOR WITH COULOMB SINGULARITY

Bernard Helffer*
Wissenschaftskolleg zu Berlin
Wallotstraße 19
D-1000 Berlin 33

Andreas Knauf
TU Berlin
Fachbereich Mathematik
D-1000 Berlin 12

Heinz Siedentop† and Rudi Weikard
Department of Mathematics
University of Alabama at Birmingham
Birmingham, AL 35294, USA

Contents

*Address as of September 1, 1991: DMI-ENS, 45 rue d'Ulm, F-75230 Paris Cédex

†Partially supported by the NSF under grant DMS-9000544. Address as of August 15, 1991: Institutt for matematiske fag, Norges Tekniske Høgskole, N-7034 Trondheim

1 Introduction

The Riesz mean problem for certain pseudodifferential operators with smooth symbols has been of recent interest [5], i.e., given, e.g., the Weyl symbol[1] $p(h;x,\xi) = p(x,\xi) = \xi^2 + V(x)$ of a Schrödinger operator with smooth potential V the problem is to compute

$$R_\gamma(h,E) := \sum_{e_j(h)\le E} (E - e_j(h))^\gamma, \tag{1}$$

where γ is a non-negative number, $e_1(h), e_2(h), \ldots$ are eigenvalues of the Schrödinger operator $P(h) = Op_h^W(p) := -h^2\Delta + V$ and E is some real number (energy) such that the energy surface $p_0^{-1}(\{E\})$ is compact. In particular a leading expression of order h^{-n}, n the dimension of the underlying space, is obtained under the assumption that E is a non-critical value of the principal symbol, plus correction terms $o(h^{-n+1})$, if the corresponding hamiltonian flow has few periodic orbits.

However, if V has a Coulomb singularity, there are counterexamples to such a claim in the case $\gamma = 1$. This is known as Scott correction (Scott [17], Hughes [7], [20, 19, 18], Bach [2], and Ivrii and Sigal [10].

Thus it is interesting to ask whether this phenomena of a leading correction term for other values of γ persists, i.e., if there is some "Scott" correction as well. In this paper we wish to consider $\gamma = 0$ for a general potential with a Coulomb type singularity. Tamura [21] has given a partial answer to this question, however, he does not show the absence of the next order term (see also the announcements of Ivrii [9]).

To state our result we remark that the set of collision orbits, i.e., the set of orbits in $T^*(\mathbb{R}^3 \setminus \{0\})$ meeting $x = 0$, is of measure zero with respect to

$$d\Sigma_E(x,\xi) := \delta(p(x,\xi) - E)d^3\xi\, d^3x. \tag{2}$$

[1]The *Weyl quantization* $Op_h^W(p)$ of an admissible symbol p is given for $\psi \in \mathcal{S}(\mathbb{R}^n)$ by

$$Op_h^W(p)\psi(x) := (2\pi h)^{-n} \int\!\!\int \exp(i(x-y)\xi/h)p(h;\tfrac{1}{2}(x+y),\xi)\psi(y)d^n y\, d^n\xi)$$

This follows from an application of a regularization method as the one given by Moser [12].

Theorem 1 *Let y be a real valued positive function on $I\!R^3$, nonvanishing at zero such that $y \circ \phi$ and all its derivatives are bounded $C^\infty(I\!R^4)$ functions, where ϕ denotes the Kustaanheimo-Stiefel transform (20), and E be a strictly negative noncritical value of $y/|\cdot|$.*

Then the number $N(h,E) := R_0(h,E)$ of eigenvalues of the operator $Op_h^W(p)$ on $L^2(I\!R^3)$ with Weyl symbol $p(r,k) := k^2 - y(r)/|r|$ meets the estimate

$$N(h,E) = (2\pi h)^{-3} \int d^3k \int d^3r \theta(E - p(r,k)) + \mathcal{O}(h^{-2}), \tag{3}$$

where θ is the characteristic function of the interval $(0,\infty)$.

Moreover, if the set of initial conditions which lead to periodic orbits is of measure zero with respect to $d\Sigma_E$ given in (2), the error in (3) is $o(h^{-2})$.

We remark that this result can presumably be also obtained by the techniques of Ivrii [9] which are being developed in a series of preprints. We prefer to give a different approach based on a regularization procedure of the potential. More precisely the strategy of our proof is as follows: We first show that the solutions of the singular problem correspond uniquely to certain invariant solutions of a smooth problem. The relation between these two is given through the Kustaanheimo-Stiefel transform and the Birman-Schwinger principle.

Applying a suitably modified version of the calculus developed in [3] (see also Robert [16]) together with a refined tauberian argument from Ivrii [8] and Petkov and Robert [14] yields the desired result. The modification concerns a trivial need. Instead of taking traces of functions of the given operator on the whole space, we need to take the trace only over a subspace, namely the space of functions that are gauge invariant under the gauge group of the Kustaanheimo-Stiefel transform. We will comment on the necessary changes in the Appendix B. In particular we shall explain how to apply [6] to our case (see also [4] and references given therein).

To make the paper more self-contained, we collect some facts for the Kustaanheimo-Stiefel transform in Appendix A.

Note that the second part of our theorem has an application to hamiltonians in atomic physics.

Theorem 2 *Let f be the solution of the Thomas-Fermi equation $f''(r) = f(r)^{3/2}/r^{1/2}$ with boundary $f(0) = 1$ and $f(\infty) = 0$, c a positive constant, and $y(r) = f(c|r|)$. Then the strengthened hypothesis of Theorem 1 applies.*

Proof: Without loss of generality set $c := 1$.

For $E < 0$ the energy shell

$$\Sigma_E := \{(r,k) \in T^*(I\!R^3 \setminus \{0\}) \mid p(r,k) = E\}$$

is a smooth manifold, since E is a regular value of the smooth function p, with $p(r,k) = k^2 - y(r)/|r|$. E is a regular value since

$$\nabla p(r,k) = 2k - \nabla \frac{y(r)}{|r|},$$

and the gradient of the potential does not vanish.

The motion in the central potential is integrable in the sense that for angular momentum $L(r,k) := r \times k$ the phase space functions p, L^2 and L_z Poisson-commute and are independent on Σ_E up to a set of Liouville measure zero. We may assume that $L^2 > 0$, disregarding the collision orbits.

Then in the orbital configuration space plane perpendicular to L we introduce polar coordinates (r,φ) and consider the reduced system given by the hamiltonian $h_0 : T^*(\mathbb{R}^2 \setminus \{0\}) \to \mathbb{R}$,

$$h_0(p_r, r; l) := p_r^2 + V_l(r) \qquad \text{with } V_l(r) := \frac{l^2}{r^2} - \frac{f(r)}{r}.$$

Let $L_m(E) := \inf\{L > 0 \mid \forall r > 0 : V_l(r) \geq E\}$ be the maximal value of the angular momentum for given energy $E < 0$.

Then for $0 < l^2 < L_m^2(E)$ the motion is organized on non-degenerate two-tori which are given as the level sets

$$T^2_{E,l} := \{y \in T^*(\mathbb{R}^2 \setminus \{0\}) \mid h_0(y) = E, L(y) = l\}.$$

This follows from Lemma 3 of [19] which states that for the given values of l the function $V_l(r)$ has exactly one minimum (which is negative and non-degenerate) and one maximum (which is positive), and no saddle point. We are to calculate the ratio $R(E,l)$ of the two basic frequencies of the motion, restricted to $T^2_{E,l}$, given by the motion in the φ direction and the radial motion. R has the explicit form

$$\begin{aligned} R(E,l) &= 2\int_{r_-(E,l)}^{r_+(E,l)} \frac{d\varphi}{dr} dr/2\pi = \frac{1}{\pi}\int_{r_-(E,l)}^{r_+(E,l)} \frac{\dot\varphi}{\dot r} dr \\ &= \frac{1}{\pi}\int_{r_-(E,l)}^{r_+(E,l)} \frac{l/r^2}{\sqrt{E - V_l(r)}} dr, \end{aligned} \tag{4}$$

with $0 < r_-(E,l) < r_+(E,l)$ uniquely determined by the equation

$$V_l(r_\pm(E,l)) = E.$$

The motion on $T^2_{E,l}$ is periodic if and only if the frequency ratio is rational, i.e., $R(E,l) \in \mathbb{Q}$.

If we can show that for a given $E < 0$,

$$\frac{\partial R}{\partial l}(E,l) \neq 0$$

up to a measure zero set in $l \in (0, L_m(E))$, then the Liouville measure of the periodic orbits vanishes. $R(E,l)$ is a real-analytic function of l. So we need only show that $R(E,l)$ is not independent of l (as would be the case if we had a Coulomb potential).

To prove the last assertion, we show that

$$R(E,0) := \lim_{l \searrow 0} R(E,l) = 1 \tag{5}$$

and

$$R(E, L_m(E)) := \lim_{l \nearrow L_m(E)} R(E,l) > 1. \tag{6}$$

Equation (5) follows since the collision orbits are regularized by the prescription that they are scattered backwards. In a more formal manner, one easily performs the limit in (5), starting from (4).

To prove (6), we notice that $r_+(E,l)$ and $r_-(E,l)$ have the same limit $\hat{r}$ so that

$$R(E, L_m(E)) = \frac{L_m(E)}{\hat{r}^2} \cdot \left(\tfrac{1}{2}\tfrac{\partial^2}{\partial r^2} V_{L_m(E)}(\hat{r})\right)^{-1/2}. \tag{7}$$

We have

$$\frac{\partial^2}{\partial r^2} V_l(r) = \frac{6l^2}{r^4} - \frac{r^2 f''(r) - 2rf'(r) + 2f(r)}{r^3}$$

and

$$\frac{\partial}{\partial r} V_{L_m(E)}(\hat{r}) = -2\frac{L_m(E)}{\hat{r}^3} - \frac{rf'(\hat{r}) - f(\hat{r})}{r^2}$$

so that

$$\frac{\partial^2}{\partial r^2} V_{L_m(E)}(\hat{r}) = 2\frac{L_m(E)}{\hat{r}^4} - \frac{f''(\hat{r})}{\hat{r}} = 2\frac{L_m(E)}{\hat{r}^4} - \left(\frac{f(\hat{r})}{\hat{r}}\right)^{3/2}, \tag{8}$$

using the Thomas-Fermi differential equation $f''(r) = f^{3/2}(r)/r^{1/2}$. By substitution of (8) in (7) we obtain

$$R(E, L_m(E)) = \left(1 - \frac{\hat{r}}{2L_m^2(E)}(\hat{r}f(\hat{r}))^{3/2}\right)^{-1/2} > 1,$$

proving (6). ∎

Remarks:

1. As can be seen from the above proof, the statement of Theorem 2 holds true even for energy $E = 0$.

2. Petkov and Safarov [15] have announced the following interesting result: For a real analytic hamiltonian A, either all hamiltonian trajectories lying on a non degenerate surface $A = const$ are periodic, or the measure of the set of periodic points on this surface equals zero. Another interesting reference is the paper by A. V. Volovoy [22].

2 Regularization of the Singular Operator

Let W_E be the Friedrichs extension in $L^2(\mathbb{R}^4, d^4x)$ of the operator which acts on $C_0^\infty(\mathbb{R}^4)$ as

$$f \mapsto \left(-\frac{h^2}{4}\Delta_4 - y \circ \phi(x) - Ex^2\right) f(x), \tag{9}$$

where $y \circ \phi$ is a positive bounded C^∞-function on $\mathbb{R}^4$ and $E < 0$.

Proposition 3 *The number of eigenvalues of W_E less than or equal to zero with gauge invariant eigenfunctions equals the number of eigenvalues of $P(h) = -h^2\Delta_3 - \frac{y(r)}{|r|}$, less than or equal to E.*

Proof: First we prove that the number of eigenvalues λ of $P(h)$ less than or equal to E is equal to the number of values λ less than or equal to E such that W_λ is not injective on the intersection of the domain of W_λ and of the subspace of the gauge invariant functions. To this end note the following fact. If ψ is twice continuously differentiable at $r = \phi(x) \in \mathbb{R}^3$, then $\Delta_4(\psi \circ \phi)(x) = 4x^2((\Delta_3\psi) \circ \phi)(x)$. In particular $W_\lambda(\psi \circ \phi)(x) = 0$ is equivalent to $P(h)\psi(r) = E\psi(r)$ for $|r| \neq 0$.

Now let ψ be an eigenfunction of $P(h)$ with eigenvalue λ, in particular, since the potential is Laplacian compact, the domain of $P(h)$ is $H^2(\mathbb{R}^3)$, so that $|\cdot|^{-1/2}\psi(\cdot) \in L^2(\mathbb{R}^3)$. This implies that we do not only have $\psi \circ \phi \in L^2(\mathbb{R}^4, \frac{4}{\pi}x^2 d^4x)$ but also $\psi \circ \phi \in L^2(\mathbb{R}^4)$. Hence $W_\lambda(\psi \circ \phi)$ is a distribution in $H_{loc}^{-2}(\mathbb{R}^4)$. Moreover, by elliptic regularity and by the above computation outside the origin, its support is confined to the origin and therefore is the zero distribution.[2] Now, by global elliptic regularity we conclude, that $\psi \circ \phi$ is in the domain of W_λ and $W_\lambda\psi \circ \phi$ vanishes.

To prove the reverse direction, assume u to be in the kernel of W_λ and gauge invariant. In particular there exists a ψ such that $u = \psi \circ \phi$ and such that $\psi/|\cdot| \in L^2(\mathbb{R}^3)$. Since u is also square integrable with respect to the measure $\frac{4}{\pi}x^2 d^4x$, ψ is square integrable with respect to d^3r.

Suppose we knew that ψ belonged to $H_{loc}^s(\mathbb{R}^3)$ for some $s \geq 1/2$ then we were done, since $(-\Delta - y/r - \lambda)\psi$ can have support at the origin at most and therefore would vanish by Footnote 2. Furthermore, since $|\cdot|^{-1}\psi$ is square integrable with respect to Lebesgue measure (which is a consequence of $|\cdot|^{-1/2}u \in L^2(\mathbb{R}^4)$), we would get that ψ is in H^2. Therefore we will prove $\psi \in H_{loc}^1(\mathbb{R}^3)$.

Define $w = \nabla\psi$ on $\mathbb{R}^3 \setminus \{0\}$. The function w is square integrable by the above computations for the Laplacian in this domain. By construction

[2] Note the following fact: If $s \geq -n/2$ then the only distribution in $H_{loc}^s(\mathbb{R}^n)$ with support at the origin is the zero distribution.

$\partial_k w_i(r) = \partial_i w_k(r)$ for $r \neq 0$. But since $\partial_k w_i - \partial_i w_k \in H^{-1}(\mathbb{R}^3)$ with support at the origin at most, we have $\partial_k w_i - \partial_i w_k = 0$ in $H^{-1}(\mathbb{R}^3)$. In this situation there exists a potential $v \in H^1_{loc}(\mathbb{R}^3)$ such that $w = \nabla v$.

Again, we obtain that $\nabla(\psi - v)(r) \in H^{-1}(\mathbb{R}^3)$ and $\nabla(\psi - v)(r) = 0$ for $r \neq 0$. Recalling Footnote 2, this implies $\nabla(\psi - v) = 0$ and therefore $(\psi - v) \in H^1_{loc}(\mathbb{R}^3)$.

Moreover by monotonicity of

$$W_{\mu,E} := -\frac{h^2}{4}\Delta_4 - \mu y \circ \phi(x) - Ex^2$$

in μ as used, e.g., in the Birman-Schwinger principle, and the fact that the space of gauge invariant functions is left invariant by $W_{\mu,E}$ the claim follows. (See Tamura [21] for a similar argument.) ∎

3 Functional Calculus with Projections

Section 2 shows that we need to compute $tr(\Pi\chi_{(-\infty,0]}(W_E))$ for the proof of our main result, Theorem 1, where Π (defined in (25)) is the projection onto the gauge invariant functions.

We use a decomposition of the form

$$\chi_{(-\infty,0]}(W_E) = f_1(W_E) + f_2(W_E)\chi_{(-\infty,0]}(W_E),$$

where f_1, f_2 are suitable non-negative functions in C_0^∞ such that $supp\, f_1 \cap (-\varepsilon/2, \infty) = \emptyset$ and $supp\, f_2 \subset (-\varepsilon, \varepsilon)$ for some sufficiently small $\varepsilon > 0$.

f_1 can be chosen to be compactly supported since W_E is bounded below uniformly in h.

Note that the principal symbol w_E^0 of W_E in the Weyl calculus is given by

$$w_E^0(x,\xi) = \frac{1}{4}\xi^2 + V_E(\phi(u)),$$

with

$$V_E(r) := -y(r) - E|r|, \tag{10}$$

and that the subprincipal symbol vanishes.

We treat $tr(\Pi f_1(W_E))$ and $tr(\Pi f_2(W_E)\chi_{(-\infty,0]}(W_E))$ separately. The first term will be analyzed below by methods of pseudodifferential calculus. For the estimates of the second term we will use Fourier integral operator techniques which will be explained in Appendix B.

Proposition 4 *Under the above assumptions*

$$tr(\Pi f_1(W_E)) = \frac{1}{(2\pi h)^3}\int d^3r \int d^3p f_1(p^2 r + V_E(r)) + o(h^{-2}). \tag{11}$$

Proof: Repeating the functional calculus of Helffer and Robert [3] yields the following.

We write the Weyl symbol $\sigma(f_1(W_E))$ in the form

$$\sigma(f_1(W_E)) = f_1(w_E^0) + h^2 P_{2,f_1} + \mathcal{O}(h^3).$$

Thus modulo $\mathcal{O}(h^{-1})$ there are two contributions to the l.h.s. of (11) to be analyzed. The main term is given by

$$\frac{1}{4\pi}(2\pi h)^{-4} \int \exp(i(x - \Theta_\sigma x) \cdot \xi / h) q_0(x, \xi, \sigma) d^4x \; d^4\xi \; d\sigma \tag{12}$$

with $q_0(x, \xi, \sigma) := f_1(w_E^0(\frac{1}{2}(\xi, x + \Theta_\sigma(x)))$, whereas the "remainder term" has the form

$$\frac{1}{4\pi}(2\pi)^{-4} h^{-2} \int \exp(i(x - \Theta_\sigma x) \cdot \xi / h) q_2(x, \xi, \sigma) d^4x \; d^4\xi \; d\sigma \tag{13}$$

with $q_2(x, \xi, \sigma) := P_{2,f_1}(\frac{1}{2}(x + \Theta_\sigma(x)), \xi)$.

Let us first prove that the second contribution (13) is $o(h^{-2})$ as $h \searrow 0$.

After eliminating an error of order $\mathcal{O}(h^\infty)$, we may assume that q_2 is a bounded C^∞ function in all variables with compact support. We decompose the integral (13) in two parts using a partition of unity on $T^*\mathbb{R}^4$ χ_1^ϵ, χ_2^ϵ where χ_1^ϵ has support in the ball of radius ϵ around the origin, χ_1^ϵ and χ_2^ϵ are nonnegative and add up to one.

We discuss first

$$\int \exp(i(x - \Theta_\sigma x)\xi / h) \chi_2^\epsilon q_2(x, \xi, \sigma) d^4x \; d^4\xi \; d\sigma. \tag{14}$$

The stationary phase argument is valid, because the support of χ_2^ϵ does not contain $(0,0)$.

The critical set of the phase $(x - \Theta_\sigma(x))\xi$ is in our case a submanifold of codimension two in $T^*\mathbb{R}^4 \times \mathbb{R}$ given by $\sigma = 0$ and $x_1\xi_2 - x_2\xi_1 + x_3\xi_4 - x_4\xi_3 = 0$. Moreover the transversal hessian is nondegenerate. Thus we obtain the estimate $C_\epsilon h$ for (14).

The first term obtained from the partition of unity in (13) yields the estimate $C\epsilon^8$ using the boundedness of the integrand.

Optimizing of ϵ gives the desired result, and we have

$$\begin{aligned} tr\left(\Pi(f_1(W_E))\right) &= \frac{1}{(2\pi h)^4} \int d^4x \frac{1}{4\pi} \int_0^{4\pi} d\sigma' \int d^4\xi \exp\left(\frac{i}{h}\xi(x - \Theta_{\sigma'} x)\right) \\ &\qquad f_1\left(w_E^0(\xi, (x + \Theta_{\sigma'} x)/2)\right) + o(h^{-2}). \end{aligned} \tag{15}$$

To evaluate the first term on the right hand side of (15), i.e. (12), we compute the following integral.

With V_E defined in (10), we get $f_1\left(w_E^0(\xi, u)\right) = f_1(\xi^2/4 + V_E(\phi(u))$. Then (12) equals $I(0)$, with

$$\begin{aligned} I(\varepsilon) &:= \frac{1}{(2\pi h)^4}\int d^4x \frac{1}{4\pi}\int_{-2\pi+\varepsilon}^{2\pi-\varepsilon} d\sigma' \int d^4\xi \\ &\qquad \exp(\frac{i}{h}\xi(x-\Theta'_\sigma x))f_1(\xi^2/4+V_E(\phi((x+\Theta_{\sigma'}x)/2))). \end{aligned}$$

Let

$$u := \frac{x+\Theta_{\sigma'}x}{2}. \tag{16}$$

Hence

$$x = \frac{1}{\cos\frac{\sigma'}{4}}\Theta_{-\frac{\sigma'}{2}}u, \quad \Theta_{\sigma'}x - x = 2\tan\frac{\sigma'}{4}\Theta_\pi u$$

and

$$d^4x = \frac{1}{(\cos\frac{\sigma'}{4})^4}d^4u.$$

Furthermore, by substituting $\frac{1}{h}\tan\frac{\sigma'}{4} = \alpha$, we get $I(\varepsilon) = J(\beta(\varepsilon))$ with

$$\begin{aligned} J(\beta) &:= \frac{h}{\pi(2\pi h)^4}\int d^4u \int_{-\beta}^{\beta} d\alpha \\ &\qquad (1+h^2\alpha^2)\int d^4\xi \exp(2i\alpha\xi\cdot\Theta_\pi u)f_1(\xi^2/4+V_E(\phi(u))) \end{aligned}$$

and $\beta(\varepsilon) := \frac{1}{h}\tan\frac{2\pi-\varepsilon}{4}$.

Observing that

$$\alpha^2\exp(2i\alpha\xi\cdot\Theta_\pi u) = -\frac{h^2}{4u^2}\Delta_\xi \exp(2i\alpha\xi\cdot\Theta_\pi u)$$

and integrating by parts, we get

$$\begin{aligned} J(\beta) &= \frac{4h}{(2\pi h)^4}\int d^4u \frac{1}{4\pi}\int_{-\beta}^{\beta} d\alpha \int d^4\xi \\ &\qquad \exp(2i\alpha\xi\cdot\Theta_\pi u)\left(1+\frac{h^2}{4u^2}\Delta_\xi\right) f_1(\xi^2/4+V_E(\phi(u))). \end{aligned}$$

We observe that

$$(r,\xi)\mapsto \left(1+\frac{h^2}{4|r|}\Delta_\xi\right) f_1(\xi^2/4+V_E(r))$$

is radial with respect to ξ which permits us to define on $\mathbb{R}^3\times\mathbb{R}^+$ the function

$$H\left(r,\frac{\xi^2}{4}\right) := f_1(\frac{\xi^2}{4}+V_E(r)) + \frac{h^2}{4|r|}\left(2f_1'(\frac{\xi^2}{4}+V_E(r)) + \frac{\xi^2}{4}f_1'(\frac{\xi^2}{4}+V_E(r))\right). \tag{17}$$

So

$$J(\beta) = \frac{h}{(2\pi h)^4}\frac{1}{\pi}\int d^4u \int_{-\beta}^{\beta} d\alpha \int d^4\xi \exp(2i\alpha\xi\cdot\Theta_\pi u)H\left(\phi(u),\frac{\xi^2}{4}\right).$$

Note that $\xi \cdot \Theta_\pi u = \sqrt{kr}\sqrt{\frac{1+\cos\sphericalangle(r,k)}{2}}\sin(\frac{\sigma_k}{2}+\gamma)$ where $k = \phi(\xi), r = \phi(u)$, $\sphericalangle(r,k)$ is the angle between k and r, σ_r and σ_k are the gauge variables of u and ξ, respectively and γ is some function not depending on σ_k.

Therefore

$$\begin{aligned}
J(\beta) &= \frac{h}{(2\pi h)^4}\frac{4}{\pi}\int d^3r \frac{1}{16r}\int_0^{4\pi} d\sigma_r \int_{-\beta}^{\beta} d\alpha \int d^3k \frac{1}{16k}\int_0^{4\pi} d\sigma_k \\
&\qquad \exp\left(2i\alpha\left(kr\left(\frac{1+\cos\sphericalangle(r,k)}{2}\right)\right)^{\frac{1}{2}}\sin\left(\frac{\sigma_k}{2}+\gamma\right)\right) H\left(r,\frac{k}{4}\right) \\
&= \frac{8h}{\pi(2\pi h)^4}\int d^3r \frac{1}{16r}\int_0^{4\pi} d\sigma_r \int_{-\beta}^{\beta} d\alpha \int_0^{\infty} dk \int_0^{2\pi} d\varphi_k \frac{k^2}{16k}\int_0^{\pi} d\theta_k \sin\theta_k \\
&\qquad \int_{-\pi}^{\pi} d\sigma_k \exp\left(2i\alpha\left(kr\frac{1+\cos\theta_k}{2}\right)^{\frac{1}{2}}\sin\sigma_k\right) H\left(r,\frac{k}{4}\right),
\end{aligned}$$

where we shifted and dilated the σ_k-integration using the periodicity of the integrand, where we picked the k-coordinate system such that the k_3-axis points in direction of r, and where θ_k is the polar angle of k. We integrate σ_r and recomplete the volume integral of k.

$$\begin{aligned}
J(\beta) &= \frac{h}{64(2\pi h)^4}\int d^3r \frac{1}{r}\int_{-\beta}^{\beta} d\alpha \int d^3k \frac{1}{k}\int_0^{\pi} d\theta \sin\theta \\
&\qquad \int_{-\pi}^{\pi} d\sigma_k \exp\left(2i\alpha\left(kr\frac{1+\cos\theta}{2}\right)^{1/2}\sin\sigma_k\right) H\left(r,\frac{k}{4}\right).
\end{aligned}$$

performing the σ_k-integration yields the Bessel function J_0. We substitute $z := \cos\theta$ and obtain

$$J(\beta) = \frac{2\pi h}{64(2\pi h)^4}\int d^3r \int_{-\beta}^{\beta} d\alpha \int d^3k \frac{1}{kr}\int_{-1}^{1} dz J_0\left(2\alpha\left(kr\frac{1+z}{2}\right)^{1/2}\right) H\left(r,\frac{k}{4}\right).$$

Doing the α-integration using $\int_0^\infty J_0(t)dt = 1$, the z-integration, and taking β to infinity yields

$$J(\infty) = \frac{1}{16(2\pi h)^3}\int d^3r \int d^3k (kr)^{-\frac{3}{2}} H\left(r,\frac{k}{4}\right).$$

Now we substitute $k = 4p^2 r$ and get

$$\begin{aligned}
J(\infty) &= \frac{1}{(2\pi h)^3}\frac{1}{16}\int d^3r \int d^3p \; 16p^2r^2 8pr \frac{1}{(4p^2r^2)^{\frac{3}{2}}} H\left(r,p^2 r\right) \\
&= \frac{1}{(2\pi h)^3}\int d^3r \int d^3p \, H\left(r,p^2 r\right).
\end{aligned}$$

Using the definition of H in (17), we obtain

$$\begin{aligned} I(0) &= \frac{1}{(2\pi h)^3}\int d^3r \int d^3p f_1(p^2r + V_E(r)) + \qquad (18)\\ &\frac{h^2}{4(2\pi h)^3}\int d^3r \int d^3p (f_1''(p^2|r| + V_E(r))p^2 + 2f_1'(p^2|r| + V_E(r))/|r|) \end{aligned}$$

This proves the proposition. ∎

Proposition 5 *Under the above assumptions*

$$tr(\Pi f_2(W_E)\chi_{(-\infty,0]}(W_E)) = \qquad (19)$$
$$\frac{1}{(2\pi h)^3}\int d^3r \int d^3p\, f_2(p^2r + V_E(r)) \cdot \chi_{(-\infty,0]}(p^2r + V_E(r)) + \mathcal{O}(h^{-2}),$$

and if the set of initial conditions which lead to periodic orbits is of measure zero with respect to $d\Sigma_E$, the error in (19) is $o(h^{-2})$.

We shall prove this proposition in Appendix B.

Proof of Theorem 1: Adding (11) and (19), we get

$$\begin{aligned} tr(\Pi\chi_{(-\infty,0]}(W_E)) &= \frac{1}{(2\pi h)^3}\int d^3r \int d^3p\, \chi_{(-\infty,0]}(p^2r + V_E(r)) + \mathcal{O}(h^{-2}) \\ &= \frac{1}{(2\pi h)^3}\int d^3r \int d^3k\, \theta(E - p(r,k)) + \mathcal{O}(h^{-2}), \end{aligned}$$

and similarly with $o(h^{-2})$. Thus Theorem 1 follows immediately from Proposition 3. ∎

A The Kustaanheimo-Stiefel Transform and All That

We shall follow partially an unpublished manuscript of R. Jost. The *Kustaanheimo-Stiefel* transform $\phi : I\!R^4 \to I\!R^3$ is given by

$$x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} \mapsto \phi(x) = r = \begin{pmatrix} 2x_1x_3 + 2x_2x_4 \\ -2x_1x_4 + 2x_2x_3 \\ x_1^2 + x_2^2 - x_3^2 - x_4^2 \end{pmatrix}. \qquad (20)$$

In particular

$$\phi(x) = \phi\begin{pmatrix} r^{1/2}\cos\frac{\vartheta}{2}\cos\frac{\sigma+\varphi}{2} \\ r^{1/2}\cos\frac{\vartheta}{2}\sin\frac{\sigma+\varphi}{2} \\ r^{1/2}\sin\frac{\vartheta}{2}\cos\frac{\sigma-\varphi}{2} \\ r^{1/2}\sin\frac{\vartheta}{2}\sin\frac{\sigma-\varphi}{2} \end{pmatrix} = r = r\begin{pmatrix} \sin\vartheta\cos\varphi \\ \sin\vartheta\sin\varphi \\ \cos\vartheta \end{pmatrix}, \qquad (21)$$

i.e., r, ϑ, φ are the spherical polar coordinates. Note that every choice of σ leads to the same r and, moreover, that $x^2 = |r|$.

We now have a closer look at this fact. As it turns out, the Kustaanheimo-Stiefel transform is invariant under the following set of transformations.

Definition 6 *The one-dimensional subgroup of the orthogonal group in $\mathbb{R}^4$ given by*

$$\begin{aligned} \Theta_\sigma : \mathbb{R}^4 &\to \mathbb{R}^4 \\ x &\mapsto \begin{pmatrix} \cos\frac{\sigma}{2} & -\sin\frac{\sigma}{2} & 0 & 0 \\ \sin\frac{\sigma}{2} & \cos\frac{\sigma}{2} & 0 & 0 \\ 0 & 0 & \cos\frac{\sigma}{2} & -\sin\frac{\sigma}{2} \\ 0 & 0 & \sin\frac{\sigma}{2} & \cos\frac{\sigma}{2} \end{pmatrix} x \end{aligned} \tag{22}$$

for $\sigma \in [-2\pi, 2\pi)$ is called the KS-gauge group and is denoted by G.

Then $\phi^{-1}(\{r\}) = \{\Theta_\sigma x | \phi(x) = r, \Theta_\sigma \in G\}$ for every $r \in \mathbb{R}^3$. In particular $\phi^{-1}(\{r\})$ is exactly one orbit of G.

The pull-back by ϕ of complex valued functions on $\mathbb{R}^3$ to complex valued functions on $\mathbb{R}^4$ is denoted by

$$\phi^* f := f \circ \phi. \tag{23}$$

Note that ϕ^* is linear and injective but not surjective. Now restrict the domain of ϕ^* to $L^2(\mathbb{R}^3)$ and call the function $\phi^* f$ *gauge invariant* with respect to G. Thus restricting the target space to gauge invariant functions and noting that

$$(f,g) = \int \overline{f(r)} g(r) d^3 r = \frac{4}{\pi} \int |x|^2 \overline{\phi^*(f)(x)} \phi^*(g)(x) d^4 x$$

we obtain the following unitary map

$$\begin{aligned} \phi^* : L^2(\mathbb{R}^3) &\to L_0^2(\mathbb{R}^4, \frac{4}{\pi} x^2 d^4 x) \\ f &\mapsto f \circ \phi \end{aligned} \tag{24}$$

where $L_0^2(\mathbb{R}^4, \frac{4}{\pi} x^2 d^4 x)$ denotes the subspace of gauge invariant functions in $L^2(\mathbb{R}^4, \frac{4}{\pi} x^2 d^4 x)$.

Let U be the unitary transformation

$$\begin{aligned} U : L^2(\mathbb{R}^4, 4x^2/\pi \; d^4 x) &\to L^2(\mathbb{R}^4, d^4 x) \\ f &\mapsto (4x^2/\pi)^{1/2} f. \end{aligned}$$

Again we call the functions in $U(L_0^2(\mathbb{R}^4, 4x^2/\pi \; d^4 x))$ gauge invariant, and we denote the orthogonal projection onto this space by Π.

Let $d\Theta$ denote the Haar measure on the KS-gauge group. We may write $\Pi : L^2(\mathbb{R}^4, d^4x) \mapsto L^2(\mathbb{R}^4, d^4x)$ as

$$(\Pi f)(x) := \int_G f(\Theta x)d\Theta = \frac{1}{4\pi}\int_{-2\pi}^{2\pi} f(\Theta_\sigma x)d\sigma. \tag{25}$$

B Some Remarks on a Result of Petkov and Robert on the Counting Function in the Context of Compact Group Actions

B.1 Introduction and Principal Statements

We make a mixture between [6] and Petkov and Robert [14] in the context of the application we need here.

Let $P(h)$ be an h-admissible pseudo-differential operator, essentially self-adjoint on $\mathbb{R}^n$ with principal symbol p_0. Let I be some compact interval such that

$$\exists \varepsilon > 0 \text{ such that } p_0^{-1}(I + [-\varepsilon, \varepsilon]) \text{ is compact in } T^*(\mathbb{R}^n). \tag{26}$$

Under these conditions we want to analyze the asymptotic behavior as h tends to zero of the counting function:

$$N_h(I) := \#\{j | \lambda_j(h) \in I\}, \tag{27}$$

where $(\lambda_j(h))$ is the increasing sequence of the eigenvalues of $P(h)$ contained in I. Let G be a compact Lie group of dimension p and $\mathcal{G}$ its Lie algebra. Let us denote by $A_1, ..., A_p$ a basis of $\mathcal{G}$. We assume that there exists an action $g \mapsto M(g)$, M of G on $\mathbb{R}^n$ with

$$M(g) \in SO(n). \tag{28}$$

We then get a natural symplectic action of G on $T^*(\mathbb{R}^n)$ defined by

$$(x, \xi) \mapsto M^*(g)(x, \xi) := (M(g)x, M(g)\xi). \tag{29}$$

Let us denote by $\tilde{M}$ the group action of G associated to M in $L^2(\mathbb{R}^n)$ and defined for $u \in L^2(\mathbb{R}^n)$ by

$$(\tilde{M}(g)u)(x) := u(M(g)^{-1}x). \tag{30}$$

We denote by $\hat{G}$ the set of (equivalence classes of) irreducible representations ρ of G and by χ_ρ the associated character. Let $(\Pi_\rho)_{\rho\in\hat{G}}$ be the family of orthogonal projectors associated to $\tilde{M}$ by

$$\Pi_\rho u := n_\rho \int_G \overline{\chi_\rho(g)}(\tilde{M}(g)u)dg \quad \text{for all } u \in L^2(\mathbb{R}^n). \tag{31}$$

We assume that

$$P(h) \text{ commutes with } \tilde{M}. \tag{32}$$

Let us introduce

$$P(\rho, h) := P(h)|L^2_\rho(I\!R^n) \text{ where } L^2_\rho(I\!R^n) := \Pi_\rho(L^2(I\!R^n)). \tag{33}$$

Let $(\lambda_{j,\rho}(h))$ be the sequence of the eigenvalues of $P(\rho, h)$. If J is an interval contained in I, then we can define

$$N_{h,\rho}(J) := \#\{\lambda_{j,\rho}(h), \lambda_{j,\rho} \in J\}. \tag{34}$$

Let q_i be the functions on $T^*(I\!R^n)$ defined by

$$q_i(x,\xi) := \langle M(A_i)x, \xi\rangle \tag{35}$$

where

$$M(A_i)x = \frac{d(M(e^{tA_i})x)}{dt}\Big|_{t=0} \text{ for } x \in I\!R^n \text{ and } i = 1, ..., p \tag{36}$$

and let Ω be the set in $T^*(I\!R^n)$ defined by

$$\Omega := \bigcap_{i=1,\dots,p} q_i^{-1}(0). \tag{37}$$

Let Γ be the set defined in $T^*(I\!R^n) \times G$ by

$$\Gamma := \{(x,\xi,g) \in \Omega \times G | M^*(g)(x,\xi) = (x,\xi)\}, \tag{38}$$

and for every interval J let

$$\Omega^J := \{(x,\xi) \in \Omega | p_0(x,\xi) \in J\}, \tag{39}$$

$$\Gamma^J := \{(x,\xi,g) \in \Omega \times G | M^*(g)(x,\xi) = (x,\xi)\}. \tag{40}$$

Let us assume that for a given interval $I = [\lambda_1, \lambda_2]$

$$0 \text{ is a } \textit{weakly regular value} \text{ of } \vec{q} = (q_1, ..., q_p), \tag{41}$$

by which we mean that

- Ω^I is a smooth submanifold of $p_0^{-1}(I)$ and
- $T_{(x,\xi)}\Omega^I = Ker(d\vec{q}(x,\xi))$ for $(x,\xi) \in \Omega^I$.

The notion of weak regularity has been introduced by Marsden and Weinstein [11] to cover applications like the states of zero angular momentum in the two-body problem.

Denote by k the rank of the system of the differentials $\{dq_i\}$ which is in this case constant[3] and require that

[3]Because it is homogeneous with respect to the dilations $(x,\xi) \mapsto (tx, t\xi)$, $t \in I\!R$, the form of these conditions can be of course simplified, but the homogeneity is lost, if we consider more general group actions or if we work on a manifold.

$$\text{all the isotropy sub-groups attached to points}$$
$$\text{in a neighborhood of } \Omega^I \text{ are conjugated.} \tag{42}$$
$$p_0|\Omega \text{ is not critical at } \lambda_1 \text{ and } \lambda_2. \tag{43}$$

Under these assumptions the following theorem is proved in [6].

Theorem 7 *Under the assumptions (26), (32), (41), (42) and (43)*

$$N_{h,\rho}(I) = n_\rho (2\pi h)^{k-n} c^I_\rho(p_0) + \mathcal{O}(h^{1+k-n}), \tag{44}$$

as h tends to zero, where

$$c^I_\rho(p_0) := \int_{\Gamma^I} \overline{\chi_\rho(g)} |Det\ (Hess\ \Psi/N\Gamma^I)|^{-1/2} dv_\Gamma,$$

$\Psi(x,\xi,g) := \langle x - M(g)x, \xi\rangle$, $N\Gamma^I$ *is the normal fiber bundle to* Γ^I *in* $T^*(I\!R^n) \times G$, *and* dv_Γ *is the density induced by the riemannian density of* $T^*(I\!R^n) \times G$ *on* Γ^I.

The assumptions (41) and (42) are in fact too restrictive and for example imply always that the point $(0,0)$ is not in $p_0^{-1}(I)$. But we can consider weaker assumptions, in particular, if $(0,0)$ is the only point where the condition is not satisfied. We have already observed that there is some homogeneity in the assumptions (41) and (42) and the weaker assumptions (45) and (46) correspond only to the assumption that (41) and (42) are satisfied on $|x|^2 + |\xi|^2 = 1$. Another way to write it is

$$0 \text{ is a weakly regular value of } \vec{q} = (q_1, \dots, q_p) \text{ in } I\!R^{2n} \setminus \{(0,0)\}. \tag{45}$$

$$\text{All the isotropy sub-groups attached to points}$$
$$\text{in } I\!R^{2n} \setminus \{(0,0)\} \text{ are conjugated.} \tag{46}$$

Let us now introduce the additional assumption[4]

$$p_0(\{(0,0)\}) \neq \lambda_1, \lambda_2. \tag{47}$$

Then Theorem 7 is improved in the following way.

Theorem 8 ([6]) *Under the assumptions (26), (32), (43), (45), (46) and (47), we have*

$$N_{h,\rho}(I) = n_\rho (2\pi h)^{k-n} c^I_\rho(p_0) + \mathcal{O}(h^{\delta+k-n}), \tag{48}$$

as h tends to zero, $\delta = 1$ if $n > k+1$ and δ is any number less than 1, if $n = k+1$.

---

[4] In Theorem 7 condition (47) was automatically satisfied.

What we need – at least in our particular case – to improve the error estimate is the following. We shall say that a point (x,ξ) is *periodic modulo* G, if there exists $t \neq 0$ and $g \in G$ such that

$$M^*(g)\Phi_t(x,\xi) = (x,\xi). \tag{49}$$

Here Φ_t is the hamiltonian flow associated to p_0, that means the flow generated by the vector field $H_{p_0} = (\partial_\xi p_0, -\partial_x p_0)$.

Under conditions (45) and (46), $(\Omega\backslash\{(0,0)\})/G$ is a regular symplectic manifold and the definition we give simply says that, if we denote by π_G the projection of $(\Omega\backslash\{(0,0)\})$ onto $(\Omega\backslash\{(0,0)\})/G$, a point (x,ξ) is periodic modulo G, if the point $\pi_G(x,\xi)$ is periodic for the hamiltonian flow $\tilde{\Phi}$ canonically associated to the hamiltonian

$$\tilde{p}_0 : (\Omega\backslash\{(0,0)\})/G \rightarrow I\!R \quad \text{defined by } p_0 = \tilde{p}_0 \circ \pi_G. \tag{50}$$

For these definitions, we refer for example to [4] and to Marsden and Weinstein [11].

The new assumption which has a sense under Assumptions (43), (47), (45) and (46)) is now

$$\begin{array}{l}\text{The measure of the set of periodic points modulo } G \text{ in} \\ p_0^{-1}(\{\lambda_i\} \cap \tilde{q}^{-1}(\{0\}) \text{ is zero for } i = 1,2.\end{array} \tag{51}$$

We will analyze the link with the condition in Theorem 1 in Subsection B.3.

Thus we have the following extension of the result of Petkov and Robert [14].

Theorem 9 *Under the assumptions (26), (32), (43), (45), (46), (47) and (51), and if* $n > k+1$

$$N_{h,\rho}(I) = n_\rho(2\pi h)^{k-n}c_\rho^I(p_0) + h^{k-n+1}c_{1,\rho}^I(p_0) + o(h^{1+k-n}), \tag{52}$$

as h *tends to zero.*

Remark: By use of the functional calculus, and according to the techniques used in [6] in the general case (or in our particular case, see Proposition 4) we need to prove only

Theorem 10 *Let us assume (26), (32), (43), (45), (46), (47) and (51). Then, for each function* $f \in C_0^\infty(I\!R, I\!R)$ *with support in a small neighborhood of* λ_1 *or* λ_2*, we have*

$$N_{h,\rho}^f(I) = n_\rho(2\pi h)^{k-n}c_\rho^{I,f}(p_0) + h^{k-n+1}c_{1,\rho}^{I,f}(p_0) + o(h^{1+k-n}), \tag{53}$$

as h *tends to zero, where*

$$N_{h,\rho}^f(I) := \sum_{\lambda_{j,\rho}(h)\in I} f(\lambda_{j,\rho}(h)) \tag{54}$$

and

$$c_\rho^{I,f}(p_0) := \int_{\Gamma^I} \overline{\chi_\rho(g)} f(p_0) |Det\ (Hess\ \Psi/N\Gamma^I)|^{-1/2} dv_\Gamma. \tag{55}$$

The following remark can be useful to prove the vanishing of the second term in (53).

Remark: Suppose we are in a situation where, for every $f \in C_0^\infty(\lambda_1 - \varepsilon_0, \lambda_1 + \varepsilon_0)$,

$$\sum f(\lambda_{j,\rho}(h)) = \alpha_0(f)(2\pi h)^{k-n} + o(h^{1+k-n}), \tag{56}$$

it is possible to prove as in [14], that

$$N_{h,\rho}^f(I) = n_\rho (2\pi h)^{k-n} c_\rho^{I,f}(p_0) + o(h^{1+k-n}), \tag{57}$$

as h tends to zero. This is in fact a way to prove that the second term vanishes, if the subprincipal symbol is zero ([14], p. 380–381). We shall give a proof of that fact in Appendix B.4.

In our case, it is not clear by the general arguments that this second term vanishes in general, but the computation explicitly given in the particular case shows that it is true (see Section 3).

As is known, this type of theorem can be usually proved by Fourier-integral techniques. We shall give a sketch of the proof in the next subsection but let us finish this part by proving Proposition 5.

Proof of Proposition 5: The operator we consider is an h-pseudodifferential operator on $I\!R^4$ whose Weyl symbol is $\xi^2/4 + V_E(\phi(x))$ with $V_E(r) = -y(r) - E|r|$, see (10).

We must check that the assumptions of Theorem 10 are met. We take for ρ the trivial representation. So Π_ρ defined in (31) is the projector Π from (25), and $\chi_\rho \equiv 1$.

We observe that $y \circ \phi$ is a positive bounded C^∞ function whose derivatives are bounded, too, and $E < 0$. (If the C^∞ function is only bounded, there is probably a way to reduce to the other case, using Agmon type estimates.)

We have the linear action of the KS-gauge group $G \approx S^1$ on $I\!R^4$: $[-2\pi, 2\pi) \ni \sigma \to \Theta_\sigma$ given by (22).

It is clear that this circle action is regular on $I\!R^4$ outside of 0 and that the corresponding action on the cotangent fiber bundle is regular outside (0,0). Condition (26) is satisfied because $E < 0$. Condition (32) is satisfied because of the invariance of $V_E \circ \phi$. Conditions (45) and (46) are satisfied and we have $k = 1$. We take $\lambda_1 := -\infty$, $\lambda_2 := 0$. In this case, the only condition for (43) is at energy 0. If we assume that $g := y \circ \phi$ is positive, we find that the condition (43) is equivalent to: if $-Ex^2 = g(x)$, then $-2Ex - \nabla g(x) \neq 0$.

An easy computation proves that it is equivalent to the condition: E is not a critical value of $y(r)/r$. That property is true in our application to the atomic physics problem, as shown in the proof of Theorem 2.

Condition (47) is satisfied, if $g(0) \equiv y(0) \neq 0$ (which is an assumption of Theorem 1). Condition (51) will be analyzed in Subsection 3.

Using Theorem 10, we see that

$$tr(\Pi f_2(W_E)\chi_{(-\infty,0]}(W_E)) = c_1 h^{-3} + c_2 h^{-2} + \mathcal{O}(h^{-2})$$

resp. $o(h^{-2})$ if assumption (51) holds. To identify c_1 and to prove that $c_2 = 0$, we use the above remark or Appendix B.4, and Proposition 4. ∎

B.2 Sketch of a Proof of Theorem 10

We follow the sketch of the proof of [13]. We work near λ_2 which we call λ and with a function f with support in $(\lambda - \varepsilon_0, \lambda + \varepsilon_0)$.

Step 1: For each real T_1, we introduce

$$\begin{aligned} K_{T_1} := \{(x,\xi) \in p_0^{-1}([\lambda - \varepsilon_0, \lambda + \varepsilon_0]) |\ &\text{there exists } t \neq 0, |t| \leq T_1, \\ &\text{there exists } g \in G \text{ such that } M^*(g)\Phi_t(x,\xi) = (x,\xi)\}. \end{aligned} \tag{58}$$

The set K_{T_1} is a closed in $p_0^{-1}([\lambda - \varepsilon_0, \lambda + \varepsilon_0])$. Let $\mathcal{O}_{T_1}$ be an open neighborhood of K_{T_1} to be determined later. Let $\omega_1 \in C_0^\infty(\mathcal{O}_{T_1})$ such that $0 \leq \omega_1 \leq 1$, $\omega_1 = 1$ on K_{T_1}. Define $\omega_2 \in C_0^\infty(I\!R^{2n})$ such that $\omega_2^2 = 1 - \omega_1^2$ on $p_0^{-1}([\lambda - \varepsilon_0, \lambda + \varepsilon_0])$. If needed we can assume that the ω_j have group invariance properties.

For $j = 1, 2$ introduce

$$\sigma_h^{j,\rho}(\mu) := \sum_{\lambda_{j,\rho} \leq \mu} f(\lambda_{j,\rho}) \| Op_h^W(\omega_j) u_{j,\rho}(h) \|^2 \tag{59}$$

where $u_{j,\rho}(h)$ is the corresponding normalized eigenfunction associated to $\lambda_{j,\rho}$. First observe that

$$\sigma_h^{1,\rho}(\mu) + \sigma_h^{2,\rho}(\mu) = \sum_{\lambda_{j,\rho} \leq \mu} f(\lambda_{j,\rho})(1 + \mathcal{O}(h^2)). \tag{60}$$

This is essentially a consequence of the Weyl calculus (Lemma 4.1 in [14]).

Step 2: Following the classical method we study

$$\frac{d\sigma_h^{j,\rho} * \theta_{h,T}}{d\tau}(\tau) \tag{61}$$

where $\theta_{h,T}$ (with $T \geq T_0, h \in (0, h_0]$) is an approximation of the identity

$$\theta_{h,T}(\tau) = (2\pi h)^{-1} T \hat{\rho}_1(-h^{-1}T\tau) = (2\pi h)^{-1} \hat{\rho}_T(-h^{-1}\tau) \tag{62}$$

with $\rho_1 \in C^\infty$, $\rho_1(0) = 1$, ρ_1 even, $supp\,\rho_1 \subset [-1, 1]$ and there exists $\delta_0 > 0$ and $\varepsilon_0 > 0$ such that $\hat{\rho}_1(\tau) \geq \delta_0$ for all $\tau \in [-\varepsilon_0, \varepsilon_0]$. Then we have

$$\frac{d\sigma^j_{h,\rho} * \theta_{h,T}}{d\tau}(\tau) = \tag{63}$$
$$(2\pi h)^{-1}\, tr\left[\int \exp(it\tau/h)\rho_T(t)\omega_j^*\omega_j f(P(\rho,h))\exp(-itP(\rho,h)/h)dt\right].$$

We can study such an expression as in [6] following the ideas of [3] and [14]. For $j = 1$ we get by [6], Proposition 5.4, the following complete expansion. This is not explicitly written in [6] but is in fact a consequence of the generalized stationary phase argument which is used there. For $T = T_0$ with T_0 small enough

$$\frac{d\sigma^1_{h,\rho} * \theta_{h,T_0}}{d\tau}(\tau) = \gamma_0^1(\tau,\rho)h^{-n+k} + \gamma_1^1(\tau,\rho)h^{-n+k+1} + \mathcal{O}(h^{-n+k+2}). \tag{64}$$

For the second one we use the fact that there is no critical point corresponding to t such that $0 < |t| < T_1$, so by adding a nonstationary phase argument, we get with $T = T_1$

$$\frac{d\sigma^2_{h,\rho} * \theta_{h,T_1}}{d\tau}(\tau) = \gamma_0^2(\tau,\rho)h^{-n+k} + \gamma_1^2(\tau,\rho)h^{-n+k+1} + \mathcal{O}_{T_1}(h^{-n+k+2}). \tag{65}$$

The $\gamma_0^j(\tau,\rho)$ are explicitly computable. The explicit computation of the second coefficient is not necessary, but we have to notice the independence with respect to T. Using [6] we get

$$\gamma_0^i(\tau,\rho) = n_\rho(2\pi h)^{k-n} f(\tau) L^i_\rho(\tau)$$

with

$$L^i_\rho(\tau) := \int \overline{\chi_\rho(g)}\omega_j^2(x,\xi)|D_\tau|^{-1/2}d\nu_{\Gamma^\tau}.$$

L_ρ is a C^∞ function in τ on the support of f, $d\nu_{\Gamma^\tau}$ is the induced riemannian density of $G \times T^*I\!R^n$ on Γ^τ, and D_τ is a C^∞ function defined in a neighborhood of λ. The map

$$f \mapsto \gamma_1^1(\tau,\rho) + \gamma_1^2(\tau,\rho)$$

is in fact a Radon measure.

Step 3: We apply now the tricky tauberian theorem of Ivrii whose detailed proof is given in [13]. Following the proof of [13] this theorem implies an estimate on $N^f_{h,\rho}(I)$ (see(54))

$$\left|N^f_{h,\rho}(I) - (2\pi h)^{k-n}c_\rho^{I,f}(p_0) - h^{k-n+1}c_{1,\rho}^{I,f}(p_0)\right| \leq \tag{66}$$
$$Cf(\lambda)\left(L^1_\rho(\lambda)/T_0 + L^2_\rho(\lambda)/T_1\right)h^{1+k-n} + \tilde{C}(\rho,T_0,T_1,\lambda)h^{2+k-n}$$

as $h \searrow 0$, where C is independent of T_0, T_1 and h.

Firstly proceed by choosing T_1 to make the second coefficient of h^{1+k-n} small enough (independent of the partition of unity ω_i^2). Secondly choose

ω_1 such that the measure of its support is small enough to make the first coefficient small. Note that the third term in (66) contains one additional power of h. ∎

B.3 On the Initial Conditions Yielding Periodic Orbits of Regularized and Unregularized Hamiltonians

Here we fill a gap in the proof of Proposition 5. We are to show that, under the condition of Theorem 1, Condition (51) of Theorem 9 is met for the symbol of the lifted operator W_E defined in (9). More precisely, we want

Lemma 11 *Assume that the $d\Sigma_E$-measure of the set of points in Σ_E lying on periodic orbits is zero. Then the measure of the periodic points modulo G*

$$\{(x,\xi) \in (w_E^0)^{-1}(\{0\}) \cap \Omega \mid \exists t \neq 0 \, \exists \Theta \in G : \Theta^* \circ \Phi_t(x,\xi) = (x,\xi)\}$$

vanishes, too.

Proof. First we relate the flow on Σ_E generated by the hamiltonian function p of Theorem 1 to the flow Φ_t, restricted to $(w_E^0)^{-1}(\{0\}) \cap \Omega$. Using the KS-transform ϕ, we can pull back by ϕ^* one-forms on $\mathbb{R}^3 \setminus \{0\}$ to one-forms on $\mathbb{R}^4 \setminus \{0\}$. A simple computation leads to the conclusion that

$$\phi^*(T^*(\mathbb{R}^3 \setminus \{0\})) = \{(x,\xi) \in T^*(\mathbb{R}^4 \setminus \{0\}) \mid q(x,\xi) = 0\}$$

with

$$q(x,\xi) := (x_1\xi_2 - x_2\xi_1) + (x_3\xi_4 - x_4\xi_3). \tag{67}$$

Moreover, these (x,ξ) project to points $(r,k) \in T^*(\mathbb{R}^3 \setminus \{0\})$ with $r = \phi(x)$ and

$$k = \frac{1}{2|x|} \begin{pmatrix} x_3 & x_4 & x_1 & x_2 \\ -x_4 & x_3 & x_2 & -x_1 \\ x_1 & x_2 & -x_3 & -x_4 \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \\ \xi_4 \end{pmatrix}. \tag{68}$$

This shows that

$$w_E^0(\phi^*(r,k)) = |r| \cdot (p(r,k) - E).$$

Thus the flow $\Phi_t(x_0,\xi_0) \equiv (x(t,x_0,\xi_0), \xi(t,x_0,\xi_0))$ on $(w_E^0)^{-1}(\{0\}) \cap \Omega$ projects to the flow on Σ_E with reparametrized time

$$s(t,(x_0,\xi_0)) := (2E)^{-1/2} \int_0^t x^2(t',(x_0,\xi_0))dt',$$

except for the collision orbits for which $x(t,(x_0,\xi_0)) = 0$ for some t. But the set of these collision orbits has the form of an immersed submanifold of codimension two, so that their measure vanishes.

As one concludes from (68), for $(r,k) \in \Sigma_E$, the pull-back

$$\phi^*(\{(r,k)\}) \subset (w_E^0)^{-1}(\{0\}) \cap \Omega$$

consists of precisely one orbit of the action of the KS-gauge group G. Thus the (non-colliding) orbits of Φ_t which are periodic modulo G project to the periodic orbits in Σ_E.

Moreover, the action of the gauge group G on $(w_E^0)^{-1}(\{0\}) \cap \Omega$ is free and proper, since this set does not contain $(0,0) \in T^*\mathbb{R}^4$ and since $G \approx S^1$ is compact. Thus by Proposition 4.1.23 of Abraham and Marsden [1]

$$\left((w_E^0)^{-1}(\{0\}) \cap \Omega\right)/G \tag{69}$$

is a smooth manifold. If one excludes from (69) the points over the singularity, then the resulting manifold is naturally diffeomorphic to Σ_E, and the natural measure on these manifolds are absolutely continuous with respect to each other (with a function only depending on the radius $|r|$ for $r \in \mathbb{R}^3 \setminus \{0\}$). This shows the validity of our lemma. ∎

B.4 On the Vanishing of the Second Coefficient

The purpose of this section is to justify a statement given in the proof of Proposition 5. In fact, we provide two different proofs of the vanishing of the second coefficient in the asymptotic expansion of the counting function when the subprincipal symbol of the operator under consideration vanishes. This is already well-known in the case where there is no group action (Petkov and Robert [13] and Ivrii and Sigal [10]).

The first one is based on the explicit computations of Proposition 4. The second one seems to be more easily generalized.

Proof 1: The two informations we have until now are the following (we assume that $\lambda_1 = -\infty$ and $\lambda = \lambda_2$).

For every $f \in C_0^\infty(]-\infty, \lambda + \epsilon[)$ with positive but small enough ϵ we have

$$tr(f(P(h, \rho = 0))) = h^{-3} d_0(f) + o(h^{-2}) \tag{70}$$

(see Proposition 4).

On the other hand we have seen (cf. Theorem 10) that for each C^∞ function f with support in a small neighborhood of λ, we have

$$N_{h,0}^f(I) = n_0 (2\pi h)^{k-n} c_0^{I,f}(p_0) + h^{k-n+1} c_{1,0}^{I,f}(p_0) + o(h^{1+k-n}), \tag{71}$$

as $h \searrow 0$, where $I =]-\infty, \lambda]$ (but possibly $I =]-\infty, \tau]$ with τ near λ), $n = 4$, and $k = 1$.

What we want to prove under these conditions is that $c_{1,0}^{I,f}(p_0) = 0$. To this end we go back to the details of the proof leading to (71). The basic idea in the study of the counting function by FIO techniques is to analyze

$$J(f,\tau) := \frac{1}{2\pi h} tr\left[\int\int M(g) \exp(it\tau/h) \rho_{T_0}(t) f(P(h,0)) \exp(-itP(h,0)/h) dt\, dg\right]$$

for f with support in a small neighborhood of λ.

Up to some error of order $\mathcal{O}(h^{-n+k+2})$, this function is equal to

$$2\pi h\left(\frac{d\sigma^1_{h,0}*\theta_{h,T_0}}{d\tau}(\tau)+\frac{d\sigma^1_{h,0}*\theta_{h,T_1}}{d\tau}(\tau)\right)$$

(see (60) - (65), and the stationary phase argument). For this quantity we obtain an expansion of the form

$$J(f,\tau)=h^{k-n}f(\tau)L_0(\tau)+h^{1+k-n}c_1(\tau,f)+\mathcal{O}(h^{2+k-n}) \qquad (72)$$

given by a stationary phase theorem.

We have now to understand the link between the coefficients appearing in (70), (71) and (72). We define $N(f,\tau):=N^f_{h,0}(I)$ with $I:=]-\infty,\tau]$. The result given by the tauberian theorem finally gives that

$$c^{I,f}_{1,0}(p_0)=\int_{-\infty}^{\tau}c_1(\sigma,f)d\sigma \quad \text{for any } f\in C_0^\infty(]\lambda-2\epsilon_0,\lambda+2\epsilon_0[). \qquad (73)$$

Considering the case where $\tau_0:=\lambda+2\epsilon_0$ and $f\in C_0^\infty(]-\infty,\tau_0[)$ with $2\epsilon_0<\epsilon$, we observe that

$$tr(f(P(h,0)))=N(f,\tau_0).$$

Consequently we get from (70)

$$\int_{-\infty}^{\tau_0}c_1(\sigma,f)d\sigma=0 \quad \text{for any } f\in C_0^\infty(]-\infty,\tau_0[). \qquad (74)$$

We want to link (73) and (74). Because of the support properties, (74) does not imply immediately that

$$c^{I,f}_{1,\rho}(p_0)=0 \quad \text{for } f\in C_0^\infty(]\lambda-\epsilon_0,\lambda+\epsilon_0[) \qquad (75)$$

with $I=]-\infty,\lambda]$. But it will be true by density, if we prove that

$$C_0^\infty((\lambda-\epsilon_0,\lambda+\epsilon_0))\ni f\mapsto\int_{-\infty}^{\tau}c_1(\sigma,f)d\sigma \qquad (76)$$

is a measure.

Let us return to $J(f,\tau)$. Let us introduce a fixed $\tilde f$ with compact support in $(\lambda-2\epsilon_0,\lambda+2\epsilon_0)$ and equal to 1 on $[\lambda-\epsilon_0,\lambda+\epsilon_0]$.

We shall analyze for f with support in $(\lambda-\epsilon_0,\lambda+\epsilon_0)$ the expression $J(f,\tau)-f(\tau)J(\tilde f,\tau)$.

We have

$$J(f,\tau) \;=\; (2\pi h)^{-1}\sum\int\exp(it(\tau-\lambda_{j,0})/h)\rho_{T_0}(t)f(\lambda_{j,0})dt$$

$$\begin{aligned}
&= (2\pi h)^{-1}\sum\int \exp(it(\tau-\lambda_{j,0})/h)\rho_{T_0}(t)\tilde{f}(\lambda_{j,0})f(\lambda_{j,0})dt \\
&= f(\tau)J(\tilde{f},\tau)+ \\
&\quad (2\pi h)^{-1}\sum\int \exp(it(\tau-\lambda_{j,0})/h)\rho_{T_0}(t)\tilde{f}(\lambda_{j,0})(f(\lambda_{j,0})-f(\tau))dt \\
&= f(\tau)J(\tilde{f},\tau)+ \\
&\quad (2\pi h)^{-1}(ih)\sum\int \exp(it(\tau-\lambda_{j,0})/h)\rho'_{T_0}(t)\tilde{f}(\lambda_{j,0})\psi(\lambda_{j,0},\tau)dt
\end{aligned}$$

with $\psi(\lambda,\tau) := (f(\lambda)-f(\tau))/(\lambda-\tau)$.

Next consider

$$h\left(\frac{1}{2\pi h}\, tr\left[\int\int M(g)\exp(it\tau/h)\rho'_{T_0}(t)\psi(P,\tau)\tilde{f}(P)\exp(-itP/h)dt\, dg\right]\right).$$

This is a term of the same type as for the study of $J(f,\tau)$, but we have gained a power of h in front of the expression. Moreover, the principal term in the application of the stationary phase theorem vanishes because $\rho'_{T_0}(0)=0$. Thus we get

$$J(f,\tau)-f(\tau)J(\tilde{f},\tau)=\mathcal{O}(h^{2+k-n}),$$

which means that the first two coefficients in the expansion of $J(f,\tau)$ are measures which proves (76) and consequently (75). ∎

Proof 2: This proof gives simultaneously some independent proof of property (70). To simplify we limit ourselves to this last proof and hope the reader can get after the general argument. Also to simplify we just prove (70) for $f\in C_0^\infty((\lambda-\epsilon_0,\lambda+\epsilon_0))$. Following [6], we observe that if the pseudodifferential operator has vanishing subprincipal symbol, then

$$\begin{aligned}
&tr(f(P(h,\rho=0))) = \qquad (77)\\
&\quad h^{-n}\int\int\int \exp(i(g\cdot x-x)\xi/h)f(p_0(\tfrac{1}{2}(x+g\cdot x),\xi))dx\,d\xi\,dg+\mathcal{O}(h^{2+k-n})
\end{aligned}$$

for $P(h,0)=Op_h^W(p)$ and $p(h;x,\xi)=p_0(x,\xi)+\mathcal{O}(h^2)$.

From the general study of [6] we know that

$$tr(f(P(h,\rho=0))) = h^{-n+k}d_0(f)+h^{-n+k+1}d_1(f)+\mathcal{O}(h^{2+k-n}), \qquad (78)$$

and the important remark is now that $d_1(f)$ is *real.*

To prove the vanishing of the second term is thus equivalent to prove that it is purely imaginary.

The computation of the coefficients in (78) is deduced from the integral in the right hand side in (78) by application of the generalized stationary phase theorem to the expression

$$\int\int\int \exp(i(g\cdot x-x)\xi/h)f(p_0(\tfrac{1}{2}(x+g\cdot x),\xi))dx\,d\xi\,dg.$$

Here we observe that the amplitude $f(p_0(\frac{1}{2}(x + g \cdot x), \xi))$ is real and that the phase $(g \cdot x - x)\xi$ has a regular critical set of codimension $2k$, and that the signature of the hessian of the phase space restricted to the critical set is 0. In this situation, the proof of the stationary phase theorem gives immediately that the coefficients of the expansion are alternatively real and purely imaginary. In particular, the coefficient of h^{k+1} is purely imaginary.

The study of the vanishing of the second term in $J(f, \tau)$ is based on the same type of argument with a different phase (see the Fourier integral constructions in [6]). ∎

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