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AROUND SCOTT CORRECTION TERM(S)[†]

VICTOR IVRII

In this talk I would like to present the final version of my investigation concerning semi-classical asymptotics for Riesz' means of the spectral function for operators with singularities.

1. Origins of the problem. In mathematical physics the problem of the ground state energy of the large Coulomb system is considered as pretty important. There is a very large number N of electrons moving around few heavy nuclei and the final system is assumed to be neutral. With some errors one can modify this problem by the following way: the interaction between electrons is replaced by interaction with the "electron cloud" of the shape obtained in frames of the Thomas-Fermi theory. So, the multiparticle Hamiltonian is now the sum of one particle Hamiltonians and since electrons are fermions the ground state energy (the lowest eigenvalue) is replaced by the sum of negative eigenvalues of this one particle Schrödinger operator. One can find in [L],[IS],[GS] this reduction in the different aspects and in [I2] discussion of the problem from the point of view of the theory of semi-classical spectral asymptotics.

After rescaling the problem is reduced to the problem of semi-classical spectral asymptotics of the sum of negative eigenvalues for operator $-h^2\Delta + V(x)$. There is no trouble with infinity since potential $V(x)$ is quickly decreasing but there are problems with the singular points of $V(x)$: namely in the points (y_j) (centers of nuclei) $V(x) = -z_j|x-y_j|^{-1} + O(1)$ and this generate the correction term known in mathematical physics as *Scott correction*. This is the background of this my work. Now I want to present a problem in its general form.

2. Problem. consider a (matrix) h-differential operator $A = A_h$ with the Weyl symbol

$$A(x,\xi) = \sum_{|\alpha|\le m} a_\alpha(x)\xi^\alpha, \tag{1}$$

Hermitian and such that in $B(0,1)$

$$|D^\beta a_\alpha| \le c|x|^{\mu(m-|\alpha|)-|\beta|} \qquad \forall \alpha : |\alpha| \le m \quad \forall \beta : |\beta| \le K \tag{2}$$

with

$$\mu > \max\bigl(-1, -\frac{d}{m}\bigr). \tag{3}$$

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Moreover, we assume that

$$\langle a(x,\xi)v,v\rangle \ge \epsilon_0|\xi|^m|v|^2 \qquad \forall(x,\xi)\in T^*B(0,1)\quad \forall v\in\mathbb{K} \tag{4}$$

where $a(x,\xi)=\sum_{|\alpha|=m}a_\alpha(x)\xi^\alpha$ is the senior symbol of A. Here $|.|$ and $\langle .,.\rangle$ are the norm and inner product in $\mathbb{K}=\mathbb{C}^D$.

Let us consider operator A in the domain $X\subset\mathbb{R}^d$ assuming that

$$B(0,1)\subset X,\quad d\ge 2 \tag{5}$$

and

(6) A is the self-adjoint operator with $\mathfrak{D}(A)\supset C_0^m\bigl(B(0,1),\mathbb{K}\bigr)$.

We are interested in semi-classical asymptotics of the Riesz' mean

$$\int \operatorname{tr}\psi(x)e_\vartheta(x,x,0)dx$$

where $\psi\in C_0^K\bigl(B(0,\frac{1}{2})\bigr)$ and $e_\vartheta(.,.,\tau)$ is the Riesz' mean of order ϑ of the Schwartz kernel $e(.,.,\tau)$ of the spectral projector A, $\vartheta>0$:

$$e_\vartheta(.,.,\tau)=\int_0^\tau(\tau-\lambda)^\vartheta d_\lambda e(.,.,\lambda).$$

It was proven in [I1], section 10.1 that under appropriate condition linked with the microhyperbolicity[1)] asymptotics

$$\int \operatorname{tr}\psi(x)e_\vartheta(x,x,0)dx=\sum_{0\le j\le J}\kappa_{\vartheta,j}h^{-d+j}+O\bigl(R_1(\tau)\bigr) \tag{7}$$

holds where

$$R_1(\tau)=\begin{cases} h^{-d+\vartheta+1} & \text{for } \vartheta<\bar\vartheta_0,\\ h^{-d+\vartheta+1}\log h & \text{for } \vartheta=\bar\vartheta_0,\\ h^l & \text{for } \vartheta>\bar\vartheta_0\end{cases} \tag{8}$$

$$\begin{aligned} &\bar\vartheta_0=(d-1)(\mu+1)(-m\mu+\mu+1)^{-1} && \text{for } m\mu<\mu+1\\ &\bar\vartheta_0=+\infty && \text{for } m\mu\ge\mu+1,\\ &l=m\mu\vartheta(\mu+1)^{-1}, \end{aligned} \tag{9}$$

$\kappa_{\vartheta,j}$ are standard Weylian coefficients and $J=[\vartheta]+1$ for $\vartheta\le\bar\vartheta_0$, $J=d+[l]$ for $\vartheta\ge\bar\vartheta_0$ excluding the case $\vartheta=\bar\vartheta_0\in\mathbb{N}$ when $J=\vartheta$. Moreover, for $\vartheta>\bar\vartheta_0$ and $l\in\mathbb{N}$ one should replace the term with $j=d+l$ of the right-hand expression of (7) by $\kappa_{\vartheta,d+l}h^l$ by $\kappa_{\vartheta,d+l}h^l\log h$.

Furthermore, if $\vartheta<\bar\vartheta_0$ and standard condition (Ψ) to Hamiltonian trajectories is fulfilled at the energy level $\tau=0$ then one can replace in asymptotics (12.4.7) $O(h^{-d+\vartheta+1})$ by $o(h^{-d+\vartheta+1})$.

The principal part of asymptotics is $O(h^{-d})$ for $m\mu\vartheta>-d(\mu+1)$ and $O(h^{-d}\log h)$ for $m\mu\vartheta=-d(\mu+1)$ and $O(h^l)$ for $m\mu\vartheta<-d(\mu+1)$[2)]; so in the last case we have the estimate instead of the asymptotics. As pretty often, applied general machinery was powerful enough to get the most accurate Weyl asymptotics.

[1)] One can skip it for the Schrödinger operator.

[2)] Under obvious conditions there are equivalence relations.

3. Scott Correction Term. I. The next goal is to treat the case $\vartheta \ge \bar\vartheta_0$ and to improve this remainder estimate. This better estimate obtained under appropriate conditions requires additional non-Weylian term ωh^l in asymptotics. Physicists call this term "Scott correction". In some cases we'll obtain more than one such term for large ϑ. To achieve the goal we need to assume that

$$|D^\beta(a_\alpha - a^0_\alpha)| \le c|x|^{\mu(m-|\alpha|)+\nu-|\beta|} \qquad \forall\alpha : |\alpha| \le m \quad \forall\beta : |\beta| \le K \tag{10}$$

with $\nu > 0$ and a^0_α positively homogeneous of degrees $\mu(m-|\alpha|)$. Then three years ago I proved the following

Theorem 1. *Let operator A satisfy conditions* (12.4.2) – (12.4.6)*. Moreover, let $\vartheta \ge 1$ and $b_\alpha = a_\alpha - a^0_\alpha$ satisfy* (12.4.10) *with the positively homogeneous of degrees $(m-|\alpha|)\mu$ (matrix-valued) coefficients a^0_α. Let $\vartheta \ge \max(\bar\vartheta_0, 1)$. Then asymptotics*

$$\int \psi(x)\,\mathrm{tr}\, e_\vartheta(x,x,0)\,dx = \sum_{0\le j\le[\vartheta]+1} \kappa_{\vartheta,j} h^{-d+j} \omega h^l + R^* \tag{11}$$

holds with some coefficients $\kappa_{\vartheta,j}$ and coefficient ω and with the remainder estimate

$$R^* = \begin{cases} h^{-d+\vartheta+1}|\log h| & \text{for } \vartheta = \bar\vartheta_0,\\ h^{l''} & \text{for } \bar\vartheta_0 < \vartheta < \bar\vartheta_1,\\ h^{l'}|\log h| & \text{for } \vartheta = \bar\vartheta_1,\\ h^{l'} & \text{for } \vartheta > \bar\vartheta_1 \end{cases} \tag{12}$$

$$\begin{aligned} l' &= (m\mu\vartheta + \nu)(\mu+1)^{-1},\\ l'' &= \bigl(m\mu\vartheta - (d-\vartheta-1)\nu\bigr)(\mu+\nu+1)^{-1},\\ \bar\vartheta_1 &= \bigl(d(\mu+1)+\nu\bigr)(\mu+1-m\mu)^{-1} \end{aligned} \tag{13}$$

Remark 2. (i) Actually, there should be condition $l \ne -d+j$. If $l = -d+j$ then one should include a factor $\log h$ in term $\kappa_{\vartheta,j}h^{-d+j}$.

(ii) Coefficients $\kappa_{\vartheta,j}$ with $-d+j < l$ are Weylian.

(iii) For $l \notin \mathbb{Z}$ non-Weylian term is equal to

$$\omega h^l = \int_{\mathbb{R}^d} \bigl(\mathrm{tr}\, e^0_\vartheta(x,x,0) - \mathrm{Weyl}(x)\bigr)\,dx \tag{14}$$

where integral convergres while both integral $\int \mathrm{tr}\, e^0_\vartheta(x,x,0)$ and $\int \mathrm{Weyl}(x)dx$ diverge at infinity.

This old theorem fails to be correct for $\vartheta < 1$ and fails to be maximally precise for $\vartheta > 1$.

4. Scott Correction Term(s). II.

Theorem 3. *Let all the conditions of theorem 1 be fulfilled excluding may be condition $\vartheta \geq 1$. Let*

(i) Moreover, let condition

(15) $a_\alpha - a^0_\alpha$ *are positively homogeneous of degrees* $\mu(m - |\alpha|)$

be fulfilled. Then asymptotics

$$\int \psi(x) e_\vartheta(x,x,\tau)\,dx = \sum_{p:p<d+L} \kappa_{\vartheta,p} h^{-d+p} + \sum_{p<d+L,q:-d+p=(m\mu\vartheta+\nu j)(\mu+1)^{-1}} \kappa'_{\vartheta,p} h^{-d+p} \log h + \sum_{q:(m\mu\vartheta+\nu q)(\mu+1)^{-1}<L} \omega_{\vartheta,q} h^{(m\mu\vartheta+\nu q)(\mu+1)^{-1}} + O\bigl(R^{**}(h)\bigr) \tag{16}$$

holds with $R^{**}(h)$ given by

$$R^{**} = \begin{cases} h^{l''} & \text{for } (m\mu+\nu)\vartheta + (d-1)(\mu+1) > 0, \\ & \quad \vartheta - (\mu+1)(d-1)(\mu+\nu+1)^{-1} \notin \mathbb{Z}^+ \\ h^{l'''}|\log h| & \text{for } (m\mu+\nu)\vartheta + (d-1)(\mu+1) > 0, \\ & \quad \vartheta - (\mu+1)(d-1)(\mu+\nu+1)^{-1} \in \mathbb{Z}^+ \\ h^{l'''}\log h & \text{for } (m\mu+\nu)\vartheta + (d-1)(\mu+1) = 0 \\ h^{l'''} & \text{for } (m\mu+\nu)\vartheta + (d-1)(\mu+1) < 0 \end{cases} \tag{17}$$

with

$$l''' = (m\mu+\nu)\vartheta(\mu+1)^{-1}, \qquad L = \min(l'', l'''). \tag{18}$$

$p, q \in \mathbb{Z}^+$ everywhere.

(ii) Moreover, for $\vartheta \leq \bar{\vartheta}_1$ one can reject condition (15).

(iii) Let us assume that

$$|D^\beta(a_\alpha - a^0_\alpha - b^0_\alpha)\| \leq c|x|^{(m-|\alpha|)\mu+\nu'-|\beta|} \tag{19}$$

where a^0_α, b^0_α are positively homogeneous of degrees $(m-|\alpha|)\mu$, $(m-|\alpha|)\mu+\nu$ respectively, $\nu' > \nu$. Then asymptotics (16) *holds with R^{**} replaced by $R^{**} + O(h^s)$ with $s = (m\mu\vartheta + \nu')(\mu+1)^{-1}$.*

Remark 4. One can express coefficients $\omega_{\vartheta,q}$ in terms of operators A^0, B with quasihomogeneous symbols. For example,

$$\omega_{\vartheta,1} = -\vartheta \int \bigl(\operatorname{tr}(B_x e^0_{\vartheta-1})(x,x,0 - \mathrm{Weyl}\bigr)dx \tag{20}$$

with all the remarks concerning ω.

5. Accurate asymptotics. To improve all these remainder estimates one need to involve propagation of singularities. Let us assume that

Let us assume that

(T) There exist closed in $(\mathbb{R}^d \setminus 0) \times \mathbb{R}^d$ quasi-conical sets Λ^+ and Λ^- and numbers $T_0 > 0$, $\epsilon_1 > 0$ such that

$$\Lambda^+ \cup \Lambda^- = \Sigma^0 = \bigl\{(x,\xi) \in (\mathbb{R}^d \setminus 0) \times \mathbb{R}^d : \det A^0(x,\xi) = 0\bigr\} \tag{21}$$

and for every point $(\bar{x},\bar{\xi})$ belonging to ϵ_1-neighborhood of $\Lambda^\pm$ intersected with $\bigl\{(x,\xi) : |x| = 1\bigr\} \cap \Sigma^0$ all the generalized bicharacteristics of the symbol $-A^0(x,\xi)$ passing through $(\bar{x},\bar{\xi})$ in the direction of $\pm t > 0$ are infinitely long with respect to t and along them

$$(x(t),\xi(t)) \in \Lambda^\pm, \quad |x(t)| \geq 2|\bar{x}| \qquad \forall t : \pm t \geq T_0; \tag{22}$$

these conditions should be fulfilled for every sign "$\pm$" separately.

Theorem 5. *Let conditions of theorem 1 and condition* (T) *be fulfilled.*

(i) Moreover, let condition (10) *be fulfilled. Then asymptotics*

$$\begin{aligned}\int \psi(x) e_\vartheta(x,x,\tau)\,dx = \sum_{p:p<d+L} \kappa_{\vartheta,p} h^{-d+p} + \\ \sum_{p<d+L,\, q: -d+p=(m\mu\vartheta+\nu q)(\mu+1)^{-1}} \kappa'_{\vartheta,p} h^{-d+p} \log h + \\ \sum_{q:(m\mu\vartheta+\nu q)(\mu+1)^{-1}<L} \omega_{\vartheta,q} h^{(m\mu\vartheta+\nu q)(\mu+1)^{-1}} + O\bigl(R^\#(h)\bigr)\end{aligned} \tag{23}$$

holds with remainder estimate

$$R^\# = h^L, \qquad L = \min(-d+1+\vartheta, l''') \tag{24}$$

and l''' defined by (18). *Moreover, condition* (15) *is not necessary provided $m\mu\vartheta + \nu \geq L$.*

(ii) Furthermore, let conditions of (i) be fulfilled. Let

$$\vartheta(m\mu + \nu - \mu - 1) + (d-1)(\mu+1) > 0 \tag{25}$$

(then (i) yields the remainder estimate $O(h^{-d+1+\vartheta})$) and condition (Ψ) *for operator A in $B(0,1)$ be fulfilled. Then one can replace remainder estimate $O\bigl(h^{-d+\vartheta+1}\bigr)$ by $o\bigl(h^{-d+\vartheta+1}\bigr)$.*

(iii) Replacing condition (15) *by* (19) *one should replace $R^\#$ by $R^\# + O(h^s)$ with $s = (m\mu\vartheta + \nu')(\mu+1)^{-1}$.*

6. Final Remarks. Let us discuss condition (T) and some generalizations of our results.

Remark 6. (i) One can see easily that for $A^0 = \bigl(|\xi|^2 - |x|^{2\mu}\bigr)^{\frac{m}{2}}$ with $\mu \in \bigl(-1,0\bigr) \cup \bigl(0,(m-1)^{-1}\bigr)$ condition (T) is fulfilled (because we treat energy level 0) and therefore one can apply theorem 5. For $\mu = -\frac{1}{2}$, $d=3$, $\vartheta = 1$ the numerical value of the coefficient ω_0 is well-known (see [IS] for example).

(ii) One can extend easily theorems 1,3 to the case when X is the conical domain (in the neighborhood of 0) and on ∂X the Dirichet boundary condition are given. Moreover, one could extend theorem 5 under nice propagation of singularities results. Namely, in condition (T) was important the following corollaries:

(26) For $t = T_0$ and $(x,\xi) \in \Lambda^{\pm}_{\epsilon_1} \cap \{|x| = 1\}$ $K^{\pm}_t(x,\xi) \subset \Lambda^{\pm} \cap \{|x| \geq 2\}$ where $K^{\pm}_t$ mean propagation of singularities "cones" at the energy level 0 for A^0 (see sections 2.2,3.3 of [I1]). Moreover, this property is stable with respect to small perturbations of A^0.

and

(27) $(x,\xi) \notin K^{\pm}_t(x,\xi)$ for $t > 0$. Moreover, this property is also stable.

Exactly these conditions with the stability condition fits for boundary-value problems. Due to geometric interpretation (see section 3.3[I1]) one can replace $K_t(x,\xi)$ by the union of the generalized bicharacteristics (and then stability is achieved automatically).

(iii) Let us consider $\mu = 0$ and $A^0(x,\xi)$ $(1,0)$-homogeneous of degree m on (x,ξ) and the energy level $\tau = 1$ instead of $\tau = 0$. We obtain this problem when we treat asymptotics of the Riesz' means when spectral parameter τ tends to $+\infty$. In order to prove condition (T) let us notice that one can take function $\phi = \langle x,\xi\rangle$ in the analysis of the propagation of singularities in section 3.1[I1]. For $x \in \partial X$ this function is constant at layers $\{(x,\xi + n\lambda), \lambda \in \mathbb{R}\}$ where n is a normal to ∂X at x and we assume that X is conical set; moreover, the microhyperbolicity conditions are fulfilled with $\mathcal{T} = H_\phi$. Therefore, for $(x,\xi) \in \Sigma_{1,f}$, $(y,\eta) \in K^{\pm}(x,\xi)$ (see definitions of $\Sigma_{\tau,b}$, $\Sigma_{\tau,f}$ in chapter 3 [I1]) inequality $\pm\langle y,\eta\rangle \geq \pm\langle x,\xi\rangle + \epsilon_0 t$ holds. Therefore condition (27) is fulfilled. Moreover, ellipticity yields that ξ is bounded at Σ_1 and $\langle x,\xi\rangle |x|^{-1}$ is bounded at $\Sigma_{1,b}$. Therefore, picking $\Lambda^{\pm} = \{\pm\langle x,\xi\rangle \geq -\epsilon_1|x|\}$ with sufficiently small ϵ_1 we obtain $K^{\pm}_t(x,\xi) \subset \{(y,\eta), |y| \geq \epsilon(|x| + t)\}$ for $t \geq 0$ and therefore condition (26) is fulfilled also. Note, that condition (25) is now "$(\nu - 1)\vartheta > 1 - d$. Moreover, that non-Weylian terms are $\omega_q \tau^{\vartheta - \frac{1}{m}\nu q}$ while the Weylian terms are $\kappa_p \tau^{\vartheta + \frac{1}{m}(d-p)}$ and the logarithmic factor appear as soon as these exponents coincide or one of them vanishes. For $\nu = 1$ condition (25) is fulfilled for all ϑ and there is a lot of terms with logarithms.

(iv) All these arguments in (ii),(iii) fit for other boundary conditions provided for fixed h the problem is elliptic in the classical sense and operator is semi-bounded from below.

Remark 7. Let us assume that $X = \mathbb{R}^d$ (or X is a cone). Moreover, let the stabilization condition (10) be fulfilled as $|x| \to \infty$ as well but with an operator A^∞

and exponents $\mu' \in (-1,0), \nu' < 0$ instead of A^0 and μ, ν. Moreover, let us assume that condition (T) is fulfilled for this operator A^∞ as well with the sets $\Lambda^\pm_\infty$ instead of $\Lambda^\pm$. Let us define sets $\Lambda^\pm_1$ as small quasi-conical vicinities of $\Lambda^\pm$, $\Lambda^\pm_\infty$ intersected with $\Sigma = \bigl\{(x,\xi) \in (\mathbb{R}^d \setminus 0) \times \mathbb{R}^d : \det A(x,\xi) = 0\bigr\}$; these sets we define for $|x| \le \epsilon$ and $|x| \ge R$ with $\epsilon > 0$ very small and R very large. Finally, let us assume that there exists t_0 such that if $(x(0), \xi(0))$ lies in the (small) $\Lambda^\pm_1 \cap \{|x| \le \epsilon\}$ then $(x(\pm t_0), \xi(\pm t_0)) \in \Lambda^\pm_1 \cap \{|x| \ge R\}$.

Under these assumptions we control propagation of singularities for very large T ($\asymp h_{\text{eff}}^{-s}$ with an arbitrarily large s) and therefore *in frames of theorem 5 and these assumptions the remainder estimate is* $O\bigl(h^{l'''}\bigr)$ with l''' defined above even if $l''' > -d + 1 + \vartheta$. Moreover, *for* $(\mu + 1)d + m\mu\vartheta < 0$ *one can take* $\psi = 1$.

As an example one can consider $X = \mathbb{R}^d$ and a Schrödinger operator with the potential $W(|x|)$ where $W(r)$ is positively homogeneous of degrees 2μ and $2\mu'$ for $|x| \le \epsilon$ and $|x| \ge R$ respectively $-1 < \mu' \le \mu < 0$ and $W(r) < 0$, $\frac{d}{dr} r^2 W(r) < 0 \quad \forall r$. Moreover, one can perturb slightly this Schrödinger operator and get rid of its spherical symmetry and homogeneity.

One can find the detailed exposition of all these results and their proofs in the *revised version* of section 12.4 [I1].

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