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Riesz means of bounded states and semi-classical limit connected with a Lieb-Thirring conjecture II

by

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ABSTRACT. — Let: $e_1(h) \leqq e_2(h) \leqq \ldots \leqq e_i(h) \leqq \ldots < 0$ be the negative eigenvalues of $P(h) = -h^2 \Delta + V$ where V is a C^∞ potential such that $\lim\limits_{|x| \to +\infty} \inf V(x) > 0$ and consider the quantity: $r_\gamma(h, V) = \sum(-e_j(h))^\gamma$, $\gamma > 0$.

Lieb and Thirring proved, under the condition $\gamma > \text{Max}(0, 1 - n/2)$, the existence of a universal, best constant, $L_{\gamma, n}$, satisfying: $h^n r_\gamma(h, V) \leqq L_{\gamma, n} \int (-V_-)^{\gamma + n/2} dx$.

A natural problem is to compare $L_{\gamma, n}$ with the classical limit:

$$L_{\gamma, n}^{cl} = \lim_{h \downarrow 0} \left(\left[\int (-V_-)^{\gamma + n/2} dx \right]^{-1} . h^n r_\gamma(h, V) \right)$$

By a very accurate study of harmonic oscillators we prove here that $L_{\gamma, n}^{cl} < L_{\gamma, n}$ for every $\gamma < 1$ and $n \geqq 1$.

RÉSUMÉ. — Soit : $e_1(h) \leqq e_2(h) \leqq \ldots \leqq e_j(h) \leqq \ldots < 0$ les valeurs propres négatives de $P(h) = -h^2 \Delta + V$ où V est un potentiel C tel que : $\lim\limits_{|x| \to +\infty} \inf V(x) > 0$ et considérons la quantité : $r_\gamma(h, V) = \sum(-e_j(h))^\gamma$, $\gamma > 0$.

Lieb et Thirring ont montré, sous la condition $\gamma > \text{Max}(0, 1 - n/2)$, l'existence d'une meilleure constante universelle, $L_{\gamma, n}$, satisfaisant : $h^n r_\gamma(h, V) \leqq L_{\gamma, n} \int (-V_-)^{\gamma + n/2} dx$.

Il est alors naturel de comparer $L_{\gamma,n}$ avec sa limite classique:

$$L^{cl}_{\gamma,n} = \lim_{h \downarrow 0} \left(\left[\int (-V_-)^{\gamma+n/2}\, dx \right]^{-1} . h^n r_\gamma (h, V) \right)$$

Par une étude fine d'oscillateurs harmoniques nous prouvons ici que $L^{cl}_{\gamma,n} < L_{\gamma,n}$ pour tout $\gamma < 1$ et $n \geqq 1$.

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0. INTRODUCTION

This paper is a continuation of $[\text{HE-RO}]_2$ where we have stated results related with some Lieb-Thirring's conjectures, using semi-classical methods.

Let us briefly recall the problem. Consider the Schrödinger operator in $\mathbb{R}^n$:

$$P(h) = -h^2 \Delta + V \tag{0.1}$$

where V is a C^∞ potential such that $\lim\limits_{|x| \to +\infty} \inf V(x) > 0$.

Let: $e_1(h) \leqq e_2(h) \leqq \ldots \leqq e_j(h) \leqq \ldots < 0$ be the negative eigenvalues of $P(h)$ and consider the quantity:

$$r_\gamma(h, V) = \sum (-e_j(h))^\gamma, \qquad \gamma > 0. \tag{0.2}$$

r_γ is the Riesz mean of order γ [HO]. This quantity appears in some physical problem ([HE-SJ], [LA], [PE], [SO-WI]).

Denote: $V_- = \text{Min}(V, 0)$.

Lieb and Thirring [LI-TH] proved, under the condition $\gamma > \text{Max}(0, 1 - n/2)$, the existence of a universal, best constant, $L_{\gamma,n}$, satisfying:

$$h^n, r_\gamma(h, V) \leqq L_{\gamma,n} \cdot \int (-V_-)^{\gamma+n/2}\, dx \quad \text{for every V and } h > 0. \tag{0.3}$$

Of course, by scaling, we can reduce to $h = 1$ but it is easier for us to introduce the Planck constant h. A natural problem is to compare $L_{\gamma,n}$ with the classical limit:

$$L^{cl}_{\gamma,n} = \lim_{h \downarrow 0} \left(\left[\int (-V_-)^{\gamma+n/2}\, dx \right]^{-1} . h^n r_\gamma (h, V) \right) \tag{0.4}$$

For V smooth, $\lim_{|x| \to +\infty} \inf V > 0$, one can prove that $L^{cl}_{\gamma, n}$ exists and has the numerical value:

$$L^{cl}_{\gamma, n} = [(2\sqrt{\pi})^n \Gamma(\gamma + 1 + n/2)]^{-1} . \Gamma(\gamma + 1)$$

Γ being the gamma function.

Clearly we have:

$$(0.5) \qquad L_{\gamma, n} \geqq L^{cl}_{\gamma, n}$$

and it was proved in [AI-LI] that:

(0.6) $\gamma \to L_{\gamma, n}/L^{cl}_{\gamma, n}$ is monotone, non increasing. So a natural question is to compute the smallest γ_c such that:

$$(0.7) \qquad L_{\gamma, n} = L^{cl}_{\gamma, n}$$

If (0.7) holds for γ_c, then, from (0.6), we have also (0.7) for every $\gamma > \gamma_c$. In [HE-RO]$_2$, using Lieb-Thirring's results and functional calculus in the context of h-dependent pseudodifferential case, we have got another proof of the inequality: $L_{\gamma, 1} > L^{cl}_{\gamma, 1}$ for every $\gamma < 3/2$ (the first proof of that is due to Lieb and Thirring [LI-TH]). In this paper we prove a result valid in all dimensions:

THEOREM 0.1. – *For every $n \geqq 1$ and every real $\gamma < 1$ we have:*

$$L_{\gamma, n} > L^{cl}_{\gamma, n}. \quad \blacksquare$$

This result seems to be in contradiction with some conjectures given in [LI-TH] (p. 272 it was conjectured that $\gamma_{c, 3} \cong 0.863$ and $\gamma_{c, n} \cong 0$ for $n \geqq 8$).

In the last section we try to clarify the limit case $\gamma = 1$. The proof of theorem (0.1) consists in an accurate computation of $R(h, V)$ for the harmonic oscillator: $V(x) = x^2 - 1$. For that we use expansions in h implicitly proved in the physical litterature ([SO-WI], [CA]) in the context of De Haas-Van Alphen effect (*see* [HE-SJ] for a mathematical proof).

Remark that we have, using (1.2), (1.3), (1.4):

$$\lim_{h \downarrow 0} h . r_\gamma(h) = \frac{\alpha_0}{\Gamma(\gamma + 2)} = \frac{\Gamma(\gamma + 1)}{2\Gamma(\gamma + 2)} = \frac{1}{2(\gamma + 1)}$$

We can also compute this limit using general results proved in [HE-RO]$_1$:

$$\lim_{h \downarrow 0} h r_\gamma(h) = \frac{1}{2\pi} \iint (1 - x^2 - \xi^2)^\gamma_+ \, dx \, d\xi$$

$$= \int_0^W r(1 - r^2)^\gamma \, dr = \frac{1}{2(\gamma + 1)}$$

the two computations agree!

1. PROOF OF THEOREM (0.1): PRELIMINARY RESULTS IN THE $n=1$ CASE

First of all, we recall some results previously used in the study of the de Haas-Van Alphen effect in [HE-SJ]. Let us denote:

$$r_\gamma(h) = \sum_{j \geqq 0} (1-(2j+1)h)_+^\gamma \tag{1.1}$$

From [He-Sj] [Lemma (2.1)] we have the following asymptotic as $h \to 0$:

$$r_\gamma(h) = \Gamma(\gamma+1)\left(h^\gamma \rho_\gamma\left(\frac{1}{h}\right) + h^{-1}\sigma_\gamma(h)\right) + O(h^\infty) \tag{1.2}$$

where:

$$\rho_\gamma(s) = \sum_{j>0} (\pi j)^{-\gamma-1} \cos\left(j\pi(s+1) - \frac{\pi}{2}(\gamma+1)\right) \tag{1.3}$$

ρ_γ is a 2-periodic function.

$$\sigma_\gamma(h) = \frac{1}{2}\sum_{j=0}^{\infty} \frac{\alpha_j}{\Gamma(\gamma+2-2j)} h^{2j} (\operatorname{mod} O(h^\infty)) \tag{1.4}$$

The coefficients α_i are given by the expansion:

$$t(sht)^{-1} = \sum_{j \geqq 0} \alpha_j t^{2j}, \qquad t \to 0 \tag{1.5}$$

In particular we have:

$$\alpha_0 = 1, \qquad \alpha_1 = -\frac{1}{6} \tag{1.6}$$

We consider first the one dimensional case to see how the proof will work in the general case. For $\gamma < 1$, we have the following asymptotic for $r_\gamma(h)$:

$$r_\gamma(h) = \frac{1}{2(\gamma+1)h} + h^\gamma \Gamma(\gamma+1)\rho_\gamma\left(\frac{1}{h}\right) + O(h) \tag{1.7}$$

If for some $s_0 \in \mathbb{R}$ we have $\rho_\gamma(s_0) > 0$, then clearly we get a contradiction with the equality: $L_{\gamma,1} = L_{\gamma,1}^{cl}$ by choosing a sequence $h_k \downarrow 0$ such that: $\frac{1}{h_k} = q_0 (\operatorname{mod} 2)$.

We have no general proof of this property of ρ_γ but it is sufficient for us to prove it for γ near 1:

LEMMA (1.1). – *There exist real numbers s_0, s_1 and $\varepsilon_0 > 0$ such that for $|1-\gamma| \leqq \varepsilon_0$ we have:*

$$\rho_\gamma(s_0) > 0 \quad \textit{and} \quad \rho_\gamma(s_1) < 0. \quad \blacksquare$$

As a consequence we get $L_{\gamma,1} > L^{cl}_{\gamma,1}$ if $\gamma < 1$. Recall that we gave a proof for this property when $\gamma < 3/2$ in [HE-RO]$_1$, but the proof here is much simpler and will work in any dimension.

Proof of Lemma (1.1). – It is sufficient to consider the case $\gamma = 1$ (the result follows by perturbation). We have:

$$\begin{aligned}\rho_1(s) &= \sum_{j \geq 1} (j\pi)^{-2} \cos(j\pi(s+1) - \pi) \\ &= \sum_{j \geq 1} (-1)^{j+1} (j\pi)^{-2} . \cos(j\pi s)\end{aligned}$$

But ρ_1 is the Fourier serie of a 2-periodic parabolic function: $f(s) = a + bs^2$ $(-1 < s < 1)$. (We have to thank J. P. Guillement for this remark.) Elementary calculus gives:

$$f(s) = a + \frac{b}{3} + 4b . \sum_{j \geq 1} (-1)^j (j^2 \pi^2)^{-1} \cos(j\pi s)$$

So $\rho_1(s)$ has the simple form:

$$\rho_1(s) = \frac{1}{12} - \frac{s^2}{4}, \qquad -1 < s < 1$$

Then we can take:

$$s_0 = 0 \left(\rho_1(s_0) = \frac{1}{12} \right) \quad \text{and} \quad s_1 = 1 \left(\rho_1(s_1) = -\frac{1}{6} \right).$$

2. PROOF OF THEOREM (0.1): THE *n*-DIMENSIONAL CASE

We have to consider:

$$\begin{aligned}r^{(n)}_\gamma(h) &= \sum_{j_1, \ldots, j_n : j_l \in \mathbb{N}} (1 - 2(j_1 + \ldots + j_n) h - nh)^\gamma_+ \\ &= \sum_{l \in \mathbb{N}} \Big(\sum_{j_1 + j_2 + \ldots + j_n = l} 1 \Big) (1 - 2lh - nh)^\gamma_+\end{aligned}$$

By induction on l, we get:

$$\sum_{j_1 + j_2 + \ldots + j_n = l} 1 = \sum_{k=0}^{l} C^{n-2}_{n-2+k} = C^{n-1}_{n+l-1}$$

(Pascal triangle rule)

Finally we have:

$$r^{(n)}_\gamma(h) = \sum_{l \geq 0} C^{n-1}_{l+n-1} (1 - 2lh - nh)^\gamma_+ \tag{2.1}$$

Now the game is to compute $r_\gamma^{(n)}(h)$ in term of some $r_\delta^{(1)}(g)$ where:

$$g=\frac{h}{1-(n-1)h} \qquad (h \text{ small})$$

we have:

$$(1-2lh-nh)_+^\gamma=(1-(n-1)h)^\gamma.(1-(2l+1)g)_+^\gamma$$

and

$$\text{(2.2)} \qquad C_{n-1+l}^{n-1}=\sum_{k=0}^{n-1}\alpha_n^k.(2l+1)^k$$

Now write:

$$\begin{aligned}((2l+1)g)^k&=(1-(2l+1)g-1)^k(-1)^k\\ &=\sum_{0\leq m\leq k} C_k^m(-1)^m(1-(2l+1)g)^m\end{aligned}$$

Using (2.1) and (2.2) we get:

$$\text{(2.3)} \qquad r_\gamma^{(n)}(h)=(1-(n-1)h)^\gamma.\sum_{k=0}^{n-1}\sum_{m=0}^{k}\beta_m^k g^{-k} r_{m+\gamma}(g)$$

with: $\beta_m^k=(-1)^m.\alpha_n^k.C_k^m$.

We can apply to $r_\gamma^{(n)}(h)$ the general result stated in [HE-RO]$_1$:

$$\text{(2.4)} \qquad \begin{aligned}&r_\gamma^n(h)=h^{-n}.C_{n,\gamma}+O(h^{-n+1+\gamma})\\ &\text{for } \gamma\leq 1 \text{ (the coefficient of } h^{-n+1} \text{ vanishes)}\end{aligned}$$

From (2.3) we compute an asymptotic for $r_\gamma^{(n)}(h)$ with remainder $O(h^{-n+2})$; using (1.2) and (2.4) we have only to consider the oscillating coefficient of $g^{-n+1+\gamma}$. This coefficient comes from (2.3) by the contribution corresponding to $k=n-1$ and $m=0$. This gives:

$$\text{(2.5)} \qquad r_\gamma^n(h)=h^{-n}.c_{n,\gamma}+\alpha_n^{n-1}.\Gamma(\alpha+1)\,\rho_\gamma(g^{-1})g+O(h^{-n+2})$$

From (2.2) we have:

$$\alpha_n^{n-1}=(2^{n-1}.(n-1)!)^{-1}$$

Suppose n odd. As in section 2, consider a sequence $h_k\downarrow 0$, $g_k^{-1}\equiv s_1 \pmod 2$ and we get the same conclusion. This finishes the proof of theorem (0.1) for every n.

3. THE $\gamma=1$ CASE $n\geq 2$

The same computation as in section 2 gives:

$$\text{(3.1)} \quad \begin{aligned}&h^n.r_1^{(n)}(h)\\ &=c_{0,1}^{(n)}+h^2(c_{2,1}^{(n)}+(-1)^{n-1}.(2^{n-1}.(n-1)!)^{-1}\rho_1(g))+O(h^3)\end{aligned}$$

From $[\text{HE-RO}]_2$ we have:

$$c_{2,1}^{(n)} = -\frac{1}{24}(2\pi)^{-n}\operatorname{vol}(S^{n-1}).\int (-V)_+^{(n/2)-1}.\Delta V(x)\,dx$$

where $V(x) = x^2 - 1$ so $\Delta V = 2n$ and:

$$c_{2,1}^{(n)} = -\frac{1}{24}(2n)(2\pi)^{-n}(\operatorname{vol} S^{n-1})^2\int_0^1 (1-r^2)^{1/2-1}\,r^{n-1}\,dr$$

$n=2$:

$$c_{2,1}^{(2)} = -\frac{1}{6}\int_0^1 (1-r^2)^0.r\,dr = -\frac{1}{12}$$

So, the coefficient of h^2 in (3.1) is non positive and we have no contradiction with $L_{1,2}^{cl} < L_{1,2}$

$n=3$:

$$c_{2,1}^{(3)} = -\frac{6}{24}(2\pi)^{-3}(4\pi)^2\int_0^1 (1-r^2)^{1/2}\,r^2\,dr$$

$$\int_0^1 (1-r^2)^{1/2}\,r^2\,dr = \frac{\pi}{16}\left(=\frac{1}{2}B\left(\frac{3}{2},\frac{3}{2}\right)=\frac{1}{4}\left(\Gamma\left(\frac{3}{2}\right)\right)^2\right)$$

then: $C_{2,1}^{(3)} = -\dfrac{1}{32}$.

So the coefficient of h^2 in (3.1) can be written as: $-\dfrac{1}{32}+\dfrac{\delta_1(h)}{8}<0$ which don't give any contradiction with $L_{1,3}^{cl} < L_{1,3}$.

General case:

$$\int_0^1 (1-r^2)^{n/2-1}\,r^{n-1}\,dr = \frac{1}{2}B\left(\frac{n}{2},\frac{n}{2}\right) = \frac{[\Gamma(n/2)]^2}{2(n-1)!}$$

and:

$$\operatorname{vol}(S^{n-1}) = \frac{n.\pi^{n/2}}{\Gamma(n/2)+1)} = \frac{2\pi^{n/2}}{\Gamma(n/2)}$$

Then: $C_{2,1}^{(n)} = -\dfrac{n}{6.2^n(n-1)!}$.

The coefficient of h^2 in (3.1) is:

$$\frac{1}{2^{n-1}(n-1)!}\left(-\frac{n}{12}+\rho_1(g)\right)<0 \quad \text{for every } n \geqq 2.$$

In conclusion we are not able to decide something about the Lieb-Thirring conjecture for $\gamma = 1$, $n \geqq 2$. Anyhow we know from Theorem (0.1) that, for every $n \geqq 2$, the critical constant $\gamma_{c,n}$ satisfies: $\gamma_{c,n} \geqq 1$.

4. FURTHER COMPUTATIONS FOR THE HARMONIC OSCILLATOR

For $\gamma \geqq 1$, integer, it is possible to get a more accurate formula for $r_\gamma^{(n)}(h)$ related to $P(h) = -\Delta + x^2$.

First of all, we have an explicit formula for $r_\gamma(h) = r_\gamma^{(1)}(h)$. To see that we start with:

$$r_\gamma(h) = h^\gamma f_\gamma(h^{-1}),$$

$$(4.1) \qquad f_\gamma(s) = (4i\pi)^{-1}\,\Gamma(\gamma+1)\int_{c+i\mathbb{R}} t^{-\gamma-1}\,e^{st}\,(sht)^{-1}\,dt, \qquad c>0$$

Remember that $z e^{zx}(e^z-1)^{-1} = 1 + \sum_{j\geqq 1} (j!)^{-1}\,B_j(x).z^j$ where the B_j are the Bernouilli's polynomials ([DI], p. 298); then the residue theorem gives:

$$(4.2) \qquad \begin{cases} f_\gamma(s) = \Gamma(\gamma+1).(\rho_\gamma(s) + 2^\gamma(\gamma+1)^{-1}\,B_{\gamma+1}((s+1)/2) \\ \rho_\gamma(s) = \sum_{j\geqq 1} (j\pi)^{-\gamma-1}\cos((s+1)j\pi - (\gamma+1)\pi/2) \end{cases}$$

By a known property of the Bernouilli's polynomials we have also:

$$(4.3) \qquad \rho_\gamma(s) = -2^\gamma((\gamma+1)!)^{-1}\,B_{\gamma+1}((s+1)/2) \qquad \text{for} \quad 0 \leqq s \leqq 1$$

Of course, we can extend (4.3) using:

$$B_j(x+1) - B_j(x) = jx^{j-1}, \qquad B_j(1-x) = (-1)^j B_j(x)$$

For $\gamma = 1$ we have already remark in section 1 that:

$$(4.4) \qquad \rho_1(s) = 1/12 - s^2/4 \qquad \text{for} \quad 0 \leqq s \leqq 1$$

Using the explicit knowledge of Bernouilli's polynomials we get:

$$(4.5) \qquad \rho_2(s) = -s(s^2-1)/12, \qquad 0 \leqq s \leqq 1$$

$$(4.6) \qquad \rho_3(s) = -s^4/48 + s^2/24 - 7/720, \qquad 0 \leqq s \leqq 1$$

We can apply this to precise the sign of $r_1^{(n)}(h) - h^{-n} c_{0,1}^{(n)}$ for $n = 2, 3$. We have

$$r_1^{(2)}(h) = (2g)^{-1}\,r_1(g) - (2g(1+g))^{-1}\,r_2(g^{-1}),$$
$$(g = h(1-h)^{-1})$$

Using (4.2) we get:

$$r_1^{(2)}(h) = (24)^{-1}\,h^{-2} - (12)^{-1} + 2^{-1}\,\rho_1(g^{-1}) - h\,\rho_2(g^{-1})$$

From (4.4) and (4.6) we see easily that $r_1^{(2)}(h) - (24)^{-1}\,h^2 < 0$ for every h in $]0, 1/2]$, hence for every $h > 0$ because from (2.1) we get $r_1^{(2)}(h) = 0$ if $h > 1/2$.

By an easy computation we get:

$$r_1^{(3)}(h)=(1-2h)g^{-2}r_3(g)/8 \\ -(g^{-2}/4+g^{-1}/2)r_2(g)+(g^{-2}+4g^{-1}+4g^{-1}+3)r_1(g)/8$$

with $g=h(1-2h)^{-1}$.

From (4.2) we know that $r_1^{(3)}$ has a natural decomposition into a sum of a rational function and an oscillating function in $h: r_1^{(3)}(h)=\mathrm{Rat}_3(h)+\mathrm{Osc}_3(h)$. We have explicitely:

$$(4.7)\quad \begin{cases} \mathrm{Rat}_3(h)=(192)^{-1}h^{-3}-(32)^{-1}h^{-1}+17(960)^{-1}h \\ \mathrm{Osc}_3(h)=(3h/4)\rho_3(g^{-1})-(1/2)\rho_2(g^{-1})+(1-h^2)\rho_1(g^{-1})/8 \end{cases}$$

Now, using (4.4), (4.5), (4.6) we get: $r_1^{(3)}(h)-(192)^{-1}h^{-3}\leqq 0$ for every h in $]0,1/2]$, hence for every $h>0$ because from (2.1) we get $r_1^{(3)}(h)=0$ if $h>1/3$.

Note added in proof: After this paper was accepted we heard about the paper by A. Martin, New Results on the Moments of the Equivalues of the Schrödinger Hamiltonian and Applications, *Commun. Math. Phys.*, n° 129, 1990, pp. 161-168, which gives an improvement of the Lieb-Thirring bound in the case $n=3$.

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