A SEMICLASSICAL HEAT TRACE EXPANSION FOR THE PERTURBED HARMONIC OSCILLATOR

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Abstract. In this paper we study the heat trace expansion of the perturbed harmonic oscillator by adapting to the semiclassical setting techniques developed by Hitrick-Polterovich in [HP]. We use the expansion to obtain certain inverse spectral results.

1. Introduction

Hitrik and Polterovich obtained in [HP] a simple formula for the on-diagonal heat kernel expansion of the Schrödinger operator, $-\Delta + V$, with $V \in C^\infty(\mathbb{R}^n)$ a bounded real-valued potential. In this paper we apply their techniques to study the semiclassical behavior of the on-diagonal heat kernel expansion for the perturbed semi-classical harmonic oscillator

$$H = \sum_{i=1}^{n} \left(-\frac{\hbar^2}{2} \frac{\partial^2}{\partial x_i^2} + \frac{x_i^2}{2} - \frac{\hbar}{2} \right) + \hbar^2 V. \tag{1.1}$$

More precisely, we consider the kernel of the operator e^{-tH} but with ordinary time t replaced by

$$t = \frac{1}{\hbar} \log \frac{1+\hbar s}{1-\hbar s} = 2s \left(1 + \frac{\hbar^2 s^2}{3} + \frac{\hbar^4 s^4}{5} + \cdots \right), \tag{1.2}$$

which greatly simplifies the calculations in the semiclassical regime.

Our first result is:

Theorem 1.1. *Assume that $V \in C^\infty(\mathbb{R}^n)$ is bounded below and that it and all its derivatives have at most polynomial growth at infinity. Then, on the diagonal, the Schwartz kernel of the operator e^{-tH}, where t is given by (1.2), has an asymptotic expansion as $\hbar$ tends to zero of the form*

$$\hbar^2 \sum_{k=0}^{\infty} \hbar^{2k}\, \Upsilon_k(s,x). \tag{1.3}$$

Moreover, the first three coefficients in this expansion, integrated over $\mathbb{R}^n$, determine the following quantities:

$$\int_{\mathbb{R}^n} V(x)\, e^{-s|x|^2}\, dx, \quad \int_{\mathbb{R}^n} V^2(x)\, e^{-s|x|^2}\, dx, \quad \int_{\mathbb{R}^n} \left(V^3(x) - V\Delta V\right)\, e^{-s|x|^2}\, dx. \tag{1.4}$$

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The Hitrik-Polterovich method, adapted to the present situation, results in a procedure to compute the Υ_k. In particular $\Upsilon_0(s,x) = 2sV(x)e^{-|x|^2 s}$.

For $\hbar$ sufficiently small the spectrum of H is discrete and the quantities (1.4) are *spectral invariants* of V associated to the $\hbar$-dependent spectrum of H. By analyzing these invariants we obtain several inverse spectral results, namely:

Corollary 1.2. *Let $S_r = \{x \in \mathbb{R}^n \;;\; |x| = r\}$. The following properties of V can be detected from the $\hbar$-dependent spectrum of H:*

(a) *Whether V is constant on a given sphere S_r, and if so the value of the constant.*
(b) *Whether V is compactly supported, and if so the the smallest annulus about the origin containing the support of V.*
(c) *Within the class of odd functions V, one can determine whether the restriction of V to any annulus about the origin is linear on that annulus.*

Remark 1.3. Item (c) is a consequence of a much stronger but slightly more technical result (see Proposition 7.1.)

The basic ingredients in the derivation of the expansion (1.3) are a variant of Mehler's formula and the Kantorovitz formula for expressing the heat expansion of the sum of two operators, A and B, in terms of the heat expansion of B alone. (The latter is also the basic ingredient in the proof of the Hitrik-Polterovich result.) We will discuss Mehler's formula in §2 and the Hitrik-Polterovich formula in §3. Then in §4 we will describe what this formula looks like if one replaces the standard heat kernel, $(4\pi t)^{-\frac{n}{2}} e^{-\frac{|x-y|^2}{4t}}$, by the semi-classical Mehler kernel. As mentioned, the expansion of this formula in powers of $\hbar^2$ generates a sequence of heat trace invariants, and in §5 we will discuss a symbolic method for computing these invariants. In §6 we will illustrate these methods by computing the first three of these invariants, and finally in §7 we will prove the aforementioned inverse spectral results.

2. Mehler's formula

Let L be the operator

$$L = \frac{1}{2}\sum\left(-\frac{\partial^2}{\partial x_i^2} + x_i^2 - 1\right). \tag{2.1}$$

Mehler's formula for the Schwartz kernel of e^{-tL} is

$$e^{-tL}(x,y) = \pi^{-\frac{n}{2}}(1-e^{-2t})^{-\frac{n}{2}} \exp\left\{-\frac{1}{1-e^{-2t}}\left[\frac{|x|^2+|y|^2}{2}(1+e^{-2t}) - 2e^{-t}x\cdot y\right]\right\} \tag{2.2}$$

(see for instance [Sim] page 38). Rescaling the variables x and y by the factor $1/\sqrt{\hbar}$ and t by the factor $\hbar$ we get, for the heat kernel of the semi-classical harmonic oscillator

$$A = -\frac{\hbar^2}{2}\Delta + \frac{|x|^2}{2} - \frac{n\hbar}{2},$$

the expression

(2.3)
$$e^{-tA}(x,y)=\pi^{-\frac{n}{2}}(1-e^{-2\hbar t})^{-\frac{n}{2}}\exp\left\{-\frac{1}{\hbar(1-e^{-2\hbar t})}\left[\frac{|x|^2+|y|^2}{2}(1+e^{-2\hbar t})-2e^{-t\hbar}x\cdot y\right]\right\}.$$

The term in square brackets can be rewritten as

$$\frac{|x|^2+|y|^2}{2}(1-e^{-t\hbar})^2+e^{-t\hbar}|x-y|^2,$$

and hence the term in curly braces is equal to

$$-\frac{|x|^2+|y|^2}{2\hbar}\frac{1-e^{-t\hbar}}{1+e^{-t\hbar}}-\frac{e^{-t\hbar}}{\hbar(1-e^{-t\hbar})(1+e^{-t\hbar})}|x-y|^2. \tag{2.4}$$

Now introduce the new time scale

$$s=\frac{1}{\hbar}\frac{1-e^{-t\hbar}}{1+e^{-t\hbar}}=\frac{t}{2}\left(1+O(t^2\hbar^2)\right) \tag{2.5}$$

or, alternatively,

$$e^{-t\hbar}=\frac{1-\hbar s}{1+\hbar s}. \tag{2.6}$$

Then the expression (2.4) becomes

$$-\frac{|x|^2+|y|^2}{2}s-\frac{1}{4}\left(\frac{1}{\hbar^2}\frac{1}{s}-s\right)|x-y|^2$$

or

$$-\frac{|x-y|^2}{4\hbar^2 s}-\frac{|x+y|^2}{4}s, \tag{2.7}$$

and hence for the Schwartz kernel of heat operator e^{-tA} we get the formula

$$e^{-tA}(x,y)=(4\pi\hbar)^{-\frac{n}{2}}s^{-\frac{n}{2}}(1+s\hbar)^n\exp\left(-\frac{|x-y|^2}{4\hbar^2 s}-\frac{|x+y|^2}{4}s\right). \tag{2.8}$$

3. The Kantorovitz formula

Let A and B be linear operators on an appropriately defined Hilbert (Banach, Frechet, $\cdots$) space which generate strongly continuous semigroups e^{tA} and e^{tB} and such that the sets of C^∞ vectors satisfy: $D^\infty(A)\subset D^\infty(A+B)$. (Both conditions will be satisfied automatically in what follows.) Then according to Kantorovitz, [Ka], $e^{t(A+B)}$ can be expressed as a series

$$e^{t(A+B)}=(I+tX_1+\frac{t^2}{2}X_2+\cdots)e^{tA}, \tag{3.1}$$

where the X_i's are defined by

$$X_0=I,\quad X_1=B,\quad X_2=B^2+[A,B] \tag{3.2}$$

and in general

$$X_m=BX_{m-1}+[A,X_{m-1}]. \tag{3.3}$$

There is also a simple closed form expression for X_m: Letting $H = A + B$,

$$X_m = H^m - mH^{m-1}A + \binom{m}{2} H^{m-2}A^2 + \cdots . \tag{3.4}$$

Example: ([HP]) Let $A = -\Delta_{\mathbb{R}^n}$ and $H = -\Delta_{\mathbb{R}^n} + V$. Then

$$e^{-tA}(x,y) = (4\pi t)^{-\frac{n}{2}} e^{-\frac{|x-y|^2}{4t}} \tag{3.5}$$

and hence

$$e^{-tH}(x,y) = (4\pi t)^{-\frac{n}{2}} \sum_{m=0}^{\infty} (-1)^m \frac{t^m}{m!} a_m(x,y,t), \tag{3.6}$$

where

$$a_m(x,y,t) = \sum_{l+j=m} \binom{m}{l} H_x^l \Delta_x^j e^{-\frac{|x-y|^2}{4t}}. \tag{3.7}$$

From this identity it is relatively easy to get an asymptotic expansion of $e^{-tH}(x,x)$ as a Taylor series in t for which the summands are (at least in principle) computable. (See [HP], §2 for details.)

In the spirit of this example, let

$$A = \sum_{i=1}^{n} \left(-\frac{\hbar^2}{2} \frac{\partial^2}{\partial x_i^2} + \frac{x_i^2}{2} - \frac{\hbar}{2} \right) \tag{3.8}$$

and let $H = A + \hbar^2 V$. Then, as above,

$$e^{-tH}(x,y) = \sum_{m=0}^{\infty} (-1)^m \frac{t^m}{m!} a_m(x,y,t,\hbar), \tag{3.9}$$

where

$$a_m(x,y,t,\hbar) = \sum_{l+j=m} (-1)^j \binom{m}{l} H_x^l A_x^j e^{-tA}(x,y). \tag{3.10}$$

By (2.8) the computation of this sum reduces to computing

$$\sum_{l+j=m} (-1)^j \binom{m}{l} H^l A^j \exp\left(-\frac{|x-y|^2}{4\hbar^2 s} \right) f(x,y,s) t^m, \tag{3.11}$$

where s is given by (2.5) and

$$f(x,y,s) = \exp\left(-s \frac{|x+y|^2}{4} \right). \tag{3.12}$$

The expression above is similar to the Hitrik-Polterovich expression

$$\sum_{l+j=m} \binom{m}{l} (-\Delta + V)^l \Delta^j \exp\left(-\frac{|x-y|^2}{4t} \right) t^m,$$

except for the presence of the factor (3.12). However, since we'll mainly be interested in the $\hbar$ dependence of the expression (3.11), and (3.12) depends in an explicit way on $\hbar$, our computations will be very similar to theirs.

4. Computations

As above let A be the operator

$$\sum_{i=1}^{n}\left(-\frac{\hbar^2}{2}\frac{\partial^2}{\partial x_i^2}+\frac{x_i^2}{2}-\frac{\hbar}{2}\right),$$

B the operator, $\hbar^2 V$, and $X_m, m=0,1,2,\cdots$ the operators defined inductively by

$$X_m = BX_{m-1}+[A,X_{m-1}] \tag{4.1}$$

and $X_0 = \mathrm{I}$. It will be convenient to write this formula as

$$X_m = \hbar^2 V X_{m-1} - \hbar^2[\frac{\Delta}{2},X_{m-1}]+[\frac{x^2}{2},X_{m-1}]. \tag{4.2}$$

From this formula one gets:

Proposition 4.1. *The operators X_m are of the form*

$$X_m = \hbar^m \sum_{\substack{i=1\\ i\equiv m \ mod(2)}}^{m} \hbar^i X_m^{i-1}, \tag{4.3}$$

where X_m^{i-1} is a differential operator of degree $i-1$ not depending on $\hbar$. Moreover, these operators satisfy

$$X_{m+1}^i = -\left[\frac{\Delta}{2},X_m^{i-1}\right]+\left[\frac{x^2}{2},X_m^{i+1}\right]+VX_m^{i-1}. \tag{4.4}$$

The proof is a simple inductive argument.

To compute the m^{th} summand in the Kantorovitz expansion (3.1), we must apply X_m to the Mehler kernel

$$e(x,y,s,\hbar)=\exp\left(-\frac{|x-y|^2}{4\hbar^2 s}-\frac{|x+y|^2}{4}s\right) \tag{4.5}$$

and then set $x=y$.

Proposition 4.2.

$$X_m\left(e(x,y,s,\hbar)\right)|_{x=y} = \hbar^m \sum_{\substack{i=1\\ i\equiv m \ mod(2)}}^{m} \hbar^i X_m^{i-1}\left(e(x,y,s,\hbar)\right)|_{x=y}$$

is equal to: For m odd and with $l=\frac{m-1}{2}$,

$$\hbar^{m+1}\left(\sum_{r=0}^{l} e_{m,r}(x,s)\hbar^{2r}\right)s^{-l}e^{-s|x|^2} \tag{4.6}$$

and for m even and with $l=\frac{m}{2}-1$,

$$\hbar^{m+2}\left(\sum_{r=0}^{l} e_{m,r}(x,s)\hbar^{2r}\right)s^{-l}e^{-s|x|^2}, \tag{4.7}$$

where in all cases the $e_{m,r}$ are polynomials in s of degree at most $2r$.

Proof. We first note that for multi-indices, μ,

$$\partial_x^\mu e^{-\frac{|x-y|^2}{4\hbar^2 s}}\bigg|_{x=y} = c_\mu \hbar^{-|\mu|} s^{-\frac{|\mu|}{2}} \tag{4.8}$$

for even μ and 0 for non-even μ, where $c_\mu = (-\frac{1}{4})^{|\nu|}\frac{\mu!}{\nu!}$ for $\mu = 2\nu$. The result follows from this, Leibniz' formula, and the properties of the operators X_m^{i-1}. □

Thus making the substitution

$$t = \frac{1}{\hbar}\log\frac{1+\hbar s}{1-\hbar s} = 2s\left(1 + \frac{\hbar^2 s^2}{3} + \frac{\hbar^4 s^4}{5} + \cdots\right), \tag{4.9}$$

the $t^m X_m e(x,y,t,\hbar)|_{x=y}$ term in the Kantorovitz formula gets converted into

$$2^m \hbar^{m+1} s^{l+1}\left(\sum_{r=0}^{l} e_{m,r}(x,s)\hbar^{2r}\right)\left(1 + \frac{\hbar^2 s^2}{3} + \frac{\hbar^4 s^4}{5} + \cdots\right)^m, \tag{4.10}$$

$l = \frac{m-1}{2}$, for m odd, and

$$2^m \hbar^{m+2} s^{l+2}\left(\sum_{r=0}^{l} e_{m,r}(x,s)\hbar^{2r}\right)\left(1 + \frac{\hbar^2 s^2}{3} + \frac{\hbar^4 s^4}{5} + \cdots\right)^m, \tag{4.11}$$

$l = \frac{m}{2} - 1$, for m even.

5. Symbolic features of the expansions (4.6)-(4.7)

We showed above that there exist functions $\rho_m(x,s)$, $m = 0,1,\ldots$ such that

$$X_m e(x,y,s,\hbar)\big|_{x=y} = \hbar^{m+1}\rho_m(x,s) + O(\hbar^{m+3}) \tag{5.1}$$

for m odd and

$$X_m e(x,y,s,\hbar)\big|_{x=y} = \hbar^{m+2}\rho_m(x,s) + O(\hbar^{m+4}) \tag{5.2}$$

for m even. We will show in this section that for m odd, $\rho_m(x,s)$ is computable purely by "symbolic" techniques and will prove a somewhat weaker form of this assertion for m even.

Let

$$X_{m+1}^i = \sum_{|\alpha|\le i} a_{i,m+1}^\alpha(x) D^\alpha \tag{5.3}$$

and let

$$p_{m+1}^i = \sum_{|\alpha|\le i} a_{i,m+1}^\alpha(x)\xi^\alpha \tag{5.4}$$

be the full symbol of X_{m+1}^i From (4.4) and standard composition formula for left Kohn-Nirenberg symbols one gets

(5.5)

$$p_{m+1}^i = \left(\sum_{r=1}^n \frac{\xi_r}{\sqrt{-1}}\frac{\partial}{\partial x_r} - \frac{1}{2}\frac{\partial^2}{\partial x_r^2}\right)p_m^{i-1} + \left(\sum_{r=1}^n \sqrt{-1}x_r\frac{\partial}{\partial \xi_r} + \frac{1}{2}\frac{\partial^2}{\partial \xi_r^2}\right)p_m^{i+1} + V(x)p_m^{i-1}.$$

In particular, if

$$\sigma_{m+1}^i = \sum_{|\alpha|=i} a_{i,m+1}^{\alpha}(x)\xi^{\alpha}$$

is the principal symbol of X_{m+1}^i and

$$\tilde{\sigma}_{m+1}^i = \sum_{|\alpha|=i-1} a_{i,m+1}^{\alpha}(x)\xi^{\alpha}$$

the subprincipal symbol, we get from (5.5) that

$$\sigma_{m+1}^i = \frac{1}{\sqrt{-1}} \sum_{r=1}^n \left(\xi_r \frac{\partial}{\partial x_r} \sigma_m^{i-1} - x_r \frac{\partial}{\partial \xi_r} \sigma_m^{i+1} \right) \tag{5.6}$$

and

$$\tilde{\sigma}_{m+1}^i = \frac{1}{\sqrt{-1}} \sum_{r=1}^n \left(\xi_r \frac{\partial}{\partial x_r} \tilde{\sigma}_m^{i-1} - x_r \frac{\partial}{\partial \xi_r} \tilde{\sigma}_m^{i+1} \right) - \frac{1}{2} \sum_{r=1}^n \left(\frac{\partial^2}{\partial x_r^2} \sigma_m^{i-1} - \frac{\partial^2}{\partial \xi_r^2} \sigma_m^{i+1} \right) + V \sigma_m^{i-1}. \tag{5.7}$$

Letting

$$\sigma_m = \hbar^m \sum_{\substack{i=1 \\ i \equiv m \bmod(2)}}^m \hbar^i \sigma_m^{i-1},$$

and letting $\mathcal{U}$ be the raising operator

$$\mathcal{U} \hbar^i \sigma = \hbar^{i+2} \sigma$$

for $i \geq 0$, we can write these formulas more succinctly in the form

$$\sigma_m = \frac{1}{\sqrt{-1}} \sum_{r=1}^n \left(\xi_r \frac{\partial}{\partial x_r} \mathcal{U} - x_r \frac{\partial}{\partial \xi_r} \right) \sigma_{m-1} \tag{5.8}$$

and

$$\tilde{\sigma}_m = \frac{1}{\sqrt{-1}} \sum_{r=1}^n \left(\xi_r \frac{\partial}{\partial x_r} \mathcal{U} - x_r \frac{\partial}{\partial \xi_r} \right) \tilde{\sigma}_{m-1} + \sum_{r=1}^n \left(-\frac{1}{2} \frac{\partial^2}{\partial x_r^2} \mathcal{U} + \frac{1}{2} \frac{\partial^2}{\partial \xi_r^2} \right) \sigma_{m-1} + V \mathcal{U} \sigma_{m-1}. \tag{5.9}$$

In particular, iterating (5.8) we get

$$\sigma_m = \left[\frac{1}{\sqrt{-1}} \sum_{r=1}^n \left(\xi_r \frac{\partial}{\partial x_r} \mathcal{U} - x_r \frac{\partial}{\partial \xi_r} \right) \right]^{m-1} \hbar^2 V \tag{5.10}$$

and, as special cases of (5.10),

$$\sigma_m^{m-1} = \left(\frac{1}{\sqrt{-1}} \sum_{r=1}^n \xi_r \frac{\partial}{\partial x_r} \right)^{m-1} V. \tag{5.11}$$

As applications of these formulas let m be odd and consider the ith summand of

$$X_m e(x,y,s,\hbar)|_{x=y} = \hbar^m \sum_{\substack{i=1 \\ i \equiv m \bmod(2)}}^m \hbar^i X_m^{i-1} e(x,y,s,\hbar) \Bigg|_{x=y}.$$

By (5.3) this is equal to

$$\hbar^{m+i}\sum_{|\alpha|=i-1} a^{\alpha}_{i-1,m}(x) D^{\alpha}_x e^{-\frac{|x-y|^2}{4\hbar^2 s}}\Big|_{x=y} e^{-s|x|^2} \tag{5.12}$$

plus terms of order $O(\hbar^{m+3})$ and by (4.8), (5.12) is equal to

$$\hbar^{m+1}\left(\sum_{|\alpha|=i-1} a^{\alpha}_{i-1,m}(x) c_\alpha\right) s^{-\frac{i-1}{2}} e^{-s|x|^2}. \tag{5.13}$$

To summarize:

Proposition 5.1. *For m odd, the leading term ρ_m in (5.1) is given by*

$$\rho_m(x,s) = e^{-s|x|^2} \sum_{\substack{i=1 \\ i\equiv m \mod(2)}}^{m} s^{\frac{1-i}{2}} \sum_{|\alpha|=i-1} a^{\alpha}_{i-1,m}(x) c_\alpha.$$

For each i, the quantity $\sum_{|\alpha|=i-1} a^{\alpha}_{i-1,m}(x) c_\alpha$ is obtained from the principal symbol of X^{i-1}_m by substituting every monomial ξ^α by the constant c_α.

For m even the computation above is similar, however one gets $\hbar^{m+2}$ contributions to (5.2) from both the terms

$$\hbar^{m+i}\sum_{|\alpha|=i-1} a^{\alpha}_{i-1,m}(x) D^{\alpha} e^{-\frac{|x-y|^2}{4\hbar^2 s}} e^{-\frac{s}{4}|x+y|^2}\Big|_{x=y}$$

<u>and</u> the terms

$$\hbar^{m+i}\sum_{|\alpha|=i-2} a^{\alpha}_{i-1,m}(x) D^{\alpha} e^{-\frac{|x-y|^2}{4\hbar^2 s}}\Big|_{x=y} e^{-s|x|^2}.$$

The second summand (involving the subprincipal symbol of X^{i-1}_m) is as before,

$$\hbar^{m+2}\sum_{|\alpha|=i-2} a^{\alpha}_{i-1,m}(x) c_\alpha s^{-\frac{i-2}{2}} e^{-s|x|^2}, \tag{5.14}$$

but the first summand (involving the principal symbol of X^{i-1}_m) becomes

$$\hbar^{m+2}\sum_{\substack{|\alpha|=i-1 \\ 1\le r\le n}} a^{\alpha}_{i-1,m}(x) c_{\alpha^{(r)}} s^{-\frac{i-4}{2}} x_r e^{-s|x|^2}, \tag{5.15}$$

where $\alpha^{(r)} = (\alpha_1,\cdots,\alpha_r - 1,\cdots,\alpha_n)$. This proves:

Proposition 5.2. *For m even the leading term of (5.2) depends only on the principal and subprincipal symbols of X_m.*

We now explore some spectral consequences of the previous results.

Proposition 5.3. *For m odd the quantities $\int \rho_m(x,s)\,dx$ are spectral invariants of V.*

Proof. For m odd we can, by (5.10), express $\rho_m(x,s)$ as a sum of terms of the form $x^\alpha \frac{\partial^\beta V}{\partial x^\beta} e^{-s|x|^2}$, where $|\alpha|+|\beta| \leq m-1$. The associated contribution to the heat trace

$$\int x^\alpha \frac{\partial^\beta V}{\partial x^\beta} e^{-s|x|^2} dx \tag{5.16}$$

can, by integration by parts, be written as sums of integrals of the form

$$\int x^\gamma V e^{-s|x|^2} dx, \qquad |\gamma| \leq m-1.$$

Thus

$$\int \rho_m(x,s) e^{-s|x|^2} dx = \int p(x,s) V e^{-s|x|^2} dx, \tag{5.17}$$

where $p(x,s)$ is a *universal* polynomial of degree $m-1$ in x. Moreover, for every $A \in SO(n)$ the heat trace expansion for the potentials V and V^A, where $V^A(x) = V(Ax)$, are the same. Hence by averaging over $SO(n)$ we can assume that $p(x,s)$ is $SO(n)$ invariant, i.e.

$$p(x,s) = \sum_{i=0}^{k} \chi_i(s)|x|^{2i}, \qquad k = \frac{m-1}{2}$$

and thus (5.17) becomes

$$\int \rho_m(x,s) e^{-s|x|^2} dx = \int_0^\infty dr \sum_{i=1}^{k} \chi_i(s) r^{2i} e^{-sr^2} \int_{|x|=r} V(x) d\sigma_r, \tag{5.18}$$

where $d\sigma_r$ is the standard volume form on the $(n-1)$-sphere $|x|=r$. We will see below however that, for each $r>0$, the integral

$$\int_{|x|=r} V(x) d\sigma_r \tag{5.19}$$

is itself a spectral invariant of the perturbed harmonic oscillator and hence the terms $\hbar^{m+1}\int \rho_m(x,s)dx$ in the heat trace expansion above can be read off from it. □

In the case m even one also gets a similar description of the contributions of (5.2) to the heat trace. The contribution coming from the term (5.15) only depends on σ_m^{i-1} and hence as above is expressible in terms of (5.18); and as for the contributions coming from (5.14) one can prove by induction that these give rise to heat trace invariants which are sums of expressions of the form (5.16) and of the form

$$\int x^\alpha V \frac{\partial^\beta V}{\partial x^\beta} e^{-s|x|^2}\ dx. \tag{5.20}$$

Indeed the second summand in (5.7) is purely symbolic; so as we've just seen it contributes terms of type (5.16) to the heat trace. Similarly the third summand contributes terms of type (5.20) and by a simple induction on m one can show that the first summand of (5.7) is a linear combination of terms of the form

$$\xi^\alpha x^\beta \frac{\partial^\gamma V}{\partial x^\gamma} \frac{\partial^\delta V}{\partial x^\delta}$$

and

$$\xi^\alpha x^\beta \frac{\partial^\gamma V}{\partial x^\gamma}.$$

These give rise to contributions to the heat trace of the form (5.16) and

$$\int x^\mu \frac{\partial^\nu V}{\partial x^\nu} \frac{\partial^\gamma V}{\partial x^\gamma} e^{-s|x|^2} dx,$$

which by integration by parts can be written as expressions of the form (5.20). Finally, the $O(n)$ invariance of the heat trace enables one to simplify these further and rewrite them as sums of the form

$$\int |x|^{2j} V (\sum x_i \frac{\partial}{\partial x_i})^k \Delta^l V dx.$$

6. The first heat invariants

It is easy to see (either by direct computation or by the symbolic formulas in the preceding section) that for $m \leq 4$ the X_m^{i-1}'s are given by

$$X_1^0 = V, \tag{6.1}$$

$$X_2^1 = -\sum \frac{\partial V}{\partial x_i} \frac{\partial}{\partial x_i} + V^2 - \frac{\Delta V}{2}, \tag{6.2}$$

$$X_3^2 = \sum \frac{\partial^2 V}{\partial x_i \partial x_j} \frac{\partial^2}{\partial x_i \partial x_j} + \sum \frac{\partial}{\partial x_i} (\Delta V - \frac{3}{2} V^2) \frac{\partial}{\partial x_i} + \frac{\Delta^2}{4} V - \frac{\Delta}{2} V^2 + V^3 - \frac{V \Delta V}{2}, \tag{6.3}$$

$$X_3^0 = \sum x_i \frac{\partial V}{\partial x_i}, \tag{6.4}$$

$$X_4^3 = [-\frac{\Delta}{2}, \sum \frac{\partial^2 V}{\partial x_i \partial x_j} \frac{\partial^2}{\partial x_i \partial x_j} + \sum \frac{\partial}{\partial x_i} (\Delta V - \frac{3}{2} V^2) \frac{\partial}{\partial x_i}] + \sum V \frac{\partial^2 V}{\partial x_i \partial x_j} \frac{\partial^2}{\partial x_i \partial x_j} \tag{6.5}$$

plus terms of degree less than two, and

$$X_4^1 = -\left[\frac{\Delta}{2}, \sum x_i \frac{\partial V}{\partial x_i}\right] + \left[\frac{x^2}{2}, \sum \frac{\partial^2 V}{\partial x_i \partial x_j} \frac{\partial^2}{\partial x_i \partial x_j} + \sum \frac{\partial}{\partial x_i} (\Delta V - \frac{3}{2} V^2) \frac{\partial}{\partial x_i}\right] + \frac{1}{2} \sum x_i \frac{\partial}{\partial x_i} V^2. \tag{6.6}$$

Thus the $\hbar^2$ term in the heat trace expansion determines

$$\int V e^{-s|x|^2} dx, \tag{6.7}$$

and hence by the inverse Laplace transform determines the integral

$$\int_{|x|=r} V d\sigma_r. \tag{6.8}$$

for each $r > 0$.

The $\hbar^4$ term involves the $m = 3$ contribution of (5.1), but as we saw above this is expressible in terms of (6.8). As for the contribution of (5.2) to the $\hbar^4$ term, the first and third summands can be converted by integration by parts into integrals which are expressible in terms of (6.8) and the second summand gives a new heat invariant,

$$\int V^2 e^{-s|x|^2} dx, \tag{6.9}$$

which, by the inverse Laplace transform, is convertible into

$$\int_{|x|=r} V^2 d\sigma_r. \tag{6.10}$$

The $\hbar^6$ term in the heat trace expansion involves the $m = 5$ contribution of (5.1) which, as we saw in the previous section, is expressible in terms of (6.8), the $m = 4$ contribution of (5.2), which is subprincipal and hence only involves the terms in (6.6) (all of which can be converted, by integration by parts, into expressions in (6.8) and (6.10)), and the cubic and quadratic terms in (6.5) all of which, except for the term

$$\sum V \frac{\partial^2 V}{\partial x_i \partial x_j} \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j}, \tag{6.11}$$

can be converted by integration by parts into expressions in (6.8) and (6.10). Finally the $\hbar^6$ terms coming from (6.3) and (6.4) are all convertible by integration by parts into expressions in (6.8) and (6.10) except for the last summand of (6.3): the term

$$V^3 - \frac{V \Delta V}{2}. \tag{6.12}$$

The term (6.11) gives, by (5.14) and (4.11) a contribution

$$-\hbar^6 s^2 \frac{V \Delta V}{2} e^{-s|x|^2} \tag{6.13}$$

to the heat trace expansion, and the term (6.12) gives, by (4.10), a contribution

$$\hbar^6 s^2 (V^3 - \frac{V \Delta V}{2}) e^{-s|x|^2} \tag{6.14}$$

to the heat trace expansion; hence the sum of these two terms gives rise to a new heat trace invariant

$$\int (V^3 - V \Delta V) e^{-s|x|^2} dx \tag{6.15}$$

which, by the inverse Laplace transform, can be converted into the invariant

$$\int_{|x|=r} (V^3 - V \Delta V) d\sigma_r. \tag{6.16}$$

This finishes the proof of Theorem 1.1.

7. Applications to inverse spectral problems

In this section we apply the first heat invariants (6.8), (6.10) and (6.16) above to the inverse spectral problems of recovering information about V from the $\hbar$-dependent spectrum of H.

Fix any $r > 0$. First let's consider V which minimize the second invariant (6.10) subject to the constraint

$$\int_{|x|=r} V d\sigma_r = \text{constant}. \tag{7.1}$$

According to the Cauchy-Schwartz inequality, the minimizers are exactly those functions V that are constant on the sphere $|x| = r$. It follows that the set of potentials V that are constant on a given sphere $|x| = r$ is intrinsically defined by its spectral properties. Moreover, one can spectrally determine the constant value for each potential in this set. This proves parts (a) and (b) of Corollary 1.2.

Next let's assume that V is an odd potential. (Using band invariant techniques, one can show that being odd is also a spectral property, c.f. [GUW].) As we have seen that the invariants determines $\|V\|^2_{L^2(S_r)}$ for each r. Taking the r derivative of the second invariant, we get that $\langle V, \frac{\partial V}{\partial r}\rangle_{L^2(S_r)}$ is a spectral invariant. On the other hand, since V is odd, the third invariant (6.15) becomes

$$-\int V\Delta V e^{-sr^2} r^{n-1} dr d\sigma_r. \tag{7.2}$$

Recall that in spherical coordinates

$$\Delta V = \frac{\partial^2 V}{\partial r^2} + \frac{n-1}{r}\frac{\partial V}{\partial r} + \frac{1}{r^2}\Delta_{S_r} V.$$

A simple computation shows that

$$-\int V \frac{n-1}{r}\frac{\partial V}{\partial r} e^{-sr^2} r^{n-1} dr d\sigma_r = \frac{n-1}{2}\int V^2 \frac{d}{dr}\left(e^{-sr^2} r^{n-2}\right) dr d\sigma_r$$

which is a spectrally determined quantity, since we know the integrals (6.10) for all r. Similarly,

$$-\int V \frac{\partial^2 V}{\partial r^2} e^{-sr^2} r^{n-1} dr d\sigma_r = \int \left(\frac{\partial V}{\partial r}\right)^2 e^{-sr^2} r^{n-1} dr d\sigma_r + \int V \frac{\partial V}{\partial r}\frac{d}{dr}(e^{-sr^2} r^{n-1}) dr d\sigma_r,$$

and again the second term on the right

$$\int V \frac{\partial V}{\partial r}\frac{d}{dr}(e^{-sr^2} r^{n-1}) dr d\sigma_r$$

is also spectrally determined according to (6.10). It follows from (7.2) that the integral

$$\int \left(\frac{\partial V}{\partial r}\right)^2 e^{-sr^2} r^{n-1} dr d\sigma_r - \int \frac{1}{r^2} V \Delta_{S_r} V e^{-sr^2} r^{n-1} dr d\sigma_r \tag{7.3}$$

is spectrally determined, which, by the inverse Laplace transform, gets converted to the invariant $\|\frac{\partial V}{\partial r}\|^2_{L^2(S_r)} + \frac{1}{r}\langle V, -\Delta_{S_r} V\rangle_{L^2(S_r)}$ for each $r > 0$. Note next that for every V one has the following inequality

$$\|V\|^2_{L^2(S_r)}\left(\|\frac{\partial V}{\partial r}\|^2_{L^2(S_r)} + \frac{1}{r}\langle V, -\Delta_{L^2(S_r)} V\rangle_{L^2(S_r)}\right) \geq \langle V, \frac{\partial V}{\partial r}\rangle^2_{L^2(S_r)} + \frac{\lambda_1}{r}\|V\|^4_{L^2(S_r)},$$

where λ_1 is the first eigenvalue of the (non-negative) Laplacian on S_r. Both sides of the inequality are spectral invariants, and equality holds if and only if V satisfies the conditions

$$\frac{\partial V}{\partial r}|_{S_r} = \chi V|_{S_r} \quad \text{and} \quad V|_{S_r} \text{ is a spherical harmonic of degree one} \tag{7.4}$$

where χ is a constant, and if so one can determine χ. This proves the first part of the following

Proposition 7.1. *The class of functions defined by the conditions (7.4) is spectrally determined. Moreover, for any V in this class one can determine the ratio*

$$\chi = \frac{\partial V}{\partial r}/V$$

on a given sphere S_r.

The determination of χ (which of course can depend on r) is done by looking at the quotient of $\langle V, \frac{\partial V}{\partial r}\rangle_{L^2(S_r)}/\|V\|^2_{L^2(S_r)}$.

As a consequence, one can determine whether a potential is of the form

$$V(x) = f(r)g(\sigma)$$

on a given annulus $r_1 \leq |r| \leq r_2$, where $g(\sigma)$ is a spherical harmonic of degree one, and if so, determine the function $f(r)$. In particular, one can spectrally determine linear potentials on any annular region $r_1 \leq |r| \leq r_2$: They are just the potentials in the previous class with $\chi = r$.

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