J. DIFFERENTIAL GEOMETRY
91 (2012) 103-128

SEMICLASSICAL SPECTRAL INVARIANTS FOR SCHRÖDINGER OPERATORS

Victor Guillemin & Zuoqin Wang

Abstract

In this article we show how to compute the semiclassical spectral measure associated with the Schrödinger operator on $\mathbb{R}^n$, and, by examining the first few terms in the asymptotic expansion of this measure, obtain inverse spectral results in one and two dimensions. (In particular we show that for the Schrödinger operator on $\mathbb{R}^2$ with a radially symmetric electric potential, V, and magnetic potential, B, both V and B are spectrally determined.) We also show that in one dimension there is a very simple explicit identity relating the spectral measure of the Schrödinger operator with its Birkhoff canonical form.

1. Introduction

Let

$$S_\hbar = -\frac{\hbar^2}{2}\Delta + V(x) \tag{1.1}$$

be the semiclassical Schrödinger operator with potential function, $V(x) \in C^\infty(\mathbb{R}^n)$, where Δ is the Laplacian operator on $\mathbb{R}^n$. We will assume that V is nonnegative and that for some $a > 0$, $V^{-1}([0,a])$ is compact. By Friedrich's theorem these assumptions imply that the spectrum of $S_\hbar$ on the interval $[0,a)$ consists of a finite number of discrete eigenvalues

$$\lambda_i(\hbar), \quad 1 \le i \le N(\hbar), \tag{1.2}$$

with $N(\hbar) \to \infty$ as $\hbar \to 0$. We will show that for $f \in C^\infty(\mathbb{R})$, with $\operatorname{supp}(f) \subset (-\infty, a)$, one has an asymptotic expansion (see also [**DiS**], [**HeR**])

$$(2\pi h)^n \sum_i f(\lambda_i(\hbar)) \sim \sum_{k=0}^\infty \nu_k(f)\hbar^{2k} \tag{1.3}$$

with principal term

$$\nu_0(f) = \int f(\frac{\xi^2}{2} + V(x))\ dx\ d\xi \tag{1.4}$$

Received 2/26/2010.

and subprincipal term

$$\nu_1(f) = -\frac{1}{24}\int f^{(2)}(\frac{\xi^2}{2}+V(x))\sum_i \frac{\partial^2 V}{\partial x_i^2}\, dx\ d\xi. \tag{1.5}$$

We will also give an algorithm for computing the higher order terms and will show that the k^{th} term is given by an expression of the form

$$\nu_k(f) = \int \sum_{j=[\frac{k}{2}+1]}^{k} f^{(2j)}(\frac{\xi^2}{2}+V(x))p_{k,j}(DV,\cdots,D^{2k}V)dxd\xi, \tag{1.6}$$

where $p_{k,j}$ are universal polynomials, and the D^kV's the k^{th} partial derivatives of V. Moreover, to illustrate how this algorithm works we will compute the terms, $\nu_k(f)$, $k=2,3$, in §3.3. (However, to simplify these computations slightly we will confine ourselves to the case $n=1$.)

One way to think about the result above is to view the left hand side of (1.3) as defining a measure, $\mu_\hbar$, on the interval $[0,a)$, and the right hand side as an asymptotic expansion of this spectral measure as $\hbar\to 0$,

$$\mu_\hbar \sim \sum \hbar^{2k}\left(\frac{d}{dt}\right)^{2k}\mu_k, \tag{1.7}$$

where μ_k is a measure on $[0,a)$ whose singular support is the set of critical values of the function, V. This "semiclassical" spectral theorem is a special case of a semiclassical spectral theorem for elliptic operators which we will describe in §2, and in §3 we will derive the formulas (1.4) and (1.5) and the algorithm for computing (1.6) from this more general result. More explicitly, we'll show that this more general result gives, more or less immediately, an expansion similar to (1.7), but with a "$(\frac{d}{dt})^{4k}$" in place of the $(\frac{d}{dt})^{2k}$. We'll then show how to deduce (1.7) from this expansion by judicious integrations by parts.

In one dimension our results are closely related to recent results of [**Col05**], [**Col08**], [**CoG**], and [**Hez**]. In particular, the main result of [**CoG**] asserts that if $c\in[0,a)$ is an isolated critical value of V and $V^{-1}(c)$ is a single non-degenerate critical point, p, then the first two terms in (1.7) determine the Taylor series of V at p, and hence, if V is analytic in a neighborhood of p, determine V itself in this neighborhood of p. In [**Col08**] Colin de Verdière proves a number of much stronger variants of this result (modulo stronger hypotheses on V). In particular, he shows that for a single well potential the spectrum of $S_\hbar$ determines V up to "pointwise reflection" $V(x)\leftrightarrow V(-x)$ without any analyticity assumptions, provided one makes certain asymmetry assumptions on V:

Theorem 1.1 (Colin de Verdière [**Col08**]). *Suppose the potential function V is a single well potential; then the semiclassical spectrum of $S_\hbar$ modulo $o(\hbar^2)$ determines V near 0 up to $V(x)\leftrightarrow V(-x)$. In* *particular, if V satisfies asymmetric conditions like* (4.1),[1] *then V is spectrally determined.*

Colin de Verdière's proof is based on a close examination of the principal and subprincipal terms in the "Bohr-Sommerfeld rules to all orders" formula that he derives in [**Col05**]. However, we'll show in §4 that this result is also easily deducible from the one-dimensional versions of (1.4) and (1.5).

The algorithm we will introduce in §2 to calculate the semiclassical spectral invariants applies to more general semiclassical differential operators. In §5 we will show that for the perturbed Schrödinger operator

$$P_\hbar = -\frac{\hbar^2}{2}\Delta + V(x) + \hbar^2 V_1(x) \tag{1.8}$$

the first three invariants, $\nu_k(f), 0 \leq k \leq 2$, give a similar inverse spectral result:

Theorem 1.2. *Suppose the potential function V is a single well potential, and $V(x)$ and $V_1(x)$ satisfy either of the following:*
(a) $V(x)$ is even and $V_1(x)$ satisfies asymmetry conditions like (4.1)*;*
(b) $V_1(x)$ is odd and $V(x)$ satisfies asymmetry conditions like (4.1)*,*
then the semiclassical spectrum of $P_\hbar$ modulo $o(\hbar^4)$ determines $V(x)$ and $V_1(x)$.

We conjecture that the invariants, $\nu_k(f), 0 \leq k < \infty$, give one inverse result for Schrödinger operators with *semiclassical* potentials, i.e. potentials of the form

$$V_\hbar \sim \sum \hbar^{2k} V_k$$

modulo parity and/or asymmetry conditions. We will also show in §6 (by slightly generalizing a counter-example of Colin de Verdière) that if one drops his asymmetry assumptions, one can construct uncountable sets, $\{V_\alpha, \alpha \in (0,1)\}$, of single well potentials, the V_α's all distinct, for which the μ_k's in (1.7) are the same, i.e. which are isospectral modulo $O(\hbar^\infty)$. We will also show that in dimensions two or higher there exist infinite parameter families of potentials which are isospectral modulo $O(\hbar^\infty)$.[2]

[1]The asymmetric condition we listed is a very simple and special one. We would like to refer to [**Col08**] for a more general and complicated asymmetric condition.

[2]We remark that in a very recent joint work [**GuH**] by H. Hezari and one of the authors, it has been proved that the potentials in Colin de Verdière's example are isospectral *only* up to $O(\hbar^\infty)$ and are not actually isospectral: in fact, for *most* $\hbar$, the ground states of the Colin de Verdière's semiclassical isospectral pair are different. A similar conclusion will also apply to our semiclassical isospectral families.

We also study the analogues of results (1.3)–(1.7) in the presence of a magnetic field. In this case the Schrödinger operator becomes

$$S_\hbar^{(m)} = \sum_{k=1}^{n} \left(\frac{\hbar}{i} \frac{\partial}{\partial x_k} + a_k(x) \right)^2 + V(x), \tag{1.9}$$

where $\alpha = \sum a_k dx_k$ is the vector potential associated with the magnetic field and the field itself is the two form

$$B = d\alpha = \sum B_{ij} dx_i \wedge dx_j. \tag{1.10}$$

For the operator (1.9) the analogues of (1.3)–(1.7) are still true, although the formula (1.6) becomes considerately more complicated. We will show that the subprincipal term (1.5) is now given by

$$\frac{1}{48} \int f^{(2)}(\frac{1}{2} \sum (\xi_i + a_i)^2 + V(x))(-2 \sum \frac{\partial^2 V}{\partial x_k^2} + \|B\|^2) dx d\xi. \tag{1.11}$$

As a result, we will show

Theorem 1.3. *In dimension 2, if both V and B are radially symmetric, then they are spectrally determined.*

The last part of this paper is devoted to studying the relation of the spectral measure (1.7) and the Birkhoff canonical forms; the latter has been proved to be very useful in proving inverse spectral results. In §9 we will prove the following "quantum Birkhoff canonical form" theorem:

Theorem 1.4. *If V is a simple single well potential on the interval $V^{-1}([0, a))$, then on this interval $S_\hbar$ is unitarily equivalent to an operator of the form*

$$H_{QB}(S_\hbar^{har}, \hbar^2) + O(\hbar^\infty), \tag{1.12}$$

where $S_\hbar^{har}$ is the semiclassical harmonic oscillator, i.e. the 1-D Schrödinger operator with potential, $V(x) = \frac{x^2}{2}$, and H_{QB} the quantum Birkhoff canonical form that we will define in §9.

Then in §10 we will show that the spectral measure, $\mu_\hbar$, on the interval, $(0, a)$, is given by

$$\mu_\hbar(f) = \int_0^a f(t) \frac{dK}{dt}(t, \hbar^2)\, dt, \tag{1.13}$$

where

$$H_{QB}(s, \hbar^2) = t \iff s = K(t, \hbar^2). \tag{1.14}$$

In other words,

Theorem 1.5. *The spectral measure determines the Birkhoff canonical forms and vice-versa.*

We will end this introduction with a few words on the organization of this paper. We will prove the asymptotic expansion (1.7) in §2 for general semiclassical differential operators, with a focus on describing how to calculate the spectral invariants iteratively. Then in §3 we will apply our method to calculate the first several semiclassical spectral invariants of the Schrödinger operator, which will be used to give a simple proof of Theorem 1.1 in §4. In §5 we consider the perturbed Schrödinger operator and prove Theorem 1.2. In §6 we will construct families of potentials that are semiclassical isospectral. §7 and §8 are devoted to the magnetic Schrödinger operator, and we will prove Theorem 1.3. Finally, in §9 and §10 we study the relations between the Birkhoff canonical form and the spectral measure (1.7), and we will prove Theorem 1.4 and Theorem 1.5.

Acknowledgements. The results in this paper were, in large part, inspired by conversations with Shlomo Sternberg. We would like to express to him our warmest thanks. We would also like to express our warmest thanks to Shijun Zheng for suggestions on Schrödinger operators with magnetic fields.

Victor Guillemin is supported in part by NSF grant DMS-1005696.

2. The Semiclassical Trace Formula

Let

$$P_\hbar = \sum_{|\alpha|\le r} a_\alpha(x,\hbar)(\hbar D_x)^\alpha \tag{2.1}$$

be a semiclassical differential operator on $\mathbb{R}^n$, where $a_\alpha(x,\hbar) \in C^\infty(\mathbb{R}^n \times \mathbb{R})$. Recall that the Kohn-Nirenberg symbol of $P_\hbar$ is

$$p(x,\xi,\hbar) = \sum_\alpha a_\alpha(x,\hbar)\xi^\alpha \tag{2.2}$$

and its Weyl symbol is

$$p^w(x,\xi,\hbar) = \exp(-\frac{\hbar}{2}D_\xi\partial_x)p(x,\xi,\hbar). \tag{2.3}$$

We assume that p^w is a real-valued function, so that $P_\hbar$ is self-adjoint. Moreover, we assume that for the interval $[a,b]$, $(p^w)^{-1}([a,b])$, $0\le\hbar\le h_0$, is compact. Then by Friedrich's theorem, the spectrum of $P_\hbar$, $\hbar<h_0$, on the interval $[a,b]$, consists of a finite number of eigenvalues,

$$\lambda_i(\hbar), \quad 1\le i\le N(\hbar), \tag{2.4}$$

with $N(\hbar)\to\infty$ as $\hbar\to 0$. Let

$$p(x,\xi,0) = p^w(x,\xi,0) \tag{2.5}$$

be the principal symbols of $P_\hbar$.

Suppose $f \in C_0^\infty(\mathbb{R})$ is smooth and compactly supported on (a, b). Then

$$f(P_\hbar) = \frac{1}{\sqrt{2\pi}} \int \hat{f}(t) e^{itP_\hbar}\, dt,$$

where $\hat{f}$ is the Fourier transform of f.

Theorem 2.1 ([**DiS**], [**HeR**])**.** *The operator $f(P_\hbar)$ is a semiclassical pseudodifferential operator with left Kohn-Nirenberg symbol*

$$b_f(x, \xi, \hbar) \sim \sum_k \hbar^k \left(\sum_{l \le 2k} b_{k,l}(x, \xi) \left((\frac{1}{i}\frac{d}{ds})^l f \right) (p_0(x, \xi)) \right), \tag{2.6}$$

where $b_{k,l}$ is described as follows.

It follows that

$$\mathrm{trace} f(P_\hbar) = \hbar^{-n} \int b_f(x, \xi, \hbar)\, dx d\xi + O(\hbar^\infty). \tag{2.7}$$

The coefficients $b_{k,l}(x, \xi)$ in (2.6) can be computed as follows: Let Q_α be the operator

$$Q_\alpha = \frac{1}{\alpha!} \left(\partial_x + it \frac{\partial p_0}{\partial x} \right)^\alpha, \tag{2.8}$$

and let $b_k(x, \xi, t)$ be defined iteratively by means of the equation

$$\frac{1}{i}\frac{\partial b_m}{\partial t} = \sum_{|\alpha| \ge 1} \sum_{j+k+|\alpha|=m} D_\xi^\alpha p_j Q_\alpha b_k + \sum_{j \ge 1} p_j b_{m-j} \tag{2.9}$$

with initial conditions

$$b_0(x, \xi, t) = 1 \tag{2.10}$$

and

$$b_m(x, \xi, 0) = 0 \tag{2.11}$$

for $m \ge 1$, where the p_j's are defined by $p = \sum p_j \hbar^j$. We will show that $b_k(x, \xi, t)$ is a polynomial in t of degree $2k$. The functions $b_{k,l}(x, \xi)$ are just the coefficients of this polynomial,

$$b_k(x, \xi, t) = \sum_{l \le 2k} b_{k,l}(x, \xi) t^l. \tag{2.12}$$

2.1. Proof of Theorem 2.1. We will only focus on symbolic calculus that leads to (2.6), with coefficients described by (2.9)–(2.12), and refer to ([**DiS**], [**HeR**]) for more technical details on the remainder estimates and trace class properties of the remainder. We look for a family $U(t)$ of semiclassical pseudodifferential differential operators depending smoothly on t which satisfies the differential equation

$$\frac{1}{i}\frac{\partial}{\partial t} U(t) = P_\hbar U(t) \tag{2.13}$$

with initial condition

$$U(0) = \mathrm{Id}. \tag{2.14}$$

Let $\mu(x, y, t, \hbar)$ be the Schwartz kernel of $U(t)$. For this to be the kernel of a pseudodifferential operator, it must have the form

$$\mu(x, y, t, \hbar) = (2\pi\hbar)^{-n} \int a(x, \xi, t, \hbar) e^{i\frac{(x-y)\cdot\xi}{\hbar}} d\xi. \tag{2.15}$$

Our initial condition (2.14) amounts to saying that

$$a(x, \xi, 0, \hbar) = 1. \tag{2.16}$$

Set

$$a(x, \xi, t, \hbar) = e^{itp_0(x,\xi)} b(x, \xi, t, \hbar),$$

and then (2.16) becomes

$$b(x, \xi, 0, \hbar) = 1 \tag{2.17}$$

while (2.13) yields

$$\frac{1}{i}\frac{\partial}{\partial t}\left(e^{itp_0(x,\xi)} b(x, \xi, t, \hbar)\right) = p(x, \xi, \hbar) \star \left(e^{itp_0(x,\xi)} b(x, \xi, t, \hbar)\right), \tag{2.18}$$

where $\star$ is the *star product* defining the symbol of the composition of two pseudodifferential operators. We can expand (2.18) out as

$$e^{itp_0}\left(\frac{1}{i}\frac{\partial b}{\partial t} + p_0 b\right) \sim \sum_\alpha \frac{\hbar^\alpha}{\alpha!} D_\xi^\alpha p \partial_x^\alpha (e^{itp_0} b),$$

write

$$\partial_x^\alpha (e^{itp_0} b) = e^{itp_0}(e^{-itp_0}\partial_x^\alpha e^{itp_0} b),$$

and cancel the factor e^{itp_0} from both sides of the preceding equation to get

$$\frac{1}{i}\frac{\partial b}{\partial t} + p_0 b \sim \sum_\alpha \frac{\hbar^\alpha}{\alpha!} D_\xi^\alpha p Q^\alpha b,$$

where Q is the operator

$$Q = \partial_x + it\frac{\partial p_0}{\partial x}.$$

Since $Q^0 = I$, we can rewrite the previous equation as

$$\frac{1}{i}\frac{\partial b}{\partial t} \sim \sum_{|\alpha|\geq 1} \frac{\hbar^\alpha}{\alpha!} D_\xi^\alpha p Q^\alpha b + (p - p_0) b. \tag{2.19}$$

Let us expand b and p in powers of $\hbar$,

$$b \sim \sum_k b_k(x, \xi, t)\hbar^k, \quad p \sim \sum_k p_k \hbar^k,$$

and equate powers of (2.19). This gives us the series of equations

$$\frac{1}{i}\frac{\partial b_m}{\partial t} = \sum_{|\alpha|\geq 1} \sum_{j+k+|\alpha|=m} \frac{1}{\alpha!} D_\xi^\alpha p_j Q^\alpha b_k + \sum_{j\geq 1} p_j b_{m-j} \tag{2.20}$$

with initial conditions

$$b_0(x,\xi,t) \equiv 1, \quad b_m(x,\xi,0) \equiv 0 \text{ for } m \geq 1,$$

and we can solve these equations recursively by integration.

Proposition 2.2. *$b_m(x,\xi,t)$ is a polynomial in t of degree at most $2m$.*

Proof. Proof by induction. We know this for $m=0$. For $j+k+|\alpha| = m$, we know by induction that $Q^\alpha b_k$ is a polynomial in t of degree at most $|\alpha|+2k = m-j+k \leq m+k < 2m$, so integration shows that b_m is a polynomial in t of degree at most $2m$. q.e.d.

3. Spectral Invariants for Schrödinger Operators

In this section we will focus on the operators (1.1), so that

$$p(x,\xi,\hbar) = p_0(x,\xi) = \frac{\xi^2}{2} + V(x). \tag{3.1}$$

We would like to compute trace$f(S_\hbar)$ for $f \in C_0^\infty(-a,a)$ via the semi-classical trace formula (2.7). Notice that from (2.6), (2.7), and (2.10) it follows that the first trace invariant is

$$\int f(p(x,\xi))\, dx d\xi,$$

which implies Weyl's law, ([**GuS**] §9.8), for the asymptotic distributions of the eigenvalues (2.4).

To compute the next trace invariant, we note that for the Schrödinger operator (1.1), the operator Q_α has the form

$$Q_\alpha = \frac{1}{\alpha!}\left(\partial_x + it\frac{\partial V}{\partial x}\right)^\alpha. \tag{3.2}$$

It follows from (2.9) that

$$\begin{aligned}\frac{1}{i}\frac{\partial b_m}{\partial t} &= \sum_{|\alpha|\geq 1}\sum_{k+|\alpha|=m} D_\xi^\alpha p_0 Q^\alpha b_k \\ &= \sum_k \frac{\xi_k}{i}\left(\frac{\partial}{\partial x_k} + it\frac{\partial V}{\partial x_k}\right) b_{m-1} - \frac{1}{2}\sum_k \left(\frac{\partial}{\partial x_k} + it\frac{\partial V}{\partial x_k}\right)^2 b_{m-2}.\end{aligned}$$

Since $b_0(x,\xi,t) = 1$ and $b_1(x,\xi,0) = 0$, we have

$$b_1(x,\xi,t) = \frac{it^2}{2}\sum_l \xi_l \frac{\partial V}{\partial x_l},$$

and thus

$$\begin{aligned}\frac{1}{i}\frac{\partial b_2}{\partial t} &= \sum_k \frac{\xi_k}{i}\left(\frac{\partial}{\partial_{x_k}} + it\frac{\partial V}{\partial x_k}\right)\left(\frac{it^2}{2}\sum_l \xi_l \frac{\partial V}{\partial x_l}\right) \\ &\quad - \frac{1}{2}\sum_k \left(\frac{\partial}{\partial x_k} + it\frac{\partial V}{\partial x_k}\right)^2 (1) \\ &= \frac{t^2}{2}\sum_{k,l}\xi_k\xi_l\left(\frac{\partial^2 V}{\partial x_k \partial x_l} + it\frac{\partial V}{\partial x_k}\frac{\partial V}{\partial x_l}\right) \\ &\quad - \frac{1}{2}\sum_k \left(it\frac{\partial^2 V}{\partial x_k^2} - t^2\frac{\partial V}{\partial x_k}\frac{\partial V}{\partial x_k}\right).\end{aligned}$$

It follows that

$$\begin{aligned} b_2(x,\xi,t) &= \frac{t^2}{4}\sum_k \frac{\partial^2 V}{\partial x_k^2} + \frac{it^3}{6}\left(\sum_k \left(\frac{\partial V}{\partial x_k}\right)^2 + \sum_{k,l}\xi_k\xi_l\frac{\partial^2 V}{\partial x_k\partial x_l}\right) \\ &\quad - \frac{t^4}{8}\sum_{k,l}\xi_k\xi_l\frac{\partial V}{\partial x_k}\frac{\partial V}{\partial x_l}. \end{aligned} \tag{3.3}$$

Thus the next trace invariant will be the integral

$$\begin{aligned} \int -\frac{1}{4}\sum_k \frac{\partial^2 V}{\partial x_k^2} f''\left(\frac{\xi^2}{2}+V(x)\right) - \frac{1}{6}\sum_k\left(\frac{\partial V}{\partial x_k}\right)^2 f^{(3)}\left(\frac{\xi^2}{2}+V(x)\right) \\ - \frac{1}{6}\sum_{k,l}\xi_k\xi_l\frac{\partial^2 V}{\partial x_k\partial x_l} f^{(3)}\left(\frac{\xi^2}{2}+V(x)\right) \\ - \frac{1}{8}\sum_{k,l}\xi_k\xi_l\frac{\partial V}{\partial x_k}\frac{\partial V}{\partial x_l} f^{(4)}\left(\frac{\xi^2}{2}+V(x)\right)\, dxd\xi. \end{aligned} \tag{3.4}$$

We can apply to these expressions the integration by parts formula,

$$\int \frac{\partial A}{\partial x_k} B\left(\frac{\xi^2}{2}+V(x)\right)\, dxd\xi = -\int A(x)\frac{\partial V}{\partial x_k}B'\left(\frac{\xi^2}{2}+V(x)\right)\, dxd\xi \tag{3.5}$$

and

$$\int \xi_k\xi_l A(x) B'\left(\frac{\xi^2}{2}+V(x)\right)\, dxd\xi = -\int \delta_k^l A(x) B\left(\frac{\xi^2}{2}+V(x)\right)\, dxd\xi. \tag{3.6}$$

Applying (3.5) to the first term in (3.4), we get

$$\int \frac{1}{4}\sum_k\left(\frac{\partial V}{\partial x_k}\right)^2 f^{(3)}\left(\frac{\xi^2}{2}+V(x)\right)\, dxd\xi,$$

and by applying (3.6), the fourth term in (3.4) becomes

$$\int \frac{1}{8}\sum_k\left(\frac{\partial V}{\partial x_k}\right)^2 f^{(3)}\left(\frac{\xi^2}{2}+V(x)\right)\, dxd\xi.$$

Finally, applying both (3.6) and (3.5), the third term in (3.4) becomes

$$\int -\frac{1}{6}\sum_k (\frac{\partial V}{\partial x_k})^2 f^{(3)}(\frac{\xi^2}{2}+V(x))\ dxd\xi.$$

So the integral (3.4) can be simplified to

$$\frac{1}{24}\int \sum_k (\frac{\partial V}{\partial x_k})^2 f^{(3)}(\frac{\xi^2}{2}+V(x))\ dxd\xi.$$

We conclude

Theorem 3.1. *The first two terms of* (2.7) *are*

$$\begin{aligned} \mathrm{trace} f(S_\hbar) = \int f\left(\frac{\xi^2}{2}+V(x)\right)\ dxd\xi + \frac{1}{24}\hbar^2 \int \sum_k (\frac{\partial V}{\partial x_k})^2 f^{(3)} \\ \left(\frac{\xi^2}{2}+V(x)\right) dxd\xi + O(\hbar^4). \end{aligned} \tag{3.7}$$

In deriving (3.7) we have assumed that f is compactly supported. However, since the spectrum of $S_\hbar$ is bounded from below by zero, the left and right hand sides of (3.7) are unchanged if we replace the "f" in (3.7) by *any* function, f, with support on $(-\infty, a)$, and, as a consequence of this remark, it is easy to see that the following two integrals,

$$\int_{\frac{\xi^2}{2}+V(x)\le\lambda} dxd\xi \tag{3.8}$$

and

$$\int_{\frac{\xi^2}{2}+V(x)\le\lambda} \sum_k (\frac{\partial V}{\partial x_k})^2 dxd\xi, \tag{3.9}$$

are determined by the spectrum (2.4) on the interval $[0, a]$. Moreover, from (3.7), one reads off the Weyl law: For $0 < \lambda < a$,

$$\#\{\lambda_i(\hbar) \le \lambda\} = (2\pi\hbar)^{-n}\left(\mathrm{Vol}(\frac{\xi^2}{2}+V(x)\le\lambda) + O(\hbar)\right). \tag{3.10}$$

We also note that the second term in the formula (3.7) can, by (3.6), be written in the form

$$\frac{1}{24}\hbar^2 \int \sum_k \frac{\partial^2 V}{\partial x_k^2} f^{(2)}(\frac{\xi^2}{2}+V(x))\ dxd\xi.$$

3.1. Proof of (1.6). To prove (1.6), we notice that for m even, the lowest degree term in the polynomial b_m is of degree $\frac{m}{2}+1$; thus we can write

$$b_m = \sum_{l=-\frac{m}{2}+1}^{m} b_{m,l} t^{m+l}.$$

Putting this into the iteration formula, we will get

$$\begin{aligned}\frac{m+l}{i}b_{m,l} =&\sum \frac{\xi_k}{i}\frac{\partial b_{m-1,l}}{\partial x_k} + \sum \xi_k \frac{\partial V}{\partial x_k} b_{m-1,l-1} - \frac{1}{2}\sum \frac{\partial^2 b_{m-2,l+1}}{\partial x_k^2} \\ &- \frac{i}{2}(\frac{\partial}{\partial x_k}\frac{\partial V}{\partial x_k} + \frac{\partial V}{\partial x_k}\frac{\partial}{\partial x_k})b_{m-2,l} + \frac{1}{2}\sum (\frac{\partial V}{\partial x_k})^2 b_{m-2,l-1},\end{aligned}$$

from which one can easily conclude that for $l \geq 0$,

$$b_{m,l} = \sum \xi^\alpha (\frac{\partial V}{\partial x})^\beta p_{\alpha,\beta}(DV, \dots, D^m V) \tag{3.11}$$

where $p_{\alpha,\beta}$ is a polynomial, and $|\alpha| + |\beta| \geq 2l - 1$. It follows that, by applying the integration by parts formula (3.5) and (3.6), all the $f^{(m+l)}$, $l \geq 0$, in the integrand of the $\hbar^n$th term in the expansion (2.6) can be replaced by $f^{(m)}$. In other words, only derivatives of f of degree $\leq 2k$ figure in the expression for $\nu_k(f)$. For those terms involving derivatives of order less than $2k$, one can also use integration by parts to show that each $f^{(m)}$ can be replaced by an $f^{(m+1)}$ and an $f^{(m-1)}$. In particular, we can replace all the odd derivatives by even derivatives. This proves (1.6).

3.2. More Spectral Invariants in 1-dimension. For simplicity, we will only consider the dimension one case. One can solve the equation (2.9) for the Schrödinger operator with initial conditions (2.10) and (2.11) inductively, and get in general

$$b_{2m}(x,\xi,t) = \sum_{k=m+1}^{4m} t^k \sum_{\substack{n+t=k-m, n\leq m\\ l_1+\cdots+l_t=2m}} \xi^{2n} V^{(l_1)} \cdots V^{(l_t)} a_{n,l}, \tag{3.12}$$

and

$$b_{2m-1}(x,\xi,t) = \sum_{k=m+1}^{4m-2} t^k \sum_{\substack{n+t=k-m, n\leq m-1\\ l_1+\cdots+l_t=2m-1}} \xi^{2n+1} V^{(l_1)} \cdots V^{(l_t)} \tilde{a}_{n,l}, \tag{3.13}$$

where $a_{n,l}$ and $\tilde{a}_{n,l}$ are constants depending on n and $l_1, \cdots, l_t$. In particular,

$$\begin{aligned} b_3(x,\xi,t) =& \frac{t^3}{6}\xi V^{(3)}(x) + \frac{t^4}{3} i\xi \left(V'(x)V''(x) + \frac{1}{8}\xi^2 V^{(3)} \right) \\ &- \frac{t^5}{12}\xi \left(V'(x)^3 + \xi^2 V'(x)V''(x) \right) - \frac{t^6}{48} i\xi^3 V'(x)^3, \end{aligned} \tag{3.14}$$

and
(3.15)

$$\begin{aligned}b_4(x,\xi,t) =& -\frac{t^3}{24}iV^{(4)}(x)+t^4\left(\frac{7}{96}V''(x)^2+\frac{5}{48}V'(x)V^{(3)}(x)+\frac{1}{16}\xi^2V^{(4)}(x)\right)\\&+t^5\left(\frac{13}{120}iV'(x)^2V''(x)+\frac{13}{120}i\xi^2V''(x)^2+\frac{19}{120}i\xi^2V'(x)V^{(3)}(x)\right.\\&\left.+\frac{1}{120}i\xi^4V^{(4)}(x)\right)\\&+t^6\left(-\frac{1}{72}V'(x)^4-\frac{47}{288}\xi^2V'(x)^2V''(x)-\frac{1}{72}\xi^4V''(x)^2\right.\\&\left.-\frac{1}{48}\xi^4V'(x)V^{(3)}(x)\right)\\&-\frac{t^7}{48}\left(i\xi^2V'(x)^4+i\xi^4V'(x)^2V''(x)\right)+\frac{t^8}{384}\xi^4V'(x)^4.\end{aligned}$$

The order $\hbar^k$ term is given by integrating the above formula with t^k replaced by $\frac{1}{i^k}f^{(k)}(\frac{\xi^2}{2}+V(x))$. By integration by parts,

$$\int \xi^{2k}A(x)B^{(k)}(\frac{\xi^2}{2}+V(x))\;dxd\xi=(-1)^k(2k-1)!!\int A(x)B(\frac{\xi^2}{2}+V(x))\;dxd\xi,$$

so we can simplify the integral to

$$\int\left(\frac{V^{(4)}f^{(3)}}{240}+\frac{(V'')^2f^{(4)}}{160}+\frac{V'V'''f^{(4)}}{120}+\frac{11(V')^2V''f^{(5)}}{1440}+\frac{(V')^4f^{(6)}}{1152}\right)dxd\xi.$$

Note that

$$\int V^{(4)}f^{(3)}=-\int V'V'''f^{(4)}=\int V''V''f^{(4)}+V''V'V'f^{(5)}$$

and

$$\int V'V'V''f^{(5)}=-\int\left(2V'V'V''f^{(5)}+V'V'V'V'f^{(6)}\right),$$

so we can finally simplify the integral to

$$\int\left(\frac{1}{480}(V''(x))^2f^{(4)}(\frac{\xi^2}{2}+V(x))+\frac{7}{3456}(V'(x))^4f^{(6)}(\frac{\xi^2}{2}+V(x))\right)\;dxd\xi,$$

or

$$\frac{1}{288}\int\left(\frac{\xi^4}{5}(V''(x))^2+\frac{7}{12}(V'(x))^4\right)f^{(6)}(\frac{\xi^2}{2}+V(x))\;dxd\xi.$$

This can also be written in a more compact form as

$$\frac{1}{1152}\int(7V'V'''+\frac{47}{5}(V''(x))^2)f^{(4)}(\frac{\xi^2}{2}+V(x))\;dxd\xi.$$

It follows that

$$\int_{\frac{\xi^2}{2}+V(x)\le\lambda}(7V'V'''+\frac{47}{5}(V''(x))^2)dxd\xi$$

is spectrally determined.

4. Inverse Spectral Results: Recovering a Single Well Potential

Suppose V is a "single well potential," i.e. has a unique nondegenerate critical point at $x = 0$ with minimal value $V(0) = 0$, and V is increasing for x positive, and decreasing for x negative. For simplicity, assume in addition that

$$-V'(-x) > V'(x) \tag{4.1}$$

holds for all $x > 0$. We will show how the spectral invariants (3.8) and (3.9) enable us to recover $V(x)$.

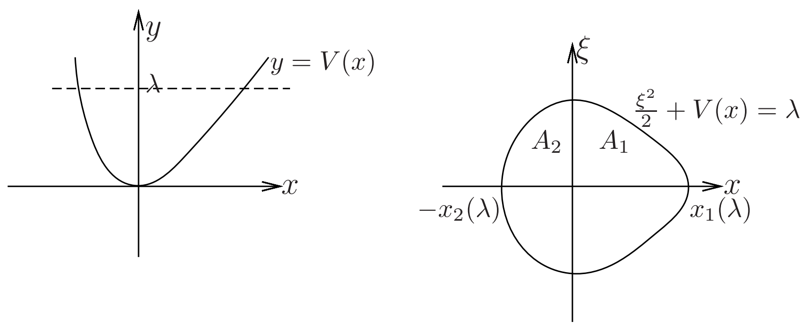

Figure 1. Single well potential.

For $0 < \lambda < a$, we let $-x_2(\lambda) < 0 < x_1(\lambda)$ be the intersections of the curve $\frac{\xi^2}{2} + V(x) = \lambda$ with the x-axis on the (x, ξ) plane. We will denote by A_1 the region in the first quadrant bounded by this curve, and by A_2 the region in the second quadrant bounded by this curve. Then from (3.8) and (3.9) we can determine

$$\int_{A_1} + \int_{A_2} dx d\xi \tag{4.2}$$

and

$$\int_{A_1} + \int_{A_2} V'(x)^2 dx d\xi. \tag{4.3}$$

Let $x = f_1(s)$ be the inverse of the function $s = V(x), x \in (0, a)$. Then

$$\begin{aligned}
\int_{A_1} V'(x)^2 \, dx d\xi &= \int_0^{x_1(\lambda)} V'(x)^2 \int_0^{\sqrt{2(\lambda - V(x))}} d\xi dx \\
&= \int_0^{x_1(\lambda)} V'(x)^2 \sqrt{2\lambda - 2V(x)} \, dx \\
&= \int_0^{\lambda} \sqrt{2\lambda - 2s} \, V'(f_1(s)) \, ds \\
&= \int_0^{\lambda} \sqrt{2\lambda - 2s} \left(\frac{df_1}{ds} \right)^{-1} ds.
\end{aligned}$$

Similarly,

$$\int_{A_2} V'(x)^2 \, dx d\xi = \int_0^{\lambda} \sqrt{2\lambda - 2s} \left(\frac{df_2}{ds} \right)^{-1} \, ds,$$

where $x = f_2(s)$ is the inverse of the function $s = V(-x), x > 0$. So the spectrum of $S_\hbar$ determines

$$\int_0^\lambda \sqrt{\lambda - s}\left((\frac{df_1}{ds})^{-1} + (\frac{df_2}{ds})^{-1}\right)\, ds. \tag{4.4}$$

Similarly, the knowledge of the integral (4.2) amounts to the knowledge of

$$\int_0^\lambda \sqrt{\lambda - s}\left(\frac{df_1}{ds} + \frac{df_2}{ds}\right)\, ds. \tag{4.5}$$

Recall now that the fractional integration operation of Abel,

$$J^a g(\lambda) = \frac{1}{\Gamma(a)}\int_0^\lambda (\lambda - t)^{a-1} g(t)\, dt \tag{4.6}$$

for $a > 0$, satisfies $J^a J^b = J^{a+b}$. Hence if we apply $J^{1/2}$ to the expression (4.5) and (4.4) and then differentiate by λ two times, we recover $\frac{df_1}{ds} + \frac{df_2}{ds}$ and $(\frac{df_1}{ds})^{-1} + (\frac{df_2}{ds})^{-1}$ from the spectral data. In other words, we can determine f_1' and f_2' up to the ambiguity $f_1' \leftrightarrow f_2'$. However, by (4.1), $f_1' > f_2'$. So we can from the above determine f_1' and f_2', and hence $f_i, i = 1, 2$. This proves Theorem 1.1.

Remark 4.1. The formula (4.5) can be used to construct lots of Zoll potentials, i.e. potentials for which the Hamiltonian flow v_H associated with $H = \xi^2 + V(x)$ is periodic of period 2π. It is clear that the potential $V(x) = x^2$ has this property and is the only even potential with this property. However, by (4.5) and the area-period relation (see Proposition 7.1), every single well potential V for which

$$f_1(s) + f_2(s) = 2s^{1/2}$$

has this property. We will discuss some implications of this in a sequel to this paper.

Remark 4.2. The same argument also shows that if V is decreasing on $(-\infty, -a)$ and is increasing on (b, ∞), and that V is known on $(-a, b)$, then we can recover V everywhere. In particular, we can recover symmetric double well potentials.

5. Inverse Spectral Results: Recovering Potentials for 1-dimensional Perturbed Schrödinger Operators

Consider the 1-dimensional perturbed Schrödinger operator

$$P_\hbar = -\frac{\hbar^2}{2}\Delta + V(x) + \hbar^2 V_1(x). \tag{5.1}$$

For this operator we have

$$p_0(x, \xi) = \frac{\xi^2}{2} + V(x)$$

and

$$p_2(x, \xi) = V_1(x).$$

By iterative use of (2.9), we get

$$b_2 = b_2^{old} + iV_1(x)t \tag{5.2}$$

and

$$b_4 = b_4^{old} + \frac{t^2}{2}(\frac{1}{2}V_1'' - V_1^2) + i\frac{t^3}{3}(\frac{1}{2}\xi^2 V_1'' + V'V_1' + \frac{3}{4}V''V_1) + \frac{t^4}{4}(-\frac{2}{3}V'V'V_1 + \frac{1}{3}\xi^2 V''V_1) + i\frac{t^5}{5}(-\frac{5}{8}\xi^2 V'V'V_1), \tag{5.3}$$

where b_2^{old} and b_4^{old} are the corresponding polynomials for the unperturbed Schrödinger operator with potential V that we computed in §3. By integration by parts, we conclude that the first three semiclassical spectral invariants for the operator (5.1) are

$$\mathrm{I}_\lambda = \int_{\frac{\xi^2}{2}+V(x)<\lambda} dx\ d\xi$$

$$\mathrm{II}_\lambda = \int_{\frac{\xi^2}{2}+V(x)<\lambda} (\frac{1}{24}V'' + \tilde{V}_1 V')dx\ d\xi$$

and

$$\mathrm{III}_\lambda = \int_{\frac{\xi^2}{2}+V(x)<\lambda} (\frac{7}{1152}V'V''' + \frac{47}{5760}V''V'' + \frac{7}{24}V'V'V_1 + \overline{W}V')dx\ d\xi,$$

where

$$\tilde{V}_1(x) = \int_0^x V_1(t)dt,$$

$$\overline{W}(x) = \int_0^x \tilde{W}(t)V'(t)dt$$

and

$$\tilde{W}(x) = \int_0^x W(t)dt = \int_0^x (-\frac{1}{12}V_1'' + \frac{1}{2}V_1^2)dt.$$

Now suppose that V is an even single well potential. Then from I_λ one can recover the potential function V. To recover the perturbation, V_1, let $x = f(s)$ be the inverse of the function $s = V(x)$ for $x > 0$. Since V is known, II_λ determines

$$\int_{\frac{\xi^2}{2}+V(x)<\lambda} \tilde{V}_1(x)V'(x)dx\ d\xi,$$

which equals

$$J^{3/2}(\tilde{V}_1(f(\lambda)) - \tilde{V}_1(-f(\lambda))),$$

where J is the fractional integral as before. It follows that one can recover the function

$$\tilde{V}_1(x) - \tilde{V}_1(-x)$$

for $0 < x < a$, and by taking the derivative, the function

$$V_1(x) + V_1(-x), \qquad x > 0. \tag{5.4}$$

Next let's extract information from the third invariant, III_λ. The first two terms in the integrand of III_λ are already known since we know V. The third term, by the same method above, gives

$$V'(x)V_1(x) - V'(-x)V_1(-x).$$

Since V is even, V' is odd. So the above expression equals

$$V'(x)(V_1(x) + V_1(-x)),$$

which is already known. So the only new information comes from the last term, which gives us

$$\overline{W}(x) - \overline{W}(-x).$$

Taking the derivative, we get the function

$$\tilde{W}(x)V'(x) + \tilde{W}(-x)V'(-x) = (\tilde{W}(x) - \tilde{W}(-x))V'(x).$$

So the function $\tilde{W}(x) - \tilde{W}(-x)$ is spectrally determined. Taking the derivative again, we recover the function

$$W(x) + W(-x) = -\frac{1}{12}(V_1''(x) + V_1''(-x)) + \frac{1}{2}(V_1^2(x) + V_1^2(-x)).$$

Since we have already determined $V_1(x) + V_1(-x)$, and thus $V_1''(x) + V_1''(-x)$, for $x > 0$, we conclude that the function

$$V_1^2(x) + V_1^2(-x), \qquad x > 0 \tag{5.5}$$

is spectrally determined. This together with (5.4) determines $V_1(x)$ modulo an asymmetry assumption of type 4.1.

Similarly, if V is a single well potential while perturbation V_1 is an odd function, then (5.4) vanishes, and thus the invariants I_λ and $\mathrm{I\!I}_\lambda$ will determine V modulo condition (4.1), and this in turn determines V_1 according to (5.5). This completes the proof of Theorem 1.2.

6. Counterexamples

Let $V \in C^\infty(\mathbb{R}^n)$ be a single well potential as in the previous section. Then we know that the spectrum of the Schrödinger operator (1.1) is discrete. The question "to what extent does this spectrum determine V?" is still an open one; however, we will show in this section

Proposition 6.1. (1) *In dimension one there exists a family of uncountable potentials for which the spectral invariants* (1.6) *are the same.*
(2) *In dimension greater than one there even exist infinite parameter families of potentials for which these invariants are the same.*

We first observe that if $A : \mathbb{R}^n \to \mathbb{R}^n$ is an orthogonal transformation, i.e. $A \in O(n)$, then

$$A^* \circ S_\hbar \circ (A^{-1})^* = S_\hbar^A,$$

where

$$S_\hbar^A = \frac{\hbar^2}{2}\Delta + V^A(x)$$

and $V^A(x) = V(Ax)$. Thus, if $K_f(x, y, \hbar)$ is the Schwartz kernel of the operator $f(S_\hbar)$, then $K_f(Ax, Ay, \hbar)$ is the Schwartz kernel of the operator $f(S_\hbar^A)$, and by (1.6), $K_f(Ax, Ax, \hbar)$ has an asymptotic expansion of the form

$$(2\pi\hbar)^{-n} \sum_k \hbar^k \int b_{k,l}(Ax, \xi) \left((\frac{1}{i}\frac{d}{ds})^l f \right) \left(\frac{|\xi|^2}{2} + V(Ax) \right) \, d\xi.$$

In particular, since the function $b_{k,l}(x, \xi)$ in the expansion (1.6) has the form

$$b_{k,l} = \sum \xi^\alpha P_{\alpha,k,l}(DV, \ldots, D^{2k}V), \tag{6.1}$$

the corresponding function for $S_\hbar^A$ has the form

$$b_{k,l}^A = \sum \xi^\alpha P_{\alpha,k,l}(DV^A, \dots, D^{2k}V^A), \tag{6.2}$$

and hence in particular

$$b_{k,l}(\xi, Ax) = \sum \xi^\alpha p_{\alpha,k,l}(DV^A, \dots, D^{2k}V^A) \tag{6.3}$$

for all $x \in \mathbb{R}^n$.

Now choose V to be rotationally symmetric and let $\rho_i(x)$ be a non-negative C^∞ function with support on the set

$$i < |x| < i+1, \quad x_1 > 0, \dots, x_n > 0$$

with $\rho_i = 0$ for i odd and $\rho_i \neq 0$ for i even. Then, fixing a sequence of rotations,

$$A = \{A_i \in O(n), i = 1, 2, 3, \dots\},$$

the potentials

$$V_A = V(x) + \sum \rho_i(A_i x)$$

have the same spectral invariants (1.6) for all sequences, A, as can be seen by writing

$$\begin{aligned}
&\int b_{k,l}(\xi, DV_A, \dots, D^{2k}V_A) f^l\left(\frac{\xi^2}{2} + V_A\right)\, dx d\xi \\
&= \sum \int_{i \leq |x| \leq i+1} b_{k,l}(\xi, DV_A, \dots, D^{2k}V_A) f^l\left(\frac{\xi^2}{2} + V_A\right)\, dx d\xi \\
&= \sum \int_{i \leq |x| \leq i+1} b_{k,l}(\xi, D(V+\rho_i)^A, \dots, \\
&\qquad D^{2k}(V+\rho_i)^{A_i}) f^l\left(\frac{\xi^2}{2} + (V+\rho_i)^{A_i}\right)\, dx d\xi
\end{aligned}$$

and observing that this is equal to

$$\sum \int_{i \leq |x| \leq i+1} b_{k,l}(\xi, D(V+\rho_i), \dots, D^{2k}(V+\rho_i)) f^l(\frac{|\xi^2|}{2} + V + \rho_i)\, dx d\xi$$

by the equation (6.3).

In dimension one this construction doesn't give us an infinite parameter family of potentials with the same spectral invariants, but it is easy to see that it does give us uncountable potentials for which these invariants are the same. Namely, for every $\alpha \in [0, 1)$ let

$$\alpha = .\alpha_1\alpha_2\alpha_3\cdots$$

be the binary expansion of α and choose A_{2i} to be the rotation $x \to -x$ if α_i is one, and $x \to x$ if α_i is zero. This example (which is a slightly modified version of a counterexample of Colin de Verdière in [**Col08**]) shows why the assumption (4.1) (or some asymmetry condition similar to (4.1)) is necessary in the hypotheses of Theorem 4.1.

7. Semiclassical Spectral Invariants for Schrödinger Operators with Magnetic Fields

In this section we will show how the results in §3 can be extended to Schrödinger operators with magnetic fields. Recall that a semiclassical Schrödinger operator with magnetic field on $\mathbb{R}^n$ has the form

$$S_\hbar^m := \frac{1}{2}\sum_j \left(\frac{\hbar}{i}\frac{\partial}{\partial x_j} + a_j(x)\right)^2 + V(x) \tag{7.1}$$

where $a_k \in C^\infty(\mathbb{R}^n)$ are smooth functions defining a magnetic field B, which in dimension 3 is given by $\vec{B} = \vec{\nabla} \times \vec{a}$, and in arbitrary dimension by the 2-form $B = d(\sum a_k dx_k)$. We will assume that the vector potential $\vec{a}$ satisfies the Coulomb gauge condition,

$$\nabla \cdot \vec{a} = \sum_j \frac{\partial a_j}{\partial x_j} = 0. \tag{7.2}$$

(In view of the definition of B, one can always choose such a Coulomb vector potential.) In this case, the Kohn-Nirenberg symbol of the operator (7.1) is given by

$$p(x,\xi,\hbar) = \frac{1}{2}\sum_j (\xi_j + a_j(x))^2 + V(x). \tag{7.3}$$

Recall that

$$Q_\alpha = \frac{1}{\alpha!}\prod_k \left(\frac{\partial}{\partial x_k} + it\frac{\partial p}{\partial x_k}\right)^{\alpha_k}, \tag{7.4}$$

so the iteration formula (2.9) becomes
(7.5)
$$\frac{1}{i}\frac{\partial b_m}{\partial t} = \sum_k \frac{1}{i}\frac{\partial p}{\partial \xi_k}\left(\frac{\partial}{\partial x_k} + it\frac{\partial p}{\partial x_k}\right) b_{m-1} - \frac{1}{2}\sum_k \left(\frac{\partial}{\partial x_k} + it\frac{\partial p}{\partial x_k}\right)^2 b_{m-2},$$

from which it is easy to see that

$$b_1(x,\xi,t) = \sum_k \frac{\partial p}{\partial \xi_k}\frac{\partial p}{\partial x_k}\frac{it^2}{2}. \tag{7.6}$$

Thus the "first" spectral invariant is

$$\int \sum_k (\xi_k + a_k(x))\frac{\partial p}{\partial x_k} f^{(2)}(p)\ dxd\xi = -\int \sum_k \frac{\partial a_k}{\partial x_k} f'(p) dxd\xi = 0,$$

where we used the fact $\sum \frac{\partial a_k}{\partial x_k} = 0$.

With a little more effort we get for the next term

$$\begin{aligned} b_2(x,\xi,t) =& \frac{t^2}{4}\sum_k \frac{\partial^2 p}{\partial x_k^2} \\ &+ \frac{it^3}{6}\left(\sum_{k,l}\frac{\partial p}{\partial \xi_k}\frac{\partial a_l}{\partial x_k}\frac{\partial p}{\partial x_l} + \sum_{k,l}\frac{\partial p}{\partial \xi_k}\frac{\partial p}{\partial \xi_l}\frac{\partial^2 p}{\partial x_k \partial x_l} + \sum_k(\frac{\partial p}{\partial x_k})^2\right) \\ &+ \frac{-t^4}{8}\sum_{k,l}\frac{\partial p}{\partial \xi_k}\frac{\partial p}{\partial x_k}\frac{\partial p}{\partial \xi_l}\frac{\partial p}{\partial x_l}, \end{aligned}$$

and, by integration by parts, the spectral invariant

$$I_2 = -\frac{1}{24}\int\left(\sum_k \frac{\partial^2 p}{\partial x_k^2} - \sum_{k,l}\frac{\partial a_k}{\partial x_l}\frac{\partial a_l}{\partial x_k}\right) f^{(2)}(p(x,\xi))dxd\xi. \tag{7.7}$$

Notice that

$$\frac{\partial^2 p}{\partial x_k^2} = \sum_j \frac{\partial^2 a_j}{\partial x_k^2}\frac{\partial p}{\partial \xi_j} + \sum_j\left(\frac{\partial a_j}{\partial x_k}\right)^2 + \frac{\partial^2 V}{\partial x_k^2}$$

and

$$\|B\|^2 = \mathrm{tr}B^2 = 2\sum_{j,k}\frac{\partial a_k}{\partial x_j}\frac{\partial a_j}{\partial x_k} - 2\sum_{j,k}(\frac{\partial a_k}{\partial x_j})^2.$$

So the subprincipal term is given by

$$\frac{1}{48}\int f^{(2)}(p(x,\xi))\left(\|B\|^2 - 2\sum_k \frac{\partial^2 V}{\partial x_k^2}\right)\, dx\ d\xi.$$

Finally, since the spectral invariants have to be gauge invariant by definition, and since any magnetic field has by gauge change a Coulomb vector potential representation, the integral

$$\int_{p<\lambda}\left(\|B\|^2 - 2\sum_k \frac{\partial^2 V}{\partial x_k^2}\right)\, dx\ d\xi$$

is spectrally determined for an arbitrary vector potential. Thus we proved

Theorem 7.1. *For the semiclassical Schrödinger operator* (7.1) *with magnetic field B, the spectral measure $\nu(f) = tracef(S_\hbar^m)$ for $f \in C_0^\infty(\mathbb{R})$ has an asymptotic expansion*

$$\nu^m(f) \sim (2\pi\hbar)^{-n}\sum \nu_r^m(f)\hbar^{2r},$$

where

$$\nu_0^m(f) = \int f(p(x,\xi,\hbar))dxd\xi$$

and

$$\nu_1^m(f) = \frac{1}{48}\int f^{(2)}(p(x,\xi,\hbar))(\|B\|^2 - 2\sum\frac{\partial^2 V}{\partial x_i^2}).$$

8. A Inverse Result for the Schrödinger Operator with a Magnetic Field

Making the change of coordinates $(x,\xi) \to (x, \xi + a(x))$, the expressions (7.1) and (7.1) simplify to

$$\nu_0^m(f) = \int f(\xi^2 + V) dx d\xi$$

and

$$\nu_1^m(f) = \frac{1}{48} \int f^{(2)}(\xi^2 + V)(\|B\|^2 - 2\sum \frac{\partial^2 V}{\partial x_i^2}) dx d\xi.$$

In other words, for all λ, the integrals

$$\mathrm{I}_\lambda = \int_{\xi^2 + V(x) < \lambda} dx d\xi$$

and

$$\mathrm{I\!I}_\lambda = \int_{\xi^2 + V(x) < \lambda} (\|B\|^2 - 2\sum \frac{\partial^2 V}{\partial x_i^2}) dx d\xi$$

are spectrally determined.

Now assume that the dimension is 2, so that the magnetic field B is actually a scalar $B = B dx_1 \wedge dx_2$. Moreover, assume that V is a radially symmetric single well potential, and the magnetic field B is also radially symmetric. Introducing polar coordinates

$$x_1^2 + x_2^2 = s,\ dx_1 \wedge dx_2 = \frac{1}{2} ds \wedge d\theta$$

$$\xi_1^2 + \xi_2^2 = t,\ d\xi_1 \wedge d\xi_2 = \frac{1}{2} dt \wedge d\psi,$$

we can rewrite the integral I_λ as

$$\mathrm{I}_\lambda = \pi^2 \int_0^{s(\lambda)} (\lambda - V(s)) ds,$$

where $V(s(\lambda)) = \lambda$. Making the coordinate change $V(s) = x \Leftrightarrow s = f(x)$ as before, we get

$$\mathrm{I}_\lambda = \pi^2 \int_0^\lambda (\lambda - x) \frac{df}{dx} dx.$$

A similar argument shows

$$\mathrm{I\!I}_\lambda = \pi^2 \int_0^\lambda (\lambda - x) H(f(x)) \frac{df}{dx} dx,$$

where

$$H(s) = B(s)^2 - 4sV''(s) - 2V'(s).$$

It follows that from the spectral data, we can determine

$$f'(\lambda) = \frac{1}{\pi^2} \frac{d^2}{d\lambda^2} \mathrm{I}_\lambda$$

and

$$H(f(\lambda)) f'(\lambda) = \frac{1}{\pi^2} \frac{d^2}{d\lambda^2} \mathrm{I\!I}_\lambda.$$

So if we normalize $V(0) = 0$ as before, we can recover V from the first equation and B from the second equation.

REMARK 8.1. In higher dimensions, one can show by a similar (but slightly more complicated) argument that V and $\|B\|$ are both spectrally determined if they are radially symmetric.

9. The Birkhoff Canonical Form Theorem for the 1-D Schrödinger Operator

Suppose that $V^{-1}([0,a])$ is a closed interval, $[c,d]$, with $c < 0 < d$ and $V(0) = 0$. Moreover, suppose that on this interval, $V'' > 0$. We will show below that there exists a semiclassical Fourier integral operator

$$\mathcal{U} : C_0^\infty(\mathbb{R}) \to C^\infty(\mathbb{R})$$

with the properties

$$\mathcal{U} f(S_\hbar)\mathcal{U}^t = f(H_{QB}(S_\hbar^{har}, \hbar)) + O(\hbar^\infty) \tag{9.1}$$

for all $f \in C_0^\infty((-\infty, a))$, and

$$\mathcal{U}\mathcal{U}^t A = A \tag{9.2}$$

for all semiclassical pseudodifferential operators with microsupport on $H^{-1}([0,a))$. To prove these assertions, we will need some standard facts about Hamiltonian systems in two dimensions: With $H(x,\xi) = \frac{\xi^2}{2} + V(x)$ as above, let $v = v_H$ be the Hamiltonian vector field

$$v_H = \frac{\partial H}{\partial \xi}\frac{\partial}{\partial x} - \frac{\partial H}{\partial x}\frac{\partial}{\partial \xi},$$

and for $\lambda < a$, let $\gamma(t,\lambda)$ be the integral curve of v with initial point $\gamma(0,\lambda)$ lying on the x-axis and $H(\gamma(0,\lambda)) = \lambda$. Then, since $L_v H = 0$, $H(\gamma(t,\lambda)) = \lambda$ for all t. Let $T(\lambda)$ be the time required for this curve to return to its initial point, i.e.

$$\gamma(t,\lambda) \neq \gamma(0,\lambda), \text{ for } 0 < t < T(\lambda)$$

and

$$\gamma(T(\lambda),\lambda) = \gamma(0,\lambda).$$

Proposition 9.1 (The area-period relation)**.** *Let $A(\lambda)$ be the area of the set $\{(x,\xi) \mid H(x,\xi) < \lambda\}$. Then*

$$\frac{d}{d\lambda}A(\lambda) = T(\lambda). \tag{9.3}$$

Proof. Let w be the gradient vector field

$$\left((\frac{\partial H}{\partial x})^2 + (\frac{\partial H}{\partial \xi})^2 \right)^{-1} \left(\frac{\partial H}{\partial x}\frac{\partial}{\partial x} + \frac{\partial H}{\partial \xi}\frac{\partial}{\partial \xi} \right) \rho(H)$$

where $\rho(t) = 0$ for $t < \frac{\varepsilon}{2}$ and $\rho(t) = 1$ for $t > \varepsilon$. Then for $\lambda > \varepsilon$ and t positive, $\exp(tw)$ maps the set $H = \lambda$ onto the set $H = \lambda + t$ and hence

$$A(\lambda + t) = \int_{H=\lambda+t} dx\, d\xi = \int_{H=\lambda} (\exp tw)^*\, dx\, d\xi.$$

So for $t = 0$,

$$\frac{d}{dt}A(\lambda+t) = \int_{H\leq\lambda} L_w\, dx\, d\xi = \int_{H\leq\lambda} d\iota(w) dx d\xi = \int_{H=\lambda} \iota(w) dx d\xi.$$

But on $H = \lambda$,

$$\iota(w) dx d\xi = \left((\frac{\partial H}{\partial x})^2 + (\frac{\partial H}{\partial \xi})^2 \right)^{-1} \left(\frac{\partial H}{\partial x} d\xi - \frac{\partial H}{\partial \xi} dx \right).$$

Hence, by the Hamilton-Jacobi equations

$$dx = \frac{\partial H}{\partial \xi}\ dt$$

and

$$d\xi = -\frac{\partial H}{\partial x}\ dt,$$

the right hand side is just $-dt$. So

$$\frac{dA}{d\lambda}(\lambda) = -\int_{H=\lambda} dt = T(\lambda).$$

q.e.d.

For $\lambda = a$, let $c = \frac{A(\lambda)}{2\pi}$ and let

$$H^0_{QB} : [0, c] \to [0, a]$$

be the function defined by the identities

$$H^0_{QB}(s) = \lambda \iff s = \frac{A(\lambda)}{2\pi}$$

and let

$$H_{CB}(x, \xi) := H^0_{QB}(\frac{x^2 + \xi^2}{2}).$$

Thus by definition

$$A_{CB}(\lambda) = \text{area}\{H_{CB} < \lambda\} = A(\lambda). \tag{9.4}$$

Now let v be the Hamiltonian vector field associated with the Hamiltonian, H, as above and v_{CB} the corresponding vector field for H_{CB}. Also as above let $\gamma(t, \lambda)$ be the integral curve of v on the level set, $H = \lambda$, with initial point on the x-axis, and let $\gamma_{CB}(t, \lambda)$ be the analogous integral curve of v_{CB}. We will define a map of the set $H < a$ onto the set $H_{CB} < a$ by requiring

(9.5)

i. $f^* H_{CB} = H$,

ii. f maps the x-axis into itself,

iii. $f(\gamma(t, \lambda)) = \gamma_{CB}(t, \lambda)$.

Notice that this mapping is well defined by Proposition 9.1. Namely, by the identity (9.4) and the area-period relation, the time it takes for the trajectory $\gamma(t, \lambda)$ to circumnavigate this level set $H = \lambda$ coincides with the time it takes for $\gamma_{CB}(t, \lambda)$ to circumnavigate the level set $H_{CB} = \lambda$. It's also clear that the mapping defined by (9.5), $\mathrm{i} - \mathrm{iii}$, is a smooth mapping except perhaps at the origin, and in fact, since it satisfies $f^* H_{BC} = H$ and $f_* v_H = v_{H_{CB}}$, is a symplectomorphism. We claim that it is a C^∞ symplectomorphism at the origin as well. This slightly non-trivial fact follows from the classical Birkhoff canonical form theorem for the *Taylor* series of f at the origin. (The proof of this is basically just a formal power series version of the proof above. See [**GPU**], §3, for details.)

Now let $\mathcal{U}_0 : C_0^\infty(\mathbb{R}) \to C^\infty(\mathbb{R})$ be a semiclassical Fourier integral operator quantizing f with the property (9.2). By Egorov's theorem, $\mathcal{U}_0 S_\hbar \mathcal{U}_0^t$ is a zeroth order semiclassical pseudodifferential operator with leading symbol $H_{QB}^0(\frac{x^2+\xi^2}{2})$ on the set $\{(x,\xi) \mid H_{QB}^0 < a\}$, and hence the operator

$$\mathcal{U}_0 S_\hbar \mathcal{U}_0^t - H^0(S_\hbar^{har})$$

is a semiclassical pseudodifferential operator on this set with leading symbol of order $\hbar^2$. We'll show next that this $O(\hbar^2)$ can be improved to an $O(\hbar^4)$. To do so, however, we'll need the following lemma:

Lemma 9.2. *Let g be a C^∞ function on the set $H^{-1}(0,a)$. Then there exists a C^∞ function, h, on this set and a function $\rho \in C^\infty(0,a)$ such that*

$$g = L_v h + \rho(H). \tag{9.6}$$

Proof. Let

$$\rho(\lambda) = \int_0^{T(\lambda)} g(\gamma(t,\lambda))\, dt$$

and let $g_1 = g - \rho(H)$. Then

$$\int_0^{T(\lambda)} g_1(\gamma(t,\lambda))\, dt = 0.$$

So one obtains a function h satisfying (9.6) by setting

$$h(\gamma(t,\lambda)) = \int_0^t g_1(\gamma(t,\lambda))\, dt.$$

q.e.d.

Remark. The identity (9.6) can be rewritten as

$$g = \{H, h\} + \rho(H). \tag{9.7}$$

Now let $-\hbar^2 g$ be the leading symbol of

$$S_\hbar - \mathcal{U}_0^t H_{QB}^0(S_\hbar^{har})\mathcal{U}_0 =: \hbar^2 R_0.$$

Then if h and ρ are the functions (9.6) and Q is a self-adjoint pseudodifferential operator with leading symbol h, one has, by (9.7),

$$\begin{aligned}\exp(i\hbar^2 Q) S_\hbar \exp(-i\hbar^2 Q) &= S_\hbar + i[Q, S_\hbar]\hbar^2 + O(\hbar^4)\\ &= S_\hbar - \hbar^2(R_0 + \rho(S_\hbar)) + O(\hbar^4).\end{aligned}$$

Hence, if we replace $\mathcal{U}_0$ by $\mathcal{U}_1 = \mathcal{U}_0 \exp(i\hbar^2 Q)$, we have

$$\begin{aligned}\mathcal{U}_1 S_\hbar \mathcal{U}_1^t &= H_{QB}^0(S_\hbar^{har}) + \hbar^2 \rho\left(H_{QB}^0(S_\hbar^{har})\right) + O(\hbar^4)\\ &= H_{QB}^0(S_\hbar^{har}) + H_{QB}^1(S_\hbar^{har}) + O(\hbar^4)\end{aligned} \tag{9.8}$$

microlocally on the set $H^{-1}(0,a)$.

As above there's an issue of whether (9.8) holds microlocally at the origin as well, or alternatively: whether, for the g above, the solutions h and ρ of (9.7) extend smoothly over $x = \xi = 0$. This, however, follows as above from known facts about Birkhoff canonical forms in a formal neighborhood of a critical point of the Hamiltonian H; for more details, cf. [**GuU**].

To summarize what we've proved above: "Quantum Birkhoff modulo $\hbar^2$" implies "Quantum Birkhoff modulo $\hbar^4$." The inductive step, "Quantum Birkhoff modulo $\hbar^{2k}$," implies "Quantum Birkhoff modulo $\hbar^{2k+2}$" is proved in exactly the same way. We will omit the details.

10. Birkhoff Canonical Forms and Spectral Measures

Let's first recall the following form of Euler-Maclaurin formula proven by S. Sternberg and the first author:

Lemma 10.1. [**GuS2**] *Let $g \in \mathcal{S}(\mathbb{R})$ be a Schwartz function, then as $N \to \infty$,*

$$\frac{1}{N}\sum_{k=0}^{\infty} g(\frac{k}{N}) \sim \int_0^{\infty} g(x)dx + \frac{g(0)}{2N} + \sum_{n=1}^{\infty}(-1)^n]\frac{B_n}{(2n)!}g^{(2n-1)}(0)N^{-2n},$$

where B_k's are the Bernoulli numbers.

In particular, if $g(s)$ is a C_0^∞ function on the interval $(0,\infty)$. Then the remainder terms in the right hand vanish, and we get

$$\sum_{n=0}^{\infty} g\left(\hbar(n+\frac{1}{2})\right) = \frac{1}{\hbar}\int_0^{\infty} g(s)\ ds + O(\hbar^\infty).$$

Hence for $f \in C_0^\infty(0,a)$,

$$\operatorname{trace} f(H_{QB}(S_\hbar^{har},\hbar)) = \frac{1}{\hbar}\int_0^{\infty} f(H_{QB}(s,\hbar))\ ds + O(\hbar^\infty).$$

Thus, by (9.1) and (9.2),

$$\mu_\hbar(f) = \operatorname{trace} f(S_\hbar) = \frac{1}{\hbar}\int_0^{\infty} f(H_{QB}(s,\hbar))\ ds + O(\hbar^\infty). \tag{10.1}$$

Thus, if $K(t,\hbar)$ is the inverse of the function $H_{QB}(s,\hbar)$ on the interval $0 < t < a$, i.e. for $0<t<a$,

$$K(t,\hbar) = s \iff H_{QB}(s,\hbar) = t,$$

then (10.1) can be rewritten as

$$\mu_\hbar(f) = \frac{1}{\hbar}\int_0^{a} f(t)\frac{dK}{dt}\ dt + O(\hbar^\infty), \tag{10.2}$$

or more succinctly as

$$\mu_\hbar = \frac{1}{\hbar}\frac{dK}{dt}\ dt + O(\hbar^\infty). \tag{10.3}$$

Hence, in view of the results of §6, this gives one an easy way to recover $H_{QB}(s,\hbar)$ from V and its derivatives via fractional integration.

References

[Abe] N. Abel, *Auflösung einer mechanichen Aufgabe,* Journal de Crelle **1** (1826), 153–157.

[AHS] J. Avron, I. Herbst & B. Simon, *Schrödinger Operators with Magnetic Fields I: General Interactions,* Duke Mathematical Journal **45** (1978), 847–883, MR 0518109, Zbl 0399.35029.

[ChS] L. Charles & V.N. San, *Spectral Asymptotics via the semiclassical Birkhoff Normal Form,* Duke Math. J. **143** (2008), 463–511, MR 2423760, Zbl 1154.58015.

[Col05] Y. Colin de Verdière, *Bohr-Sommerfeld Rules to All Orders,* Ann. Henri Poincaré **6** (2005), 925–936. MR 2219863, Zbl 1080.81029.

[Col08] Y. Colin de Verdière, *A Semi-classical Inverse Problem II: Reconstruction of the Potential,* Geometric aspects of analysis and mechanics, 97–119, Progr. Math., 292, Birkhäuser/Springer, New York, 2011, MR 2809469.

[CoG] Y. Colin de Verdière & V. Guillemin, *A Semi-classical Inverse Problem I: Taylor Expansion,* Geometric aspects of analysis and mechanics, 81–95, Progr. Math., 292, Birkhäuser/Springer, New York, 2011, MR 2809468.

[DiS] M. Dimassi & J. Sjöstrand, *Spectral asymptotics in the semi-classical limit*, London Mathematical Society Lecture Note Series 268, Cambridge University Press, Cambridge, 1999, MR 1735654, Zbl 0926.35002.

[Gra] A. Gracia-Saz, *The symbol of a function of a pseudodifferential operator,* Ann. Inst. Fourier **55** (2005), 2257–2284, MR 2709137, Zbl 1091.53062.

[Gui] V. Guillemin, *Wave Trace Invariants,* Duke Math. J. **83** (1996), 287–352, MR 1390650, Zbl 0858.58051.

[GuH] V. Guillemin & H. Hezar, *A Fulling-Kuchment theorem for the 1D Harmonic Oscillator,* preprint, available at arXiv: 1109.0967.

[GPU] V. Guillemin, T. Paul & A. Uribe, *'Bottom of the Well' Semi-classical Trace Invariants,* Math. Res. Lett. **14** (2007), 711–719, MR 2335997, Zbl 1140.58007.

[GuS] V. Guillemin & S. Sternberg, *Semi-classical Analysis*, available at Shlomomath.harvard.edu.

[GuS2] V. Guillemin & S. Sternberg, *Riemann sums over polytopes,* Annales de l'institut Fourier **57** (2007), 2183–2195. MR 2394539, Zbl 1143.52011.

[GuU] V. Guillemin & A. Uribe, *Some inverse spectral results for semiclassical Schrödinger operators,* Math. Res. Lett. **14** (2007), 623–632, MR 2335988, Zbl 1138.35006.

[HeR] B. Helffer & D. Robert, *Calcul fonctionnel par la transformation de Mellin et opérateurs admissibles,* J. Funct. Anal. **53** (1983), 246–268. MR 0724029, Zbl 0524.35103.

[HeS] B. Helffer & J. Sjöstrand, *Semiclassical analysis for Harper's equation III: Cantor Structure of the Spectrum*, Mémoires de la Société Mathématique de France (nouvelle série) **39** (1989), MR 1041490, Zbl 0725.34099.

[Hez] H. Hezari, *Inverse spectral problems for Schrödinger operators,* Comm. in Math. Phy. **288** (2009), 1061–1088, MR 2504865, Zbl 1170.81042.

[ISZ] A. Iantchenko, J. Sjöstrand & M. Zworski, *Birkhoff normal forms in semiclassical inverse problems,* Math. Res. Lett. **9** (2002), 337–362, MR 1909649, Zbl pre01804060.

[MiR] K. Miller & B. Ross, *An introduction to the fractional calculus and fractional differential equations*, John Wiley & Sons, 1993, MR 1219954, Zbl 0789.26002.

[SjZ] J. Sjöstrand & M. Zworski, *Quantum monodromy and semi-classical trace formulae,* J. Math. Pure Appl. **81** (2002), 1–33, MR 1994881, Zbl 1038.58033.

[Zel00] S. Zelditch, *Spectral determination of analytic bi-axisymmetric plane domains,* Geom. Func. Anal. **10** (2000), 628–677, MR 1779616, Zbl 0961.58012.

[Zel08] S. Zelditch, *Inverse spectral problem for analytic domains ii: $\mathbb{Z}_2$-symmetric domains,* Ann. Math. **170** (2009), 205–269, MR 2521115, Zbl 1196.58016.

Department of Mathematics
Massachusetts Institute of Technology
Cambridge, MA 02139
E-mail address: vwg@math.mit.edu

Department of Mathematics
University of Michigan
Ann Arbor, MI 48109
E-mail address: wangzuoq@umich.edu