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ON THE HIGH-ENERGY ASYMPTOTICS OF THE INTEGRATED DENSITY OF STATES

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Abstract

Assuming that the integrated density of states of a Schrödinger operator admits a high-energy asymptotic expansion, the authors give explicit formulae for the coefficients of this expansion in terms of the heat invariants.

1. Introduction

Consider the Schrödinger operator $H = (-i\nabla + A(x))^2 + V(x)$ in $L^2(\mathbb{R}^d)$, $d \geq 1$; here, the electric potential $V : \mathbb{R}^d \to \mathbb{R}$ and the magnetic vector potential $A : \mathbb{R}^d \to \mathbb{R}^d$ are infinitely smooth functions, with all the derivatives uniformly bounded in $\mathbb{R}^d$. Let $\Omega_L$ be a cube, $\Omega_L = [-L/2, L/2]^d \subset \mathbb{R}^d$, and let $\chi_L$ be the characteristic function of $\Omega_L$. One says that $H$ has a density of states measure (see, for example, [14] or [9]) if for all $g \in C_0^\infty(\mathbb{R})$ the quantity $L^{-d} \text{Tr}(\chi_L g(H))$ has a limit as $L \to \infty$. If the above limit exists for all $g$, then it can be represented as an integral

$$\lim_{L \to \infty} L^{-d} \text{Tr}(\chi_L g(H)) = \int_{-\infty}^{\infty} g(\lambda) \, dk(\lambda),$$

where the Borel measure $dk(\lambda)$ is by definition the density of states measure. It is well known that in the case of periodic potentials $V$ and $A$, the density of states measure exists.

The function

$$k(\lambda) := \int_{-\infty}^{\lambda} dk(t), \quad \lambda \in \mathbb{R},$$

is called the integrated density of states. The asymptotics of $k(\lambda)$ as $\lambda \to +\infty$ has been attracting considerable attention; see [3, 8, 16] and the references therein. For $V \equiv 0$ and $A \equiv 0$, one has $k(\lambda) = (2\pi)^{-d} \omega_d^{d/2} \lambda^{d/2}$, where $\omega_d = \pi^{d/2}/\Gamma(1 + d/2)$ is the volume of a unit ball in $\mathbb{R}^d$, and $\lambda_+ = (|\lambda| + \lambda)/2$.

If $d = 1$, $A = 0$ and $V$ is periodic, then an asymptotic expansion of $k(\lambda)$ is known (see [16]; see also related results in [10]):

$$k(\lambda) = (2\pi)^{-d} \omega_d^{d/2} \left( \sum_{j=0}^{N} Q_j \lambda^{-j} + o(\lambda^{-N}) \right), \quad \lambda \to \infty,$$

where $Q_j \in \mathbb{R}$ are some coefficients and $N > 0$ can be taken to be arbitrarily large. The asymptotic expansion of the type (2) is also valid in the case where $d = 1$, $A = 0$ and $V$ is almost periodic [13]. It is a general belief among the specialists in this area that formula (2) with some reasonably large $N$ and appropriate coefficients $Q_j$ also

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holds true in the case of an arbitrary dimension and periodic \( A \) and \( V \). However, to the authors’ knowledge, in the case where \( d \geq 2 \) and \( V \) and \( A \) are periodic, only a two-term asymptotic formula for \( k(\lambda) \) is so far known [3, 8], and the proof of this formula appears to be quite difficult.

The purpose of this paper is to discuss explicit formulae for the asymptotic coefficients \( Q_j \) in (2). We use the following simple observation. Consider the Laplace transform \( L(t) = \int_{-\infty}^{\infty} e^{-tk(\lambda)} \, d\lambda \), \( t > 0 \), of the density of states measure. It appears that for a wide class of potentials \( V \), including the periodic ones, a complete asymptotic expansion of \( L(t) \) as \( t \to +0 \) can be easily obtained, and the coefficients of this expansion can be explicitly computed in terms of the heat invariants of the operator \( H \). This expansion does not, of course, directly imply the asymptotics (2) of \( k(\lambda) \). However, if the expansion (2) holds true with some (unknown) coefficients \( Q_j \), then, comparing the expansions for \( k(\lambda) \) and its Laplace transform \( L(t) \), one immediately obtains explicit formulae for these coefficients. This argument is well known, and is frequently used in the study of the scattering phase (see, for example, [2]), the eigenvalue counting function, and the spectral function of elliptic operators. However, no application to the integrated density of states seems as yet to have appeared in the literature.

Proving the validity of the asymptotics (2) is, of course, a difficult analytic problem. However, it is often the case that the proof does not readily yield explicit formulae for the coefficients \( Q_j \). We feel therefore that a simple, independent method of computing these coefficients would be of some value. As a by-product of our calculation, we also find some integral identities for the integrated density of states.

2. Heat invariants

Consider the operator \( e^{-tH} \) and its integral kernel \( e^{-tH}(x,y) \). It is well known that the following asymptotic expansion holds true as \( t \to +0 \):

\[
e^{-tH}(x,x) \sim (4\pi t)^{-d/2} \sum_{j=0}^{\infty} t^j a_j(x),
\]

locally uniformly in \( \mathbb{R}^d \). Here, \( a_j \) are polynomials (with real coefficients) in \( V \) and \( A \) and their derivatives. The coefficients \( a_j(x) \) are called local heat invariants of the operator \( H \). Explicit formulae for \( a_j \) are known:

\[
a_j(x) = \sum_{k=0}^{j} \frac{(-1)^j \Gamma(j+d/2)}{4^k k!(k+j)!(j-k)! \Gamma(k+d/2+1)} H_y^{k+j}(|x-y|^{2k}) \bigg|_{y=x};
\]

here the notation \( H_y \) means that the operator \( H \) is applied in the variable \( y \). For the case \( A = 0 \), formula (4), to the authors’ knowledge, first appeared in [5], although this result has many precursors in the literature (see, for example, [2], [11] and the references therein). For the case \( A \neq 0 \), formula (4) can be easily derived from the results of [11]; the proof has been indicated in [4].

From (4), one obtains by a direct computation:

\[
a_0 = 1, \quad a_1 = -V, \quad a_2 = \frac{1}{2} V^2 - \frac{1}{6} \Delta V - \frac{1}{6} |B(x)|^2,
\]

where \( B(x) \) is the 2-form of the magnetic field corresponding to the vector potential \( A(x) \). (For example, \( B(x) = \text{curl} A(x) \) in dimensions two and three.)
3. Laplace transforms of \( dk(\lambda) \)

We start with a formal computation that explains the heart of the matter. Assume that all the limits
\[
\lim_{L \to \infty} L^{-d} \int_{\Omega_L} a_j(x) \, dx =: M(a_j), \quad j = 0, 1, 2, \ldots,
\]
exist. (Note that this is obviously the case for periodic \( V \) and \( A \).) By (1) and (3), we obtain (formally!)
\[
\int_{-\infty}^{\infty} e^{-t\lambda} \, dk(\lambda) = \lim_{L \to \infty} L^{-d} \text{Tr}(\chi_L e^{-tH}) \sim (4\pi t)^{-d/2} \sum_{j=0}^{\infty} t^j M(a_j).
\]

The above formal computation can easily be justified as follows.

**Theorem 1.** Let \( A, V \in C^\infty(\mathbb{R}^d) \) with all the derivatives uniformly bounded. Assume that the density of states measure \( dk(\lambda) \) for \( H = (-i\nabla + A(x))^2 + V(x) \) exists, and that the limits (5) exist for \( j = 0, 1, 2, \ldots, N \). Then
\[
\int_{-\infty}^{\infty} e^{-t\lambda} \, dk(\lambda) = (4\pi t)^{-d/2} \left( \sum_{j=0}^{N} t^j M(a_j) + O(t^{N+1}) \right), \quad t \to +0.
\]

Note that the hypothesis of Theorem 1 obviously holds true (with any \( N > 0 \)) for any periodic \( V \in C^\infty(\mathbb{R}^d) \).

In order to justify the formal computation (6), one has only to check that under our assumptions on \( V \) and \( A \), the asymptotic expansion (3) holds true uniformly in \( x \in \mathbb{R}^d \). For periodic \( V \), this is quite obvious; it is also not difficult to prove in the general case, by repeating the arguments given in the papers [1, 11, 5], and by keeping track of the remainder estimates in the asymptotic formulae. For completeness, we give the proof in Section 5.

4. Corollaries

We need the following elementary lemma.

**Lemma 2.** Let \( k : \mathbb{R} \to \mathbb{R} \) be a measurable function that is supported on a semi-axis \( [a, \infty) \) and bounded on every bounded sub-interval of \( [a, \infty) \). Suppose that \( k \) has the following asymptotics:
\[
k(\lambda) = \sum_i p_i \lambda^{-x_i} + \sum_j q_j \lambda^{-\beta_j} + o(\lambda^{-M}), \quad \lambda \to \infty,
\]
where \( \{x_i\} \subset \mathbb{R} \setminus \mathbb{N} \) and \( \{\beta_j\} \subset \mathbb{N} \) are finite sets, \( M \geq \max(\{x_i\} \cup \{\beta_j\}) \), and \( \{p_i\} \) and \( \{q_j\} \) are complex numbers. Then the following asymptotic formula for the Laplace transform of \( k \) holds true:
\[
\int_{-\infty}^{\infty} e^{-t\lambda} \, k(\lambda) \, d\lambda = \sum_i p_i \Gamma(1-x_i) t^{x_i-1} + (\log t) \sum_j q_j \frac{(-1)^{\beta_j}}{(\beta_j - 1)!} t^{\beta_j-1}
\]
\[+ \sum_{0 \leq l < M-1} c_l t^l + o(t^{M-1}|\log t|^\delta), \quad t \to +0,
\]
where \( \delta = 1 \) if \( M \in \mathbb{N} \), and \( \delta = 0 \) otherwise.
Moreover, if the second sum in (8) vanishes, then the coefficients $c_l$ in (9) can be presented in the simple form

$$c_l = \frac{(-1)^l}{l!} \int_{-\infty}^{\infty} \left( k(\lambda) - \sum_{\alpha_j < l+1} p_j \lambda^{-\alpha_j} \theta(\lambda) \right) \lambda^l d\lambda, \quad (10)$$

where $\theta(\lambda) = (1 + \text{sign}(\lambda))/2$ is the Heaviside function.

Lemma 2 was stated without proof (and without the explicit formula (10)) in [2, Lemma 5.2]. The proof is elementary, and can be obtained, for example, by separately considering the special cases

$$k(\lambda) = \lambda^{-z} \theta(\lambda - 1) \quad (z \in \mathbb{R}) \quad \text{and} \quad k(\lambda) = o(\lambda^{-M}),$$

and checking that these terms make the desired contribution to the asymptotics of the Laplace transform.

From Theorem 1 and Lemma 2, one immediately obtains the following two corollaries.

**Corollary 3.** Assume that the hypothesis of Theorem 1 holds, and suppose that the integrated density of states $k(\lambda)$ has the asymptotics (2) for some natural $N$. Then the coefficients $Q_j$ are given by

$$Q_0 = 1, \quad Q_j = \frac{d}{2} \left( \frac{d}{2} - 1 \right) \cdots \left( \frac{d}{2} - j + 1 \right) M(a_j), \quad j = 1, \ldots, N. \quad (11)$$

Note that for $d$ even and $j \geq d/2 + 1$, one has $Q_j = 0$. In all other cases, formula (11) can be recast as

$$Q_j = \frac{\Gamma(d/2 + 1)}{\Gamma(d/2 - j + 1)} M(a_j).$$

In the one-dimensional case, formulae for $Q_j$ were given in [16], although not as explicitly as in (11): the coefficients $Q_j$ are computed as integrals of a sequence of functions defined by some recurrence relation. In the case $d \geq 2$, formulae for $Q_0$ and $Q_1$ are given in [3].

**Corollary 4.** Assume that the hypothesis of Theorem 1 holds, and suppose that the integrated density of states $k(\lambda)$ has the asymptotics (2) for some $N \in \mathbb{N}$. Then the following statements hold.

(i) For $d$ odd, one has the identities

$$\int_{-\infty}^{\infty} \left( k(\lambda) - (2\pi)^{-d} \omega_d \lambda^{d/2} \sum_{j=0}^{l+(d+1)/2} Q_j \lambda^{-j} \theta(\lambda) \right) \lambda^l d\lambda = 0,$$

$$l = 0, 1, \ldots, N - (d + 1)/2 - 1. \quad (12)$$

(ii) For $d$ even, one has the identities

$$\int_{-\infty}^{\infty} \left( k(\lambda) - (2\pi)^{-d} \omega_d \lambda^{d/2} \sum_{j=0}^{d/2} Q_j \lambda^{-j} \theta(\lambda) \right) \lambda^l d\lambda = (-1)^l l! M(a_l),$$

$$l = 0, \ldots, N - d/2 - 2. \quad (13)$$
By the same pattern, one easily verifies that if the remainder term in (2) is \( O(\lambda^{-N-\delta}) \), then:

(i) for \( d \) odd and \( \delta > 1/2 \), the identity (12) holds true also with \( l = N - (d + 1)/2 \); and

(ii) for \( d \) even and \( \delta > 0 \), the identity (13) holds true also with \( l = N - d/2 - 1 \).

**Remark.** In [8, Theorem 5] it has been proved that for the case \( d = 3 \), \( A = 0 \), \( V \) periodic, \( M(a_1) = 0 \), one has

\[
(k(\lambda) = (2\pi)^{-3} \omega_3 \lambda^{3/2} + d V_0 + O(\lambda^{-\delta}),
\]

where \( \zeta > 1/130 \) and \( d V_0 \) is a constant, which was expressed as a sum of the integrals of the type (12) (with \( d = 1 \) and \( l = 0 \)) for some auxiliary one-dimensional problems. Thus, from Corollary 2 it follows that \( d V_0 = 0 \).

5. **Proof of Theorem 1**

Essentially, we repeat the arguments of [1] with combinatorial simplifications due to I. Polterovich [11, 12]. However, our proof of (3) is perhaps somewhat simpler than the proofs given in [1, 11, 12]; this is due to the fact that we use the iterated resolvent identity (16), which gives a simple explicit form for the error term in the asymptotic formulae. The connection between the iterated resolvent identity and the the expansion (3) has been pointed out in [5]; the identity itself has been proved in [7], but various versions have probably been used many times in the literature. A construction very similar to our proof is used in a recent paper [6].

Denote \( H_0 = -\Delta \) in \( L^2(\mathbb{R}^d) \). Below, we use the notation \( R_0(z) = (H_0 - z)^{-1}, R(z) = (H - z)^{-1} \).

1. On the domain \( \bigcap_{n \geq 0} \text{Dom}(H_0^n) \), define the operators \( X_m, m \geq 1 \), recursively by

\[
X_0 = I, \quad X_{m+1} = X_m H_0 - H X_m.
\]

The operators \( X_m \) are differential operators of the form

\[
X_m = \sum_{|\alpha| \leq m} b_{mx}(x)D^\alpha,
\]

where \( D^\alpha = (\partial/\partial x_1)^{\alpha_1} \cdots (\partial/\partial x_d)^{\alpha_d} \) and \( b_{mx} \) are polynomials in \( V, A \) and their derivatives.

The following identity holds true [7] for any \( M \geq 1 \):

\[
R(z) = \sum_{m=0}^M X_m R_0^{m+1}(z) + R(z)X_{M+1} R_0^{M+1}(z).
\]

In [7], the above identity has been proved in the context of Banach algebras, so strictly speaking, the proof applies only to bounded operators \( H_0 \) and \( H \). However, under our assumptions on \( V \), the identity (16) can easily be proved directly by induction in \( M \).

Let us fix \( c < 0 \), \( c < \inf \text{spec}(H) \), and \( t > 0 \). Multiplying the identity (16) by \( e^{-tz} \) and integrating over \( z \) from \( c - i\infty \) to \( c + i\infty \), one obtains [7]:

\[
e^{-tH} = \sum_{m=0}^M \frac{t^m}{m!} X_m e^{-tH_0} + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} R(z)X_{M+1} R_0^{M+1}(z)e^{-tz} dz, \quad t > 0.
\]
Multiplying (17) by \( \chi_L \) and taking traces, one obtains
\[
\text{Tr}(\chi_L e^{-tH}) = \sum_{m=0}^{M} \frac{t^m}{m!} \text{Tr}(\chi_L X_m e^{-tH_0}) + I(t),
\]
where \( I(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \text{Tr}(\chi_L R(z)X_{M+1} R_0^{M+1} R(z)) e^{-tz} \, dz. \) (18)

2. Let us first estimate the remainder term \( I(t) \). As \( \text{ord}(X_{M+1}) \leq M + 1 \), the operator \( X_{M+1} |R_0(z)|^{(M+1)/2} \) is bounded. Applying standard trace class estimates (see, for example, [15]), one obtains
\[
|\text{Tr} X_{M+1} |R_0(z)|^{(M+1)/2} \| R_0(z) \|^{(M+1)/2} \chi_{LR}(z) \|_{\mathcal{G}_1} \leq C L^d |z|^{(d-M-3)/2}, \quad \Re z \leq c, \quad (19)
\]
where \( \| \cdot \|_{\mathcal{G}_1} \) is the trace norm. Now let us shift the contour of integration in (18) to the left, transforming it into the vertical line \( (c/t - i\infty, c/t + i\infty) \). Then (19) immediately yields
\[
I(t) = O\left(L^d t^{(M-d+1)/2}\right), \quad t \to +0. \quad (20)
\]

3. Next, using (15) and the explicit formula for the integral kernel of \( e^{-tH_0} \), one easily computes the \( m \)th term in the sum in (18):
\[
t^m \text{Tr}(\chi_L X_m e^{-tH_0}) = t^{-d/2} \sum_{j=m-[m/2]}^{m} t^j \int_{\Omega_L} f_{mj}(x) \, dx, \quad t > 0, \quad (21)
\]
where \( f_{mj} \) are some polynomials in \( V \) and the derivatives of \( V \).

4. Substituting (20) and (21) into (18) and taking \( M \) large (in fact, \( M = 2N - 1 \) is sufficient), one obtains
\[
\text{Tr}(\chi_L e^{-tH}) = (4\pi t)^{-d/2} \left( \sum_{j=0}^{N-1} t^j \int_{\Omega_L} a_j(x) \, dx + O(L^d t^N) \right), \quad t \to +0. \quad (22)
\]
A detailed combinatorial analysis [11, 5] of the coefficients \( a_j(x) \) gives the explicit formulae (4).

Finally, the standard arguments (see [14, Proposition C.7.2]) show that formula (1) holds true with \( g(\lambda) = e^{-t\lambda} \) (although \( g \) is not compactly supported). Thus, multiplying (22) by \( L^{-d} \) and taking \( L \to \infty \), we arrive at (7).

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