On the high energy asymptotics of the integrated density of states

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November 2002

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.

AMS Subject classification: 35J10, 47F05, 35P20.

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

$$\lim_{L\to\infty} L^{-d}\operatorname{Tr}(\chi_L g(H)) = \int_{-\infty}^{\infty} g(\lambda)dk(\lambda), \tag{1}$$

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 $\mathbf{A}$, 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 [16, 3, 8] and references therein. For $V \equiv 0$ and $\mathbf{A} \equiv 0$, one has $k(\lambda) = (2\pi)^{-d}\omega_d\lambda_+^{d/2}$, where $\omega_d = \pi^{d/2}/\Gamma(1+\frac{d}{2})$ is the volume of a unit ball in $\mathbb{R}^d$ and $\lambda_+ = (|\lambda|+\lambda)/2$.

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

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

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where $Q_j \in \mathbb{R}$ are some coefficients and $N > 0$ can be taken arbitrary large. The asymptotic expansion of the type (2) is also valid in the case $d = 1$, $\mathbf{A} = 0$ and V 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 holds true also in the case of an arbitrary dimension and periodic $\mathbf{A}$ and V. However, to the authors' knowledge, in the case $d \geq 2$, V and $\mathbf{A}$ periodic, only a two-term asymptotic formula for $k(\lambda)$ is known so far [3, 8] and the proof of this formula appears to be quite difficult.

The purpose of this note is to discuss explicit formulae for the asymptotic coefficients Q_j in (2). We use the following simple observation. Consider the Laplace transform $L(t) = \int_{-\infty}^{\infty} e^{-t\lambda} dk(\lambda)$, $t > 0$ 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 frequently used in the study of the scattering phase (see e.g. [2]), the eigenvalue counting function, and the spectral function of elliptic operators. However, its application to the integrated density of states does not seem 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 an independent simple method of computing these coefficients is of some value. As a by-product of our calculation, we also get 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 $t \to +0$:

$$e^{-tH}(x, x) \sim (4\pi t)^{-d/2} \sum_{j=0}^{\infty} t^j a_j(x), \tag{3}$$

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

$$a_j(x) = \sum_{k=0}^{j} \frac{(-1)^j \Gamma(j + \frac{d}{2})}{4^k k!(k + j)!(j - k)!\, \Gamma(k + \frac{d}{2} + 1)} H_y^{k+j} (|x - y|^{2k}) \,|_{y=x}; \tag{4}$$

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

From (4) by a direct computation one obtains

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

where $B(x)$ is the 2-form of the magnetic field corresponding to the vector potential $\mathbf{A}(x)$ (e.g. $B(x) = \operatorname{curl} \mathbf{A}(x)$ in dimensions two and three).

3. Laplace transforms of $dk(\lambda)$ We start with a formal computation which explains the heart of the matter. Assume that all the limits

$$\lim_{L\to\infty} L^{-d}\int_{\Omega_L} a_j(x)dx =: M(a_j), \quad j=0,1,2\dots \tag{5}$$

exist (note that this is obviously the case for periodic V and $\mathbf{A}$). By (1) and (3), we obtain (formally!)

$$\int_{-\infty}^{\infty} e^{-t\lambda}dk(\lambda) = \lim_{L\to\infty} L^{-d}\operatorname{Tr}(\chi_L e^{-tH}) \sim (4\pi t)^{-d/2}\sum_{j=0}^{\infty} t^j M(a_j). \tag{6}$$

The above formal computation can be easily justified:

Theorem 1. *Let* $\mathbf{A}, V \in C^\infty(\mathbb{R}^d)$ *with all the derivatives uniformly bounded. Assume that the density of states measure* $dk(\lambda)$ *for* $H=(-i\nabla+\mathbf{A}(x))^2+V(x)$ *exists and that the limits* (5) *exist for* $j=0,1,2,\dots,N$*. Then*

$$\int_{-\infty}^{\infty} e^{-t\lambda}dk(\lambda) = (4\pi t)^{-d/2}\Big(\sum_{j=0}^{N} t^j M(a_j) + O(t^{N+1})\Big), \quad t\to +0. \tag{7}$$

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 only has to check that under our assumptions on V and $\mathbf{A}$, the asymptotic expansion (3) holds true uniformly in $x\in\mathbb{R}^d$. For periodic V, this is quite obvious; in general case, this is also not difficult to prove by repeating the arguments of the papers [1, 11, 5] and 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, which 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:*

$$k(\lambda) = \sum_i p_i\lambda^{-\alpha_i} + \sum_j q_j\lambda^{-\beta_j} + o(\lambda^{-M}), \quad \lambda\to\infty, \tag{8}$$

where $\{\alpha_i\}\subset\mathbb{R}\setminus\mathbb{N}$ *and* $\{\beta_j\}\subset\mathbb{N}$ *are finite sets,* $M\geq\max(\{\alpha_i\}\cup\{\beta_j\})$*, and* $\{p_i\}$ *and* $\{q_j\}$ *are complex numbers. Then the following asymptotic formula for the Laplace transform of* k *holds true:*

$$\begin{aligned}\int_{-\infty}^{\infty} e^{-t\lambda}k(\lambda)d\lambda &= \sum_i p_i\Gamma(1-\alpha_i)t^{\alpha_i-1} + (\log t)\sum_j q_j\frac{(-1)^{\beta_j}}{(\beta_j-1)!}t^{\beta_j-1}\\ &+ \sum_{0\leq l<M-1} c_l t^l + o(t^{M-1}|\log t|^\delta), \quad t\to+0,\end{aligned} \tag{9}$$

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*

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

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

Lemma 2 (without the explicit formula (10)) was stated without proof in [2] (Lemma 5.2). The proof is elementary and can be obtained, for example, by separately considering the special cases $k(\lambda) = \lambda^{-\alpha}\theta(\lambda - 1)$, $\alpha \in \mathbb{R}$, and $k(\lambda) = o(\lambda^{-M})$ and checking that these terms give the desired contribution into the asymptotics of the Laplace transform.

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

Corollary 1. *Assume the hypothesis of Theorem 1 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*

$$Q_0 = 1, \quad Q_j = \tfrac{d}{2}(\tfrac{d}{2} - 1)\dots(\tfrac{d}{2} - j + 1)M(a_j), \quad j = 1, \dots, N. \tag{11}$$

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

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

In the one-dimensional case, formulae for Q_j were given in [16], although not as explicit as (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 2. *Assume the hypothesis of Theorem 1 and suppose that the integrated density of states $k(\lambda)$ has the asymptotics (2) for some $N \in \mathbb{N}$. Then (i) for d odd, one has the identities*

$$\int_{-\infty}^{\infty} \Big(k(\lambda) - (2\pi)^{-d}\omega_d \lambda^{d/2} \sum_{j=0}^{l+\frac{d+1}{2}} Q_j \lambda^{-j}\theta(\lambda) \Big) \lambda^l d\lambda = 0, \quad l = 0, 1, \dots, N - \tfrac{d+1}{2} - 1; \tag{12}$$

(ii) for d even, one has the identities

$$\int_{-\infty}^{\infty} \Big(k(\lambda) - (2\pi)^{-d}\omega_d \lambda^{d/2} \sum_{j=0}^{d/2} Q_j \lambda^{-j}\theta(\lambda) \Big) \lambda^l d\lambda = (-1)^l l! M(a_l), \quad l = 0, \dots, N - \tfrac{d}{2} - 2. \tag{13}$$

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 $l = N - \frac{d+1}{2}$; (ii) for d even and $\delta > 0$, the identity (13) holds true also with $l = N - \frac{d}{2} - 1$.

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

$$k(\lambda) = (2\pi)^{-3}\omega_3\lambda^{3/2} + d_V^0 + O(\lambda^{-\zeta}),$$

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 of [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 proven in [7], but its different 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 $\cap_{n\geq 0} \operatorname{Dom}(H_0^n)$ define the operators X_m, $m \geq 1$, recursively by

$$X_0 = I, \quad X_{m+1} = X_m H_0 - H X_m. \tag{14}$$

The operators X_m are differential operators of the form

$$X_m = \sum_{|\alpha|\leq m} b_{m\alpha}(x) D^\alpha, \tag{15}$$

where $D^\alpha \equiv (\partial/\partial x_1)^{\alpha_1} \dots (\partial/\partial x_d)^{\alpha_d}$ and $b_{m\alpha}$ are polynomials in V, $\mathbf{A}$ and in their derivatives.

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

$$R(z) = \sum_{m=0}^{M} X_m R_0^{m+1}(z) + R(z) X_{M+1} R_0^{M+1}(z). \tag{16}$$

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

Let us fix $c < 0$, $c < \inf \operatorname{spec}(H)$, 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]:

$$e^{-tH} = \sum_{m=0}^{M} \frac{t^m}{m!} X_m e^{-tH_0} + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} R(z) X_{M+1} R_0^{M+1}(z) e^{-tz} dz, \quad t > 0. \tag{17}$$

Multiplying (17) by χ_L and taking traces, one obtains:

$$\begin{aligned} \operatorname{Tr}(\chi_L e^{-tH}) &= \sum_{m=0}^{M} \frac{t^m}{m!} \operatorname{Tr}(\chi_L X_m e^{-tH_0}) + I(t), \\ \text{where} \quad I(t) &= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \operatorname{Tr}\big(\chi_L R(z) X_{M+1} R_0^{M+1}(z)\big) e^{-tz} dz. \end{aligned} \tag{18}$$

2. Let us first estimate the remainder term $I(t)$. As $\operatorname{ord}(X_{M+1}) \leq M + 1$, the operator $X_{M+1} |R_0(z)|^{(M+1)/2}$ is bounded. Applying standard trace class estimates (see e.g. [15]), one gets

$$\begin{aligned} &|\operatorname{Tr}(\chi_L R(z) X_{M+1} R_0^{M+1}(z))| \\ &\quad \leq \|X_{M+1} |R_0(z)|^{(M+1)/2}\| \| |R_0(z)|^{(M+1)/2} \chi_L R(z)\|_{\mathfrak{S}_1} \leq C L^d |z|^{(d-M-3)/2}, \quad \operatorname{Re} z \leq c, \end{aligned} \tag{19}$$

where $\|\cdot\|_{\mathfrak{S}_1}$ 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

$$I(t) = O(L^d t^{(M-d+1)/2}), \quad t \to +0. \tag{20}$$

3. Next, using (15) and explicit formula for the integral kernel of e^{-tH_0}, one easily computes the m'th term in the sum in (18):

$$t^m \operatorname{Tr}(\chi_L X_m e^{-tH_0}) = t^{-d/2} \sum_{j=m-[m/2]}^{m} t^j \int_{\Omega_L} f_{mj}(x) dx, \quad t > 0, \tag{21}$$

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

$$\mathrm{Tr}(\chi_L e^{-tH}) = (4\pi t)^{-d/2}\Big(\sum_{j=0}^{N-1} t^j \int_{\Omega_L} a_j(x)dx + O(L^d t^N)\Big), \quad t \to +0. \tag{22}$$

A detailed combinatorial analysis [11, 5] of the coefficients $a_j(x)$ gives explicit formulae (4).

Finally, the standard arguments (cf. [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). ∎

6. Acknowledgments The authors are grateful to A. Sobolev and Yu. Karpeshina for useful discussions and ecouragement. The final version of the paper was prepared during the authors' visit to the Mittag-Leffler Institute, Stockholm; the authors are grateful to the Insitute for the hospitality.

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