A remark on the high energy asymptotics of the integrated density of states

E. Korotyaev* and A. Pushnitski†

19 March 2002

Abstract

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

1. Introduction Let $H = -\Delta + V(x)$ in $L^2(\mathbb{R}^d)$, $d \geq 1$, where $V \in C^\infty(\mathbb{R}^d)$ is a real-valued potential such that V and all the derivatives of V are uniformly bounded in $\mathbb{R}^d$. Let $\Omega_L = [-L/2, L/2]^d \subset \mathbb{R}^d$ and let χ_L be the characteristic function of Ω_L. One says that H *has a density of states measure* (see e.g. [11] or [7]) 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 and almost-periodic potentials V, the density of states measure exists.

The function

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

is called the *integrated density of states*. The asymptotics of $k(\lambda)$ as $\lambda \to +\infty$ has been attracting considerable attention — see [13, 3, 6] and references therein. For $V \equiv 0$, 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 $\lambda_+ = (|\lambda|+\lambda)/2$. For an arbitrary bounded V by a simple variational argument [14] one obtains

$$k(\lambda) = (2\pi)^{-d}\omega_d\lambda^{d/2}(1+O(\lambda^{-1})), \quad \lambda \to \infty. \tag{2}$$

Moreover, if $d = 1$ and V is periodic, an asymptotic expansion of $k(\lambda)$ is known [13] (see also related results in [8]):

$$k(\lambda) = (2\pi)^{-d}\omega_d\lambda^{d/2}\Big(\sum_{j=0}^{N-1} Q_j\lambda^{-j} + O(\lambda^{-N})\Big), \quad \lambda \to \infty, \tag{3}$$

*Institut für Mathematik, Humboldt Universität zu Berlin, Rudower Chaussee 25, 12489, Berlin, Germany. e-mail: ek@mathematik.hu-berlin.de

†Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, U.K. e-mail: a.b.pushnitski@lboro.ac.uk

where $Q_j \in \mathbb{R}$ are some coefficients and $N > 0$ can be taken arbitrary large. However, in the case $d \geq 2$, V periodic, only a two-term asymptotic formula for $k(\lambda)$ is known [3, 6] 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 (3). We use the following simple observation which is probably known to some specialists but does not seem to have appeared explicitly in the literature. 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 (3) of $k(\lambda)$. However, if the expansion (3) holds true with some (unknown) coefficients Q_j, then we immediately obtain explicit formulae for these coefficients.

Proving the validity of the asymptotics (3) 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.

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 $t \to +0$:

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

locally uniformly in $\mathbb{R}^d$. Here a_j are polynomials (with real coefficients) in V and the derivatives of V. The coefficients $a_j(x)$ are called *local heat invariants* of the operator H. Explicit formulae for a_j are given in [4] (see also [2, 9]):

$$a_j(x) = \sum_{k=0}^{j-1} \frac{(-1)^j \Gamma(j + \frac{d}{2})}{4^k k!(k + j)!(j - 1 - k)!\, \Gamma(k + \frac{d}{2} + 1)} (-\Delta_y + V(y))^{k+j} (|x - y|^{2k}) \,|_{y=x} \,. \tag{5}$$

In particular,

$$a_0 = 1, \quad a_1 = -V, \quad a_2 = \tfrac{1}{2}V^2 - \tfrac{1}{6}\Delta V, \quad a_3 = -\tfrac{1}{6}V^3 + \tfrac{1}{6}V\Delta V + \tfrac{1}{12}(\Delta V)^2 - \tfrac{1}{6}\Delta^2 V.$$

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

$$\lim_{L\to\infty} L^{-d} \int_{\Omega_L} a_j(x) dx =: M(a_j), \quad j = 0, 1, 2 \ldots \tag{6}$$

exist (note that this is obviously the case for periodic V). By (1) and (4), we obtain (formally!)

$$\int_{-\infty}^{\infty} e^{-t\lambda} dk(\lambda) = \lim_{L\to\infty} L^{-d} \operatorname{Tr}(\chi_L e^{-tH}) \sim (4\pi t)^{-d/2} \sum_{j=0}^{\infty} t^j M(a_j). \tag{7}$$

The above formal computation can be easily justified:

Theorem 1. *Let $V \in C^\infty(\mathbb{R}^d)$ and suppose that V and all the derivatives of V are uniformly bounded. Assume that the density of states measure $dk(\lambda)$ for $H = -\Delta + V(x)$ exists and that the limits* (6) *exist for $j = 0, 1, 2, \dots, N-1$. Then*

$$\int_{-\infty}^{\infty} e^{-t\lambda} dk(\lambda) = (4\pi t)^{-d/2} \Big(\sum_{j=0}^{N-1} t^j M(a_j) + O(t^N) \Big), \quad t \to +0. \tag{8}$$

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 (7), one only has to check that under our assumptions on V, the asymptotic expansion (4) 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, 9, 4] and keeping track of the remainder estimates in the asymptotic formulae. For completeness, below we give the proof.

4. Corollary Theorem 1 immediately gives explicit formulae for the coefficients Q_j of the asymptotics (3):

Corollary. *Assume the hypothesis of Theorem 1. Suppose that the integrated density of states $k(\lambda)$ has the asymptotics* (3). *Then the coefficients Q_j are given by*

$$Q_0 = 1, \quad Q_j = \tfrac{d}{2}(\tfrac{d}{2} - 1) \dots (\tfrac{d}{2} - j + 1) M(a_j), \quad j = 1, \dots, N-1. \tag{9}$$

Note that for d even and $j \geq \frac{d}{2} + 1$, one has $Q_j = 0$. In all other cases, formula (9) can be recast as

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

The proof of the Corollary is obtained by a direct application of Lemma 5.2 of [2].

Note that in the one-dimensional case, formulae for Q_j were given in [13], although not as explicit as (9): 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].

5. Proof of Theorem 1 Essentially, we repeat the arguments of [1] with combinatorial simplifications due to I. Polterovich [9, 10]. However, our proof of (4) is perhaps somewhat simpler than the proofs of [1, 9, 10]; this is due to the fact that we use the iterated resolvent identity (12) (discovered in [5]), 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 (4) has been pointed out in [4].

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

$$X_0 = I, \quad X_{m+1} = X_m H_0 - H X_m. \tag{10}$$

The operators X_m are differential operators of the form

$$X_m = \sum_{|a| \leq m-1} b_{m\alpha}(x) D^\alpha, \tag{11}$$

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 and the derivatives of V.

The following identity holds true [5] for any $M \geq 1$:

$$R(z) = \sum_{m=0}^{M} X_m R_0^{m+1}(z) + R(z) X_{M+1} R_0^{M+1}(z). \tag{12}$$

In [5], 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 (12) 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 (12) by e^{-tz} and integrating over z from $c - i\infty$ to $c + i\infty$, one obtains [5]:

$$e^{-tH} = \sum_{m=0}^{M} \frac{t^m}{m!} X_m e^{-tH_0} + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} R(z) X_{M+1} R_0^{M+1}(z) e^{-tz} dz, \quad t > 0. \tag{13}$$

Multiplying (13) by χ_L and taking traces, one obtains:

$$\begin{aligned} \operatorname{Tr}(\chi_L e^{-tH}) &= \sum_{m=0}^{M} \frac{t^m}{m!} \operatorname{Tr}(\chi_L X_m e^{-tH_0}) + I(t), \\ \text{where} \quad I(t) &= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \operatorname{Tr}\big(\chi_L R(z) X_{M+1} R_0^{M+1}(z)\big) e^{-tz} dz. \end{aligned} \tag{14}$$

2. Let us first estimate the remainder term $I(t)$. As $\operatorname{ord}(X_{M+1}) \leq M$, the operator $X_{M+1}|R_0(z)|^{M/2}$ is bounded. Applying standard trace class estimates (see e.g. [12]), one gets

$$\begin{aligned} &|\operatorname{Tr}(\chi_L R(z) X_{M+1} R_0^{M+1}(z))| \\ &\leq \|X_{M+1}|R_0(z)|^{M/2}\| \||R_0(z)|^{M/2+1} \chi_L R(z)\|_{\mathfrak{S}_1} \leq C L^d |z|^{\frac{d}{2} - \frac{M}{2} - 2}, \quad \operatorname{Re} z \leq c, \end{aligned} \tag{15}$$

where $\|\cdot\|_{\mathfrak{S}_1}$ is the trace norm. It follows that for sufficiently large M, the integral $I(t)$ converges absolutely for all $t \geq 0$. Moreover, as the trace in the integrand is analytic in z for $\operatorname{Re} z \leq c$, by the deformation of contour argument it follows that $I(0) = 0$. The same reasoning can be applied to the derivatives of $d^k I(t)/dt^k$ of the order $k < \frac{M-d}{2} + 1$. Thus,

$$I(t) = O(L^d t^k), \quad t \to +0, \tag{16}$$

for any $k \in \mathbb{N}$, $k < \frac{M-d}{2} + 1$.

3. Next, using (11) and explicit formula for the integral kernel of e^{-tH_0}, one easily computes the m'th term in the sum in (14):

$$t^m \operatorname{Tr}(\chi_L X_m e^{-tH_0}) = t^{-d/2} \sum_{j=[m/2]+1}^{m} t^j \int_{\Omega_L} f_{mj}(x) dx, \quad t > 0, \tag{17}$$

where f_{mj} are some polynomials in V and the derivatives of V.

4. Substituting (16) and (17) into (14) and taking M large (in fact $M = 2N - 2$ is sufficient), one obtains

$$\operatorname{Tr}(\chi_L e^{-tH}) = (4\pi t)^{-d/2} \Big(\sum_{j=0}^{N-1} t^j \int_{\Omega_L} a_j(x) dx + O(L^d t^N) \Big), \quad t \to +0. \tag{18}$$

A detailed combinatorial analysis [9, 4] of the coefficients $a_j(x)$ gives explicit formulae (5).

Finally, recall (see e.g. [11, Proposition C.7.2]) that formula (1) holds true with $g(\lambda) = e^{-t\lambda}$ (although g is not compactly supported). Thus, multiplying (18) by L^{-d} and taking $L \to \infty$, we arrive at (8). ∎

6. Acknowledgments The authors are grateful to A. Sobolev for useful discussions.

References

[1] S. Agmon, Y. Kannai, *On the asymptotic behavior of spectral functions and resolvent kernels of elliptic operators.* Israel J. Math. **5** (1967), 1–30.

[2] Y. Colin de Verdière, *Une formule de traces pour l'opérateur de Schrödinger dans* $\mathbf{R}^3$, Ann. Sci. École Norm. Sup. **14**, (1981), 27–39.

[3] B. Helffer, A. Mohamed, *Asymptotic of the density of states for the Schrödinger operator with periodic electric potential.* Duke Math. J. **92** (1998), no. 1, 1–60.

[4] M. Hitrik, I. Polterovich, *Regularized traces and Taylor expansions for the heat semigroup,* preprint September 2001.

[5] S. Kantorovitz, C^n*-operational calculus, noncommutative Taylor formula and perturbation of semigroups,* J. Funct. Anal. **113** (1993), no. 1, 139–152.

[6] Yu. Karpeshina, *On the density of states for the periodic Schrödinger operator,* Ark. Mat. **38** (2000), no. 1, 111–137.

[7] W. Kirsch, *Random Schrödinger operators. A course.* in: Schrödinger operators (Sønderborg, 1988), 264–370, Lecture Notes in Phys., 345, Springer, Berlin, 1989.

[8] V. A. Marchenko, *Sturm-Liouville operators and applications.* Birkhäuser Verlag, Basel, 1986

[9] I. Polterovich, *Heat invariants of Riemannian manifolds,* Israel J. Math. **119** (2000), 239–252.

[10] I. Polterovich, *A commutator method for computation of heat invariants,* Indag. Math. (N.S.) **11** (2000), no. 1, 139–149.

[11] B. Simon, *Schrödinger semigroups,* Bull. Amer. Math. Soc. (N.S.) **7** (1982), no. 3, 447–526.

[12] B. Simon, *Trace ideals and their applications.* Cambridge University Press, Cambridge-New York, 1979.

[13] D. Shenk, M. A. Shubin, *Asymptotic expansion of state density and the spectral function of the Hill operator,* Math. USSR-Sb. **56** (1987), no. 2, 492–515.

[14] M. A. Shubin, *Spectral theory and the index of elliptic operators with almost-periodic coefficients,* Russian Math. Surveys **34** (1979), no. 2, 109–158.