Integrated density of states for random Schrödinger operators on manifolds[1]

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Abstract

We consider a Riemannian manifold X admitting a compact quotient X/Γ, i.e., Γ is a cocompact subgroup of the isometries acting properly discontinuously on X. We show, under certain conditions on Γ, that it is possible to define an integrated density of states for Γ-ergodic random Schrödinger operators on X (see Theorem 7). These conditions are, e.g., satisfied if Γ has polynomial growth.

Physical and geometrical setting

The integrated density of states (IDS) is a quantity introduced in the quantum theory of solids corresponding to the number of electron states per unit volume in a given energy interval $]-\infty, E[$. The electron levels correspond to eigenvalues of a Schrödinger operator which models the motion of an electron in condensed matter. For the medium one assumes a certain form of homogeneity, which is mathematically encoded in the ergodicity of the electrostatic potential which is produced by the medium. For the physical and mathematical background see, e.g., [4, 8, 5, 13].

For Euclidean configuration spaces the IDS is introduced mathematically as follows:

1. Let $\Lambda_l \subset \mathbb{R}^d$ be a cube of lenght l and centered at 0.
2. Consider a family of Schrödinger operators $H^\omega = -\Delta + V^\omega, \omega \in \Omega$, with ergodic potential V^ω. (Precise definition of ergodicity will follow.) Note that we use the sign convention that $-\Delta$ is a positive operator.
3. Restrict H^ω to Λ_l with Dirichlet boundary conditions to get H_l^ω.

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4. Call $N_l^\omega(E) := \#\{i \mid \lambda_i(H_\omega^l) < E\}$ the eigenvalue counting function of H_l^ω. Here $\lambda_i(H_\omega^l)$ are the eigenvalues of H_l^ω, enumerated in non-decreasing order and including multiplicities.

5. Under certain conditions on the family of ergodic potentials $V^\omega, \omega \in \Omega$ one can show that, for almost all ω, say, in the set Ω' of full measure, the limit

$$\lim_{l\to\infty} \frac{N_l^\omega(E)}{l^d} = N^\omega(E) = N(E) \tag{1}$$

exists for all continuity points of N and is independent of $\omega \in \Omega'$.

The limit (1) is called the IDS of the family H^ω. Note that, by definition, the functions $N_l^\omega(\cdot)$ are non-negative, monotone increasing and left-continuous. Since, in the thermodynamic limit ($l \to \infty$), the randomness disappears, the IDS $N(E)$ is called self-averaging. Once the non-randomness of the IDS has been established, one relates it to the spectrum of the operators $H^\omega, \omega \in \Omega$. In the Euclidean case it is known [7] that the set of points of increase

$$\{\lambda \in \mathbb{R} \mid \ N(\lambda + \epsilon) - N(\lambda - \epsilon) > 0 \ \forall \epsilon > 0\} \tag{2}$$

contains the spectrum of H^ω, which is independent of ω almost surely.

The Euclidean Laplace operator and the associated fundamental operators from physics can be naturally generalized to Riemannian manifolds. The spectrum of these physical operators then also reflects local and global geometric properties of the underlying manifold. In 1992, Adachi and Sunada [2] carried over techniques developed by mathematical physicists (cf. e.g. [15, 9]) to define an IDS of an periodic Schrödinger operator on a Riemannian manifold. In this new situation one encounters the nontrivial problem how to replace the cubes Λ_l, $l \to \infty$, which exhaust the Euclidean space. Actually, in $\mathbb{R}^d$ one is allowed to choose much more general exhaustions to define the (same) IDS.

In [2] the following geometrical setting is considered:

- Let X be a d-dimensional, non-compact, complete, connected Riemannian manifold.

- Let $\Gamma \subset$ be a discrete, amenable subgroup of the isometries acting freely and properly discontinously on X such that the quotient $M := X/\Gamma$ is compact. Then Γ is finitely generated.

Our geometric setting is the same as in [2]. However, instead of a single periodic operator we consider a random family of Schrödinger operators $H^\omega := -\Delta + V^\omega, \omega \in \Omega$, with the following properties.

- $(\Omega, \mathcal{A}, \mathbb{P})$ is a probability space with a group of ergodic measure perserving transformations $T_\gamma, \gamma \in \Gamma$. Ergodicity of the group of measure preserving transformations means that the only sets $A \in \mathcal{A}$ which are invariant under all $T_\gamma, \gamma \in \Gamma$ are those with $\mathbb{P}(A) = 0$ or $\mathbb{P}(A) = 1$.

- The potential is a jointly measurable stochastic process $V : \Omega \times X \to \mathbb{R}$ and, for technical reasons, we require $V^\omega \in C^\infty(X), \forall \omega$ and a uniform bound on the derivatives

$$\|\nabla^k V^\omega\|_\infty \leq C \text{ for all } \omega \in \Omega, k \leq \frac{1}{2}\dim(X) + 2 \ . \tag{3}$$

- The Γ-action on the potential and on X are consistent in the following sense: For all $\gamma \in \Gamma$ we have

$$V^\omega(\gamma x) = V^{T_\gamma \omega}(x) \ . \tag{4}$$

  This property is called ergodicity of the stochastic process V^ω.

Already earlier Sznitman [16, 17] studied the IDS for the Schrödinger operator with a random Poissonian potential on a hyperbolic manifold. This setting however differs from ours, both regarding the geometry of the manifold, as well as the ergodicity properties of the random potential.

If we define $U_\gamma f(x) := f(\gamma x)$ as the unitary operator on $L^2(X)$ corresponding to the isometry $\gamma : X \to X$, (4) can be written in the form $U_\gamma V^\omega U_\gamma^* = V^{T_\gamma \omega}$. Since $-\Delta$ is invariant under the operators U_γ one gets

$$U_\gamma H^\omega U_\gamma^* = H^{T_\gamma \omega}. \tag{5}$$

There are two approaches at hand to prove the convergence in (1). Either one uses the Laplace transform of the normalised eigenvalue counting function, which can be written in terms of the trace of the corresponding heat equation semigroup. In this case one applies a pointwise ergodic theorem for additive (w.r.t. domains) processes. Or one uses Dirichlet-Neumann bracketing to show that the eigenvalue counting functions form themselves a superadditive process. For such processes there are also ergodic theorems avaliable [3, 10]. However only in the abelian case they assure the pointwise existence of a limit. In our non-abelian setting we would get just a limit in mean.

Thus we rely on the first alternative and therefore need some tools from the theory of heat equation semigroups.

Heat kernel bounds

Under the above assumptions H^ω is a densely defined selfadjoint operator on $L^2(X)$. By the spectral theorem we can define the operator $\exp(-tH^\omega)$ which has an integral kernel $k^\omega(t, \cdot, \cdot)$. Let $D \subset X$ be a regular domain, i.e., a connected subset with compact closure and smooth boundary. We denote the restriction of H^ω to D with Dirichlet boundary conditions by H_D^ω and the corresponding heat kernel of $\exp(-tH_D^\omega)$ by $k_D^\omega(t, \cdot, \cdot)$.

Since the heat kernel depends monotonously on the domain (see [6, 18]), we have

$$0 \leq k_D^\omega(t, x, y) \leq k^\omega(t, x, y) \ \forall \ t > 0; x, y \in D \ . \tag{6}$$

We need, however, more information about the integral kernels. Firstly, we would like to bound the rhs of (6) by some constant independent on x, y and ω. Furthermore we would like to control the difference between the heat kernel on the whole manifold and the one restricted to the domain D. We collect this information in the following lemma.

Lemma 1 *Let k^ω, k^ω_D be the heat kernels as above. Then we have*
(a) $k^\omega(t,x,y) \le C(t),\ \forall x,y;\omega,$
(b) $\forall t, \epsilon > 0\ \exists h = h(t,\epsilon) < \infty$ such that, for all regular domains D and all $\omega \in \Omega$, we have

$$0 \le k^\omega(t,x,y) - k^\omega_D(t,x,y) \le \epsilon \quad \forall x,y \in D \setminus \partial_h D, \tag{7}$$

where $\partial_h D := \{x \in D |\ d(x, \partial D) \le h\}$.

The proof of (a) for a fixed potential V^ω can be infered from section 3 in [11]. Actually the dependence of the heat kernel on the potential can be bounded by a function of the sup-norm of the potential only. Since our family of potentials has an uniform norm bound we can choose the constant $C(t)$ to be independent of ω. The proof of (b) uses a result about unit propagation speed of the wave equation with potential, as it can be found, for example, in [18]. The bound on the difference of the two heat kernels is then obtained by an argument of U. Bunke as outlined in Theorem 2.26 of [12]. See also [14].

Assumptions on the group Γ

In the Euclidean case, any monotone exhaustion of $\mathbb{R}^d$ by cubes $\Lambda_{l_1}, \Lambda_{l_2}, \dots$ guaranteed the existence of a nonrandom IDS by an application of an abelian ergodic theorem. Actually there is much more freedom. One is even allowed to shift the cubes a little bit on each scale, so that the cubes do not contain the preceeding ones any more; one can choose balls instead of cubes or other convex domains as long as they satisfy some very reasonable growth conditions, cf. [9, 10].

On a Riemannian manifold one has to deal with the problem to find an adequate substitute for the cubes Λ_l. This problem already appeared in [2] for a single operator with periodic potential. If one considers a Γ-ergodic family of potentials and wants to prove existence of the IDS there is need for a non-abelian ergodic theorem. We will use an ergodic theorem due to Tempelman [19, 20]. This theorem is only applicable for exhaustions or summing sequences (the analoga of $\Lambda_{l_1}, \Lambda_{l_2}, \dots$) which satisfy much more restrictive conditions than those imposed in abelian ergodic theorems. The following definition lays the grounds to apply Tempelman's ergodic theorem (in the version given in [10]).

Definition 2 *A sequence of subsets $\{I_n\}_{n \in \mathbb{N}}$ of Γ is called an admissible sum-*

ming sequence if

$$\begin{array}{ll} (P0) & I_n \subset I_{n+1}\,,\ ,0<|I_n|<\infty\ \forall n\in\mathbb{N}, \\ (P1) & \forall\gamma:\ |I_n\Delta I_n\gamma|/|I_n|\longrightarrow 0\ \textit{for}\ n\to\infty, \\ (P2) & \exists K<\infty:\ |I_n^{-1}I_n|\le K|I_n|\ . \end{array}$$

Here $|A|$ denotes the cardinality of a finite set A.

The condition (P1) is an formulation of Følner's condition for discrete groups. (P2) is a growth condition which can be understood best, e.g., in the particular case where the sets I_n are combinatorial balls of radius n (w.r.t. a word metric): Doubling the radius increases the cardinality of the ball by only a constant multiple. Admissible summing sequences are the main input in Tempelman's ergodic theorem applied to the group $T_\gamma, \gamma \in \Gamma$. In the next section, we construct, to a given admissible summing sequence, a corresponding sequence of subsets of the Riemannian manifold to which we will restrict our Schrödinger operators.

Admissible exhaustions and the main result

As explained in section 3 of [2], there exists a smooth triangulation of the compact manifold M and, by lifting the simplices to X in a suitable manner, we obtain a connected polyhedral Γ-fundamental domain $\mathcal{F}$. Particularly $\mathcal{F}$ consists of finitely many smooth images of d-dimensional simplices which can overlap only at their boundaries.

Definition 3 *For an admissible summing sequence $\{I_n\}_{n\in\mathbb{N}}$ we define*

$$D_n = \bigcup_{\gamma\in I_n} \gamma\mathcal{F} \tag{8}$$

where $\mathcal{F}$ is a fundamental domain as explained above. We call $\{D_n\}_{n\in\mathbb{N}}$ an admissible exhaustion if, additionally,

$$(P) \qquad \textit{For all } h>0: \frac{vol(\partial_h D_n)}{vol(D_n)} \longrightarrow 0 \ \ \textit{for } n\to\infty\ . \tag{9}$$

It was shown in [1, 2] that the geometric condition (P) is automatically satisfied if $|I_nA^n - I_n| \le |I_n|/(n|A^n|)$, for all $n \in \mathbb{N}$, where $A \subset \Gamma$ is the following particular set of generators: $A = \{\gamma : \overline{\gamma\mathcal{F}} \cap \overline{\mathcal{F}} \neq \emptyset\}$.

Lemma 4 *For an admissible exhaustion $\{D_n\}_{n\in\mathbb{N}}$ and any $\delta>0$ there exists a sequence $\{M_n\}_{n\in\mathbb{N}}$ of regular domains such that:*

$$D_n \setminus \partial_\delta D_n \subset M_n \subset D_n\,,\ \partial M_n \subset \partial_\delta D_n\,,\ \forall n, \tag{10}$$

and, for $n \to \infty$, we have

$$\left| |D_n|^{-1} \int_{D_n} k^\omega(t,x,x)dx - |M_n|^{-1} \int_{M_n} k^\omega_{M_n}(t,x,x)dx \right| \longrightarrow 0 \ . \qquad (11)$$

We call $\{M_n\}_{n\in\mathbb{N}}$ a regularisation of $\{D_n\}_{n\in\mathbb{N}}$.

For the proof of (11) one uses Lemma 1(b) to bound the difference of the kernels by some arbitrary small number $\epsilon > 0$ away from the boundary of D_n. The region near the boundary, where this estimate is not valid, is small by property (P). There we use Lemma 1(a) and the fact that the symmetric difference of M_n and D_n is small, as well.

The ergodicity of V^ω implies (5). An analogous relation is valid for the spectral projections of H^ω as can be inferred from [21, Theorem 7.15] and the uniqueness of the spectral projection.

$$U_\gamma E(\lambda,\omega) U_\gamma^* = E(\lambda, T_\gamma\omega) \ . \qquad (12)$$

This relation also holds for $\exp(-tH^\omega)$ and thus its kernel $k^\omega(t,x,y)$ is an ergodic stochastic process in the following sense

$$k^\omega(t,\gamma x,\gamma x) = k^{T_\gamma\omega}(t,x,x) \ . \qquad (13)$$

This enables us to apply later the next lemma to the heat kernels.

Lemma 5 *Let $\{D_n\}_{n\in\mathbb{N}}$ be an admissible exhaustion and $f : \Omega \times X \to \mathbb{R}$ be a Γ-ergodic stochastic process. Then*

$$\lim_{n\to\infty} |D_n|^{-1} \int_{D_n} f(\omega,x)dx = |\mathcal{F}|^{-1}\, \mathbb{E}\left[\int_{\mathcal{F}} f(\bullet,x)dx\right] \ . \qquad (14)$$

Here $\mathbb{E}$ denotes the expectation with respect to the measure $\mathbb{P}$.

Proof: Set $F(\omega) = |\mathcal{F}|^{-1}\int_{\mathcal{F}} f(\omega,x)dx$. Now transform the term on the lhs of (14).

$$\begin{aligned} |D_n|^{-1}\int_{D_n} f(\omega,x)dx &= |I_n|^{-1}\sum_{\gamma\in I_n} |\mathcal{F}|^{-1}\int_{\gamma\mathcal{F}} f(\omega,x)dx \\ &= |I_n|^{-1}\sum_{\gamma\in I_n} |\mathcal{F}|^{-1}\int_{\mathcal{F}} f(\omega,\gamma x)dx \\ &= |I_n|^{-1}\sum_{\gamma\in I_n} |\mathcal{F}|^{-1}\int_{\mathcal{F}} f(T_\gamma\omega,x)dx \\ &= |I_n|^{-1}\sum_{\gamma\in I_n} F(T_\gamma\omega) \longrightarrow \tilde{f}(\omega) \end{aligned}$$

for $n \to \infty$ and a measurable $\tilde{f} : \Omega \to \mathbb{R}$. Here we used that

1. D_n can be written as an union of translates of the fundamental domain $\mathcal{F}$,

2. γ is an isometry and thus preserves the volume element dx,

3. we can transfer the action of γ from the geometric to the random parameter by the ergodicity of the process f,

4. admissible summing sequences satisfy the conditions of Tempelman's ergodic theorem.

We additionally know from this ergodic theorem that the function $\tilde{f}$ is invariant under all $T_\gamma, \gamma \in \Gamma$. By assumption, these transformations are ergodic and, thus, $\tilde{f}$ is constant almost surely. The convergence calculated above implies that this constant has to be equal to $\mathbb{E}(F)$.
□

In order to prove our main result (Theorem 7) we need, finally, the following lemma (see [15, Lemma 5.2]). It will be used to derive convergence of the normalized eigenvalue counting function from convergence of the corresponding heat kernels.

Lemma 6 (Šubin) *Let $N_n : \mathbb{R} \to \mathbb{R}^+$ be a sequence of left-continuous, monotone increasing functions such that*

1. *there exists a $c \in \mathbb{R}: \ N_n(\lambda) = 0 \quad \forall \lambda \leq c, \, n \in \mathbb{N}$,*

2. *there exists a $C : \mathbb{R}^+ \to \mathbb{R} : \psi_n(t) := \int e^{-\lambda t} dN_n(\lambda) \leq C(t) \ \ \forall n \in \mathbb{N}, \, t > 0$,*

3. *$\lim_{n\to\infty} \psi_n(t) =: \psi(t)$ exists for all $t > 0$.*

Then the limit

$$N(\lambda) := \lim_{n\to\infty} N_n(\lambda)$$

exists at all continuity points. N is a non-negative, monotone increasing, left-continuous function of λ, and its Laplace transform is ψ.

Theorem 7 *Let $\{D_n\}_{n\in\mathbb{N}}$ be an admissible exhaustion and $\{M_n\}_{n\in\mathbb{N}}$ a regularisation of $\{D_n\}$. Define*

$$\phi_n^\omega(\lambda) := \#\{ \text{ eigenvalues of } H^\omega_{M_n} \leq \lambda\}, \ N_n^\omega = |M_n|^{-1} \phi_n^\omega \ . \tag{15}$$

Then, for almost all $\omega \in \Omega$, the limit

$$N(\lambda) = \lim_{n\to\infty} N_n^\omega(\lambda) \tag{16}$$

exists at all continuity points of $N(\cdot)$. Moreover, N is a non-negative, monotone increasing, left-continuous function (independent of ω).

Proof: We check Šubin's hypotheses:

1. $\phi_n^\omega(\lambda) = 0$ for all $\omega \in \Omega, n \in \mathbb{N}$, if $\lambda < -\|V^\omega\|_\infty$.
2.

$$\begin{aligned} |M_n|^{-1} \int e^{-t\lambda} d\phi_n^\omega(\lambda) &= |M_n|^{-1} \sum_{\lambda_n \in \sigma(H^\omega_{M_j})} e^{-t\lambda_n} \\ &= |M_n|^{-1} \operatorname{Tr} e^{-tH^\omega_{M_j}} \\ &= |M_n|^{-1} \int_{M_n} k^\omega_{M_n}(t,x,x)dx \\ &\leq |M_n|^{-1} \int_{M_n} k^\omega(t,x,x)dx \\ &\leq C(t). \end{aligned}$$

3.

$$\begin{aligned} \lim_{n\to\infty} |M_n|^{-1} \int e^{-t\lambda} d\phi_n^\omega(\lambda) &= \lim_{n\to\infty} |M_n|^{-1} \int_{M_n} k^\omega_{M_n}(t,x,x)dx \\ &= \lim_{n\to\infty} |D_n|^{-1} \int_{D_n} k^\omega(t,x,x)dx \\ &= |\mathcal{F}|^{-1}\, \mathbb{E} \left[\int_{\mathcal{F}} k^\bullet(t,x,x)dx \right] . \end{aligned}$$

Here we used the Lemmata 4 and 5.

□

An Example

We supply a non-abelian example of a pair (X, Γ) which satisfies all necessary conditions to define an IDS in the above manner.

For any Riemannian manifold with a polynomially bounded cocompact discrete group of isometries an admissible exhaustion $\{D_n\}_{n\in\mathbb{N}}$ can be constructed. In particular, this is the case for nilpotent groups. Thus, an example is given by the Heisenberg group

$$X = \left\{ \begin{pmatrix} 1 & x & y \\ 0 & 1 & z \\ 0 & 0 & 1 \end{pmatrix} \mid x,y,z \in \mathbb{R} \right\} \tag{17}$$

with a left-invariant metric, and $\Gamma = X \cap M(3, \mathbb{Z})$. X is diffeomorphic to $\mathbb{R}^3$, but non-abelian. Note that the discrete group Γ acts, by isometries, from the left on X and that the quotient $\Gamma\backslash X$ is compact.

An example for a Γ-ergodic potential on (X, Γ) is the analogue of the one which is called alloy-type potential in the Euclidean setting.

Let $u : X \to \mathbb{R}$ be a smooth function supported in $\mathcal{F}$. We choose $\Omega = \bigotimes_{\gamma\in\Gamma} \mathbb{R}$, equipped with the product measure $\mathbb{P} := \bigotimes_{\gamma\in\Gamma} \mu$, where μ is a probability measure on $\mathbb{R}$. Consider the independent, identically distributed random variables $\pi_\gamma : \Omega \to \mathbb{R}, \pi_\gamma(\omega) := \omega_\gamma, \gamma \in \Gamma$ and the measure preserving transformations $(T_\gamma(\omega))_\beta := \omega_{\gamma\beta}$. Then the potential, given by

$$V^\omega(x) := \sum_{\gamma\in\Gamma} \omega_\gamma u(\gamma x), \tag{18}$$

is Γ-ergodic and satisfies the required regularity assumptions (3) to define the IDS. Actually, it seems that by using probabilistic estimates for the heat kernels, instead, these regularity assumptions can be relaxed to the "natural" ones. These are formulated in terms of the expectation of some local L^p-norm of V^ω, cf. [9].

Discussion

The IDS is a quantity related to the restrictions of Schrödinger operators in a familiy $H^\omega, \omega \in \Omega$, to suitable exhaustions of a non-compact Riemannian manifold X. It should be possible to use the same functional analytic arguments as in the Euclidean case to establish the equality of its points of increase (2) with the spectrum of H^ω.

The definition of an admissible exhaustion contains assumptions about both the sequence of subsets I_n of the group Γ as well as the geometry of the domains D_n. It would be desirable to formulate the conditions in terms of either group-theoretic or geometric properties only. Recently, we observed, in the case of a polynomially bounded group Γ, that Theorem 7 is also valid for a sequence $M_n \subset X$ of regularized geodesic balls with increasing radii satisfying condition (P). Thus for this choice one obtains via (16) a non-random IDS. It is natural to ask for more general classes of exhaustions of X, for which the normalised eigenvalue counting functions converge and whether they give rise to the same IDS.

The remark in Krengel [10] after the statement of Tempelman's theorem implies the uniqueness of the IDS in the following sense. Let $I_n, n \in \mathbb{N}$ be a sequence of subsets of Γ, not necessarily admissible in our sense and $D_n, n \in \mathbb{N}$ as in (8). Assume that it satisfies condition (P) and that a regularisation $M_n, n \in \mathbb{N}$ exists. If the N_n^ω defined in (15) converge to a non-random limit N, then this has to be equal to the IDS defined in Theorem 7 by an admissible summing sequence. In particular any two admissible exhaustions give rise to the same IDS.

Note also that our choice of the admissible exhaustion depends on the pair (X, Γ) only. This means particularly, that it is independent of the properties of the family of Schrödinger operators$H_\omega, \omega \in \Omega$. If one would allow for admissible exhaustions depending on the stochastic process V^ω, too, the convergence (16) of the normalised eigenvalue counting functions to an IDS could be achieved in more general geometric situations.

Finally, it should be possible to study an ergodic family of operators where higher order parts of the operators depend on the random parameter ω and to carry through the same procedure as in this paper. Such a situation would occur if ω were related to the change of a magnetic field or to the change of the metric of the underlying Riemannian manifold.

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