A

Properties of the Spectral Shift Function

In this appendix certain properties of the spectral shift function which are relevant for the study of the integrated density of states are collected. Let us note that this function is sometimes called Lifshitz-Krein SSF since Lifshitz and Krein were the first to devote attention to it, see e.g. the discussion in the introduction of [50].

For an exposition of the theory of the spectral shift function (SSF) see [50, 293].

An survey of the role played by the SSF in scattering theory can be found in the last chapter of [499]. The SSF has proven useful in the study of random operators, particularly in problems related to surface models, e.g. the definition of the density of surface states [82, 83, 297, 298]. In [443] it is used in the analysis of rank one perturbations of operators, in particular in the random context. More recently, it has found applications in the study of quantum graphs, cf. [299, 209, 295, 210].

Various of the properties of the SSF are discussed in the literature: monotonicity and concavity [182, 193, 294], the asymptotic behaviour in the large coupling constant limit [400, 418, 401] and semiclassical limit [372], and some other bounds [397, 398, 399]. For magnetic Schrödinger operators the SSF is analysed in [68, 164, 67, 402, 403].

A.1 The SSF for Trace Class Perturbations

For two selfadjoint operators A, B such that the difference $A-B$ is trace class the SSF $\xi(\cdot, A, B)$ may be defined (up to an additive constant) by the formula

$$\mathrm{Tr}(\rho(A) - \rho(B)) = \int \rho'(\lambda)\, \xi(\lambda, A, B)\, d\lambda \tag{A.1}$$

for all functions $\rho \in C^1(\mathbb{R})$ such that ρ' is the Fourier transform of a complex measure on $\mathbb{R}$ with finite total variation, cf. Theorem 3.2 in [50] or Theorem

8.3.3 in [499]. Actually, the assumption that ρ is in the Besov space $B^1_{\infty,1}(\mathbb{R})$ is sufficient to guarantee that $\rho(A) - \rho(B)$ is trace class and that the relation (A.1) holds, see [391] for details. Equality (A.1) is called *Krein trace formula.* If the operators A, B are semi-bounded, the mentioned additive constant can be normalised to be equal to zero, and thus the SSF becomes unique.

The SSF is related to the perturbation determinant from scattering theory by the formula

$$\xi(\lambda, A, B) = \frac{1}{\pi} \lim_{\varepsilon \searrow 0} \arg \det[1 + (A - B)(B - \lambda - i\varepsilon)^{-1})] \tag{A.2}$$

for almost all values of $\lambda \in \mathbb{R}$. For the right side to be well defined it is actually sufficient to assume only that $(A - B)(B + i)^{-1}$ is trace class. So one can interpret (A.2) as an extension of the definition of the SSF to the class of relative trace class perturbations.

The SSF can be bounded in terms of Schatten-von Neumann ideal properties of $A - B$, namely

$$\|\xi(\cdot, A, B)\|_1 \leq \|A - B\|_{J_1} \tag{A.3}$$

Here J_1 denotes the ideal of trace class operators and $\| \cdot \|_{J_1}$ the *trace norm.* In particular, for trace class perturbations $A - B$, the SSF ξ is in $L^1(\mathbb{R})$. On the other hand, if $A - B$ is finite rank

$$\|\xi(\cdot, A, B)\|_\infty \leq \operatorname{rank}(A - B) \tag{A.4}$$

Since we have an estimate on ξ in the L^1 and L^∞-norms, it is natural to ask whether an estimate for the L^p-norm, $p \in]1, \infty[$, may be derived. This indeed turns out to be true and can be understood as an interpolation result, cf. the proof of Theorem 2.1 in [97].

To formulate this bound we have to introduce ideals of 'better than trace class' operators, defined in terms of summability properties of singular values. Recall that the singular values of a compact operator C are the square-roots of the eigenvalues of C^*C. We enumerate them in non-increasing order $\mu_1(C) \geq \mu_2(C) \geq \cdots \geq \mu_n(C) \cdots \geq 0, n \in \mathbb{N}$ counting multiplicities. If C is trace class, the sum of the singular values is finite and equals $\|C\|_{J_1}$. We denote by J_β the class of compact operators such that

$$\|C\|_{J_\beta} := \Big(\sum_{n \in \mathbb{N}} \mu_n(C)^\beta \Big)^{1/\beta} < \infty \tag{A.5}$$

The theory of such operators is classical for $\beta \geq 1$, see for instance [437]. However, since we want to interpolate between (A.3) and (A.4), we need to consider operators whose singular values converge not slower, but *faster* than an ℓ^1-sequence to zero. This leads us to consider operators such that $\|C\|_{J_\beta}$ is finite, for β *smaller than one.* In particular, all such operators are trace class, which explains why they are sometimes called *super-trace class* operators.

It follows that the SSF may be defined for perturbations of this type. The classes $J_\beta, \beta < 1$ have been studied in [200, 46, 48], while their relevance in the context of random operators was recognised in [97].

From these sources we infer the following properties of J_β. For any compact operator A and bounded B the singular values of the products obey the relation

$$\mu_n(AB) \leq \|B\| \, \mu_n(A) \qquad \text{and} \qquad \mu_n(BA) \leq \|B\| \, \mu_n(A) \tag{A.6}$$

If we assume that B is also compact, the Ky-Fan inequalities [158, 437] establish for the singular values of the sum $A + B$ the bounds

$$\mu_{n+m+1}(A+B) \leq \mu_{n+1}(A) + \mu_{m+1}(B) \quad \text{ for all } n, m = 0, 1, 2, \ldots \tag{A.7}$$

In particular the set J_β is a two-sided ideal in the algebra of bounded operators for all $\beta > 0$. For $\beta \geq 1$ the functional $A \mapsto \|A\|_{J_\beta}$ is a norm, which is not true for $\beta < 1$. More precisely, in the latter case we have only

$$\|A + B\|_{J_\beta}^\beta \leq \|A\|_{J_\beta}^\beta + \|B\|_{J_\beta}^\beta$$

This property implies that $\| \cdot \|_{J_\beta}$ is a *quasi-norm* and that

$$\mathrm{dist}_\beta(A, B) = \|A - B\|_{J_\beta}^\beta$$

is a well defined metric on J_β. The pair $(J_\beta, \mathrm{dist}_\beta)$ forms a complete, separable, linear metric space, in which the finite rank operators form a dense subset.

In [97] the following L^p-bound on the SSF was proven.

Theorem A.1.1. *Let $p \geq 1$ and A, B be selfadjoint operators whose difference is in J_β, where $\beta = 1/p$. Then the spectral shift function $\xi(\cdot, A, B)$ is in $L^p(\mathbb{R})$ and*

$$\|\xi(\cdot, A, B)\|_{L^p} \leq \big\|A - B\big\|_{J_\beta}^\beta \tag{A.8}$$

A sharp bound on the SSF was proven by Hundertmark and Simon in [221], which in fact includes Theorem A.1.1 as a special case.

Theorem A.1.2. *Let $F \colon [0, \infty[\to [0, \infty[$ be a convex function such that $F(0) = 0$. Let A, B be bounded and C a non-negative compact operator such that for all $N \in \mathbb{N}$*

$$\sum_{n=N}^\infty \mu_n(|A - B|) \leq \sum_{n=N}^\infty \mu_n(C) \tag{A.9}$$

Then

$$\int F\big(|\xi(\lambda, A, B)|\big) d\lambda \leq \int F\big(|\xi(\lambda, C, 0)|\big) d\lambda = \sum_{n \in \mathbb{N}} \big[F(n) - F(n-1)\big] \, \mu_n(C)$$

Condition (A.9) is in particular satisfied if $|A - B| \leq C$. Of course, to be able to apply Theorem A.1.2 one needs to have appropriate estimates on the singular values of the operator C. In the context of Schrödinger operators such estimates are derived in Sect. A.2.

In certain situations one can show that an operator C belongs to a Schatten-von Neumann class J_β by writing it as a product of operators $C_1, \dots, C_N$ for which one already knows that they belong to a larger class J_α with $\alpha > \beta$. Then the product $C = C_1 \cdots C_N$ will enjoy much better summability properties than the individual factors.

For this purpose it is useful to note that the Hölder inequality extends also to the case of exponents smaller than one: let $a_i \colon \mathbb{N} \to \mathbb{C}$, $i = 1, \dots, N$ be such that $|a_i(n)|^{p_i}$ is summable, where $p_i > 0$ for all $i = 1, \dots, N$, and set $\frac{1}{r} := \sum_{i=1}^N \frac{1}{p_i}$. Then the pointwise product $\prod_{i=1}^N a_i$ is in $\ell^r(\mathbb{N})$ and

$$\Big\| \prod_{i=1}^N a_i \Big\|_r \leq \prod_{i=1}^N \|a_i\|_{p_i}$$

By applying this to the sequence of singular values of compact operators, we obtain the following

Lemma A.1.3. *Let $C_i \in J_{p_i}$ for $i = 1, \dots, N$, then $\prod_{i=1}^N C_i$ is in J_r where $\frac{1}{r} := \sum_{i=1}^N \frac{1}{p_i}$ and*

$$\Big\| \prod_{i=1}^N C_i \Big\|_{J_r} \leq \prod_{i=1}^N \|C_i\|_{J_{p_i}} \tag{A.10}$$

See also [48], Corollary 11.11.

A.2 The SSF for Schrödinger Operators and the Invariance Principle

We want to apply the formalism of the SSF to Schrödinger operators. In this setting we cannot use the results of the previous section on trace class perturbations, since any potential given by a proper function is not in this class of operators.

It turns out that the SSF can be defined easily for a pair of selfadjoint, lower bounded operator with purely discrete spectrum. This would cover Schrödinger operators restricted to finite cubes Λ. In the application in Sect. 4.2 we use only the SSF for this type of operators. However, since we are not only interested in the *existence* of the SSF as a function, but also on *upper bounds*, we have to resort to more powerful techniques, which then allow us along the way to define the SSF for a pair of Schrödinger operators on the whole of $\mathbb{R}^d$, under the assumption that they differ by a compactly supported potential.

For a selfadjoint, lower bounded operator H with purely discrete spectrum the eigenvalue counting function $\mathcal{N}(H,E) := \#\{n \mid \lambda_n(H) \le \lambda\}$ is well defined. Here $\lambda_n(H), n \in \mathbb{N}$ enumerates the spectrum of H, counting multiplicities, in increasing order. Thus for two such operators H_1, H_2 the SSF can be defined as the difference of the eigenvalue counting functions,

$$\xi(\lambda, H_2, H_1) := \mathcal{N}(H_2, E) - \mathcal{N}(H_1, E)$$

If the difference $H_2 - H_1$ happens to be trace class, this definition produces (almost everywhere) the same function ξ as (A.1). To see this, one chooses in (A.1) a sequence ρ_ε of switch functions which converges to the step function $\chi_{]-\infty,E]}$ as $\varepsilon \to 0$.

Now we consider the case that the operators H_1 and H_2 are selfadjoint and lower bounded, but we neither assume that the difference $H_2 - H_1$ is trace class nor that the operators H_1 and H_1 have purely discrete spectrum. Let $g\colon \mathbb{R} \to [0,\infty[$ be a C^2-function such that g' is everywhere negative. In particular, the function g is bounded on the spectra of H_1 and H_2 and thus $g(H_2) - g(H_1)$ is a bounded operator. Assume that $g(H_2) - g(H_1)$ is trace class. Then the SSF for the operator pair $g(H_1), g(H_2)$ is well defined by (A.1) and we may set

$$\xi(\lambda, H_2, H_1) := -\xi\big(g(\lambda), g(H_2), g(H_1)\big) \tag{A.11}$$

This definition is independent of the choice of g, as long as it has the abovementioned properties, see e.g. [50, Sect. 1.4]. Formula (A.11) is called the *invariance principle* in analogy to the relation in scattering theory. This last definition will be sufficiently general to cover the type of Schrödinger operators we are considering. Natural candidates for the function g are the following families of functions

$$g(x) = (x + C)^{-k}, \ \mathbb{N} \ni k > \frac{d}{2} + 2, \ C > -\inf \sigma(H)$$

corresponding to powers of resolvents, respectively

$$g(x) = \exp(-tx), \ t > 0 \tag{A.12}$$

corresponding to semigroups of Schrödinger operators. Of course we will still have to impose certain regularity assumptions on the Schrödinger operators H_1, H_2 such that $g(H_2) - g(H_1)$ really turns out to be trace class. In the remainder of the appendix we choose the function g as in (A.12).

A.3 Singular Value Estimates

There is a short and transparent way to prove the super-trace class estimates needed for the bound of the SSF. It uses the decay of singular values of certain auxiliary operators. The basic observation is that the singular values of the difference of two Schrödinger semigroups decay almost exponentially and the semigroup difference is therefore in any super-trace class ideal. There are

essentially two ingredients in the proof of this statement: a Weyl-type bound on eigenvalues and exit time estimates for Brownian motion. We follow here the presentation from the paper [218] by Hundertmark, Killip, Nakamura, Stollmann and the author.

Weyl's law gives the asymptotic behaviour of the n^{th} eigenvalue of the Laplacian on an open ball B for large n. For our purposes it is necessary to have a lower bound of this type valid for *all* eigenvalues. It is provided in the following lemma which applies for rather general Schrödinger operators with electromagnetic field.

We consider magnetic Schrödinger operators

$$H = H_A + V, \quad H_A = (-i\nabla - A)^2 \tag{A.13}$$

acting on $\mathbb{R}^d$ with magnetic potential A and electric potential $V = V_+ - V_-$, where $V_+ := \max(0, V)$ and $V_- := \max(0, -V)$.

Lemma A.3.1. *Let H be as in* (A.13). *Assume that each component of A is in $L^2_{\text{loc}}(\mathbb{R}^d)$, that $V_+ \in L^1_{\text{loc}}(\mathbb{R}^d)$, and that V_- is $-\Delta$ bounded with relative bound $\delta < 1$. Furthermore, let $H^{\mathcal{U}}$ be the Dirichlet restriction of H to an arbitrary open set $\mathcal{U} \subset \mathbb{R}^d$ with finite volume $|\mathcal{U}|$. Then there exists a constant C, such that the n^{th} eigenvalue of $H^{\mathcal{U}}$ satisfies*

$$\lambda_n \geq \frac{2\pi(1-\delta)d}{e} \left(\frac{n}{|\mathcal{U}|}\right)^{2/d} - C \qquad \textit{for all } n \in \mathbb{N} \tag{A.14}$$

Under these assumptions on the vector and scalar potential, H can be defined by the use of quadratic forms, see for instance Sect. 2 of [222]. The Dirichlet restriction $H^{\mathcal{U}}$ to the set $\mathcal{U}$ is defined in the same way. If A and V_- vanish, we have already used this way to define Schrödinger operators in Remark 2.2.3.

Proof. Since the Sobolev space with Dirichlet b.c. $W^{1,2}_0(\mathcal{U})$ is a natural subset of $W^{1,2}(\mathbb{R}^d)$, V_- is also relatively form bounded w.r.t. $-\Delta^{\mathcal{U}}$, the Dirichlet Laplacian on $\mathcal{U}$, with relative bound δ. The diamagnetic inequality, cf. [436], then implies that V_- is also relatively form bounded with respect to the Dirichlet restriction $H^{\mathcal{U}}_A$ of H_A to $\mathcal{U}$. In other words, there exists a constant $C \in \mathbb{R}$ such that

$$V_- \leq \delta H^{\mathcal{U}}_A + C$$

in the sense of quadratic forms. In particular, since V_+ is non-negative,

$$H^{\mathcal{U}} \geq H^{\mathcal{U}}_A - V_- \geq (1-\delta) H^{\mathcal{U}}_A - C$$

which implies the bound

$$\begin{aligned}\operatorname{Tr}(\mathrm{e}^{-2tH^{\mathcal{U}}}) &\leq \mathrm{e}^{2tC}\operatorname{Tr}(\mathrm{e}^{-2t(1-\delta)H_A}) = \mathrm{e}^{2tC}\|\mathrm{e}^{-t(1-\delta)H_A}\|^2_{\mathrm{HS}} \\ &= \mathrm{e}^{2tC}\iint_{\mathcal{U}\times\mathcal{U}} |\mathrm{e}^{-t(1-\delta)H_A}(x,y)|^2 dx\, dy\end{aligned}$$

where $\|\cdot\|_{\mathrm{HS}}$ denotes as before the Hilbert-Schmidt norm. Using once more the diamagnetic inequality for Schrödinger semigroups, e.g., [436, 222], one obtains the pointwise bound $|\mathrm{e}^{-t(1-\delta)H_A}(x,y)| \leq \mathrm{e}^{t(1-\delta)\Delta^{\mathcal{U}}}(x,y)$. In particular,

$$\|\mathrm{e}^{-t(1-\delta)H_A}\|_{\mathrm{HS}}^2 \leq \|\mathrm{e}^{t(1-\delta)\Delta^{\mathcal{U}}}\|_{\mathrm{HS}}^2 = \mathrm{Tr}(\mathrm{e}^{2t(1-\delta)\Delta^{\mathcal{U}}}) \leq |\mathcal{U}| \big(8\pi t(1-\delta)\big)^{-d/2}$$

In the last line we used that by domain monotonicity the kernel of the Dirichlet semigroup $\mathrm{e}^{\beta\Delta^{\mathcal{U}}}$ on the diagonal is bounded by the heat kernel on the whole of $\mathbb{R}^d$, i.e.,

$$\mathrm{e}^{\beta\Delta^{\mathcal{U}}}(x,x) \leq \mathrm{e}^{\beta\Delta}(x,x) = (4\pi\beta)^{-d/2} \qquad \text{for all } \beta > 0 \text{ and } x \in \mathcal{U}$$

Thus

$$\mathrm{Tr}(\mathrm{e}^{-2tH^{\mathcal{U}}}) \leq |\mathcal{U}| \big(8\pi t(1-\delta)\big)^{-d/2} \tag{A.15}$$

Let $\mathcal{N}^{\mathcal{U}}(\lambda) := \#\{n \mid \lambda_n(H^{\mathcal{U}}) \leq \lambda\}$ be the number of eigenvalues of $H^{\mathcal{U}}$ smaller or equal to λ. By Čebyšev's inequality and (A.15),

$$\begin{aligned}\mathcal{N}^{\mathcal{U}}(\lambda) &\leq \mathrm{e}^{2t\lambda}\int_{-\infty}^{\lambda} \mathrm{e}^{2ts} d\mathcal{N}^{\mathcal{U}}(s) \leq \mathrm{e}^{2t\lambda}\mathrm{Tr}(\mathrm{e}^{-2tH^{\mathcal{U}}}) \\ &\leq |\mathcal{U}|\,(8\pi(1-\delta))^{-d/2}\, t^{-d/2}\mathrm{e}^{2t(\lambda+C)}\end{aligned}$$

for arbitrary $t > 0$. The last expression is for $t := \frac{d}{4(\lambda+C)}$ equal to

$$|\mathcal{U}| \left(\frac{e(\lambda+C)}{2\pi(1-\delta)d}\right)^{d/2}$$

This estimate implies together with $n \leq \mathcal{N}^{\mathcal{U}}(\lambda_n)$ the lower bound

$$\lambda_n \geq \frac{2\pi(1-\delta)d}{e}\left(\frac{n}{|\mathcal{U}|}\right)^{2/d} - C$$

on the eigenvalues. □

In the next theorem we consider a pair Schrödinger operators which obey slightly stronger assumptions regarding the negative part V_- of their scalar potential. More precisely, we assume that V_- is in the Kato class. A general discussion of the Kato-class can be found in [102]. For its relevance to the Feynman-Kac formula see, e.g., [12, 65, 438]. In particular, V_- is in the Kato-class, if it is in $L^p_{\mathrm{loc,unif}}(\mathbb{R}^d)$ for $p = 1$, if $d = 1$ and $p > d/2$, if $d \geq 2$, cf. Sect. 1.2. Under these hypotheses, one may define H via the corresponding quadratic form with core $C_c^\infty(\mathbb{R}^d)$, similarly as in Remark 2.2.3. By the same method, one can define the Dirichlet restriction H^l of H to the cube $\Lambda_l =]-l/2, l/2[^d, l \geq 1$.

Let H_1 be a Schrödinger operator of the form just described and let $H_2 = H_1 + u$. Assume that $u = u_+ - u_-$ has compact support, that $u_+ \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$

and that u_- is in the Kato class. Our aim is to obtain an estimate on the singular values of $V_{\text{eff}} := \mathrm{e}^{-H_1} - \mathrm{e}^{-H_2}$ and on the corresponding object in the finite volume case, namely $V_{\text{eff}}^l := \mathrm{e}^{-H_1^l} - \mathrm{e}^{-H_2^l}$.

Theorem A.3.2. *There exists a constant c depending only on the dimension d, and a constant C depending on the Kato-class norms of u_-, V_- and on the diameter of the support of u_+ such that the singular values of the operators V_{eff} and V_{eff}^l obey for all $n \in \mathbb{N}$ and $l \geq 1$ the relations*

$$\mu_n(V_{\text{eff}}) \leq C\,\mathrm{e}^{-cn^{1/d}} \qquad \textit{and} \qquad \mu_n(V_{\text{eff}}^l) \leq C\,\mathrm{e}^{-cn^{1/d}} \tag{A.16}$$

Remark A.3.3. (i) Note that the estimate (A.16) depends on the positive part of u only through $\operatorname{supp} u$. Thus, for $u = \kappa\tilde{u}$ where $\tilde{u} \geq 0$ and κ is a non-negative coupling constant, the estimate is independent of the choice of κ.

(ii) Actually, u may be taken to $+\infty$ on its support. In this case H_2 equals the restriction of H_1 to $\mathbb{R}^d \setminus \operatorname{supp} u$ with Dirichlet boundary conditions, provided the boundary of supp u obeys some mild regularity conditions, see for instance [455].

(iii) Similarly, H_1, H_2 may be defined on a set strictly smaller than $\mathbb{R}^d$: Let $\mathcal{U} \subset \mathbb{R}^d$ be open, $H_A^{\mathcal{U}}$ the Dirichlet restriction of H_A on $\mathcal{U}$, and $H_1 = H_A^{\mathcal{U}} + V$, $H_2 = H_A^{\mathcal{U}} + V + u$ where V and u satisfy the same conditions as before. In this case H_j^l is the Dirichlet restriction of $H_j, j = 1, 2$ to the set $\Lambda_l \cap \mathcal{U}$.

Remark A.3.4. The decay estimate in (A.16) is almost optimal with respect to the exponent. In [405] Raikov and Warzel analyse the perturbation of the free Schrödinger operator with a constant magnetic field in two dimensions, i.e. the Landau Hamiltonian, by a compactly supported potential. The results in [405] (and similarly those in [359]) show that for general magnetic Schrödinger operators one cannot obtain a faster decay than

$$\mu_n(V_{\text{eff}}) \leq C\,\mathrm{e}^{-cn^{2/d}}$$

This is explained in some detail in the first Section of [218]. See also Remark A.4.2.

Proof (of Theorem A.3.2). We give the proof for V_{eff}, the adaption to V_{eff}^l requires only minor changes. We will use the symbols c and C for constants that vary from line to line; however, their dependence on H_1 and H_2 will always be as stated in the Theorem.

Without loss of generality, we can assume that the origin is contained in the support of u. We will estimate the n^{th} singular value by Dirichlet decoupling at an n-dependent radius R. To this end, let R be sufficiently large so that $\operatorname{supp} u$ is contained strictly inside the ball of radius R centred at the origin, which we will denote by B_R.

Let H_j^R ($j = 1$ or 2) be the Dirichlet restriction of H_j to the ball B_R, and let

$$A_R := \mathrm{e}^{-H_2^R} - \mathrm{e}^{-H_1^R} \quad \text{and} \quad D_R := V_{\text{eff}} - A_R. \tag{A.17}$$

As any Kato-class potential is relatively form bounded with respect to the Laplacian with relative bound zero, we may apply Lemma A.3.1 to deduce that $\mu_n(\mathrm{e}^{-H_j^n}) \leq C \exp(-cn^{2/d} R^{-2})$ for both $j = 1$ and $j = 2$. Since A_R is the difference of two *non-negative* operators by the min-max theorem its singular values obey the same type of bound:

$$\mu_n(A_R) \leq C \exp(-cn^{2/d} R^{-2}) \tag{A.18}$$

If D_n is bounded, then $\mu_n(V_{\text{eff}}) \leq \mu_n(A_R) + \|D_n\|$. We now proceed to estimate the norm of D_n by using the Feynman-Kac-Itô formula for magnetic Schrödinger semigroups with Dirichlet boundary conditions, see [65, 436].

Let $\mathbf{E}_x$ and $\mathbf{P}_x$ denote the expectation and probability for a Brownian motion, b_t starting at x. Let $\tau_R = \inf\{t > 0 | b_t \notin B_R\}$ denote the exit time from the ball B_R and set $\tau_n := \tau_{R_n}$. Then

$$(D_n f)(x) = \mathbf{E}_x \left[\mathrm{e}^{-\mathrm{i} S_A(b)} \left(\mathrm{e}^{-\int_0^1 (V+u)(b_s) ds} - \mathrm{e}^{-\int_0^1 V(b_s) ds} \right) \chi_{\{\tau_n \leq 1\}}(b) f(b_1) \right]$$

where S_A^t is real valued stochastic process corresponding to the purely magnetic part of the Schrödinger operator. Actually, for this representation one first chooses a suitable gauge, for instance $\operatorname{div} A = 0$, and then uses gauge invariance for the general case, see [322].

By taking the modulus and using the triangle inequality, one sees that the magnetic vector potential can be eliminated:

$$|D_n f|(x) \leq \mathbf{E}_x \left[\mathrm{e}^{-\int_0^1 V(b_s) ds} \left| \mathrm{e}^{-\int_0^1 u(b_s) ds} - 1 \right| \chi_{\{\tau_n \leq 1\}}(b) |f(b_1)| \right]$$

Moreover, only Brownian paths which both visit $\operatorname{supp} u$ and leave B_{R_n} within one unit of time contribute to the expectation. Thus if τ_u is the hitting time for $\operatorname{supp} u$ and $\mathcal{B} = \{\tau_n \leq 1, \tau_u \leq 1\}$, then

$$|D_n f|(x) \leq \mathbf{E}_x \left[\mathrm{e}^{-\int_0^1 V(b_s) ds} \left| \mathrm{e}^{-\int_0^1 u(b_s) ds} - 1 \right| \chi_{\mathcal{B}}(b) |f(b_1)| \right]$$

so, applying Hölder's inequality,

$$\begin{aligned} |D_n f|(x) \leq & \left(\mathbf{E}_x \left[\mathrm{e}^{-8 \int_0^1 V(b_s) ds} \right] \right)^{1/8} \left(\mathbf{E}_x \left[\left| \mathrm{e}^{-\int_0^1 u(b_s) ds} - 1 \right|^8 \right] \right)^{1/8} \\ & \cdot \left(\mathbf{E}_x \left[\chi_{\mathcal{B}}(b) \right] \right)^{1/4} \left(\mathbf{E}_x \left[|f(b_1)|^2 \right] \right)^{1/2} \end{aligned}$$

Since V_- and u_- are in the Kato class, Kashminskii's lemma implies that the first two terms are bounded uniformly in x, see for instance [12, 438].

Levy's inequality combined with elementary estimates imply $\mathbf{P}_{x=0}\{\tau_R \leq 1\} \leq 2\mathbf{P}_{x=0}\{|b_1| \geq R\} \leq C\mathrm{e}^{-R^2/4}$. As any path in $\mathcal{B}$ must cover the distance

r between supp u and the complement of the ball B_R, we can deduce that $\mathbf{P}_x(\mathcal{B}) \leq C\mathrm{e}^{-r^2/4} \leq C\mathrm{e}^{-R^2/8}$ where we chose without loss of generality $r \geq R/\sqrt{2}$. Thus

$$|D_n f|(x) \leq C\mathrm{e}^{-R^2/32}\big\{\mathbf{E}_x|f(b_1)|^2\big\}^{1/2} = C\mathrm{e}^{-R^2/32}\big\{(\mathrm{e}^{\Delta}|f|^2)(x)\big\}^{1/2}$$

in particular, using the fact that e^{Δ} is an L^1 contraction,

$$\|D_n f\|_2 \leq C\mathrm{e}^{-R^2/32}\big\|(\mathrm{e}^{\Delta}|f|^2)\big\|_1^{1/2} \leq C\mathrm{e}^{-R^2/32}\|f^2\|_1^{1/2} = C\mathrm{e}^{-R^2/32}\|f\|_2$$

To balance the two bounds obtained for $\mu_n(A_R)$ and $\|D_n\|$ one chooses $R_n := n^{1/2d}$, which leads to (A.16). □

A.4 Bounds on the SSF for Schrödinger Operators

Let H_1, H_2 be as in the last Section. Theorem A.3.2 implies in particular that V_{eff} and V_{eff}^l are trace class. Thus the SSF for the operator pair H_1, H_2 is well defined by formula (A.11) with the choice $g(x) = \mathrm{e}^{-x}$.

The explicit estimates obtained in Theorem A.3.2 for the singular values of Schrödinger semigroups differences together with the abstract results from Sect. A.1 allow us to infer the desired bounds on the SSF for a pair of Schrödinger operators. The results and the presentation in this section are taken from the paper [218] by Hundertmark, Killip, Nakamura, Stollmann and the author.

Theorem A.4.1. *Let ξ be the spectral shift function for the pair H_1, H_2 or H_1^l, H_2^l. There exists constants K_1, K_2 depending only on d,* diam supp u_+ *and the Kato class norms of V_-, u_-, such that for any bounded compactly supported function f,*

$$\int f(\lambda)\,\xi(\lambda)\,d\lambda \leq K_1\mathrm{e}^b + K_2\,\{\log(1+\|f\|_\infty)\}^d\|f\|_1 \tag{A.19}$$

with $b = \sup\operatorname{supp} f$.

Remark A.4.2. (i) Theorem A.4.1 implies that the spectral shift function can have at most logarithmic local singularities. One might think that, at least for smooth compactly supported perturbations, the SSF should always be locally bounded. However, this is not the case. In the paper [405] already mentioned in Remark A.3.4, Raikov and Warzel consider the free Schrödinger operator with a constant magnetic field in dimension two. For a perturbation of this operator by a compactly supported potential they showed that the SSF diverges at each Landau level λ_q like

$$|\xi(\lambda_q+\lambda)| \sim \Big(\frac{|\ln(\lambda)|}{\ln|\ln\lambda|}\Big)^{d/2} \qquad \text{as } \lambda\downarrow 0 \tag{A.20}$$

See [359] for the generalisation to even dimensions.

(ii) An example without magnetic fields, where the SSF shows unexpected divergencies, was given by Kirsch in [246, 248]. Denote by Δ^l the Laplace operator on the cube Λ_l with Dirichlet b.c. For $\lambda > 0$, $u\colon \mathbb{R}^d \to \mathbb{R}$ a non-negative, bounded function with compact support, which is not identically equal to zero, and a function $a\colon [0,\infty[\to]0,\infty[$, set $\xi_l(\cdot) := \xi(\cdot, -\Delta^l, (-\Delta + a(l)u)^l)$. Then $\limsup_{l\to\infty} \xi_l(\lambda) = \infty$, for any λ, a and u as above. This result relies on the high degeneracy of eigenvalues of the pure Dirichlet Laplacian on a cube. In this respect it is related to the example in Remark (i) with the Landau Hamiltonian which has infinitely degenerate eigenvalues. Kirsch shows that there is, however, a set of full measure $\mathcal{E} \subset \mathbb{R}$ with dense complement such that

$$\lim_{\mathbb{N}\ni l\to\infty} \xi_l(\lambda) = 0, \text{ for all } \lambda \in \mathcal{E}, \text{ if } a(l) \le l^{-k}, k > 3$$

(iii) In contrast to the above unboundedness results, Sobolev, [449] showed that for the pair $H_1 = -\Delta$ and $H_2 = -\Delta + u$ with $|u(x)| \le \mathit{const.}\,(1 + |x|)^{-\alpha}$ and $\alpha > d$, the spectral shift function ξ is, indeed, locally bounded. However, this type of result seems to require very strong hypotheses on H_1, for example, a trace-class limiting absorption principle and in particular, that H_1 has absolutely continuous spectrum on the positive real axis.

(iv) For certain alloy type Schrödinger operators Combes, Hislop and Klopp obtain in Theorem 2.1 of [92] a local boundedness result for an associated *averaged* SSF.

Proof (of Theorem A.4.1). Let the two Schrödinger operators $H_2 = H_1 + u$ be as in the statement of the Theorem.

For $t > 0$ define $F_t : [0,\infty[\to [0,\infty[$ by

$$F_t(x) = \int_0^x (\exp(ty^{1/d}) - 1)\, dy \tag{A.21}$$

As the integrand is increasing, F_t is a convex function. We show first that there exists a constant K_1, depending on t, such that for small enough $t > 0$,

$$\int_{-\infty}^T F_t(|\xi(\lambda)|)\, d\lambda \le K_1 \mathrm{e}^T < \infty \tag{A.22}$$

for all $T < \infty$. To see this, we use the invariance principle and a change of variables, to obtain

$$\begin{aligned}\int_{-\infty}^T F(|\xi(\lambda, H_2, H_1)|)\, d\lambda &= \int_{-\infty}^T F(|\xi(\mathrm{e}^{-\lambda}, \mathrm{e}^{-H_2}, \mathrm{e}^{-H_1})|)\, d\lambda \\ &\le \mathrm{e}^T \int_{\mathrm{e}^{-T}}^\infty F(|\xi(s, \mathrm{e}^{-H_2}, \mathrm{e}^{-H_1})|)\, ds\end{aligned}$$

By Theorem A.1.2 the integral on the right hand side is bounded by

$$\int_{-\infty}^{\infty} F(|\xi(s, \mathrm{e}^{-H_2}, \mathrm{e}^{-H_1})|)\, ds \le \sum_{n=1}^{\infty} \mu_n(V_{\mathrm{eff}})(F(n) - F(n-1))$$
$$\le \sum_{n=1}^{\infty} \mu_n(V_{\mathrm{eff}}) \int_{n-1}^{n} (\mathrm{e}^{ts^{1/d}} - 1) ds \le C \sum_{n=1}^{\infty} \mathrm{e}^{(t-c)n^{1/d}}$$

which is finite, if we chose t smaller than the constant c from Theorem A.3.2. Thus we have proven (A.22).

Now we deduce the bound (A.19) from (A.22) with the help of Young's inequality for an appropriate pair of functions. Note that F_t is non-negative, convex with $F_t'(0) = 0$ and hence its Legendre transform G is well defined and satisfies

$$G(y) := \sup_{x \ge 0}\{xy - F(x)\} \le y\Big(\frac{\log(1+y)}{t}\Big)^d \text{ for all } y \ge 0$$

Thus, by the very definition of G, Young's inequality holds: $yx \le F(x) + G(y)$. So, with $b = \sup \operatorname{supp} f$,

$$\int f(\lambda)\xi(\lambda)\, d\lambda \le \int_{-\infty}^{b} F(|\xi(\lambda)|)\, d\lambda + \int G(|f(\lambda)|)\, d\lambda \tag{A.23}$$

Using the estimate (A.22), the first integral is bounded by $K_1 \mathrm{e}^b$. For the second integral in (A.23), we estimate

$$\int G(|f(\lambda)|)\, d\lambda \le \int |f(\lambda)| \Big(\frac{\log(1+|f(\lambda)|)}{t}\Big)^d d\lambda \le t^{-d} |\log(1 + \|f\|_\infty)|^d\, \|f\|_1$$

This finishes the proof of Theorem A.4.1. □

To apply Theorem A.4.1 in the situation of Sect. 4.2, we take f to be the the derivative of a smooth, monotone switch function $\rho_{E,\varepsilon} \colon \mathbb{R} \to [-1, 0]$. By a switch function we mean that for a positive $\varepsilon \le 1/2$ it has the following properties: $\rho_{E,\varepsilon} \equiv -1$ on $]-\infty, E-\varepsilon]$, $\rho_{E,\varepsilon} \equiv 0$ on $[E+\varepsilon, \infty[$ and $\|\rho'_{E,\varepsilon}\|_\infty \le 1/\varepsilon$, similarly as in Sect. 4.1. Theorem A.4.1 and the Krein trace formula (A.1) imply

Corollary A.4.3. *Let H_1, H_2 and $\rho_{E,\varepsilon}$ be as above. There is a constant C_E depending only on E, d,* diam supp u_+ *and the Kato class norms of V_-, u_-, such that*

$$\operatorname{Tr}\left[\rho_{E,\varepsilon}(H_2) - \rho_{E,\varepsilon}(H_1)\right] \le C_E\, |\log \varepsilon|^d \tag{A.24}$$

The function $E \mapsto C_E$ is monotone and continuous.

The estimate (A.24) improves upon a bound derived by Combes, Hislop and Nakamura in [97]. They prove that for any exponent $\alpha < 1$, there is a constant $\tilde{C}_E(\alpha)$ depending only on d, C_0, $\operatorname{diam} \operatorname{supp} u$, $E + \varepsilon$ and α such that

$$\operatorname{Tr}\left[\rho_{E,\varepsilon}(H_2) - \rho_{E,\varepsilon}(H_1)\right] \le \tilde{C}_E(\alpha)\ \varepsilon^{-\alpha} \tag{A.25}$$

Remark A.4.4. In the context of random Schrödinger operators H_1 and H_2 appear as particular members of a random family $\{H_\omega\}_\omega$. If two configurations $\omega, \omega' \in \Omega$ differ only in one coordinate $\omega_j \neq \omega'_j$ and coincide in all the others, i.e. $\omega_k = \omega'_k$ for all $k \in \mathbb{Z}^d \setminus \{j\}$, then the pair $H_1 = H_\omega$, $H_2 = H_{\omega'}$ differs only by a single site potential. If this is compactly supported, the pair H_1, H_2 fits in the framework considered in this and the preceding sections.

Specialising further, one is often interested in the case that on the lattice site $j \in \mathbb{Z}^d$ one of the operators, say H_1, has a coupling constant taking the lowest possible value, i.e.

$$\omega_j = \omega_- = \inf \operatorname{supp} \mu$$

where μ denotes as before the distribution of ω_j, and the other operator H_2 has at this site a coupling constant with the largest possible value, i.e.

$$\omega'_j = \omega_+ = \sup \operatorname{supp} \mu$$

Let $\Lambda_l \subset \mathbb{R}^d$ be a cube such that $j \in \Lambda_l^+$. Then we can write the two operators H_1 and H_2 as

$$\begin{aligned} H_1 &= H_\omega^l(\omega_j = \min) := H_\omega^l + (\omega_- - \omega_j)\, u(\cdot - j) \\ H_2 &= H_\omega^l(\omega_j = \max) := H_\omega^l + (\omega_+ - \omega_j)\, u(\cdot - j) \end{aligned} \tag{A.26}$$

and consequently the difference $H_2 - H_1 = (\omega_+ - \omega_-)\, u(\cdot - j)$ is a compactly supported potential. Note that in the formulae (A.26) it is possible to express the two operators H_1 and H_2 using only one of the two configurations ω and ω'.

The upshot of this considerations is that the trace

$$\operatorname{Tr}\big[\rho[H_\omega^l(\omega, j = \max) - E] - \rho[H_\omega^l(\omega, j = \min) - E]\big] \tag{A.27}$$

can be estimated by Corollary A.4.3. It is precisely for such a pair of operators that this corollary is used in the proof of Theorem 4.2.4.

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