Singular spectrum for multidimensional Schrödinger operators with potential barriers

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Abstract

We prove comparison criteria for the absence of absolutely continuous spectrum which have the following form: If the set $\{x; V_0(x) \neq V(x)\}$ can be divided into bounded parts with suitable geometric conditions, then

$$\sigma_{ac}(-\tfrac{1}{2}\Delta + V) \subset [\inf \sigma_{ess}(-\tfrac{1}{2}\Delta + V_0), \infty),$$

or, under somewhat stronger conditions,

$$\sigma_{ac}(-\tfrac{1}{2}\Delta + V) \subset \sigma_{ess}(-\tfrac{1}{2}\Delta + V_0).$$

The first result proves absence of absolute continuity for $-\frac{1}{2}\Delta + V$ below $\inf \sigma_{ess}(-\frac{1}{2}\Delta + V_0)$ and is a continuum analog of a result for discrete Schrödinger operators by Simon and Spencer. The second inclusion implies in addition that $-\frac{1}{2}\Delta + V$ has no absolutely continuous spectrum in arbitrary gaps of $\sigma_{ess}(-\frac{1}{2}\Delta + V_0)$. One should think of applying this to a given V by constructing V_0 suitably in order to produce prescribed gaps in $\sigma_{ess}(-\frac{1}{2}\Delta + V_0)$. Different potentials V_0 may be associated with one and the same V in order to exclude absolute continuity in varying intervals.

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1 Introduction

The study of random or quasiperiodic media in physics is the main motivation for the rising interest in the spectral theory of Schrödinger operators with irregularly varying potentials. The most striking phenomenon is the occurence of dense pure point spectrum (*localization*) in many of these models. Absence of absolutely continuous spectrum (non–existence of *extended states*) is a weaker property which, nevertheless, may be regarded as a preliminary step in this direction.

While there is by now a good understanding of the underlying mathematics in dimension $d = 1$, much less is known for $d > 1$, where most rigorous results are established for discrete Schrödinger operators. Fairly complete up to date information and references can be found in the monograph [**?**].

In the present article we wish to contribute to the study of the multidimensional continuous case, proving "comparison criteria" for the absence of absolutely continuous spectra. More precisely, we will show that if the "exceptional set" $\{x \in^d; V_0(x) \neq V(x)\}$ allows a suitable decomposition, respectively strict decomposition (the precise definition of these notions is given in Section 4), then

$$\sigma_{ac}(-\tfrac{1}{2}\Delta + V) \subset [\inf \sigma_{ess}(-\tfrac{1}{2}\Delta + V_0), \infty)$$

(Theorem **??**), respectively

$$\sigma_{ac}(-\tfrac{1}{2}\Delta + V) \subset \sigma_{ess}(-\tfrac{1}{2}\Delta + V_0)$$

(Theorem **??**).

The reader will immediately notice that these results can be viewed from two different points: On the one hand they provide a stability result saying that below or in the gaps of the essential spectrum of the unperturbed operator $-\frac{1}{2}\Delta + V_0$ the perturbed one, $-\frac{1}{2}\Delta + V$, has no absolutely continuous spectrum. On the other hand, one can start with $-\frac{1}{2}\Delta + V$ and look for a "close enough" V_0 with gaps in $\sigma_{ess}(-\frac{1}{2}\Delta + V_0)$. For example, one might define $V_0(x) = \max\{V(x), E_0\}$ in order to prove $\sigma_{ac}(-\frac{1}{2}\Delta + V) \subset [E_0, \infty)$, provided of course, the set $\{x \in^d; V(x) < E_0\}$ admits an application of Theorem **??**.

To illustrate Theorem **??** with a typical example and at the same time describe the contents of the following sections let us now sketch the following analog of a discrete result of Simon and Spencer [**?**].

Corollary 1.1 (to Theorem ??) *Assume that* $\{V_0 \neq V\} \subset \bigcup_n B_n$*, where the* B_n *are balls of radius* R_n *such that* $(B_n, \bigcup_{m\neq n} B_m) = \delta_n \geq \delta_0 > 0$*. If*

$$\sum_n (R_n + \delta_n)^{d-1} e^{-\varepsilon\delta_n} < \infty \quad \textit{for all} \quad \varepsilon > 0,$$

then $\sigma_{ac}(-\frac{1}{2}\Delta + V) \subset [\inf \sigma_{ess}(-\frac{1}{2}\Delta + V_0), \infty)$.

Our global strategy to prove such a result is taken from [?]: We want to show that $P_{J,ac} := E_J(H)P_{ac}(H) = 0$ for every compact $J \subset (-\infty, \inf \sigma_{ess}(-\frac{1}{2}\Delta + V_0)) \cap \rho(-\frac{1}{2}\Delta + V_0)$ and this will be achieved, if we can construct wave operators

$$W_\pm(H^D, H, P_{J,ac}) = s - \lim_{t\to\pm\infty} e^{itH^D} e^{-itH} P_{J,ac}$$

for an operator H^D which has no absolutely continuous spectrum below $\inf \sigma_{ess}(-\frac{1}{2}\Delta + V_0)$. The idea is to add Dirichlet boundary conditions in order to decouple the set $\{V_0 \neq V\}$ as illustrated by Figure 1.

Denote by S_n a sphere of radius $R_n + \delta_n/2$ around the center of the ball B_n and write H_n for the operator which is obtained from H by adding Dirichlet boundary conditions at the first n spheres $S_1, \ldots, S_n$. $H^D = \lim H_n$ is the operator which has Dirichlet boundary conditions at $S = \bigcup_n S_n$, and thus can be written as a direct sum (U_i is the "interior" of S_i, U_0 the rest where $V_0 = V$)

$$\bigoplus_{i\geq 1} (-\tfrac{1}{2}\Delta + V)_{U_i} \oplus (-\tfrac{1}{2}\Delta + V_0)_{U_0}.$$

Since the first summand has pure point spectrum (the U_i's are bounded!), the absolutely continuous spectrum of H^D equals $\sigma_{ac}((-\frac{1}{2}\Delta + V_0)_{U_0})$, which clearly is contained in $[\inf \sigma_{ess}(-\frac{1}{2}\Delta + V_0), \infty)$. By the invariance principle, existence of wave operators can be reduced to proving that $(e^{-H} - e^{-H^D})P_{J,ac}$ is a trace class operator. To this end, we estimate the trace norms $\|(e^{-tH_{n-1}} - e^{-tH_n})P_{J,ac}\|_{tr}$, and the summability condition in Corollary **??** above will ensure that these norms are summable. In fact, in the condition of Corollary **??** two characteristic features of the geometry of the sequence (S_n) occur: One is the size of S_n, more precisely its surface area. In Definition **??** we will provide an analog suitable for more general sets S under the name of “generalized area”, denoted by $\sigma(S)$. Section 2 will be devoted to showing that

$$\|(e^{-H} - e^{-H_{d\setminus S}})\chi\|_{tr} \leq C e^{-\eta\delta^2}\sigma(S) \tag{1}$$

where $H_{d\setminus S}$ denotes $-\frac{1}{2}\Delta + V$ with an additional Dirichlet boundary condition at S and χ is a characteristic function with $\mathrm{dist}(S, \mathrm{supp}\,\chi) \geq \delta$.

Together with the estimate

$$\|\chi_F E_J(H)\| \leq C(J) e^{-\eta(J)\delta} \tag{2}$$

found in Section 3 for sets F which satisfy $\mathrm{dist}(F, \{V_0 \neq V\}) \geq \delta$ we can then deduce that

$$\|(e^{-H_{n-1}} - e^{-H_n})P_{J,ac}\|_{tr} \leq \|(e^{-H_{n-1}} - e^{-H_n})(1-\chi_{F_n})\|_{tr} + \|e^{-H_{n-1}} - e^{-H_n})\|_{tr}\|\chi_{F_n}P_{J,ac}\|$$

has a summable majorant, setting $F_n := \{x; \mathrm{dist}(x, S_n) \leq \delta_n/2\}$.

The second parameter, entering critically in (**??**), is the distance $\delta_n/2$ from the exceptional set to the set S_n, where we add Dirichlet boundary conditions.

In view of applications, where one wants to exclude absolute continuity of $-\frac{1}{2}\Delta + V$ for a given V, it is desirable to have high flexibility in choosing the comparison potential V_0. Therefore we have made an attempt to prove our results under very general assumptions on the geometry of the exceptional set $\{V_0 \neq V\}$ and the decoupling surfaces S_n. In Theorems **??** and **??** this is reflected by the fact that assumptions can be formulated completely in terms of $\sigma(S_n)$ and $\mathrm{dist}(S_n, \{V_0 \neq V\})$, which allows quite general patterns for the decomposition of ^{d} into $\{V_0 = V\}$ and $\{V_0 \neq V\}$. We also think that Theorem **??**, which allows the use of V_0 with gaps in $\sigma_{ess}(-\frac{1}{2}\Delta + V_0)$, is of considerable interest beyond the range of applicability of Theorem **??**.

Results of the above type as well as the use of trace class methods in their proofs go back to Simon and Spencer [**?**], who treated the one-dimensional case as well as the discrete higher dimensional case. Further results for one dimension are given in [**?**] (see also [**?**] and [**?**]). The first to treat the continuous higher dimensional case were Combes and Hislop [**?**], who despite following the same general ideas (those of Simon/Spencer) employ techniques which are very different from ours.

Let us finally say a few more words about those techniques:

In contrast to the discrete case or the one-dimensional situation, adding a Dirichlet boundary condition is no longer a finite dimensional perturbation. Hence the trace class estimates, worked out in Section 2, become more involved. We use here a factorization technique (already employed in [?]) which is based on pointwise estimates of the semigroup calculated via the Feynman-Kac formula. Together with quite elementary properties of hitting probabilities this implies (??). We think that the operator theoretic part of this argument, Lemma **??**, is worth noting.

The estimate (??) is deduced by an argument which is very close to the one-dimensional situation: (??) follows from a Combes-Thomas type decay property for the resolvent, given in Lemma **??**. Since this technique has many applications, the estimates proved in Lemma **??** are of independent interest. Clearly, the geometry in ^{d} is more complex than in and this is reflected in our use of regularized distance functions.

Our methods compare to the methods of [?] as follows: In [?, Section 3] no use is made of semigroups; to some extend they are replaced by powers of the resolvent. This allows the use of more classical trace class results than ours, but will need more regularity of the potential in applications. Here, we will only need that the potentials V and V_0 are in $L_{1,loc}$ with negative parts belonging to the Kato class. Combes and Hislop in [?] are interested in proving $\sigma_{ac}(H) \cap (-\infty, E) = \emptyset$ in situations where the wells of the potentials, i.e., the regions with $V(x) < E$, are sufficiently scarce. In this case estimates of the type (??) are provided in the form of tunneling estimates by results in [?], where the Agmon metric is used to measure the size of the barriers $\{x : V(x) > E\}$. The Agmon metric is a very precise tool in this case and allows summability conditions in [?] which are more closely adapted to the geometry of V than the summability conditions in our results. For example, the effect of wide barriers and high barriers can be studied simultaneously. But the Agmon metric can not be applied to energies in a spectral gap of the comparison operator $-\frac{1}{2}\Delta + V_0$, as needed to prove $\sigma_{ac}(-\frac{1}{2}\Delta + V) \subset \sigma_{ess}(-\frac{1}{2}\Delta + V_0)$. This is our reason for using the Combes–Thomas method in Section 3, thereby replacing the Agmon distance by Euclidean distance.

The trace class estimates of Section 2 below can be extended to prove absence of absolute continuity for multidimensional Schrödinger operators with a series of high potential barriers. This is done in [?], where a proof is given which does not use tunneling estimates.

2 Trace class estimates

We start with a general trace class criterion for operators in L_2-spaces, which factorize over L_1 in an appropriate way. , $_1$ and $_2$ with norms $\|\cdot\|$, $\|\cdot\|_{tr}$ and $\|\cdot\|_{HS}$ denote the bounded operators, trace class operators and Hilbert-Schmidt operators, respectively.

Lemma 2.1 *Let $T \in (L_1, L_2)$, $S \in (L_2, L_1)$ and $\phi \in L_1$ such that*

$$|Sf(x)| \leq \phi(x)$$

for a.e. x and all $f \in L_2$ with $\|f\|_2 \leq 1$. Then $T\,S \in_1$ and

$$\|T\,S\|_{tr} \leq \|\phi\|_1 \|T\|.$$

Proof: Setting $\phi^{-1}(x) = 1/\phi(x)$ if $\phi(x) \neq 0$ and $\phi^{-1}(x) = 0$ otherwise, we have

$$T\,S = T\phi^{1/2}\phi^{1/2}\phi^{-1}S. \tag{3}$$

By assumption $\phi^{-1}S \in (L_2, L_\infty)$ and $\|\phi^{-1}S : L_2 \to L_\infty\| \leq 1$. From $\phi^{1/2} \in L_2$ and the Dunford-Pettis theorem (e.g. [**?**, Th.A.1.1]) we get $\phi^{1/2}\phi^{-1}S \in_2$ and $\|\phi^{1/2}\phi^{-1}S\|_{HS} \leq \|\phi\|_1^{1/2}$. Moreover, $T^* \in (L_2, L_\infty)$ and therefore $\|T\phi^{1/2}\|_{HS} = \|\phi^{1/2}T^*\|_{HS} \leq \|\phi\|_1^{1/2}\|T^*\| = \|\phi\|_1^{1/2}\|T\|$. The result now follows from (**??**). $\Box$

For the rest of this paper let $V = V_+ - V_-$, $V_\pm \geq 0$ with $V_+ \in L_{1,loc}(^d)$ and $V_- \in K_d$, the Kato class over ^{d}. For an open subset Ω of ^{d} let $-\frac{1}{2}\Delta_\Omega^D$ be the Dirichlet Laplacian on Ω, i.e. the Friedrichs extension of $-\frac{1}{2}\Delta|C_0^\infty(\Omega)$. V_- is infinitesimally form small with respect to $-\frac{1}{2}\Delta_\Omega^D$ ([**?**, p.459] or [**?**, Prop.2.3]), therefore we can define the selfadjoint form sum $H_\Omega = -\frac{1}{2}\Delta_\Omega^D \dot{+} V$ in $L_2(\Omega)$.

In the following $(\Omega^x, ^x, (X_t)_{t\geq 0})$ denotes Brownian motion starting at $x \in^d$ with expectation ^{x}. For $\omega \in \Omega^x$ the hitting time of S is $\tau_S(\omega) = \inf\{t > 0 : X_t(\omega) \in S\}$.

Proposition 2.2 *There exist constants $C = C(V_-)$, $A = A(V_-)$ and $\eta > 0$ such that for every compact $S \subset^d$ with Lebesgue measure zero, every open $\Omega \subset^d$ and $M_\delta := \{x : dist(x, S) \geq \delta\}$ we have*

$$\begin{aligned} &\|(e^{-2tH_\Omega} - e^{-2tH_{\Omega\setminus S}})\chi_{M_\delta}\|_{tr} \leq \\ &\quad Ce^{At}t^{-d/2}\Big\{\int_{M_{\delta/2}} (^x[\tau_S \leq t])^{1/2}\,dx + e^{-\eta\delta^2/t}\int_{d} (^x[\tau_S \leq t])^{1/2}\,dx \\ &\quad + \int_{d} (^x[\tau_S \leq t, X_t \in M_\delta])^{1/2}\,dx\Big\}. \end{aligned}$$

Remark: For the special case $\delta = 0$ this result was given in [?].

Proof: Writing $G := \Omega \setminus S$ and $D(t) := e^{-tH_\Omega} - e^{-tH_G}$ we have

$$\begin{aligned} \chi_{M_\delta} D(2t) &= \chi_{M_\delta} e^{-tH_\Omega} D(t) + \chi_{M_\delta} D(t) e^{-tH_G} \\ &= e^{-tH_\Omega} \chi_{M_\delta} D(t) + \left(\chi_{M_\delta} e^{-tH_\Omega} - e^{-tH_\Omega} \chi_{M_\delta} \right) D(t) + \chi_{M_\delta} D(t) e^{-tH_G}. \qquad (4) \end{aligned}$$

In order to estimate $\|D(2t)\chi_{M_\delta}\|_{tr} = \|\chi_{M_\delta} D(2t)\|_{tr}$ we will first show that

$$\|e^{-tH_\Omega} \chi_{M_\delta} D(t)\|_{tr} \leq C e^{At} t^{-d/2} \int_{M_\delta} ({}^x[\tau_S \leq t])^{1/2}\, dx. \qquad (5)$$

By the Feynman-Kac formula ([?], resp. [?], where it can be found in the generality needed here)

$$(e^{-tH_\Omega} f)(x) =^x \left[\exp\left(-\int_0^t V \circ X_s ds \right) \mathbf{1}_{\{\tau_{d \setminus \Omega} > t\}} f \circ X_t \right]$$

and

$$(e^{-tH_G} f)(x) =^x \left[\exp\left(-\int_0^t V \circ X_s ds \right) \mathbf{1}_{\{\tau_{d \setminus \Omega} > t\}} \mathbf{1}_{\{\tau_S > t\}} f \circ X_t \right].$$

Therefore, Cauchy-Schwarz for the Wiener measure gives

$$\begin{aligned} |(D(t)f)(x)| &= \left| {}^x \left[\exp\left(-\int_0^t V \circ X_s ds \right) \mathbf{1}_{\{\tau_{d \setminus \Omega} > t\}} \mathbf{1}_{\{\tau_S \leq t\}} f \circ X_t \right] \right| \\ &\leq \left({}^x \left[\exp\left(-2 \int_0^t V \circ X_s ds \right) |f|^2 \circ X_t \right] \right)^{1/2} ({}^x[\tau_S \leq t])^{1/2}. \end{aligned}$$

By $V \geq -V_-$ and Feynman-Kac we get

$$\begin{aligned} {}^x \left[\exp\left(-2 \int_0^t V \circ X_s ds \right) |f|^2 \circ X_t \right] &\leq \left(e^{t(\frac{1}{2}\Delta + 2V_-)} |f|^2 \right)(x) \\ &\leq \|e^{t(\frac{1}{2}\Delta + 2V_-)} : L_1 \to L_\infty\| \, \||f|^2\|_1, \end{aligned}$$

but $\|e^{t(\frac{1}{2}\Delta + 2V_-)} : L_1 \to L_\infty\| \leq C e^{At} t^{-d/2}$ ([?, p.463]), so we finally arrive at

$$|(D(t)f)(x)| \leq C e^{At} t^{-d/4} ({}^x[\tau_S \leq t])^{1/2} \qquad (6)$$

for f with $\|f\|_2 \leq 1$. The estimate (**??**) is now a consequence of Lemma **??** and $\|e^{-tH_\Omega} : L_1 \to L_2\| \leq C e^{At} t^{-d/4}$.

Our next estimate is

$$\begin{aligned} &\left\| (\chi_{M_\delta} e^{-tH_\Omega} - e^{-tH_\Omega} \chi_{M_\delta}) D(t) \right\|_{tr} \leq \\ &\quad C e^{At} t^{-d/2} \left\{ e^{-\eta \delta^2 / t} \int ({}^x[\tau_S \leq t])^{1/2}\, dx + \int_{M_{\delta/2}} ({}^x[\tau_S \leq t])^{1/2}\, dx \right\}. \qquad (7) \end{aligned}$$

To prove it, we write

$$\begin{aligned}\chi_{M_\delta} e^{-tH_\Omega} - e^{-tH_\Omega}\chi_{M_\delta} &= \chi_{M_\delta} e^{-tH_\Omega}(1-\chi_{M_{\delta/2}}) + \left(\chi_{M_\delta} e^{-tH_\Omega}\chi_{M_{\delta/2}} - e^{-tH_\Omega}\chi_{M_\delta}\right) \\ &=: T_1 + T_2.\end{aligned}$$

As in the proof of (**??**) we get

$$\|T_2 D(t)\|_{tr} \leq C e^{At} t^{-d/2} \int_{M_{\delta/2}} ({}^x[\tau_S \leq t])^{1/2}\, dx.$$

Estimate (**??**) and Lemma **??** yield

$$\|T_1 D(t)\|_{tr} \leq C e^{At} t^{-d/4} \int ({}^x[\tau_S \leq t])^{1/2}\, dx \|\chi_{M_\delta} e^{-tH_\Omega}(1-\chi_{M_{\delta/2}}) : L_1 \to L_2\|.$$

Since $\mathrm{dist}(\mathrm{supp}\,\chi_{M_\delta}, \mathrm{supp}\,(1-\chi_{M_{\delta/2}})) = \delta/2$ we know ([?, Prop. B.4.2, p. 469])

$$\|\chi_{M_\delta} e^{-tH_\Omega}(1-\chi_{M_{\delta/2}}) : L_1 \to L_2\| \leq C t^{-d/4} e^{-\left(\frac{\delta}{2}\right)^2/8t}.$$

This completes the proof of (**??**).

We finally prove

$$\begin{aligned}\|\chi_{M_\delta} D(t) e^{-tH_G}\|_{tr} &= \|e^{-tH_G} D(t)\chi_{M_\delta}\|_{tr} \\ &\leq C e^{At} t^{-d/2} \int ({}^x[\tau_S \leq t, X_t \in M_\delta])^{1/2}\, dx. \end{aligned} \tag{8}$$

For f with $\|f\|_2 \leq 1$ we get

$$\begin{aligned}|(D(t)\chi_{M_\delta} f)(x)| &= \left|{}^x\left[\exp\left(-\int_0^t V\circ X_s ds\right) \mathbf{1}_{\{\tau_S \leq t\}} (\chi_{M_\delta} f)\circ X_t\right]\right| \\ &\leq ({}^x[\tau_S \leq t, X_t \in M_\delta])^{1/2} \left({}^x\left[\exp\left(-2\int_0^t V\circ X_s ds\right) |f|^2 \circ X_t\right]\right)^{1/2} \\ &\leq C e^{At} t^{-d/4} ({}^x[\tau_S \leq t, X_t \in M_\delta])^{1/2}.\end{aligned}$$

Lemma **??** and $\|e^{-tH_G} : L_1 \to L_2\| \leq C e^{At} t^{-d/4}$ imply (**??**). The proof of Proposition **??** is completed by inserting (**??**), (**??**) and (**??**) into (**??**). □

Our applications of Proposition 2.2 will be based on the following elementary estimate for ${}^x[\tau_S \leq t]$:

Lemma 2.3 ${}^x[\tau_S \leq t] \leq 2d e^{-\frac{1}{2dt}\,\mathrm{dist}\,(x,S)^2}$.

Proof: Let Q be the hypercube inscribed into the ball of radius $\mathrm{dist}(x,S)$ with center x, i.e. $Q = (x_1 - a, x_1 + a) \times \ldots \times (x_d - a, x_d + a)$, $a = \mathrm{dist}\,(x,S)/\sqrt{d}$. Then

$${}^x[\tau_S \leq t] \leq^x [\tau_{\partial Q} \leq t] = 1 -^x [\tau_{\partial Q} > t]. \tag{9}$$

Denoting by ^{0} the Wiener measure of one-dimensional Brownian motion starting in 0, we have

$$
\begin{aligned}
{}^x[\tau_{\partial Q} > t] &= ({}^0[\tau_{\{-a,a\}} > t])^d \\
&= (1 - {}^0\,[\tau_{\{-a,a\}} \leq t])^d.
\end{aligned}
$$

A use of the reflexion principle yields

$$
\begin{aligned}
{}^0[\tau_{\{-a,a\}} \leq t] &\leq 2{}^0[\tau_{\{a\}} \leq t] = 4{}^0[X_t > a] \\
&= 4\left(\frac{1}{2\pi t}\right)^{1/2} \int_a^\infty e^{-x^2/2t} \leq 4\left(\frac{1}{2\pi t}\right)^{1/2} \int_0^\infty e^{-x^2/2t} e^{-a^2/2t}\, dx \\
&= 2e^{-a^2/2t}.
\end{aligned}
$$

Inserting into (**??**) gives

$$
{}^x[\tau_S \leq t] \leq 1 - (1 - 2e^{-a^2/2t})^d \leq 2de^{-a^2/2t}.
$$

$\square$

The following definition will provide us with high flexibility in the choice of S when applying Proposition **??**.

Definition 2.4 A compact subset S of ^{d} has *generalized area* $\sigma(S) > 0$ if there exists $\alpha \in [0, d]$ such that

$$
\text{meas}\,\{x : r \leq \text{ dist } (x, S) \leq r + 1\} \leq \sigma(S)(r^\alpha + 1)
$$

for every $r \geq 0$.

In applications one will of course aim to work with the minimal value for $\sigma(S)$. Important are the choices $\alpha = d$ and $\alpha = d - 1$, in which cases $\sigma(S)$ will correspond to a volume and a surface measure, respectively:

Examples: (i) For an arbitrary compact S we have

$$
\begin{aligned}
\text{meas}\,\{x : r \leq \text{ dist}\,(x, S) \leq r + 1\} &\leq c_d((\text{diam}\, S) + r + 1)^d \\
&\leq \tilde{c}_d((\text{diam}\, S)^d + 1)(r^d + 1),
\end{aligned}
$$

i.e. the "volume" $\sigma(S) = \tilde{c}_d((\text{diam}\, S)^d + 1)$.

(ii) For a sphere $S = \{|x| = R\}$ we get

$$\begin{aligned} \text{meas}\,\{x : r \leq \text{ dist}\,(x, S) \leq r + 1\} &\leq c_d(R + r + 1)^{d-1} \\ &\leq \hat{c}_d(R^{d-1} + 1)(r^{d-1} + 1), \end{aligned}$$

i.e. $\sigma(S) = \hat{c}_d(R^{d-1} + 1)$, a surface measure for large R. More general surfaces in ^{d} (the boundary of a cube, etc.) can be treated similarly.

Proposition 2.5 *Given $t > 0$ there exist constants $C = C(V_-, t)$ and $\eta = \eta(t) > 0$ such that*

$$\left\| \left(e^{-2tH_\Omega} - e^{-2tH_{\Omega\setminus S}} \right) \chi_{M_\delta} \right\|_{tr} \leq C\sigma(S)e^{-\eta\delta^2}$$

for every $\delta \geq 0$, every compact $S \subset^d$ with Lebesgue measure 0 and every open $\Omega \subset^d$.

Proof: Lemma **??** and the definition of $\sigma(S)$ yield

$$\begin{aligned} \int_{M_{\delta/2}} ({}^x[\tau_S \leq t])^{1/2}\,dx &= \sum_{n=0}^{\infty} \int_{n+\delta/2\leq\,\text{dist}(x,S)\leq n+\delta/2+1} ({}^x[\tau_S \leq t])^{1/2}\,dx \\ &\leq \sqrt{2d}\,\sigma(S) \sum_{n=0}^{\infty} ((n + \frac{\delta}{2})^\alpha + 1)e^{-\frac{1}{4dt}(n+\frac{\delta}{2})^2} \\ &\leq \sqrt{2d}\,\sigma(S)e^{-\frac{1}{4dt}(\delta/2)^2} \sum_{n=0}^{\infty} 2^\alpha(n^\alpha + (\delta/2)^\alpha + 1)e^{-\frac{n^2}{4dt}} \\ &\leq C_1(1 + \delta^\alpha)\sigma(S)e^{-\eta_1\delta^2} \leq C_2\sigma(S)e^{-\eta_2\delta^2}. \end{aligned}$$

In particular, we have for $\delta = 0$

$$\int_d ({}^x[\tau_S \leq t])^{1/2}\,dx \leq C_2\sigma(S).$$

Furthermore, we have

$$\begin{aligned} ({}^x[\tau_S \leq t, X_t \in M_\delta])^{1/2} &\leq ({}^x[\tau_S \leq t])^{1/4}({}^x[X_t \in M_\delta])^{1/4} \\ &\leq \min\left\{ ({}^x[\tau_S \leq t])^{1/4}, ({}^x[X_t \in M_\delta])^{1/4} \right\}, \end{aligned}$$

i.e.

$$\int_d ({}^x[\tau_S \leq t, X_t \in M_\delta])^{1/2}\,dx \leq \int_{M_{\delta/2}} ({}^x[\tau_S \leq t])^{1/4}\,dx + \int_{\text{dist}(x,S)\leq\frac{\delta}{2}} ({}^x[X_t \in M_\delta])^{1/4}\,dx.$$

The first term on the r.h.s. is estimated as above by $C_3\sigma(S)e^{-\eta_3\delta^2}$. For x with $r :=$ dist (x, M_δ) we have

$$\begin{aligned} {}^x[X_t \in M_\delta] &= (2\pi t)^{-d/2}\int_{M_\delta} e^{-|x-y|^2/2t}\,dy \le (2\pi t)^{-d/2}\int_{|y|\ge r} e^{-|y|^2/2t}\,dy \\ &= (2\pi t)^{-d/2}\int_0^\infty (u+r)^{d-1}e^{-(u+r)^2/2t}\,du \\ &\le C_4 e^{-\eta_4 r^2}(1+r^{d-1}) \le C_5 e^{-\eta_5 r^2}. \end{aligned}$$

From this we finally get, setting $[\delta/2] := \min(\cap[\delta/2,\infty))$

$$\begin{aligned} \int_{\mathrm{dist}(x,S)\le\frac{\delta}{2}} ({}^x[X_t \in M_\delta])^{1/4}\,dx &= \sum_{n=0}^{[\delta/2]} \int_{\frac{\delta}{2}-n-1\le\ \mathrm{dist}(x,S)\le\frac{\delta}{2}-n} ({}^x[X_t\in M_\delta])^{1/4}\,dx \\ &\le C_6\sigma(S)\sum_{n=0}^{[\delta/2]}((\delta/2)^\alpha+1)e^{-\eta_6(n+\delta/2)^2} \\ &\le C_7\sigma(S)e^{-\eta_7\delta^2}. \end{aligned}$$

Collecting all our estimates in Proposition **??** we have shown Proposition **??**. □

3 Localization in energy

The aim of this section is the estimate in Proposition **??** below. For our application it will be crucial that we can control the constants. From a technical point of view, this will require the construction of "cut-off functions" with universal bounds on their derivatives. For this purpose we recall the *regularized distance* (see [**?**, p. 170f.]):

There exist constants $c_1 > 0$, $c_2 > 0$ and B_α such that every closed set $F \subset^d$ admits a C^∞-function $\Theta_F :^d \backslash F \longrightarrow (0,\infty)$ with the following properties:

$$c_1\,\mathrm{dist}\,(x,F) \le \Theta_F(x) \le c_2\,\mathrm{dist}\,(x,F) \qquad \text{for } x \in^d \backslash F,$$

$$|\partial^\alpha\Theta_F(x)| \le B_\alpha(\mathrm{dist}\,(x,F))^{1-|\alpha|} \qquad \text{for } x \in^d \backslash F.$$

The point is that c_1, c_2 and the B_α are independent of F! We shall use Θ_F in the proof of the following Lemma, which is based on an argument of Combes-Thomas type (see [**?**], [**?**]) and is analogous to the proof of Lemma 1 of [**?**] and, in the discrete case, Lemma 4.2 of [**?**]. A special case can also be found in [**?**].

Here we introduce $H_0 := -\frac{1}{2}\Delta \dotplus V_0$ with $V_{0,+} \in L_{1,loc}(^d)$ and $V_{0,-} \in K_d$, which will later play the role of a comparison operator. We write $J \subset\subset U$ to indicate that J is a compact subset of U.

Lemma 3.1 *For $J \subset\subset \rho(H_0)$ there exist constants $C = C(J)$ and $\eta = \eta(J) > 0$ such that for all $\chi, \tilde{\chi} \in L_\infty$ with $\|\chi\|_\infty \leq 1$, $\|\tilde{\chi}\| \leq 1$ and* $(\operatorname{supp}\chi, \operatorname{supp}\tilde{\chi}) \geq \delta$ *and all $E \in J$, $i = 1, \dots, d$:*

$$\begin{aligned} \|\tilde{\chi}(H_0 - E)^{-1}\chi\| &\leq Ce^{-\eta\delta}, \\ \|\tilde{\chi}\partial_i(H_0 - E)^{-1}\chi\| &\leq Ce^{-\eta\delta}. \end{aligned}$$

Proof: We only give the details for the first estimate, since the proof in [?] is sufficiently analogous.

Fix a C^∞-function $u :\longrightarrow$ such that $u(x) = 0$ for $x \leq 1/2$ and $u(x) = x$ for $x \geq 1$. If Θ_F is chosen to $F := \operatorname{supp}\chi$ as above, $\rho := \rho_F = u \circ \left(\frac{1}{c_1}\Theta_F\right)$ extends by $\rho(x) = 0$ for $x \in F$ to a C^∞-function on ^{d} with

$$\|\nabla\rho_F\|_\infty, \; \|\Delta\rho_F\|_\infty \leq c',$$

where the bounds only depend on c_1, c_2, B_α and not on F.

We calculate

$$e^{\eta\rho}(H_0 - E)e^{-\eta\rho} = \left(I - \frac{1}{2}e^{\eta\rho}(\Delta e^{-\eta\rho})(H_0 - E)^{-1} - e^{\eta\rho}(\nabla e^{-\eta\rho}) \cdot \nabla(H_0 - E)^{-1}\right)(H_0 - E)$$

as operators on $D(H_0)$. J is a compact subset of $\rho(H_0)$ so that $(H_0 - E)^{-1}$ and $\partial_i(H_0 - E)^{-1}$ are bounded uniformly in $E \in J$ (recall that $D(H_0) \subset W^{1,2}$, the first order Sobolev space in L_2, since $V_{0,-} \in K_d$). Since $\|e^{\eta\rho}\Delta e^{-\eta\rho}\|_\infty, \|e^{\eta\rho}\nabla e^{-\eta\rho}\|_\infty \to 0$ for $\eta \to 0$ we find $C = C(J)$ and $\eta = \eta(J) > 0$ such that

$$\|e^{\eta\rho}(H_0 - E)^{-1}e^{-\eta\rho}\| \leq C$$

(stability of bounded invertibility).

By the uniform boundedness of $(H_0 - E)^{-1}$ and $\partial_i(H_0 - E)^{-1}$ in $E \in J$ we only have to prove the assertion for $\delta \geq 1$. Using the fact that $c_1\delta \leq c_1 \operatorname{dist}(x, F) \leq \rho(x)$ for $x \in \operatorname{supp}\tilde{\chi}$ and changing η if necessary, we arrive at

$$\|\tilde{\chi}(H_0 - E)^{-1}\chi\| \leq \|\tilde{\chi}e^{-\eta\rho}\| \, \|e^{\eta\rho}(H_0 - E)^{-1}e^{-\eta\rho}\| \, \|e^{\eta\rho}\chi\| \leq e^{-\eta\rho} \cdot C.$$

$\square$

We are now in position to prove the main result of this section. $E_J(H)$ denotes the spectral projection for H onto a subset J of .

Proposition 3.2 *For all $J \subset\subset \rho(H_0)$ and $\delta_0 > 0$ there exist $C = C(J, \delta_0)$ and $\eta = \eta(J, \delta_0) > 0$ such that for all $F \subset^d$ with $(F, \{V_0 \neq V\}) = \delta \geq \delta_0$:*

$$\|\chi_F E_J(H)\| \leq C e^{-\eta\delta}.$$

Proof: (cf. [?, Proof of Lemma 2]) It clearly suffices to prove the claim for bounded F only. Moreover, we may replace H by H_L, where

$$H_L = -\frac{1}{2}\Delta \dot{+} V \quad \text{in } L_2(|x| < L)$$

with Dirichlet boundary conditions, provided the constants do not depend on L (see loc. cit. for the respective argument; note that $H_L \to H$ in strong resolvent sense for $L \to \infty$).

For every bounded F set $\vartheta_F(x) = v(\frac{1}{\delta c_1}\Theta_F(x))$, where Θ_F is as above and v a smooth function with $v(x) = 1$ for $x \leq 1/3$ and $v(x) = 0$ for $x \geq 2/3$. We have $\vartheta_F(x) = 0$ for $(x, F) \geq \frac{2}{3}\delta$, $\vartheta_F(x) = 1$ for $(x, F) \leq \frac{c_1}{3c_2}\delta$, where $\|\nabla\vartheta_F\|_\infty$ and $\|\Delta\vartheta_F\|_\infty$ are uniformly bounded for F with $\delta \geq \delta_0$.

Fix J and let L be large enough in order to ensure $\operatorname{supp}\vartheta_F \subset \{|x| < L\}$. For every normalized eigenfunction ϕ of H_L with eigenvalue $E \in J$ we have by the first representation theorem for quadratic forms (cf. [?]) that $\vartheta_F\phi \in D(H_0)$ and

$$\begin{aligned}
(H_0 - E)\vartheta_F\phi &= \frac{1}{2}(\Delta\vartheta_F)\phi - \nabla\cdot(\nabla\vartheta_F)\phi + \underbrace{\vartheta_F(H_L - E)\phi}_{= \vartheta_F(-\frac{1}{2}\Delta + V_0 - E)\phi = 0} \\
&= \frac{1}{2}(\Delta\vartheta_F)\phi - \nabla\cdot(\nabla\vartheta_F)\phi,
\end{aligned}$$

where we have used that $\{V_0 \neq V\}$ lies outside $\operatorname{supp}\vartheta_F$. Hence

$$\begin{aligned}
|\langle\phi, \chi_F g\rangle| &= |\langle(H_0 - E)^{-1}(H_0 - E)\vartheta_F\phi, \chi_F g\rangle| \\
&\leq |\langle\phi, \nabla\vartheta_F \cdot \nabla(H_0 - \bar{E})^{-1}\chi_F g\rangle| + |\langle\phi, \frac{1}{2}(\Delta\vartheta_F)(H_0 - \bar{E})^{-1}\chi_F g\rangle| \\
&\leq C(J) e^{-\eta(J)\frac{c_1}{3c_2}\delta}\|g\|
\end{aligned}$$

by Lemma ??, since $(\operatorname{supp}\nabla\vartheta_F, \operatorname{supp}\chi_F) \geq \frac{c_1}{3c_2}\delta$ and the derivatives of ϑ_F are bounded. If $\|f\| \leq 1$ then $E_J(H_L)f = \sum_i a_i\phi_i$ for suitable normalized eigenfunctions ϕ_i of H_L and $\sum|a_i|^2 \leq 1$. Therefore we have

$$\begin{aligned}
\|\chi_F E_J(H_L)\|^2 &= \sup_{\|f\|\leq 1, \|g\|\leq 1} |\langle E_J(H_L)f, \chi_F g\rangle|^2 \\
&= \sup_{\|g\|\leq 1, \sum|a_i|^2\leq 1} \sum_i |a_i|^2 |\langle\phi_i, \chi_F g\rangle|^2 \\
&\leq C(J)^2 e^{-\frac{2c_1}{3c_2}\eta(J)\delta}
\end{aligned}$$