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THE SPECTRUM OF THE SCATTERING MATRIX NEAR RESONANT ENERGIES IN THE SEMICLASSICAL LIMIT

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Abstract. The object of study in this paper is the on-shell scattering matrix $S(E)$ of the Schrödinger operator with the potential satisfying assumptions typical in the theory of shape resonances. We study the spectrum of $S(E)$ in the semiclassical limit when the energy parameter E varies from $E_{\mathrm{res}} - \varepsilon$ to $E_{\mathrm{res}} + \varepsilon$, where E_{res} is a real part of a resonance and ε is sufficiently small. The main result of our work describes the spectral flow of the scattering matrix through a given point on the unit circle. This result is closely related to the Breit-Wigner effect.

1. Introduction

1.1. **The set-up.** We consider the Schrödinger operator

$$H = H_0 + V, \quad H_0 = -\hbar^2 \Delta \quad \text{in } L^2(\mathbb{R}^d), \quad d \geq 2, \tag{1.1}$$

where $\hbar \in (0,1)$ is the Planck constant and the potential $V = V(x)$ satisfies the short-range condition

$$|V(x)| \leq C(1+|x|)^{-\rho}, \quad x \in \mathbb{R}^d, \tag{1.2}$$

with $\rho > 1$. We will be interested in the semiclassical regime $\hbar \to +0$, although the dependence of various operators on $\hbar$ will be suppressed in our notation. For $E > 0$ we define the classically accessible region by

$$\mathcal{G}(E) = \left\{ x \in \mathbb{R}^d \;\middle|\; V(x) < E \right\}$$

and write

$$\mathcal{G}(E) = \mathcal{G}^{\mathrm{int}}(E) \cup \mathcal{G}^{\mathrm{ext}}(E),$$

where $\mathcal{G}^{\mathrm{ext}}(E)$ is the unbounded connected component of $\mathcal{G}(E)$, and $\mathcal{G}^{\mathrm{int}}(E)$ is the union of all other connected components.

In Section 2.1, we describe our assumptions on V; these are typical for the theory of shape resonances. In particular, we require that for some $E_0 > 0$ the interior domain $\mathcal{G}^{\mathrm{int}}(E_0)$ is non-empty and that for all energies E in a neighbourhood $\Delta = (E_0 - \delta, E_0 + \delta)$ of E_0 the potential V is non-trapping in $\mathcal{G}^{\mathrm{ext}}(E)$; see Assumption B below and Figure 1.

If it were not for the quantum mechanical tunnelling, the quantum particle with an energy $E \in \Delta$ would not be able to penetrate the potential barrier separating $\mathcal{G}^{\mathrm{int}}(E)$ from $\mathcal{G}^{\mathrm{ext}}(E)$. Thus, the particle would be either confined to the domain $\mathcal{G}^{\mathrm{int}}(E)$ or experience scattering in the domain $\mathcal{G}^{\mathrm{ext}}(E)$. The particles confined to

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$\mathcal{G}^{\rm int}(E)$ would then generate bound states with positive energies. Due to tunnelling, these bound states in fact become resonances with exponentially small (in the semiclassical regime) imaginary part; see e.g. [4, 8, 9, 12, 16–18]. Resonances produced in this way are called *shape resonances*.

Our purpose is to study the spectrum of the scattering matrix for the pair H_0, H for energies near the real parts of shape resonances. In order to locate these resonances, we use the following standard technique: we define an auxiliary Hamiltonian $H^{\rm int} = H_0 + V^{\rm int}$ whose eigenvalues coincide (up to an exponentially small error $O(e^{-c/\hbar})$) with the real parts of shape resonances. The potential $V^{\rm int}$ is defined such that $V^{\rm int}(x) = V(x)$ in $\mathcal{G}^{\rm int}(E_0)$ and $V^{\rm int}(x) \geq E_+ > E_0$ in $\mathbb{R}^d \setminus \mathcal{G}^{\rm int}(E_0)$; the precise assumptions are listed in Section 2.1, but to get an at-a-glance idea of our construction, the reader is advised to take a look at Figure 1. We will call the positive eigenvalues of $H^{\rm int}$ the *resonant energies*. As mentioned above, under additional assumptions one can prove that for each resonant energy $E_{\rm res}$ there exists a resonance $\mathcal{E}_{\rm res}$ of H with $|E_{\rm res} - {\rm Re}\ \mathcal{E}_{\rm res}|$ and $|{\rm Im}\ \mathcal{E}_{\rm res}|$ exponentially small in the semiclassical regime; see [4, 9, 12, 16–18]. However, it is technically convenient for us to work with real resonant energies $E_{\rm res}$ rather than with complex resonances $\mathcal{E}_{\rm res}$. Thus, although resonances provide motivation for our work and are key to interpreting our results, we will say nothing about them and instead refer to resonant energies. In fact (although this is merely a technical point) we do not assume that the resolvent of H admits an analytic continuation and so the existence of resonances under our assumptions cannot be guaranteed; see [16] for a detailed analysis of this issue.

Remark. An alternative way to construct $H^{\rm int}$, used e.g. in [4], is to impose a Dirichlet boundary condition that decouples the domains $\mathcal{G}^{\rm int}(E_0)$ and $\mathcal{G}^{\rm ext}(E_0)$ and then to define $H^{\rm int}$ as the Hamiltonian corresponding to the interior domain. We find it more convenient to work with the Hamiltonian $H^{\rm int}$ defined on the whole space.

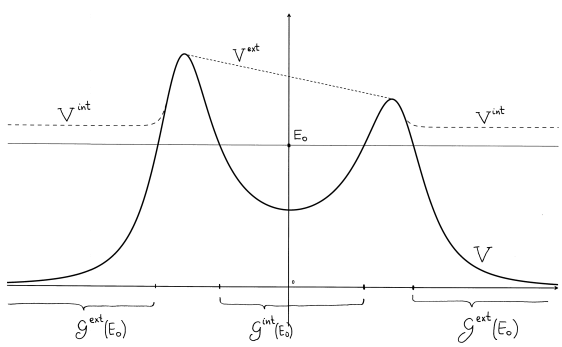

FIGURE 1. Illustrative graph of $V(x)$, $V^{\rm int}(x)$, $V^{\rm ext}(x)$

Besides $H^{\rm int}$, we also define the Hamiltonian $H^{\rm ext} = H_0 + V^{\rm ext}$, where the potential $V^{\rm ext}$ coincides with V on $\mathcal{G}^{\rm ext}(E_0)$ but is globally non-trapping, so the domain $\{x \mid V^{\rm ext}(x) < E\}$ has no bounded connected component; see Figure 1. It turns out that away from the resonant energies, the scattering matrix for the

pair H, H_0 is exponentially close to the scattering matrix for the pair H^{ext}, H_0; see Proposition 2.2. We will use the pair H^{ext}, H_0 as a reference system which has "almost" the same scattering characteristics as H, H_0, but no resonances.

1.2. **The Breit-Wigner effect.** The main object of this paper is the spectrum of the scattering matrix $S(E) = S(E; H, H_0)$, where $E > 0$ varies near resonant energies. We recall the precise definition of the scattering matrix in Section 3.1. The scattering matrix $S(E)$ is a unitary operator on $L^2(\mathbb{S}^{d-1})$ and the difference $S(E) - I$ is compact, where I is the identity operator. Thus, the spectrum of $S(E)$ consists of eigenvalues on the unit circle, and the multiplicities of all eigenvalues (apart from possibly 1) are finite. These eigenvalues may accumulate only to 1. We denote the eigenvalues of $S(E)$, enumerated with multiplicities taken into account, by $\{e^{i\theta_n(E)}\}_{n=1}^{\infty}$. The scattering matrix $S(E)$ depends continuously on the energy $E > 0$ in the operator norm.

If the potential satisfies the short range condition (1.2) with $\rho > d$, then one can define the spectral shift function $\xi(E) = \xi(E; H, H_0)$; see, e.g., [3] for an introduction to the spectral shift function theory. For $E < 0$, the spectral shift function coincides with $-N((-\infty, E); H)$; here and it what follows $N(X, H)$ denotes the number of eigenvalues of H in the interval X. Thus, if $E < 0$ is an eigenvalue of H of multiplicity m, then ξ has a discontinuity at E: $\xi(E+0) - \xi(E-0) = -m$.

For $E > 0$, the spectral shift function $\xi(E)$ is continuous in E and is related to the scattering matrix by the Birman-Krein formula

$$\det S(E) = e^{-2\pi i \xi(E)}, \quad E > 0. \tag{1.3}$$

This formula can be equivalently written in terms of the eigenvalues $\{e^{i\theta_n(E)}\}_{n=1}^{\infty}$ of $S(E)$ as

$$\xi(E) = -\frac{1}{2\pi} \sum_{n=1}^{\infty} \theta_n(E) \pmod 1. \tag{1.4}$$

Suppose E grows monotonically. Then, as E crosses a resonant energy $E_{\text{res}} > 0$ of multiplicity $m \geq 1$, the spectral shift function $\xi(E)$ experiences an exponentially fast (in the semiclassical regime) increment by $(-m)$:

Proposition 1.1 ([20]). *Let Assumptions A and B (see Section* 2.1*) hold true with $\rho > d$ in* (2.1)*, and let $H^{\text{ext}} = H_0 + V^{\text{ext}}$ and $H^{\text{int}} = H_0 + V^{\text{int}}$ be as stipulated in Section* 2.2*. Then there exist positive constants α, β, δ such that for all E satisfying $|E - E_0| < \delta$ and* $\operatorname{dist}(E, \sigma(H^{\text{int}})) > e^{-\beta/\hbar}$ *one has*

$$\left|\xi(E; H, H_0) - \xi(E; H^{\text{ext}}, H_0) + N((-\infty, E); H^{\text{int}})\right| \leq C e^{-\alpha/\hbar}.$$

Moreover, since V^{ext} is non-trapping, the behaviour of $\xi(E; H^{\text{ext}}, H_0)$ near $E = E_0$ is well understood, with an asymptotic expansion in powers of $\hbar$ ([24,25]). Thus, $\xi(E; H, H_0)$ can be approximated by a sum of the smooth component $\xi(E; H^{\text{ext}}, H_0)$ and a *step* component $-N((-\infty, E); H^{\text{int}})$. Proposition 1.1 is one of the alternative ways of describing the *Breit-Wigner effect*; see [14, Section 134] or [21, Chapter 12] for a physics discussion or [7, 17] for precise mathematical results. We emphasise that the mathematical description of the Breit-Wigner effect requires the trace class assumption $\rho > d$ in (1.2), since the spectral shift function is only defined in the trace class framework. On the other hand, the scattering matrix is well defined under the assumption $\rho > 1$.

Since $\xi(E)$ experiences a fast "jump" at resonant energies, formula (1.4) suggests that some of the phases $\theta_n(E)$ also experience jumps near $E_{\rm res}$. This leads to the following questions:

(i) What is the behaviour of individual phases $\theta_n(E)$ near resonant energies?
(ii) Can one observe some version of the Breit-Wigner effect outside the trace class scheme by looking at the phases $\theta_n(E)$?

We attempt to answer these questions, at least partially, in this paper. We study the behaviour of the phases $\{\theta_n(E)\}_{n=1}^\infty$ outside the trace class scheme (i.e. under the assumption $\rho > 1$ in (1.2)) when E varies near resonant energies. In spectral theory it is often more convenient to study an eigenvalue counting function instead of individual eigenvalues. This turns out to be the case in our problem: instead of looking at individual eigenvalues $e^{i\theta_n(E)}$ of the scattering matrix $S(E)$, we study a certain version of the eigenvalue counting function, known as the spectral flow. Our main result, Theorem 2.4, says, roughly speaking, that when E increases monotonically from $E_{\rm res}-\varepsilon$ to $E_{\rm res}+\varepsilon$, where $E_{\rm res}$ is a resonant energy of multiplicity $m \geq 1$ and $\varepsilon > 0$ is exponentially small, the spectral flow of $S(E)$ through "most" points $e^{i\theta}$ on the unit circle equals m. This means that the number of eigenvalues of $S(E)$ that cross $e^{i\theta}$ counterclockwise minus the number of eigenvalues of $S(E)$ that cross $e^{i\theta}$ clockwise equals m.

We expect that the main conclusions of our work also hold true in other models where resonances are present close to the real axis. The semiclassical set-up for us is simply a particular mechanism which produces isolated resonances with a small imaginary part.

2. Main result

2.1. **Assumptions.** Let H_0, H be as in (1.1). We will need a version of the short-range condition (1.2) which also involves the derivatives of V:

Assumption A. *$V \in C^\infty(\mathbb{R}^d)$ is a real-valued function such that for some $\rho > 1$ and any multi-index α,*

$$\left|\partial_x^\alpha V(x)\right| \leq C_\alpha \langle x\rangle^{-\rho-|\alpha|}, \quad x \in \mathbb{R}^d, \tag{2.1}$$

where $\langle x\rangle = (1+|x|^2)^{1/2}$.

Next, we make a standard non-trapping assumption; cf. e.g. [24, 25]. Let $(x(t;y,v))_{t\in\mathbb{R}}$ be the solution to the Newton equation:

$$\ddot{x}(t;y,v) = -2\nabla V(x(t;y,v)),$$
$$x(0;y,v) = y, \quad \dot{x}(0;y,v) = v.$$

Assumption B. *(i) $\mathcal{G}^{\rm int}(E_0) \neq \varnothing$.*

(ii) There exists a neighbourhood $\Delta = (E_0-\delta, E_0+\delta)$ of E_0 such that all energies $E \in \Delta$ are non-trapping in $\mathcal{G}^{\rm ext}(E)$ in the sense of Robert-Tamura, i.e., for any $R > 0$ there is $T > 0$ such that if

$$y \in \mathcal{G}^{\rm ext}(E), \quad |y| < R, \quad |v|^2 + V(y) = E,$$

then

$$|x(t;y,v)| \geq R \quad \text{for } |t| \geq T.$$

2.2. **The Hamiltonians H^{int} and H^{exter}. Resonant energies.** In order to state our results, we need to introduce two auxiliary Hamiltonians, H^{int} and H^{ext}. Let Ω_1, $\Omega_2 \subset \mathbb{R}^d$ be open sets such that

$$\mathcal{G}^{\mathrm{int}}(E_0) \Subset \Omega_1 \Subset \Omega_2 \Subset (\mathbb{R}^d \setminus \mathcal{G}^{\mathrm{ext}}(E_0)),$$

where $\Omega_1 \Subset \Omega_2$ means, as usual, that $\overline{\Omega}_1 \subset \Omega_2$ ($\overline{\Omega}_1$ is the closure of Ω_1). Let us fix $E_+ > E_0$ sufficiently close to E_0 such that

$$\inf\bigl\{V(x) \bigm| x \in \Omega_2 \setminus \Omega_1\bigr\} > E_+. \tag{2.2}$$

Next we choose V^{int} and $V^{\mathrm{ext}} \in C^\infty(\mathbb{R}^d)$ so that (see Figure 1)

$$\begin{aligned}
&V^{\mathrm{ext}}(x) = V(x), \quad \text{if } x \in \mathbb{R}^d \setminus \Omega_1,\\
&V^{\mathrm{ext}}(x) \geq V(x) \quad \text{everywhere},\\
&V^{\mathrm{ext}}(x) \geq E'_+ > E_+, \quad \text{if } x \in \Omega_1,\\
&V^{\mathrm{int}}(x) = V(x), \quad \text{if } x \in \Omega_2,\\
&V^{\mathrm{int}}(x) \geq E'_+ > E_+, \quad \text{if } x \in \mathbb{R}^d \setminus \Omega_2.
\end{aligned}$$

We assume V^{int} to be bounded; in fact, we may assume V^{int} to be constant (greater than E_+) outside a compact set. We set

$$H^{\mathrm{ext}} = H_0 + V^{\mathrm{ext}}, \quad H^{\mathrm{int}} = H_0 + V^{\mathrm{int}}.$$

By our assumptions, H^{int} has only discrete spectrum in the interval $(-\infty, E_+)$. We will call the eigenvalues of H^{int} in this interval the *resonant energies* for H. Since the above definitions do not uniquely specify V^{int}, the resonant energies are not uniquely defined. The following statement shows, however, that the discrepancy between different definitions of resonant energies is exponentially small in the semiclassical limit $\hbar \to 0$.

Proposition 2.1. *Let V_j^{int}, $j = 1, 2$, be two choices of the potential V^{int}, satisfying the above assumptions. For $j = 1, 2$, let $E_1^{(j)} \leq E_2^{(j)} \leq \cdots$ be the eigenvalues of $H_0 + V_j^{\mathrm{int}}$ in the interval $(-\infty, E_+)$, listed in non-decreasing order with multiplicities taken into account. Then there exists $\nu > 0$ such that for all n and for all sufficiently small $\hbar > 0$, the estimate*

$$|E_n^{(1)} - E_n^{(2)}| \leq e^{-\nu/\hbar} \tag{2.3}$$

holds true.

For the proof, see Appendix C. We note that a lower bound for the constant $\nu > 0$ in the estimate (2.3) is explicitly given by the Agmon distance between Ω_1 and Ω_2^c at the energy E_+.

In the problem we are discussing one has to keep in mind two scales as $\hbar \to 0$: the power scale and the exponential scale. Indeed, the number of eigenvalues of H^{int} on $(-\infty, E_+)$ grows as $\hbar^{-d}$. On the other hand, our results below are valid for energies in Δ outside exponentially small neighbourhoods of resonant energies. More precisely, we will consider the energies $E \in \Delta$ that satisfy $\operatorname{dist}(E, \sigma(H^{\mathrm{int}})) > e^{-\alpha/\hbar}$ for some $\alpha > 0$. Thus, the Lebesgue measure of the set

$$\bigl\{E \in \Delta \bigm| \operatorname{dist}(E, \sigma(H^{\mathrm{int}})) \leq e^{-\alpha/\hbar}\bigr\}$$

that we exclude from the interval Δ is exponentially small as $\hbar \to 0$. The fact that we have to exclude exponentially small neighbourhoods of resonant energies E_{res}

is a reflection of the effect that the resonances $\mathcal{E}_{\rm res}$ of H are exponentially close to $E_{\rm res}$; see e.g. [4, 9, 17].

2.3. **The scattering matrix.** The following preliminary result (which is not really new; cf. [17]) shows that away from the resonant energies the scattering matrices $S(E; H, H_0)$ and $S(E; H^{\rm ext}, H_0)$ are exponentially close to each other:

Proposition 2.2. *There exist positive constants C, α, δ such that for all E satisfying $|E - E_0| < \delta$ and $\operatorname{dist}(E, \sigma(H^{\rm int})) > e^{-\alpha/\hbar}$, one has*

$$\|S(E; H^{\rm ext}, H_0) - S(E; H, H_0)\| \le Ce^{-\alpha/\hbar}, \tag{2.4}$$

for all sufficiently small $\hbar > 0$.

The proof follows directly from Lemma 5.6 and the representation (2.9) below. Proposition 2.2, in particular, immediately implies that away from resonant energies the scattering matrix $S(E; H^{\rm ext}, H_0)$ is independent of the choice of $V^{\rm ext}$ up to an exponentially small error.

The next preliminary result shows that $S(E; H^{\rm ext}, H_0)$ varies sufficiently slowly:

Proposition 2.3. *There exist positive constants C, γ, δ such that if $E_1, E_2 \in (E_0 - \delta, E_0 + \delta)$, then*

$$\|S(E_1; H^{\rm ext}, H_0) - S(E_2; H^{\rm ext}, H_0)\| \le C\hbar^{-2-\gamma}|E_1 - E_2|^{\gamma}, \quad \hbar \in (0, 1]. \tag{2.5}$$

See Appendix B for the proof. Note that the neighbourhoods of resonant energies are not excluded in Proposition 2.3.

2.4. **Main result.** In order to state our main result, first we need to recall the definition of spectral flow for unitary operators. Let $\{U(t)\}_{t\in[0,1]}$ be a norm continuous family of unitary operators in a Hilbert space $\mathcal{H}$ such that $U(t) - I$ is compact for all $t \in [0, 1]$. We would like to define the spectral flow of $\{U(t)\}_{t\in[0,1]}$ through a point $e^{i\theta}$, $\theta \in (0, 2\pi)$. The *naïve* definition of spectral flow is

$$\begin{aligned} &\operatorname{sf}(e^{i\theta}; \{U(t)\}_{t\in[0,1]}) \\ &= \langle \text{the number of eigenvalues of } U(t) \text{ which cross } e^{i\theta} \\ &\qquad \text{in the counterclockwise direction}\rangle \\ &\quad - \langle \text{the number of eigenvalues of } U(t) \text{ which cross } e^{i\theta} \\ &\qquad \text{in the clockwise direction}\rangle \end{aligned} \tag{2.6}$$

as t grows from 0 to 1. The eigenvalues are counted with multiplicities taken into account. Of course, there may be infinitely many intersections, and so in general the r.h.s. of (2.6) may be ill-defined. We postpone the discussion of the precise definition of the spectral flow until Section 3.

Our main result is

Theorem 2.4. *Under Assumptions A and B (see Section 2.1) there exist positive constants α, β, δ such that the following statement holds true. Suppose $|E_{\rm res} - E_0| < \delta$, $E_{\rm res}$ is an eigenvalue of $H^{\rm int}$ of multiplicity $m \ge 1$ and*

$$[E_{\rm res} - e^{-\alpha/\hbar}, E_{\rm res} + e^{-\alpha/\hbar}] \cap \sigma(H^{\rm int}) = \{E_{\rm res}\}.$$

Then for all $\theta \in (0, 2\pi)$ such that

$$\operatorname{dist}\big(e^{i\theta}, \sigma(S(E_{\rm res}; H^{\rm ext}, H_0))\big) > e^{-\beta/\hbar} \tag{2.7}$$

and for all sufficiently small $\hbar > 0$ one has

$$\mathrm{sf}(e^{i\theta}; \{S(E; H, H_0)\}_{E\in[E_-,E_+]}) = m, \tag{2.8}$$

where $E_\pm = E_{\mathrm{res}} \pm e^{-\alpha/\hbar}$.

It would be interesting to obtain more detailed information about the eigenvalues of the scattering matrix near resonant energies.

Theorem 2.4 will be derived in Sections 3–5 from a more precise result, Theorem 3.1, which is stated in terms of the spectral flow of the scattering matrix when the energy E varies from some finite value to infinity.

We need to explain that Theorem 2.4 is not vacuous, i.e. that the set of angles θ satisfying (2.7) is non-empty:

Proposition 2.5. *There exist positive constants δ, η such that for any $\theta_1, \theta_2 \in (0, 2\pi)$ and any E satisfying $|E - E_0| < \delta$, one has*

$$\sum_{\theta_1<\theta<\theta_2} \dim \mathrm{Ker}(S(E; H^{\mathrm{ext}}, H_0) - e^{i\theta}) = O(\hbar^{-\eta}), \quad \hbar \to 0.$$

The proof is given in Appendix A. Proposition 2.5 shows that the Lebesgue measure of the $O(e^{-\alpha/\hbar})$-neighbourhood of the spectrum of $S(E; H^{\mathrm{ext}}, H_0)$ on any arc not containing 1 is exponentially small. Thus (2.7) holds true for a *large* set of θ.

2.5. **Method of proof.** We will use the chain rule for scattering matrices to write

$$S(E; H, H_0) = \widetilde{S}(E; H, H^{\mathrm{ext}}) S(E; H^{\mathrm{ext}}, H_0), \quad E > 0, \tag{2.9}$$

where $\widetilde{S}(E; H, H^{\mathrm{ext}})$ is unitarily equivalent to $S(E; H, H^{\mathrm{ext}})$; see (3.5), (3.6). In Section 4 we develop a version of perturbation theory for the spectral flow of products of unitaries. This allows us to estimate the spectral flow of $S(E; H, H_0)$ in terms of the spectral flows of $S(E; H, H^{\mathrm{ext}})$ and $S(E; H^{\mathrm{ext}}, H_0)$. Next, using the stationary representation for the scattering matrix (see Section 3.2) and tunnelling estimates (see Section 5), we show that if θ satisfies (2.7), then the spectral flow of $S(E; H^{\mathrm{ext}}, H_0)$ through $e^{i\theta}$ is zero and the spectral flow of $S(E; H, H^{\mathrm{ext}})$ is m.

3. The eigenvalue counting function for the scattering matrix

3.1. **Scattering theory.** Here we recall a small amount of general scattering theory, as necessary to define the basic objects of our construction. For the details, see e.g. [29]. For a self-adjoint operator A we denote by $P_{ac}(A)$ the projection onto the absolutely continuous subspace of A. The wave operators are defined, as usual, by

$$W_\pm(B, A) = \operatorname*{s-lim}_{t\to\pm\infty} e^{itB} e^{-itA} P_{ac}(A),$$

provided that the strong limits exist. The scattering operator is defined by

$$\mathbf{S}(B, A) = W_+(B, A)^* W_-(B, A). \tag{3.1}$$

If the wave operators are complete, i.e. if

$$\mathrm{Ran}\, W_+(B, A) = \mathrm{Ran}\, W_-(B, A) = \mathrm{Ran}\, P_{ac}(B),$$

then the scattering operator $\mathbf{S}(B,A)$ is unitary in $\operatorname{Ran} P_{ac}(A)$. For self-adjoint operators A, B, C, we have the chain rule

$$\mathbf{S}(C,A) = \widetilde{\mathbf{S}}(C,B)\mathbf{S}(B,A), \tag{3.2}$$

where

$$\widetilde{\mathbf{S}}(C,B) = W_+(B,A)^*\mathbf{S}(C,B)W_+(B,A), \tag{3.3}$$

provided that the wave operators $W_\pm(B,A)$ and $W_\pm(C,B)$ exist and are complete.

By the intertwining property of wave operators, viz.

$$W_\pm(B,A)A = BW_\pm(B,A)$$

(which holds on all elements of the domain of A), the scattering operator $\mathbf{S}(B,A)$ commutes with A, and therefore $\mathbf{S}(B,A)$ and A can be simultaneously diagonalized. The fibre operators of $\mathbf{S}(B,A)$ in this diagonalisation give the scattering matrix $S(E;B,A)$.

Now let us recall the details of this construction for the operators $A = H_0 = -\hbar^2\Delta$, $B = H^{\mathrm{ext}}$, $C = H$ as defined in Section 2.2. We first note that the wave operators $W_\pm(H,H_0)$, $W_\pm(H^{\mathrm{ext}},H_0)$ and $W_\pm(H,H^{\mathrm{ext}})$ exist and are complete. For $f \in L^2(\mathbb{R}^d)$ such that $\langle x\rangle^s f(x) \in L^2(\mathbb{R}^d)$, $s > 1/2$, we set

$$(\mathcal{F}_E f)(\omega) = \frac{1}{\sqrt{2}\hbar^{d/2}} E^{(d-2)/4}\hat{f}(\sqrt{E}\omega\hbar^{-1}), \quad E > 0, \quad \omega \in \mathbb{S}^{d-1}, \tag{3.4}$$

where $\hat{f}$ is the (unitary) Fourier transform of f. Then the map

$$\mathcal{F} \,:\, L^2(\mathbb{R}^d) \to L^2((0,\infty); L^2(\mathbb{S}^{d-1})), \quad (\mathcal{F}f)(E,\omega) = (\mathcal{F}_E f)(\omega),$$

is a unitary operator which diagonalises H_0:

$$(\mathcal{F}_E H_0 f)(\omega) = E(\mathcal{F}_E f)(\omega).$$

It follows that $\mathcal{F}S(H,H_0)\mathcal{F}^*$ can be represented as a direct integral of fibre operators:

$$\mathcal{F}_E\mathbf{S}(H,H_0)f = S(E;H,H_0)(\mathcal{F}_E f), \quad E > 0.$$

Here $S(E;H,H_0) : L^2(\mathbb{S}^{d-1}) \to L^2(\mathbb{S}^{d-1})$ is the scattering matrix.

In the same way, one defines the scattering matrix $S(E;H^{\mathrm{ext}},H_0)$. Finally, as in (3.2), (3.3), we denote

$$\widetilde{\mathbf{S}}(H,H^{\mathrm{ext}}) = W_+(H^{\mathrm{ext}},H_0)^*\mathbf{S}(H,H^{\mathrm{ext}})W_+(H^{\mathrm{ext}},H_0). \tag{3.5}$$

Then $\widetilde{\mathbf{S}}(H,H^{\mathrm{ext}})$ commutes with H_0 and therefore $\widetilde{\mathbf{S}}(H,H^{\mathrm{ext}})$ can also be represented as

$$\mathcal{F}_E\widetilde{\mathbf{S}}(H,H^{\mathrm{ext}})f = \widetilde{S}(E;H,H^{\mathrm{ext}})(\mathcal{F}_E f), \quad E > 0, \tag{3.6}$$

with some fibre operators $\widetilde{S}(E;H,H^{\mathrm{ext}}) : L^2(\mathbb{S}^{d-1}) \to L^2(\mathbb{S}^{d-1})$. Then, as a consequence of (3.2), (3.3), the chain rule (2.9) holds.

3.2. **The stationary representation for the scattering matrix.** Essential for our construction is the stationary representation for the scattering matrix $S(E; H, H_0)$; see e.g. [29, Section 0.7]. Let $\mathcal{F}_E$ be as in (3.4), and let $R_0(z) = (H_0 - zI)^{-1}$, $R(z) = (H - zI)^{-1}$. The stationary representation reads

$$S(E; H, H_0) = I - 2\pi i \mathcal{F}_E (V - VR(E + i0)V)\mathcal{F}_E^*. \tag{3.7}$$

This representation allows one to describe the spectrum of the scattering matrix in terms of the spectrum of the boundary values of the resolvent $R(E + i0)$. Let us denote

$$J = \operatorname{sign}(V), \qquad T_0(z) = \sqrt{|V|}R_0(z)\sqrt{|V|},$$
$$A_0(E) = \operatorname{Re} T_0(E + i0), \quad B_0(E) = \operatorname{Im} T_0(E + i0).$$

Using this notation, the resolvent identity and the identity $J^{-1} = J$, one can write (3.7) as

$$S(E; H, H_0) = I - 2\pi i \mathcal{F}_E \sqrt{|V|}\big(J - A_0(E) - iB_0(E)\big)^{-1}\sqrt{|V|}\mathcal{F}_E^*; \tag{3.8}$$

see e.g. [29, Section 7.7]. This formula has a general operator theoretic nature and is not specific to the pair H_0, H. In fact, in what follows we will apply the representation (3.8) to the pair H, H^{ext}.

3.3. **Definition of spectral flow.** First we fix the notation for an eigenvalue counting function of a unitary operator. Let U be a unitary operator such that the difference $U - I$ is compact. For $\theta_1, \theta_2 \in (0, 2\pi)$, we denote

$$N(e^{i\theta_1}, e^{i\theta_2}; U) = \sum_{\theta_1 \le \theta < \theta_2} \dim \operatorname{Ker}(U - e^{i\theta} I), \quad \text{if } \theta_1 \le \theta_2, \tag{3.9}$$

and

$$N(e^{i\theta_1}, e^{i\theta_2}; U) = -N(e^{i\theta_2}, e^{i\theta_1}; U), \quad \text{if } \theta_1 \ge \theta_2. \tag{3.10}$$

Let $\{U(t)\}_{t\in[0,1]}$ be a norm continuous family of unitary operators in a Hilbert space $\mathcal{H}$ such that $U(t) - I$ is compact for all $t \in [0, 1]$. The *naïve* definition of the spectral flow of $\{U(t)\}_{t\in[0,1]}$ through a point $e^{i\theta}$, $\theta \in (0, 2\pi)$, is given by (2.6). Let us discuss a rigorous definition of spectral flow. First we assume that there exists $\theta_0 \in (0, 2\pi)$ such that

$$e^{i\theta_0} \notin \sigma(U(t)), \quad \text{for all } t \in [0, 1]. \tag{3.11}$$

Then we set (using the notation (3.9), (3.10))

$$\operatorname{sf}(e^{i\theta}; \{U(t)\}_{t\in[0,1]}) = N(e^{i\theta}, e^{i\theta_0}; U(1)) - N(e^{i\theta}, e^{i\theta_0}; U(0)). \tag{3.12}$$

It is evident that this definition is independent of the choice of θ_0 and agrees with the *naïve* definition (2.6) whenever the latter makes sense.

In general, θ_0 as above may not exist. However, using the norm continuity of $U(t)$, one can always find values

$$0 = t_0 < t_1 < t_2 < \cdots < t_n = 1$$

such that for each of the intervals $\Delta_j = [t_{j-1}, t_j]$, a point $\theta_j \in (0, 2\pi)$ satisfying (3.11) for all $t \in \Delta_j$ can be found. Thus, the spectral flows $\operatorname{sf}(\cdot; \{U(t)\}_{t\in\Delta_j})$, $j = 1, \ldots, n$, are well defined. Now we set

$$\operatorname{sf}(e^{i\theta}; \{U(t)\}_{t\in[0,1]}) = \sum_{j=1}^{n} \operatorname{sf}(e^{i\theta}; \{U(t)\}_{t\in\Delta_j}). \tag{3.13}$$

It is not difficult to see that this definition is independent of the choice of the intervals Δ_j and the corresponding points θ_0, and agrees with the *naïve* definition (2.6) whenever the latter makes sense.

In the context of self-adjoint operators with discrete spectrum, the notion of spectral flow goes back at least to the seminal work [2]; see also [26] for a comprehensive survey. One can find many equivalent approaches to the definition of spectral flow in the literature.

The property of the spectral flow that is crucial for us in the sequel is its invariance with respect to the homotopies of the family $\{U(t)\}_{t\in[0,1]}$; see Lemma 4.2 below. The homotopy must be of a class preserving the compactness of $U(t) - I$.

3.4. **The eigenvalue counting function for $S(E)$.** For $E > 0$, let us consider the eigenvalue counting function of the scattering matrix $S(E) = S(E; H, H_0)$. For a fixed $\theta_0 \in (0, 2\pi)$, the function

$$(0, 2\pi) \ni \theta \mapsto N(e^{i\theta}, e^{i\theta_0}; S(E)) \tag{3.14}$$

is a non-increasing integer-valued function with jumps at the points $e^{i\theta} \in \sigma(S(E))$. Of course, different choices of θ_0 lead to different integer additive constants in the definition of the counting function (3.14). Below we explain how to fix this constant in a certain standard way; the resulting counting function will be denoted by $\mu(e^{i\theta}, E)$.

Recall the well-known relation

$$\|S(E) - I\| \to 0 \quad \text{as } E \to +\infty. \tag{3.15}$$

Now fix $E > 0$ and define the family

$$U(t) = S(E'), \quad E' = E + \frac{1-t}{t}, \quad t \in (0, 1], \quad \text{and } U(0) = I. \tag{3.16}$$

Then $\{U(t)\}_{t\in[0,1]}$ is a norm continuous unitary family with $U(t) - I$ compact for all $t \in [0, 1]$. We set

$$\mu(e^{i\theta}, E; H, H_0) = \mathrm{sf}(e^{i\theta}, \{U(t)\}_{t\in[0,1]}), \quad \text{where } U \text{ is given by (3.16).} \tag{3.17}$$

Then $\mu(\cdot, E; H, H_0)$ coincides with the eigenvalue counting function (3.14) up to a particular choice of the additive integer normalisation constant.

The above definition of μ can be alternatively described as follows. The function $\mu(e^{i\theta}, E)$ is the unique function which satisfies the following properties:

(i) for any $\theta_0 \in (0, 2\pi)$ and any $E > 0$ there is an integer $m(\theta_0, E)$ such that

$$\mu(e^{i\theta}, E) = N(e^{i\theta}, e^{i\theta_0}; S(E)) + m(\theta_0, E), \quad \forall \theta \in (0, 2\pi);$$

(ii) the function

$$(0, 2\pi) \ni \theta \mapsto \mu(e^{i\theta}, E) \tag{3.18}$$

considered as an element of $L^1_{\mathrm{loc}}(0, 2\pi)$ (the choice of the function space is not important here) depends continuously on $E > 0$;

(iii) the function (3.18), considered as an element of $L^1_{\mathrm{loc}}(0, 2\pi)$, converges to zero as $E \to +\infty$.

The function μ has been systematically studied in [22, 23] in an abstract operator theoretic framework. It possesses a number of natural properties; for example, $\pm\mu(e^{i\theta}, E) \geq 0$ if $\mp V \geq 0$.

3.5. **The counting function μ near resonant values.** Let the Hamiltonians $H_0, H, H^{\rm int}, H^{\rm ext}$, and the energy E_0 be as stipulated in Sections 2.1 and 2.2. Our results below involve the eigenvalue counting functions $\mu(e^{i\theta}, E; H, H_0)$, $\mu(e^{i\theta}, E; H^{\rm ext}, H_0)$ of the scattering matrices $S(E; H, H_0)$, $S(E; H^{\rm ext}, H_0)$; see definition (3.17) above.

Theorem 3.1. *There exist positive constants α, δ such that for all E satisfying $|E - E_0| < \delta$ and $\operatorname{dist}(E; \sigma(H^{\rm int})) > \frac{1}{2}e^{-\alpha/\hbar}$, and for all $\theta \in (e^{-\alpha/\hbar}, 2\pi - e^{-\alpha/\hbar})$, one has*

$$\begin{aligned}\mu(e^{i\theta_+}, E; H^{\rm ext}, H_0) + N((-\infty, E); H^{\rm int}) &\le \mu(e^{i\theta}, E; H, H_0)\\ &\le \mu(e^{i\theta_-}, E; H^{\rm ext}, H_0) + N((-\infty, E); H^{\rm int})\end{aligned} \tag{3.19}$$

if $\hbar > 0$ is sufficiently small, where $\theta_\pm = \theta \pm e^{-\alpha/\hbar}$.

We note that the factor $\frac{1}{2}$ in front of the exponential $e^{-\alpha/\hbar}$ in the statement of the theorem is of no importance; it is introduced purely for the convenience of the proof of Theorem 2.4. The proof of Theorem 3.1 is given in Sections 4 and 5.

Corollary 3.2. *There exist positive constants α, δ such that for all E satisfying $|E - E_0| < \delta$ and $\operatorname{dist}(E; \sigma(H^{\rm int})) > \frac{1}{2}e^{-\alpha/\hbar}$, and for any $\theta \in (0, 2\pi)$ such that*

$$\operatorname{dist}(e^{i\theta}, \sigma(S(E; H^{\rm ext}, H_0))) > e^{-\alpha/\hbar}, \tag{3.20}$$

one has

$$\mu(e^{i\theta}, E; H, H_0) = \mu(e^{i\theta}, E; H^{\rm ext}, H_0) + N((-\infty, E); H^{\rm int}). \tag{3.21}$$

Proof. Indeed, for all θ that satisfy (3.20) we have

$$\mu(e^{i\theta_+}, E; H^{\rm ext}, H_0) = \mu(e^{i\theta_-}, E; H^{\rm ext}, H_0) = \mu(e^{i\theta}, E; H^{\rm ext}, H_0),$$

and so (3.19) yields (3.21). □

Now using Corollary 3.2, we can prove Theorem 2.4.

Proof of Theorem 2.4. Let α, δ be as in Theorem 3.1. Using Proposition 2.3, we get for all sufficiently small $\hbar$

$$\|S(E; H^{\rm ext}, H_0) - S(E_{\rm res}; H^{\rm ext}, H_0)\| \le C\hbar^{-2-\gamma}e^{-\gamma\alpha/\hbar}, \qquad \text{if } |E - E_{\rm res}| < e^{-\alpha/\hbar}. \tag{3.22}$$

Choose $\beta > 0$ such that $\beta < \alpha$ and $\beta < \gamma\alpha$, and let θ be any angle that satisfies (2.7). Then, combining (2.7) and (3.22), we obtain

$$\operatorname{dist}(e^{i\theta}, \sigma(S(E; H^{\rm ext}, H_0))) > \frac{1}{2}e^{-\alpha/\hbar} \tag{3.23}$$

for all sufficiently small $\hbar$ and all $E \in [E_-, E_+]$. Now we can apply Corollary 3.2 to $E = E_\pm$. This yields

$$\begin{aligned}\mu(e^{i\theta}, E_+; H, H_0) - \mu(e^{i\theta}, E_-; H, H_0)&\\ = N((-\infty, E_+); H^{\rm int}) - N((-\infty, E_-); H^{\rm int}) &= m.\end{aligned} \tag{3.24}$$

Here we have used the fact that by (3.23), none of the eigenvalues of $S(E; H^{\rm ext}, H_0)$ crosses $e^{i\theta}$ as E grows from E_- to E_+, and therefore

$$\mu(e^{i\theta}, E_+; H^{\rm ext}, H_0) = \mu(e^{i\theta}, E_-; H^{\rm ext}, H_0).$$

Representing the family $\{S(E';H,H_0)\}_{E'\in[E_-,\infty)}$ as the concatenation of the families $\{S(E';H,H_0)\}_{E'\in[E_-,E_+]}$ and $\{S(E';H,H_0)\}_{E'\in[E_+,\infty)}$ and recalling the definition (3.17) of μ, we obtain

$$\mu(e^{i\theta},E_+;H,H_0)-\mu(e^{i\theta},E_-;H,H_0)=\mathrm{sf}(e^{i\theta};\{S(E;H,H_0)\}_{E\in[E_-,E_+]}). \tag{3.25}$$

From (3.24) and (3.25) we obtain (2.8). □

3.6. **The strategy of proof of Theorem 3.1.** The proof is based on the chain rule (2.9). In Section 4 we develop a perturbation theory for spectral flow of products of unitaries. This allows us to estimate the function $\mu(\cdot,E;H,H_0)$ in terms of $\mu(\cdot,E;H^{\mathrm{ext}},H_0)$ and $\mu(\cdot,E;H,H^{\mathrm{ext}})$; see Theorem 4.1. The next crucial step is to prove the equality

$$\mu(e^{i\theta},E;H,H^{\mathrm{ext}})=N((-\infty,E);H^{\mathrm{int}}) \tag{3.26}$$

for relevant values of θ. For this, we rely on an explicit formula for the function μ from [22]. This formula has an abstract operator-theoretic nature; we apply it to the pair of operators (H,H^{ext}). Denote $V_0=V^{\mathrm{ext}}-V$; by our assumptions, we have $V_0\geq 0$. Similarly to the notation of Section 3.2, let us set

$$\begin{aligned}
R^{\mathrm{ext}}(z)&=(H^{\mathrm{ext}}-zI)^{-1},\\
A^{\mathrm{ext}}(E)&=\mathrm{Re}\,\big(\sqrt{V_0}R^{\mathrm{ext}}(E+i0)\sqrt{V_0}\big),\\
B^{\mathrm{ext}}(E)&=\mathrm{Im}\,\big(\sqrt{V_0}R^{\mathrm{ext}}(E+i0)\sqrt{V_0}\big).
\end{aligned}$$

Proposition 3.3 ([22, Section 5])**.** *For any $\theta\in(0,2\pi)$ and $E>0$, one has*

$$\begin{aligned}
&\dim\mathrm{Ker}(S(E;H,H^{\mathrm{ext}})-e^{i\theta}I)\\
&\qquad=\dim\mathrm{Ker}(A^{\mathrm{ext}}(E)+\cot(\theta/2)B^{\mathrm{ext}}(E)-I),
\end{aligned} \tag{3.27}$$

$$\mu(e^{i\theta},E;H,H^{\mathrm{ext}})=N((1,\infty);A^{\mathrm{ext}}(E)+\cot(\theta/2)B^{\mathrm{ext}}(E)). \tag{3.28}$$

See also [23, Section 4] for an alternative proof. Proposition 3.3 is a consequence of the stationary representation (3.8) for the scattering matrix. This circle of ideas goes back to [27] and perhaps even to [13].

Now we can prove (3.26) as follows. According to (3.28) with $\theta=\pi$,

$$\mu(-1,E;H,H^{\mathrm{ext}})=N((1,\infty),A^{\mathrm{ext}}(E)). \tag{3.29}$$

On the other hand, by the Birman-Schwinger principle,

$$N((-\infty,E);H^{\mathrm{int}})=N\big((1,\infty);\sqrt{V_0}(H^{\mathrm{int}}+V_0-E)^{-1}\sqrt{V_0}\big). \tag{3.30}$$

We recall that by our assumptions (see Section 2.2), we have $V^{\mathrm{int}}+V_0\geq E_+$ everywhere, and therefore $H^{\mathrm{int}}+V_0\geq E_+$; thus, the inverse operator on the r.h.s. of (3.30) is well defined. Using tunnelling and non-trapping estimates, in Section 5 we prove that the right hand sides of (3.29) and (3.30) coincide for E outside exponentially small neighbourhoods of resonant energies. This yields (3.26) for relevant values of θ.

4. Perturbation theory for spectral flow

4.1. **Perturbation result.** The proof of Theorem 3.1 is achieved by applying a version of perturbation theory for unitary families to the representation (2.9). Thus, our aim in this section is to consider the unitary families of the type $M(t)=\widetilde{U}(t)U(t)$ and to prove the following statement.

Theorem 4.1. *Let $U(t)$ and $\widetilde{U}(t)$, $t \in [0,1]$, be norm continuous families of unitary operators in a Hilbert space $\mathcal{H}$ such that $U(t) - I$ and $\widetilde{U}(t) - I$ are compact for all t. Assume that $U(0) = \widetilde{U}(0) = I$. Assume also that for some $\varphi \in (0,\pi)$ one has*

$$\sigma(\widetilde{U}(1)) \subset \left\{ e^{i\chi} \;\middle|\; -\varphi \le \chi \le \varphi \right\}. \tag{4.1}$$

Denote $M(t) = \widetilde{U}(t)U(t)$ and

$$m = \mathrm{sf}(-1; \{\widetilde{U}(t)\}_{t\in[0,1]}). \tag{4.2}$$

Then for any $\theta \in (\varphi, 2\pi - \varphi)$ one has

$$\begin{aligned} \mathrm{sf}(e^{i(\theta+\varphi)}; \{U(t)\}_{t\in[0,1]}) + m &\le \mathrm{sf}(e^{i\theta}; \{M(t)\}_{t\in[0,1]}) \\ &\le \mathrm{sf}(e^{i(\theta-\varphi)}; \{U(t)\}_{t\in[0,1]}) + m. \end{aligned} \tag{4.3}$$

In Section 4.2 we prove two particular cases of Theorem 4.1 and in Section 4.3 we combine these results to obtain the full proof.

4.2. **Preliminary statements.** First we recall the homotopy invariance of the spectral flow. Both the statement below and its proof are standard facts (see e.g. [26]); we recall it here for completeness only, as homotopy invariance is crucial to our argument.

Lemma 4.2. *Let $U_0(t)$ and $U_1(t)$, $t \in [0,1]$, be norm continuous families of unitary operators such that $U_0(t) - I$ and $U_1(t) - I$ are compact for all t and such that $U_0(0) = U_1(0)$ and $U_0(1) = U_1(1)$. Assume that these families are homotopic to each other, i.e. there exists a norm continuous two parameter family $U_\tau(t)$, $(t,\tau) \in [0,1] \times [0,1]$, of unitary operators with $U_\tau(t) - I$ compact for all (t,τ) and such that $U_\tau(0) = U_0(0)$, $U_\tau(1) = U_0(1)$ for all $\tau \in [0,1]$. Then*

$$\mathrm{sf}(e^{i\theta}; \{U_0(t)\}_{t\in[0,1]}) = \mathrm{sf}(e^{i\theta}, \{U_1(t)\}_{t\in[0,1]}), \quad \theta \in (0, 2\pi). \tag{4.4}$$

Sketch of proof. This is a standard topological argument; see e.g. [15, Section 5.3]. By the continuity of $U_\tau(t)$, we can subdivide $[0,1] \times [0,1]$ into sufficiently small rectangles $[t_i, t_{i+1}] \times [\tau_i, \tau_{i+1}]$ such that for (t,τ) in each of these rectangles, one can find $\theta_0 = \theta_0(i,j)$ with the property (3.11), i.e.

$$e^{i\theta_0(i,j)} \notin \sigma(U_\tau(t)), \quad \text{for all } (t,\tau) \in [t_i, t_{i+1}] \times [\tau_i, \tau_{i+1}].$$

Using this and arguing from the definition (3.12) of the spectral flow, we can successively modify our family from $\{U_0(t)\}_{t\in[0,1]}$ to $\{U_{\tau_1}(t)\}_{t\in[0,1]}$, etc., proving that

$$\mathrm{sf}(e^{i\theta}; \{U_{\tau_i}(t)\}_{t\in[0,1]}) = \mathrm{sf}(e^{i\theta}, \{U_{\tau_{i+1}}(t)\}_{t\in[0,1]}), \quad \theta \in (0, 2\pi),$$

for each i, which eventually leads to (4.4). □

The following statement is a version of Theorem 4.1 with $\varphi = 0$.

Lemma 4.3. *Let $U(t)$ and $\widetilde{U}(t)$, $t \in [0,1]$, be norm continuous families of unitary operators such that $U(t) - I$ and $\widetilde{U}(t) - I$ are compact for all t. Assume $U(0) = \widetilde{U}(0) = \widetilde{U}(1) = I$. Denote $M(t) = \widetilde{U}(t)U(t)$ and $m = \mathrm{sf}(-1; \{\widetilde{U}(t)\}_{t\in[0,1]})$. Then for all $\theta \in (0, 2\pi)$,*

$$\mathrm{sf}(e^{i\theta}; \{M(t)\}_{t\in[0,1]}) = \mathrm{sf}(e^{i\theta}, \{U(t)\}_{t\in[0,1]}) + m. \tag{4.5}$$

Proof. We first note that since $\widetilde{U}(0) = \widetilde{U}(1) = I$, we have

$$\mathrm{sf}(e^{i\theta}; \{\widetilde{U}(t)\}_{t\in[0,1]}) = m, \quad \text{for all } \theta \in (0, 2\pi). \tag{4.6}$$

Next, in the Hilbert space $\mathcal{H} \oplus \mathcal{H}$, we consider the families

$$Q_0(t) = U(t) \oplus \widetilde{U}(t); \quad Q_1(t) = \widetilde{U}(t)U(t) \oplus I.$$

It is evident that for all $\theta \in (0, 2\pi)$,

$$\mathrm{sf}(e^{i\theta}; \{Q_0(t)\}_{t\in[0,1]}) = \mathrm{sf}(e^{i\theta}; \{U(t)\}_{t\in[0,1]}) + m, \tag{4.7}$$

$$\mathrm{sf}(e^{i\theta}; \{Q_1(t)\}_{t\in[0,1]}) = \mathrm{sf}(e^{i\theta}; \{M(t)\}_{t\in[0,1]}). \tag{4.8}$$

We note that Q_0 and Q_1 have the same end points:

$$Q_0(0) = Q_1(0) = I; \quad Q_0(1) = Q_1(1) = U(1) \oplus I.$$

Below we construct a homotopy between $\{Q_0(t)\}_{t\in[0,1]}$ and $\{Q_1(t)\}_{t\in[0,1]}$. By the homotopy invariance of the spectral flow (see Lemma 4.2), this will imply that the left hand sides of (4.7) and (4.8) coincide and therefore (4.5) holds true.

We consider the following norm continuous family of unitary operators on $\mathcal{H}\oplus\mathcal{H}$:

$$\widetilde{U}_\tau(t) = \begin{pmatrix} \cos(\tau\pi/2) & -\sin(\tau\pi/2) \\ \sin(\tau\pi/2) & \cos(\tau\pi/2) \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \widetilde{U}(t) \end{pmatrix} \begin{pmatrix} \cos(\tau\pi/2) & \sin(\tau\pi/2) \\ -\sin(\tau\pi/2) & \cos(\tau\pi/2) \end{pmatrix},$$

where $t \in [0, 1]$, $\tau \in [0, 1]$. By inspection, we learn

(i) $\widetilde{U}_0(t) = I \oplus \widetilde{U}(t)$ for $t \in [0, 1]$;
(ii) $\widetilde{U}_1(t) = \widetilde{U}(t) \oplus I$ for $t \in [0, 1]$;
(iii) $\widetilde{U}_\tau(0) = \widetilde{U}_\tau(1) = I \oplus I$ for $\tau \in [0, 1]$;
(iv) $\widetilde{U}_\tau(t) - I$ is compact for all t, τ.

It follows that the family

$$Q_\tau(t) = \widetilde{U}_\tau(t)(U(t) \oplus I) \quad \text{in } \mathcal{H} \oplus \mathcal{H}$$

provides the required homotopy between Q_0 and Q_1. □

The following statement is related to the case when $m = 0$ in the hypothesis of Theorem 4.1.

Lemma 4.4. *Let U be a unitary operator in $\mathcal{H}$ such that $U - I$ is compact. Let A be a compact self-adjoint operator in $\mathcal{H}$ with $\|A\| \le \varphi < \pi$. Then*

$$\mathrm{sf}(e^{i\theta}; \{e^{itA}U\}_{t\in[0,1]}) \le N(e^{i(\theta-\varphi)}, e^{i\theta}; U), \quad \varphi < \theta < 2\pi, \tag{4.9}$$

$$\mathrm{sf}(e^{i\theta}; \{e^{itA}U\}_{t\in[0,1]}) \ge -N(e^{i\theta}, e^{i(\theta+\varphi)}; U), \quad 0 < \theta < 2\pi - \varphi. \tag{4.10}$$

Proof. 1) Using the spectral representation of A, let us split A into the positive and negative parts:

$$A = A_+ - A_-, \quad \sigma(A_\pm) \subset [0, \varphi].$$

It is easy to see that $\{e^{itA}\}_{t\in[0,1]}$ is homotopic to the path $\{\widetilde{U}(t)\}_{t\in[0,2]}$, where

$$\widetilde{U}(t) = \begin{cases} e^{itA_+}, & 0 \le t \le 1, \\ e^{-i(t-1)A_-}e^{iA_+}, & 1 \le t \le 2. \end{cases}$$

Thus, by the homotopy invariance of the spectral flow (see Lemma 4.2), we have

$$\mathrm{sf}(e^{i\theta}; \{e^{itA}U\}_{t\in[0,1]}) = \mathrm{sf}(e^{i\theta}; \{e^{itA_+}U\}_{t\in[0,1]}) + \mathrm{sf}(e^{i\theta}; \{e^{-itA_-}e^{iA_+}U\}_{t\in[0,1]}). \tag{4.11}$$

2) We consider the family $\{e^{itA_+}U\}_{t\in[0,1]}$. Its eigenvalues are branches of analytic functions. If $\mu_n(t)$ is a simple eigenvalue of $e^{itA_+}U$ with the corresponding normalized egenvector $\psi_n(t)$, then

$$\frac{\mu_n'(t)}{i\mu_n(t)} = (A_+\psi_n(t), \psi_n(t)) \in [0, \varphi].$$

This calculation shows that as t increases, the eigenvalues of $e^{itA_+}U$ rotate counterclockwise with the angular speed of rotation $\leq \varphi$. From here it clearly follows that

$$\mathrm{sf}(e^{i\theta}; \{e^{itA_+}U\}_{t\in[0,1]}) \leq N(e^{i(\theta-\varphi)}, e^{i\theta}; U), \quad \varphi < \theta < 2\pi. \tag{4.12}$$

3) A similar argument shows that the eigenvalues of $e^{-itA_-}e^{iA_+}U$ rotate clockwise and therefore

$$\mathrm{sf}(e^{i\theta}; \{e^{-itA_-}e^{iA_+}U\}_{t\in[0,1]}) \leq 0, \quad 0 < \theta < 2\pi. \tag{4.13}$$

Combining (4.11)–(4.13), we obtain the upper bound (4.9). The lower bound (4.10) is obtained in a similar way by using the family

$$\widetilde{U}(t) = \begin{cases} e^{-itA_-}, & 0 \leq t \leq 1, \\ e^{i(t-1)A_+}e^{-iA_-}, & 1 \leq t \leq 2. \end{cases}$$

□

Lemma 4.5. *Let $\{U(t)\}_{t\in[0,1]}$ be a norm continuous family of unitary operators such that $U(t) - I$ is compact for all t. Then for all $\theta_1, \theta_2 \in (0, 2\pi)$ one has*

$$\begin{aligned} \mathrm{sf}(e^{i\theta_1}; \{U(t)\}_{t\in[0,1]}) - \mathrm{sf}(e^{i\theta_2}; \{U(t)\}_{t\in[0,1]}) \\ = N(e^{i\theta_1}, e^{i\theta_2}; U(1)) - N(e^{i\theta_1}, e^{i\theta_2}; U(0)). \end{aligned} \tag{4.14}$$

Proof. First suppose that there exists $\theta_0 \in (0, 2\pi)$ such that (3.11) holds true. Then, by the definition (3.12), the left hand side of (4.14) becomes

$$\begin{aligned} N(e^{i\theta_1}, e^{i\theta_0}; U(1)) - N(e^{i\theta_1}, e^{i\theta_0}; U(0)) - N(e^{i\theta_2}, e^{i\theta_0}; U(1)) + N(e^{i\theta_2}, e^{i\theta_0}; U(0)) \\ = N(e^{i\theta_1}, e^{i\theta_2}; U(1)) - N(e^{i\theta_1}, e^{i\theta_2}; U(0)), \end{aligned}$$

so the statement is proven. The general case follows by applying the above result to each of the intervals Δ_j (see (3.13)), which leads to telescopic sums in both the left and right hand sides of (4.14). □

4.3. **Proof of Theorem 4.1.** 1) By our assumption (4.1), we can write $\widetilde{U}(1) = e^{iA}$, where A is a compact self-adjoint operator with $\|A\| \leq \varphi$. Now set

$$\widetilde{U}(t) = e^{i(2-t)A}, \quad \text{and} \quad M(t) = \widetilde{U}(t)U(1), \quad \text{for } t \in [1, 2].$$

We obtain

$$\begin{aligned} \mathrm{sf}(e^{i\theta}; \{M(t)\}_{t\in[0,1]}) &= \mathrm{sf}(e^{i\theta}; \{M(t)\}_{t\in[0,2]}) - \mathrm{sf}(e^{i\theta}; \{M(t)\}_{t\in[1,2]}) \\ &= \mathrm{sf}(e^{i\theta}; \{M(t)\}_{t\in[0,2]}) - \mathrm{sf}(e^{i\theta}; \{e^{i(1-t)A}U(1)\}_{t\in[0,1]}) \\ &= \mathrm{sf}(e^{i\theta}; \{M(t)\}_{t\in[0,2]}) + \mathrm{sf}(e^{i\theta}; \{e^{itA}U(1)\}_{t\in[0,1]}). \end{aligned} \tag{4.15}$$

2) Since $-1 \notin \sigma(e^{itA})$ for $t \in [0, 1]$, it is easy to see that

$$\mathrm{sf}(-1; \{\widetilde{U}(t)\}_{t\in[0,2]}) = \mathrm{sf}(-1, \{\widetilde{U}(t)\}_{t\in[0,1]}) = m.$$

Since $\widetilde{U}(0) = \widetilde{U}(2) = I$, we can apply Lemma 4.3 to the family $\{M(t)\}_{t\in[0,2]}$. This yields

$$\mathrm{sf}(e^{i\theta}; \{M(t)\}_{t\in[0,2]}) = \mathrm{sf}(e^{i\theta}; \{U(t)\}_{t\in[0,1]}) + m. \tag{4.16}$$

Combining (4.15), (4.16) and the estimates of Lemma 4.4, we obtain

$$\begin{aligned} \mathrm{sf}(e^{i\theta}; \{M(t)\}_{t\in[0,1]}) &\le m + \mathrm{sf}(e^{i\theta}; \{U(t)\}_{t\in[0,1]}) \\ &\quad + N(e^{i(\theta-\varphi)}, e^{i\theta}; U(1)), \quad \varphi < \theta < 2\pi, \end{aligned} \tag{4.17}$$

$$\begin{aligned} \mathrm{sf}(e^{i\theta}; \{M(t)\}_{t\in[0,1]}) &\ge m + \mathrm{sf}(e^{i\theta}; \{U(t)\}_{t\in[0,1]}) \\ &\quad - N(e^{i\theta}, e^{i(\theta+\varphi)}; U(1)), \quad 0 < \theta < 2\pi - \varphi. \end{aligned} \tag{4.18}$$

3) By Lemma 4.5, taking into account $U(0) = I$, we get

$$\mathrm{sf}(e^{i(\theta-\varphi)}; \{U(t)\}_{t\in[0,1]}) = \mathrm{sf}(e^{i\theta}; \{U(t)\}_{t\in[0,1]}) + N(e^{i(\theta-\varphi)}, e^{i\theta}; U(1)) \tag{4.19}$$

for all $\varphi < \theta < 2\pi$. Combining (4.17) and (4.19) yields the upper bound in (4.3). The lower bound is obtained in the same way by using (4.13) instead of (4.17). □

5. Proof of Theorem 3.1

5.1. **Non-trapping and tunnelling resolvent estimates.** The analytic basis of our proof is provided by Propositions 5.1 and 5.2 below. The first of these results yields a semiclassical resolvent estimate for non-trapping potentials:

Proposition 5.1 ([6, 24, 25])**.** *Suppose that a potential $\widetilde{V}$ satisfies Assumption A with some $\rho > 0$ and let $E > 0$ be a non-trapping energy for $\widetilde{V}$ (i.e. Assumption B(ii) holds true with $\mathbb{R}^d$ instead of $\mathcal{G}^{\mathrm{ext}}(E)$). Then for any $s > 1/2$ we have the estimate*

$$\|\langle x\rangle^{-s}(H_0 + \widetilde{V} - E - i0)^{-1}\langle x\rangle^{-s}\| \le O(\hbar^{-1})$$

as $\hbar \to 0$. Furthermore, if E ranges over a compact interval in a non-trapping energy range, then the above bound is uniform in E.

The second result crucial for us is known as a tunnelling estimate; it goes back to Agmon [1] (see also [10, 19] or [5, Section 6]). Fix a compact set $K \subset \mathbb{R}^d$ and let χ_K be the characteristic function of K in $\mathbb{R}^d$. Consider a potential $\widetilde{V} \in C(\mathbb{R}^d)$, $\widetilde{V} \ge 0$, and let $E < 0$. Let $\mathbf{d}x^2 = (\widetilde{V}(x) - E)_+ dx^2$ be the Agmon metric for $\widetilde{V}$ at the energy E and let $\mathbf{d}(x, K)$ be the corresponding Agmon distance from x to K.

Proposition 5.2 ([5, Section 6])**.** *For any $\varepsilon > 0$ there exists $C_\varepsilon > 0$ such that for all sufficiently small $\hbar > 0$, the estimate*

$$\|e^{(\mathbf{d}(x,K)-\varepsilon)/\hbar}(H_0 + \widetilde{V} - E)^{-1}\chi_K\| \le C_\varepsilon$$

holds true.

Combining the above two results, we obtain the following key estimates:

Lemma 5.3. *Let $A^{\mathrm{ext}}(E)$, $B^{\mathrm{ext}}(E)$ be as defined in Section 3.6. There exist positive constants δ, α such that for all E satisfying $|E - E_0| < \delta$ one has*

$$\|B^{\mathrm{ext}}(E)\| \le e^{-2\alpha/\hbar}, \tag{5.1}$$

$$\left\|A^{\mathrm{ext}}(E) - \sqrt{V_0}(H^{\mathrm{int}} + V_0 - E)^{-1}\sqrt{V_0}\right\| \le e^{-2\alpha/\hbar}, \tag{5.2}$$

provided $\hbar > 0$ is sufficiently small.

Proof. 1) We choose $\delta > 0$ sufficiently small that $V^{\rm int}(x) + V_0(x) \geq E_0 + 2\delta$ for all $x \in \mathbb{R}^d$. Denote

$$D(E) = \sqrt{V_0}\big(R^{\rm ext}(E+i0) - (H^{\rm int} + V_0 - E)^{-1}\big)\sqrt{V_0}.$$

Since $(H^{\rm int} + V_0 - E)^{-1}$ is self-adjoint, recalling the definition of operators $A^{\rm ext}$, $B^{\rm ext}$, we obtain

$$A^{\rm ext}(E) - \sqrt{V_0}(H^{\rm int} + V_0 - E)^{-1}\sqrt{V_0} = \operatorname{Re} D(E), \quad B^{\rm ext}(E) = \operatorname{Im} D(E).$$

Thus, it suffices to prove the estimate

$$\|D(E)\| \leq e^{-\kappa/\hbar} \tag{5.3}$$

for $|E - E_0| < \delta$ and $\hbar > 0$ sufficiently small.

2) Let us prove (5.3). By the second resolvent equation, we have

$$\begin{aligned} D(E) &= -\sqrt{V_0}R^{\rm ext}(E+i0)(V - V^{\rm int})(H^{\rm int} + V_0 - E)^{-1}\sqrt{V_0} \\ &= -\sqrt{V_0}R^{\rm ext}(E+i0)\langle x\rangle^{-s}\cdot\langle x\rangle^{s}(V - V^{\rm int})(H^{\rm int} + V_0 - E)^{-1}\sqrt{V_0}, \end{aligned} \tag{5.4}$$

where $s > 1/2$. By Proposition 5.1, we have

$$\|\sqrt{V_0}R^{\rm ext}(E+i0)\langle x\rangle^{-s}\| \leq C\hbar^{-1} \tag{5.5}$$

for small $\hbar > 0$. Next, let $\mathbf{d}x^2 = (V^{\rm int} + V_0 - E)dx^2$ be the Agmon metric for the potential $V^{\rm int} + V_0$, and let $\mathbf{d}_E(x, K)$ be the corresponding Agmon distance from $x \in \mathbb{R}^d$ to the set $K = \operatorname{supp} V_0$. By Proposition 5.2, we have

$$\|e^{-(\mathbf{d}_E(x,K)-\varepsilon)/\hbar}(H^{\rm int} + V_0 - E)^{-1}\chi_K\| \leq C_\varepsilon. \tag{5.6}$$

Now note that

$$\operatorname{supp} V_0 \cap \operatorname{supp}(V - V^{\rm int}) \subset \Omega_1 \cap \Omega_2^c = \varnothing.$$

Thus, (5.6) yields

$$\|\langle x\rangle^{s}(V - V^{\rm int})(H^{\rm int} + V_0 - E)^{-1}\sqrt{V_0}\| \leq C_\varepsilon e^{-(\mathbf{d}-\varepsilon)/\hbar} \tag{5.7}$$

with any $\varepsilon > 0$, where

$$\mathbf{d} = \inf\{\mathbf{d}_E(x, K) \mid x \in \operatorname{supp}(V - V^{\rm int}), \quad |E - E_0| < \delta\} > 0.$$

Combining (5.4), (5.5) and (5.7), we obtain (5.3) with any $\alpha < \mathbf{d}/2$. □

5.2. Relating $\mu(\cdot, E; H, H^{\rm exter})$ to $H^{\rm int}$.

Lemma 5.4. *Let the constants α, δ be as in Lemma 5.3. Then for all E satisfying $|E - E_0| < \delta$ and $\operatorname{dist}(E, \sigma(H^{\rm int})) > e^{-\alpha/\hbar}$, one has*

$$\mu(-1, E; H, H^{\rm ext}) = N((-\infty, E); H^{\rm int}), \tag{5.8}$$

provided $\hbar > 0$ is sufficiently small.

Proof. 1) Assume $\operatorname{dist}(E, \sigma(H^{\rm int})) > e^{-\alpha/\hbar}$; our aim is to show that the right hand sides of (3.29) and (3.30) coincide for small $\hbar$.

2) We use the operator identity

$$\big(I - \sqrt{V_0}(H^{\rm int} + V_0 - E)^{-1}\sqrt{V_0}\big)\big(I + \sqrt{V_0}(H^{\rm int} - E)^{-1}\sqrt{V_0}\big) = I. \tag{5.9}$$

Using our assumption $\operatorname{dist}(E, \sigma(H^{\rm int})) > e^{-\alpha/\hbar}$, we obtain

$$\begin{aligned} \big\|I + \sqrt{V_0}(H^{\rm int} - E)^{-1}\sqrt{V_0}\big\| &\leq 1 + \big\|\sqrt{V_0}\big\|\cdot\|(H^{\rm int} - E)^{-1}\|\cdot\big\|\sqrt{V_0}\big\| \\ &\leq 1 + e^{\alpha/\hbar}\|V_0\|. \end{aligned}$$

Therefore, by (5.9),

$$\left\| \left(I - \sqrt{V_0}(H^{\mathrm{int}} + V_0 - E)^{-1}\sqrt{V_0} \right)^{-1} \right\| \le 1 + e^{\alpha/\hbar}\|V_0\|.$$

It follows that

$$\operatorname{dist}\bigl(1, \sigma\bigl(\sqrt{V_0}(H^{\mathrm{int}} + V_0 - E)^{-1}\sqrt{V_0}\bigr)\bigr) \ge \frac{1}{1 + e^{\alpha/\hbar}\|V_0\|} > \frac{e^{-\alpha/\hbar}}{1 + \|V_0\|}. \tag{5.10}$$

3) By the estimates (5.2) and (5.10), for all sufficiently small $\hbar$ we have

$$\begin{aligned} \bigl\| A^{\mathrm{ext}}(E) - \sqrt{V_0}(H^{\mathrm{int}} + V_0 - E)^{-1}\sqrt{V_0} \bigr\| &\le e^{-2\alpha/\hbar} < \frac{e^{-\alpha/\hbar}}{1 + \|V_0\|} \\ &< \operatorname{dist}\bigl(1, \sigma\bigl(\sqrt{V_0}(H^{\mathrm{int}} + V_0 - E)^{-1}\sqrt{V_0}\bigr)\bigr), \end{aligned}$$

and so, applying the elementary perturbation theory for compact self-adjoint operators, we get that the right hand sides of (3.29) and (3.30) coincide. □

5.3. **An estimate for $S(E; H, H^{\mathrm{exter}}) - I$.** We will need a corollary of Proposition 3.3:

Lemma 5.5. *Let $a = \operatorname{dist}(1, \sigma(A^{\mathrm{ext}}(E))) > 0$. Then*

$$\|S(E; H, H^{\mathrm{ext}}) - I\| \le 2a^{-1}\|B^{\mathrm{ext}}(E)\|\bigl(1 + a^{-2}\|B^{\mathrm{ext}}(E)\|^2\bigr)^{-1/2}. \tag{5.11}$$

Proof. By the identity (3.27) and elementary perturbation theory for self-adjoint operators,

$$\text{if } |\cot(\theta/2)| \cdot \|B^{\mathrm{ext}}(E)\| < a, \quad \text{then } e^{i\theta} \notin \sigma(S(E; H, H^{\mathrm{ext}})).$$

Let $\theta_0 \in (0, \pi)$ be such that $\cot(\theta_0/2)\|B^{\mathrm{ext}}(E)\| = a$. Then

$$\sigma(S(E; H, H^{\mathrm{ext}})) \subset \bigl\{ e^{i\theta} \bigm| -\theta_0 < \theta < \theta_0 \bigr\},$$

and so

$$\|S(E; H, H^{\mathrm{ext}}) - I\| \le |e^{i\theta_0} - 1|.$$

Now an elementary calculation shows that

$$|e^{i\theta_0} - 1| = 2\bigl(1 + a^2\|B^{\mathrm{ext}}(E)\|^{-2}\bigr)^{-1/2},$$

which proves (5.11). □

Lemma 5.6. *Let δ, α be the constants from Lemma 5.3. Then for all E satisfying $|E - E_0| < \delta$ and $\operatorname{dist}(E, \sigma(H^{\mathrm{int}})) > e^{-\alpha/\hbar}$, one has*

$$\|S(E; H, H^{\mathrm{ext}}) - I\| \le Ce^{-\alpha/\hbar} \tag{5.12}$$

for all sufficiently small $\hbar > 0$.

Proof. Let $\operatorname{dist}(E, \sigma(H^{\mathrm{int}})) > e^{-\alpha/\hbar}$. Then, as in the proof of Lemma 5.4 (see (5.10)), we get

$$\operatorname{dist}\bigl(1, \sigma\bigl(\sqrt{V_0}(H^{\mathrm{int}} + V_0 - E)^{-1}\sqrt{V_0}\bigr)\bigr) > c\, e^{-\alpha/\hbar}.$$

Combining this with the estimate (5.2) of Lemma 5.3, we obtain, for sufficiently small $\hbar$:

$$\operatorname{dist}(1, \sigma(A^{\mathrm{ext}}(E))) \ge c\, e^{-\alpha/\hbar} - e^{-2\alpha/\hbar} \ge (c/2)e^{-\alpha/\hbar}.$$

Combining this with the estimate (5.1) of Lemma 5.3 and with Lemma 5.5, we obtain:

$$\begin{aligned}\|S(E;H,H^{\rm ext})-I\| &\le 2\|B^{\rm ext}(E)\|\cdot(\operatorname{dist}(1,\sigma(A^{\rm ext}(E))))^{-1}\\ &\le 2e^{-2\alpha/\hbar}2c^{-1}e^{\alpha/\hbar}\le (4/c)e^{-\alpha/\hbar},\end{aligned}$$

as required. □

5.4. **Proof of Theorem 3.1.** We use Theorem 4.1 with

$$\begin{aligned}&U(t)=S(E';H^{\rm ext},H_0),\\ &\widetilde U(t)=\widetilde S(E';H,H^{\rm ext}),\quad E'=E+\frac{1-t}{t},\quad t\in(0,1],\end{aligned}$$

and $U(0)=\widetilde U(0)=I$. Here $\widetilde S(E;H,H^{\rm ext})$ is as defined in Section 3.1; see (3.6). Then, according to the chain rule (2.9), we have

$$M(t)=\widetilde U(t)U(t)=S(E;H,H_0).$$

By Lemma 5.6, the hypothesis (4.1) of Theorem 4.1 is satisfied with $\varphi=O(e^{-\alpha/\hbar})$ as $\hbar\to 0$. By Lemma 5.4,

$$m=N((-\infty,E);H^{\rm int}).$$

Now the conclusion of Theorem 4.1 yields the desired estimates. □

Appendix A. Proof of Proposition 2.5

1) Without loss of generality we assume $\theta_2=2\pi-\theta_1$. Then is suffices to prove that

$$N((-\infty,\cos\theta_1);\operatorname{Re}S(E;H^{\rm ext},H_0))=O(\hbar^{-\eta}),\quad \hbar\to 0.$$

We denote the q-th Schatten trace ideal class by S_q. Due to the estimate

$$N((-\infty,-a);A)\le a^{-q}\|A\|_{S_q}^q\quad \text{for all } a>0,\ q\ge 1,$$

it suffices to prove that

$$\|\operatorname{Re}S(E;H^{\rm ext},H_0)-I\|_{S_q}^q=O(\hbar^{-b}),\quad \hbar\to 0, \tag{A.1}$$

with some exponents $q\ge 1$ and $b>0$.

2) According to the stationary representation (3.7) for the scattering matrix, we have

$$\operatorname{Re}S(E;H^{\rm ext},H_0)-I=2\pi\operatorname{Im}\Big(\mathcal{F}_EV^{\rm ext}R^{\rm ext}(E+i0)V^{\rm ext}\mathcal{F}_E^*\Big). \tag{A.2}$$

In order to estimate the norm of the operator on the r.h.s. of (A.2), we use the non-trapping resolvent estimate of Proposition 5.1 and also the following Schatten class estimate:

$$\|\mathcal{F}_E\langle x\rangle^{-s}\|_{S_q}\le C\hbar^{-r}, \tag{A.3}$$

if $\frac12<r<s$ and $q=2(d-1)/(2r-1)$. (A.3) follows from an interpolation between

$$\|\mathcal{F}_E\langle x\rangle^{-s_0}\|\le C\hbar^{-1/2}\quad \text{if } s_0>1/2 \tag{A.4}$$

and

$$\|\mathcal{F}_E\langle x\rangle^{-s_1}\|_{S_2}\le C\hbar^{-d/2}\quad \text{if } s_1>d/2.$$

Proposition 5.1 and the estimate (A.3) imply

$$\|\mathcal{F}_EV^{\rm ext}R^{\rm ext}(E+i0)V^{\rm ext}\mathcal{F}_E^*\|_{S_q}\le C\hbar^{-1-2r}$$

with $\frac{1}{2} < r < s = \rho/2$, and $q = (d-1)/(2r-1)$, where $\rho > 1$ is the constant in the assumption (2.1). This proves (A.1) with $b = 1 + 2r$. □

Appendix B. Proof of Proposition 2.3

Let $s > \frac{1}{2}$ and $\gamma = (s - \frac{1}{2})(s + \frac{1}{2})$. Then we have

$$\|\langle x\rangle^{-s} R^{\mathrm{ext}}(E_1)\langle x\rangle^{-s} - \langle x\rangle^{-s} R^{\mathrm{ext}}(E_2)\langle x\rangle^{-s}\| \le C\hbar^{-1-\gamma}|E_1 - E_2|^{\gamma} \tag{B.1}$$

if $E_1, E_2 \in (E_0 - \delta, E_0 + \delta)$ with small $\delta > 0$. (B.1) is shown by observing the $\hbar$-dependence of the constants in the proofs of the key statements of the Mourre theory. See, e.g., [11], Section 2. There the $\hbar$-dependence of the Hölder continuity is not investigated, but we easily observe the estimate by scaling.

Similarly, we have

$$\|\mathcal{F}_{E_1}\langle x\rangle^{-s} - \mathcal{F}_{E_2}\langle x\rangle^{-s}\|^2 \le C\hbar^{-1-\gamma}|E_1 - E_2|^{\gamma}.$$

Now combining these estimates, (A.4), and Proposition 5.1 with the stationary representation formula of the scattering matrix (3.7), we conclude the proof of the assertion. □

Appendix C. Proof of Proposition 2.1

We use an argument which is essentially due to [4].

Lemma C.1. *Let A_1, A_2 be self-adjoint operators and let $\lambda \in \mathbb{R}$ be such that $\varepsilon = \mathrm{dist}(\lambda, \sigma(A_1)) > 0$. Suppose that*

$$\|(A_1 - \lambda - i\varepsilon)^{-1} - (A_2 - \lambda - i\varepsilon)^{-1}\| < \frac{1}{2\varepsilon}. \tag{C.1}$$

Then $\lambda \notin \sigma(A_2)$.

Proof. For simplicity of notation, assume $\lambda = 0$. Set

$$N_j(z) = ((A_j - i\varepsilon)^{-1} - (z - i\varepsilon)^{-1})^{-1}, \quad j = 1, 2, \quad z \in \mathbb{C}.$$

By a direct calculation,

$$N_j(z) = -(z - i\varepsilon) - (z - i\varepsilon)^2 (A_j - z)^{-1}. \tag{C.2}$$

Using the last formula and our assumptions $\varepsilon = \mathrm{dist}(\lambda, \sigma(A_1))$, we get

$$\|N_1(0)\| \le \varepsilon + \varepsilon^2 \|A_1^{-1}\| \le 2\varepsilon. \tag{C.3}$$

By (C.2), it suffices to check the boundedness of the norm of $N_2(z)$ as $z \to 0$. Using the resolvent identity, we get

$$N_2(z)(I - DN_1(z)) = N_1(z),$$

where $D = (A_1 - i\varepsilon)^{-1} - (A_2 - i\varepsilon)^{-1}$. By (C.1) and (C.3) we get $\|DN_1(0)\| < 1$, and so the norm of $N_2(z)$ is bounded when $z \to 0$. □

Proof of Proposition 2.1. 1) For $j = 1, 2$, let $\widetilde{V}_j$ be the smooth function given by

$$\widetilde{V}_j(x) = \begin{cases} V^{\mathrm{ext}}(x) & \text{if } x \in \Omega_2, \\ V_j^{\mathrm{int}}(x) & \text{if } x \in \mathbb{R}^d \setminus \Omega_2. \end{cases}$$

We note that $\widetilde{V}_j \geq E'_+ > E_+$ everywhere, and therefore

$$\|(H_0 + \widetilde{V}_j - z)^{-1}\| \leq C \quad \text{uniformly in } \operatorname{Re} z \leq E_+. \tag{C.4}$$

Next, let $W = V_2^{\mathrm{int}} - V_1^{\mathrm{int}}$, which is supported inside $\mathcal{G}^{\mathrm{ext}}(E_+)$, and let χ_W be the characteristic function of supp W. We have

$$(H_0 + V_j^{\mathrm{int}} - z)^{-1} - (H_0 + \widetilde{V}_j - z)^{-1} = (H_0 + V_j^{\mathrm{int}} - z)^{-1}(\widetilde{V}_j - V_j^{\mathrm{int}})(H_0 + \widetilde{V}_j - z)^{-1},$$

and therefore

$$\begin{aligned}
&\|(H_0 + V_j^{\mathrm{int}} - z)^{-1}\chi_W\| \\
&\leq \|(H_0 + V_j^{\mathrm{int}} - z)^{-1}\chi_W\| + \|(H_0 + V_j^{\mathrm{int}} - z)^{-1}\|\|(\widetilde{V}_j - V_j^{\mathrm{int}})(H_0 + \widetilde{V}_j - z)^{-1}\chi_W\|.
\end{aligned}$$

Note that the supports of W and $\widetilde{V}_j - V_j^{\mathrm{int}}$ are disjoint. Thus, if $\operatorname{Re} z \leq E_+$, then by a tunnelling estimate (a version of Proposition 5.2 with complex E; see [19, Theorem 2.5]) there exists $\nu > 0$ such that

$$\|(\widetilde{V}_j - V_j^{\mathrm{int}})(H_0 - \widetilde{V}_j - z)^{-1}\chi_W\| \leq Ce^{-\nu/\hbar}.$$

Using (C.4), we obtain that

$$\|(H_0 + V_j^{\mathrm{int}} - z)^{-1}\chi_W\| \leq C' \tag{C.5}$$

for some $C' > 0$, provided that $\operatorname{Re} z \leq E_+$ and $\|(H_0 + V_j^{\mathrm{int}} - z)^{-1}\| \leq e^{-\nu/\hbar}$.

2) Now we use a *zooming argument* of [4, Section IV] to compare the eigenvalues of $H_0 + V_1^{\mathrm{int}}$ and $H_0 + V_2^{\mathrm{int}}$. Let $\lambda < E_+$ be such that $\operatorname{dist}(\lambda, \sigma(H_0 + V_1^{\mathrm{int}})) > e^{-\nu/\hbar}$, and set $\varepsilon = e^{-\nu/\hbar}$. By (C.5), we get

$$\begin{aligned}
&\|(H_0 + V_1^{\mathrm{int}} - \lambda - i\varepsilon)^{-1} - (H_0 + V_2^{\mathrm{int}} - \lambda - i\varepsilon)^{-1}\| \\
&\qquad = \|(H_0 + V_1^{\mathrm{int}} - \lambda - i\varepsilon)^{-1} W (H_0 + V_2^{\mathrm{int}} - \lambda - i\varepsilon)^{-1}\| \leq C.
\end{aligned}$$

Now using Lemma C.1 with $A_j = H_0 + V_j^{\mathrm{int}}$ and $\varepsilon = e^{-\nu/\hbar}$, we get that $\lambda \notin \sigma(H_2 + V_2^{\mathrm{int}})$. Finally, using a standard argument involving continuous deformation of V_1^{int} into V_2^{int}, we get the required statement. □

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