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Resolvent Estimates and Time-Decay in the Semiclassical Limit

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1. Introduction.

In this note we study the Schrödinger operator :

$$H = -(\hbar^2/2)\Delta + V(x), \qquad \text{on} \quad L^2(\mathbf{R}^d), \quad \hbar > 0$$

in the semiclassical limit: $\hbar \to 0$. In particular, we are interested in the scattering theory and long time behaviors of the time evolution: $e^{-itH/\hbar}\varphi$. Boundary value of the resolvent: $\lim_{\varepsilon\to+0}(H-\lambda\pm i\varepsilon)^{-1} = (H-\lambda\pm i0)^{-1}$ plays essential roles in the scattering theory, and various observable quantities, e.g., scattering amplitude, time-delay, etc., are represented by it ([RS]). In studying the boundary value of the resolvent, the theory of Mourre is quite powerful and has been applied to many problems (e.g., [M], [PSS], [CFKS]). Jensen, Mourre and Perry extended the theory using multiple commutators, and proved the existence of boundary values of *powers* of the resolvent ([JMP]). Using the result they also obtained time-decay results (see also [J1]).

In a series of papers [RT1]–[RT4], Robert and Tamura systematically studied the semiclassical limit of the scattering process for nontrapping energies. In their arguments, an estimate of the form:

$$\left\| \langle x\rangle^{-\alpha} (H-\lambda\pm i0)^{-1} \langle x\rangle^{-\alpha} \right\| \le C_\alpha \hbar^{-1}, \qquad \hbar > 0, \alpha > 1/2,$$

which is called *semiclassical resolvent estimate*, plays a crucial role. Here we have used the standard notation: $\langle x\rangle = \left(1+|x|^2\right)^{1/2}$. They proved it using a parametrix for the time evolution. The proof was simplified and generalized by several authors with the aid of the Mourre theory ([GM], [HN], [G], [W2], etc.). Moreover, Wang proved semiclassical estimates for powers of the resolvent ([W1], [W2]):

$$\left\| \langle x\rangle^{-\alpha} (H-\lambda\pm i0)^{-n} \langle x\rangle^{-\alpha} \right\| \le C_\alpha \hbar^{-n}, \qquad \hbar > 0, \alpha > n - 1/2.$$

We also want to mention works on semiclassical resolvent estimates for high energies ([Y], [J2]).

On the other hand, motivated by works on the barrier top resonances ([BCD], [S]), the author generalized the semiclassical resolvent estimate to the simplest trapping energy, namely the barrier top energy ([N1]). In this case, the estimate has the form:

$$\left\| \langle x \rangle^{-\alpha} (H - \lambda \pm i0)^{-1} \langle x \rangle^{-\alpha} \right\| \le C_\alpha \hbar^{-2}, \qquad \hbar > 0, \alpha > 1/2,$$

where λ is the barrier top energy.

The aim of this note is to construct a semiclassical analogue of the multiple commutator method of Jensen, Mourre and Perry, and apply it to the barrier top energy and nontrapping energies. We note that for the nontrapping energy case, this was done by Wang ([W2]). Roughly speaking, our abstract result is as follows: Let A and H be a pair of self-adjoint operators satisfying certain regularity conditions (cf. (H1)–(H4) in Section 2). If, in addition, they satisfy

$$E_\Delta(H)[H, iA]E_\Delta(H) \ge c\hbar^\beta E_\Delta(H), \qquad \hbar > 0,$$

for some $1 \le \beta \le 2$, where Δ is a neighborhood of an energy E, then we can show

$$\left\| \langle A \rangle^{-\alpha} (H - E \pm i0)^{-n} \langle A \rangle^{-\alpha} \right\| \le C_\alpha \hbar^{-n\beta}, \qquad \hbar > 0, \alpha > n - 1/2.$$

$\beta = 1$ corresponds to the nontrapping case, and $\beta = 2$ to the barrier top case. We don't know any concrete examples with $1 < \beta < 2$. Even though the restriction $\beta \le 2$ doesn't seem crucial, our proof dosn't work for the case $\beta > 2$. Time-decay results in the semiclassical limit follow from the above result (Theorem 3). In particular, it follows that if $f \in C_0^\infty(\mathbf{R})$ is supported in a small neighborhood of the barrier top energy, then

$$\left\| \langle x \rangle^{-s} e^{-itH} f(H) \langle x \rangle^{-s} \right\| \le C\hbar^{-s} \langle t \rangle^{-s'}, \qquad t \in \mathbf{R},$$

for $s > s' > 0$.

This note is organized as follows: In Section 2 we state the abstract results, and it is proved in Section 4. Applications to Schrödinger operators are discussed in Section 3.

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2. Abstract Results.

Let H and A be $\hbar$-dependent self-adjoint operators on a Hilbert space $\mathcal{H}$ ($\hbar \in (0, \infty)$). We first suppose

(H1) $D(A) \cap D(H)$ is dense in $D(H)$ with respect to the graph norm.

Let $B_0 = H$. We wish to define B_j inductively by

$$B_j = [B_{j-1}, iA], \qquad j = 1, 2, \cdots,$$

at least formally. In order that we suppose

(H2) $B_1 = [H, iA]$, defined as a form on $D(H) \cap D(A)$, is extended to a bounded operator from $D(H)$ to $\mathcal{H}$. Inductively, $B_{j+1} = [B_j, iA]$, defined as a form on $D(H) \cap D(A)$, is extended to a bounded operator from $D(H)$ to $\mathcal{H}$ for any $j \geq 1$.

In this sense, H is C^∞-smooth with respect to A. We suppose the following $\hbar$-dependence of these commutators:

(H3) For each $j \geq 1$ there is $C_j > 0$ such that

$$\left\| B_j (H + i)^{-1} \right\| \leq C_j \hbar^j, \qquad \hbar > 0.$$

(H4) There is $C > 0$ such that

$$\left\| (H + i)^{-1} [H, [H, iA]] (H + i)^{-1} \right\| \leq C\hbar^2, \qquad \hbar > 0.$$

In applications, (H1)–(H4) follow easily from the symbol calculus. See Section 3.

Now let us fix an energy $E_0 \in \mathbf{R}$. The next inequality, a semiclassical variation of the Mourre estimate, is essential. Let $\beta \geq 1$.

(H5:β) There is an interval $\Delta \ni E_0$ and $C > 0$ such that

$$E_\Delta(H)[H, iA]E_\Delta(H) \geq C\hbar^\beta E_\Delta(H), \qquad \hbar > 0,$$

where $E_\Delta(H)$ is the spectral projection of H and Δ.

We prove the next theorem in Section 4.

THEOREM 1. *Suppose (H1)–(H5:β) with $1 \leq \beta \leq 2$. Then there is an interval $\Delta \ni E_0$ satisfying the following: Let $n \geq 1$ an integer, and let $s > n - 1/2$, then for any $\lambda \in \Delta$,*

$$\lim_{\delta \to +0} \langle A \rangle^{-s} (H - \lambda \pm i\delta)^{-n} \langle A \rangle^{-s} \equiv \langle A \rangle^{-s} (H - \lambda \pm i0)^{-n} \langle A \rangle^{-s}$$

exists and satisfies

$$\left\| \langle A \rangle^{-s} (H - \lambda \pm i0)^{-n} \langle A \rangle^{-s} \right\| \leq C\hbar^{-n\beta}, \qquad \hbar > 0, \lambda \in \Delta. \tag{1}$$

REMARK: Condition (H4) is missing in Lemma 2.3 of [N2], but we need it even for $n = 1$ if $\beta > 1$. On the other hand, it is not necessary if $\beta = 1$ (cf. Proof of Lemma 6).

The next result on time-decay is a direct consequence of Theorem 1.

THEOREM 2. *Suppose (H1)–(H5:β) with $1 \le \beta \le 2$. Then there is an interval $\Delta \ni E_0$ such that for any $f \in C_0^\infty(\Delta)$ and for any constants $s > s' > 0$, $s'' > s'(\beta - 1)$,*

$$\left\| \langle A \rangle^{-s} e^{-itH/\hbar} f(H) \langle A \rangle^{-s} \right\| \le C \hbar^{-s''} \langle t \rangle^{-s'}, \qquad \hbar > 0, t \in \mathbf{R}. \tag{2}$$

PROOF: We follow the argument of Theorem 4.2 in [JMP]. Since

$$\begin{aligned}\left(\frac{d}{d\lambda}\right)^j E'_\lambda(H) &= \frac{1}{2\pi i}\left(\frac{d}{d\lambda}\right)^j \left((H-\lambda-i0)^{-1} - (H-\lambda+i0)^{-1}\right) \\ &= \frac{j!}{2\pi i}\left((H-\lambda-i0)^{-j-1} - (H-\lambda+i0)^{-j-1}\right),\end{aligned}$$

it follows from Theorem 1 that

$$\left\| \langle A \rangle^{-s} \left(\frac{d}{d\lambda}\right)^j E'_\lambda \langle A \rangle^{-s} \right\| \le C \hbar^{-\beta(j+1)}$$

if $s > j + 1/2$. By integration by parts and the functional calculus, we have

$$\begin{aligned} t^j e^{-itH/\hbar} f(H) &= \int_{-\infty}^{\infty} \left(t^j e^{-it\lambda/\hbar}\right) f(\lambda) E'_\lambda d\lambda \\ &= \int_{-\infty}^{\infty} e^{-it\lambda/\hbar} \left(-it\hbar \frac{d}{d\lambda}\right)^j \left(f(\lambda)E'_\lambda\right) d\lambda. \end{aligned}$$

Thus

$$t^j \left\| \langle A \rangle^{-s} e^{-itH/\hbar} f(H) \langle A \rangle^{-s} \right\| \le C \hbar^{-\beta} \hbar^{-(\beta-1)j},$$

and hence

$$\left\| \langle A \rangle^{-s} e^{-itH/\hbar} f(H) \langle A \rangle^{-s} \right\| \le C \langle t \rangle^{-j} \hbar^{-\beta} \hbar^{-(\beta-1)j}$$

if $s > j + 1/2$. Now (2) follows by interpolation. ∎

3. Applications.

Here we apply the results of Section 2 to Schrödinger operators:

$$H = -\frac{1}{2}\hbar^2 \Delta + V(x) \qquad \text{on} \quad \mathcal{H} = L^2(\mathbf{R}^d)$$

with $d \ge 1$, $\hbar > 0$. Throughout this section we assume the potential $V(x)$ satisfies the following condition:

(P) $V \in C^\infty(\mathbf{R}^d)$ and for any multi-index α,

$$\left| \left(\frac{d}{dx}\right)^\alpha V(x) \right| \le C_\alpha \langle x \rangle^{-|\alpha|}, \qquad x \in \mathbf{R}^d.$$

Let $h(x,p) = \frac{1}{2}p^2 + V(x)$ be the corresponding classical Hamiltonian. We denote the solutions of the Newton equation:

$$x'(t) = p(t), \qquad p'(t) = -\frac{\partial V}{\partial x}(x(t))$$

with the initial condition: $x(0) = x_0$, $p(0) = p_0$ by $x(x_0, p_0; t)$ and $p(x_0, p_0; t)$. We write the ω-limit set as

$$\omega\text{-}\lim(x_0,p_0) = \bigcap_{M=1}^{\infty} \overline{\{(x(x_0,p_0;t), p(x_0,p_0;t))\,|t \geq M\}}.$$

Now we fix an energy $E_0 \in \mathbf{R}$. E_0 is called *nontrapping* if the following condition is satisfied:

(NT) There is $\varepsilon > 0$ such that for any $(x,p) \in \mathbf{R}^d \times \mathbf{R}^d$ satisfying $h(x,p) \in [E_0 - \varepsilon, E_0 + \varepsilon]$, $\omega\text{-}\lim(x,p) = \emptyset$.

We also suppose that $V(x)$ satisfies the virial condition near $x = \infty$, i.e.,

(V) There are $R > 0$ and $\delta > 0$ such that

$$(E_0 - V(x)) - \frac{1}{2}x \cdot \frac{\partial V}{\partial x}(x) \geq \delta \qquad \text{for} \quad |x| \geq R.$$

THEOREM 3. *Suppose (P), (NT) and (V). Then there is Δ : a neighborhood of E_0, such that:*

(i) *For any $n \geq 1$ and $s > n - 1/2$, the limit*

$$\lim_{\delta \to +0} \langle x\rangle^{-s} (H - \lambda \pm i\delta)^{-n} \langle x\rangle^{-s} \equiv \langle x\rangle^{-s} (H - \lambda \pm i0)^{-n} \langle x\rangle^{-s}$$

exists for $\lambda \in \Delta$ and sufficiently small $\hbar > 0$. Moreover it satisfies

$$\left\| \langle x\rangle^{-s} (H - \lambda \pm i0)^{-n} \langle x\rangle^{-s} \right\| \leq C\hbar^{-n}, \qquad \lambda \in \Delta, \hbar > 0. \tag{3}$$

(ii) *For any $f \in C_0^\infty(\Delta)$ and $s > s' > 0$, $\varepsilon > 0$,*

$$\left\| \langle x\rangle^{-s} e^{-itH/\hbar} f(H) \langle x\rangle^{-s} \right\| \leq C\hbar^{-\varepsilon} \langle t\rangle^{-s'}, \qquad t \in \mathbf{R}, \hbar > 0. \tag{4}$$

REMARK: Theorem 3 was first proved by Wang ([W1] Theorem 2) using different methods. See also [W2], where the estimate (3) is proved for N-body Schrödinger operators. We note (4) is not optimum. In fact Wang showed that if $V(x)$ is short range then the estimate holds with $s = s'$ and $\varepsilon = 0$ ([W1]

Theorem 1). It seems difficult to obtain such an estimate from (3). We expect that the optimum estimate can be proved by more direct method.

Now we turn to the barrier top energy case. If V attain its maximum at a point, then $E_0 = \sup V$ is clearly trapping energy in the classical sense. We call it the *barrier top energy*, and we suppose:

(BT-i) The origin is the unique nondegenerate maximum of $V(x)$, i.e.,

$$E_0 = \sup_x V(x) = V(0), \qquad \det\left(\frac{\partial^2 V}{\partial x \partial x}(0)\right) \neq 0.$$

(BT-ii) There is $\varepsilon > 0$ such that any classical particle with the energy in $[E_0 - \varepsilon, E_0 + \varepsilon]$ has no ω-limit set except for $(0,0)$, i.e.,

$$\bigcup_{h(x,p)\in[E_0-\varepsilon, E_0+\varepsilon]} \omega\text{-}\lim(x,p) = \{(0,0)\}.$$

(BT-iii) There are no homoclinic orbits with the energy E_0, i.e., if $x(t) \to 0$ as $t \to \pm\infty$ then $x(t) \equiv 0$.

THEOREM 4. *Let E_0 be the barrier top energy and suppose (P), (V) and (BT). Then there is Δ : a neighborhood of E_0, such that:*

(i) *For any $n \geq 1$ and $s > n - 1/2$, the limit*

$$\lim_{\delta\to+0} \langle x\rangle^{-s} (H - \lambda \pm i\delta)^{-n} \langle x\rangle^{-s} \equiv \langle x\rangle^{-s} (H - \lambda \pm i0)^{-n} \langle x\rangle^{-s}$$

exists for $\lambda \in \Delta$ and sufficiently small $\hbar > 0$. Moreover it satisfies

$$\left\| \langle x\rangle^{-s} (H - \lambda \pm i0)^{-n} \langle x\rangle^{-s} \right\| \leq C\hbar^{-2n}, \qquad \lambda \in \Delta, \hbar > 0. \tag{5}$$

(ii) *For any $f \in C_0^\infty(\Delta)$ and $s > s' > 0$,*

$$\left\| \langle x\rangle^{-s} e^{-itH/\hbar} f(H) \langle x\rangle^{-s} \right\| \leq C\hbar^{-s} \langle t\rangle^{-s'}, \qquad t \in \mathbf{R}, \hbar > 0. \tag{6}$$

REMARK: (6) implies that it takes at most time of order $O(\hbar^{s/s'})$ for a quantum particle with the energy near E_0 to escape from a bounded region. As in Theorem 3, we expect that (6) holds with $s = s'$.

In the proof, we use the symbol class $S(m,g)$ with $m = m(\hbar; x, \xi)$, $g = dx^2/\langle x\rangle^2 + d\xi^2/\langle \xi\rangle^2$. $S(m,g)$ is the set of functions: $f(\hbar; x, \xi) \in C^\infty(\mathbf{R}^n \times \mathbf{R}^n)$ with a parameter $\hbar > 0$ such that for any α and β,

$$\left| \left(\frac{\partial}{\partial x}\right)^\alpha \left(\frac{\partial}{\partial \xi}\right)^\beta f(\hbar; x, \xi) \right| \leq C_{\alpha\beta}\, m(\hbar; x, \xi) \langle x\rangle^{-|\alpha|} \langle \xi\rangle^{-|\beta|}, \quad x, \xi \in \mathbf{R}^d.$$

The Weyl operator with the symbol $b(\hbar; x, \xi)$ (or the $\hbar$-pseudodifferential operator with the Weyl symbol $b(\hbar; x, \xi)$) is defined (formally) by

$$b^w(\hbar; x, \hbar D)\psi(x) = (2\pi\hbar)^{-n} \int e^{i(x-y)\xi/\hbar}\, b\left(\hbar; \frac{x+y}{2}, \xi\right) \psi(y)\, dy d\xi.$$

Conversely, we denote the Weyl symbol of an $\hbar$-pseudodifferential operator by $\sigma^w(\cdot)$, i.e., $\sigma^w\left(b^w(\hbar; x, \hbar D)\right) = b(\hbar; x, \xi)$. (cf. [H]; see also [R], [G], [N1] for the calculus of $\hbar$-pseudodifferential operators.)

It is easy to see that $h(x,\xi) = \frac{1}{2}\xi^2 + V(x) \in S(\langle\xi\rangle^2, g)$ is the symbol of H.

Lemma 1. *Let $a \in S(\langle x\rangle \langle\xi\rangle, g)$ and suppose $A = a^w(\hbar; x, \hbar D)$ is essentially self-adjoint on the Schwartz space $\mathcal{S}$. Then the pair of operators H and A satisfies the conditions (H1)–(H4).*

Proof: (H1) is clear since $\mathcal{S}$ is dense in $D(H) = H^2(\mathbf{R}^d)$. For any $B = b^w(\hbar; x, \hbar D)$, $b \in S(\langle\xi\rangle^2, g)$, we have

$$\sigma^w([B, iA]) \in S(\langle x\rangle \langle\xi\rangle \cdot \langle\xi\rangle^2 \cdot \hbar \langle x\rangle^{-1} \langle\xi\rangle^{-1}, g) = S(\hbar \langle\xi\rangle^2, g),$$

and hence $\left\|[B, iA](H+i)^{-1}\right\| \le C\hbar$. In particular,

$$\sigma^w(B_1) = \sigma^w([H, iA](H+i)^{-1}) \in S(\hbar\langle\xi\rangle^2, g); \qquad \left\|B_1(H+i)^{-1}\right\| \le C\hbar.$$

Inductively, we have

$$\sigma^w(B_j) = \sigma^w([B_{j-1}, iA]) \in S(\hbar^j \langle\xi\rangle^2, g); \qquad \left\|B_j(H+i)^{-1}\right\| \le C\hbar^j,$$

for $j \ge 2$. This proves (H2) and (H3). Similarly, we have

$$\sigma^w([H, [H, iA]]) \in S(\hbar^2 \langle x\rangle^{-1} \langle\xi\rangle^3, g),$$

and hence

$$\left\|(H+i)^{-1}[H, [H, iA]](H+i)^{-1}\right\| \le C\hbar^2. \qquad \blacksquare$$

In order to prove Theorems 3 and 4, it remains to show that there is $a \in S(\langle x\rangle\langle\xi\rangle, g)$ such that (H5:β) holds with $\beta = 1$ and 2, respectively. For the nontrapping case, such $a(x,\xi)$ was constructed by Gérard and Martinez [GM]:

Lemma 2. *Suppose (P), (NT) and (V). Then there is a real-valued symbol: $a \in C_0^\infty(\mathbf{R}^d \times \mathbf{R}^d)$ such that:*

(i) $a(x,\xi) - x\cdot\xi \in C_0^\infty(\mathbf{R}^d \times \mathbf{R}^d)$;

(ii) *There are* $\varepsilon > 0$ *and* $\delta > 0$ *such that for any* $(x, \xi) \in \mathbf{R}^d \times \mathbf{R}^d$ *with* $h(x, \xi) \in [E_0 - \varepsilon, E_0 + \varepsilon]$,

$$\{h, a\}(x, \xi) \geq \delta, \tag{7}$$

where $\{\cdot, \cdot\}$ *is the Poisson bracket:*

$$\{a, b\} \equiv \sum_{i=1}^{d} \left(\frac{\partial a}{\partial \xi_i} \frac{\partial b}{\partial x_i} - \frac{\partial a}{\partial x_i} \frac{\partial b}{\partial \xi_i} \right).$$

Let $a_0(x, \xi) = x \cdot \xi$. then $A_0 = a_0^w(x, \hbar D)$ is the generator of the dilation group, and hence it is essentially self-adjoint on $\mathcal{S}$. It follows from Lemma 2-(i) that $a \in S(\langle x \rangle \langle \xi \rangle, g)$ and $A = a^w(x, \hbar D)$ is also essentially self-adjoint. Thus A satisfies the conditions of Lemma 1. The next lemma follows from (7) and the functional calculus:

LEMMA 3. *Let* $a(x, \xi)$, ε *and* δ *as in Lemma le:a2. Then for any* $\delta > \delta' > 0$ *and* $f \in C_0^\infty(E_0 - \varepsilon, E_0 + \varepsilon)$,

$$f(H)[H, iA]f(H) \geq \delta' \hbar f(H)^2, \qquad \hbar > 0. \tag{8}$$

For the detail, we refer [GM]. See [G] for the 3-body case, and [W2] for the N-body case. See also [HN] and [N2] for similar discussions.

PROOF OF THEOREM 3: By these lemmas, H and A satisfy (H1)–(H5:1). Thus Theorems 1 and 2 apply to obtain (3) and (4), respectively, with the weight $\langle A \rangle^{-s}$ instead of $\langle x \rangle^{-s}$. We note that

$$\left\| \langle x \rangle^{-s} (H + i)^{-n} \langle A \rangle^{s} \right\| \leq C$$

if $s \leq 2n$. If $s = 2n$, the above estimate follows from the observation:

$$\sigma^w \left(\langle x \rangle^{-2n} (H + i)^{-n} \langle A \rangle^{2n} \right) \in S \left(\langle x \rangle^{-2n} \cdot \langle \xi \rangle^{-2n} (\langle x \rangle \langle \xi \rangle)^{2n}, g \right) = S(1, g),$$

and it is extended to $0 \leq s \leq 2n$ by complex interpolation (cf. [PSS], Lemma 8.2). Combining these we obtain the conclusion. ∎

For the barrier top energy case, such $a(x, \xi)$ was constructed in [N2]:

LEMMA 4. *Suppose (P), (V) and (BT). Then there is a real-valued symbol:* $a(x, \xi) \in C^\infty(\mathbf{R}^d \times \mathbf{R}^d)$ *such that:*

(i) $a(x, \xi) - x \cdot \xi \in C_0^\infty(\mathbf{R}^d \times \mathbf{R}^d)$;

(ii) *There are* $\varepsilon, \alpha, \beta > 0$ *such that for any* $(x, \xi) \in \mathbf{R}^d \times \mathbf{R}^d$ *with* $h(x, \xi) \in [E_0 - \varepsilon, E_0 + \varepsilon]$,

$$\{h, a\}(x, \xi) \geq \min\left(\alpha(|x|^2 + |\xi|^2), \beta\right). \tag{9}$$

The next lemma follows from (9) analogously to Lemma 3:

LEMMA 5. *Let $a(x,\xi)$, ε as in Lemma 4. Then for any $f \in C_0^\infty(E_0-\varepsilon, E_0+\varepsilon)$, there is $c>0$ such that*

$$f(H)[H,iA]f(H) \geq c\hbar^2 f(H)^2, \qquad \hbar > 0. \tag{10}$$

For the detail, we refer [N2]. Now Theorem 4 follows from Lemmas 1 and 5, analogously to Theorem 3.

4. Proof of Theorem 1.

Throughout this section we assume (H1)–(H5:β) hold with $1 \leq \beta \leq 2$. We trace arguments in [JMP] and [CFKS], Section 4.3. Let $f \in C_0^\infty(\mathbf{R})$ be supported in Δ of (H5:β), and $f=1$ in a neighborhood of E_0. Then (H5:β) implies

$$f(H)[H,iA]f(H) \geq c\hbar^\beta f(H)^2. \tag{11}$$

We often write $f = f(H)$ and $\widetilde{f} = 1-f$ for simplicity. We also write $\rho = \langle A \rangle^{-1}$. For $\varepsilon \geq 0$ and $z \in \mathbf{C}\setminus\mathbf{R}$, we let

$$G_\varepsilon^M(z) = G_\varepsilon^M = (H - i\varepsilon M^2 - z)^{-1}; \qquad M^2 = f(H)[H,iA]f(H) \geq 0.$$

We fix a neighborhood of E_0: $\Delta' \subset\subset \{\lambda | f(\lambda) = 1\}$, and let

$$\Omega_\pm = \{z \in \mathbf{C} | \mathrm{Re}\, z \in \Delta', \pm \mathrm{Im}\, z > 0\}.$$

LEMMA 6. *For $\varepsilon \geq 0$, Im $z > 0$, $\big(H - i\varepsilon M^2 - z\big)$ is invertible. The inverse is continuous in ε for $\varepsilon \geq 0$ and smooth for $\varepsilon > 0$. Moreover, there are $\varepsilon_0 > 0$ and $C > 0$ such that*

$$\left\|fG_\varepsilon^M\varphi\right\| \leq C\hbar^{-\beta/2}\varepsilon^{-1/2}\left|\langle\varphi, G_\varepsilon^M\varphi\rangle\right|^{1/2}, \tag{12}$$

$$\left\|fG_\varepsilon^M\right\| + \left\|HfG_\varepsilon^M\right\| \leq C\hbar^{-\beta}\varepsilon^{-1}, \tag{13}$$

$$\left\|\widetilde{f}G_\varepsilon^M\right\| + \left\|H\widetilde{f}G_\varepsilon^M\right\| \leq C \tag{14}$$

for $0 < \varepsilon \leq \varepsilon_0$, $0 < \hbar \leq 1$ and $z \in \Omega_\pm$.

PROOF: For $z = \mu + i\delta$, $\mu \in \Delta'$, $\delta > 0$,

$$\begin{aligned}\left\|\left(H - i\varepsilon M^2 - z\right)\varphi\right\|^2 &= \left\|\left(H - i\varepsilon M^2 - \mu\right)\varphi\right\|^2 + \delta^2\|\varphi\|^2 + 2\varepsilon\delta\|M\varphi\|^2 \\ &\geq \delta^2\|\varphi\|^2, \qquad \varphi \in D(H).\end{aligned}$$

Hence $G_\varepsilon^M(z)$ exists and it is easy to see that it is smooth in ε if $\varepsilon > 0$ because M^2 is bounded. Now we use the Mourre estimate (11):

$$\begin{aligned}\left\|fG_\varepsilon^M\varphi\right\|^2 &= \langle\varphi, G_\varepsilon^{M*}f^2G_\varepsilon^M\varphi\rangle \\ &\le C\hbar^{-\beta}\langle\varphi, G_\varepsilon^{M*}M^2G_\varepsilon^M\varphi\rangle \\ &\le C\hbar^{-\beta}\varepsilon^{-1}\langle\varphi, G_\varepsilon^{M*}\left(2\varepsilon M^2 + 2\mathrm{Im}\ z\right)G_\varepsilon^M\varphi\rangle \\ &= C\hbar^{-\beta}\varepsilon^{-1}\langle\varphi, i\left(G_\varepsilon^{M*} - G_\varepsilon^M\right)\varphi\rangle \\ &\le 2C\hbar^{-\beta}\varepsilon^{-1}\left|\langle\varphi, G_\varepsilon^M\varphi\rangle\right|.\end{aligned}$$

This proves (12). Estimate (12) implies

$$\left\|fG_\varepsilon^M\right\| \le C\hbar^{-\beta/2}\varepsilon^{-1/2}\left\|G_\varepsilon^M\right\|^{1/2}. \tag{15}$$

Now we decompose G_ε^M as

$$\begin{aligned}\left\|G_\varepsilon^M\right\| &\le \left\|fG_\varepsilon^M\right\| + \left\|\widetilde{f}G_\varepsilon^M\right\| \\ &\le C\hbar^{-\beta/2}\varepsilon^{-1/2}\left\|G_\varepsilon^M\right\|^{1/2} + \left\|\widetilde{f}(H-z)^{-1}\right\| + \left\|\widetilde{f}(H-z)^{-1}\varepsilon M^2G_\varepsilon^M\right\| \\ &\le C\hbar^{-\beta/2}\varepsilon^{-1/2}\left\|G_\varepsilon^M\right\|^{1/2} + C\left(1 + \hbar\varepsilon\left\|G_\varepsilon^M\right\|\right).\end{aligned}$$

By solving the quadratic inequality in $\left\|G_\varepsilon^M\right\|^{1/2}$, we obtain

$$\left\|G_\varepsilon^M\right\| \le C\hbar^{-\beta}\varepsilon^{-1} \tag{16}$$

if $\hbar\varepsilon$ is sufficiently small. We set $\varepsilon_0 > 0$ so small that it holds for any $0 < \hbar \le 1$. (13) follows immediately from (16).

In order to prove (14), we first note that by the resolvent equation,

$$\begin{aligned}\left\|\widetilde{f}G_\varepsilon^M\right\| &\le \left\|\widetilde{f}(H-z)^{-1}\right\| + \left\|\widetilde{f}(H-z)^{-1}\left(i\varepsilon M^2\right)G_\varepsilon^M\right\| \\ &\le C\left(1 + \hbar\varepsilon\cdot C\hbar^{-\beta}\varepsilon^{-1}\right) \le C\hbar^{1-\beta}.\end{aligned} \tag{17}$$

We take $\widetilde{g} \in C_0^\infty(\mathbf{R})$ so that $\widetilde{g} = 0$ in a neighborhood of Δ' and $\widetilde{g}\widetilde{f} = \widetilde{f}$. Then (17) holds for $\widetilde{g}G_\varepsilon^M$ also. We decompose $\widetilde{f}G_\varepsilon^M$ as

$$\widetilde{f}G_\varepsilon^M = \widetilde{f}(H-z)^{-1}\left(i\varepsilon M^2\right)\widetilde{g}(H)G_\varepsilon^M + \widetilde{f}(H-z)^{-1}\left[\widetilde{g}(H), i\varepsilon M^2\right]G_\varepsilon^M.$$

Since (H4) implies

$$\begin{aligned}\left\|\left[\widetilde{g}, i\varepsilon M^2\right]\right\| &= \varepsilon\left\|f\left[\widetilde{g},[H,iA]\right]f\right\| \\ &\le \varepsilon\left\|\left[(1-\widetilde{g}),[H,iA]\right]\right\| \le C\hbar^2\varepsilon,\end{aligned}$$

and $\beta \le 2$, we have

$$\left\|\widetilde{f}G_\varepsilon^M\right\| \le C + C\hbar\varepsilon\cdot C\hbar^{1-\beta} + C\hbar^2\varepsilon\cdot\hbar^{-\beta}\varepsilon^{-1} \le C\left(1 + \hbar^{2-\beta}\right) \le C.$$

$\left\|H\widetilde{f}G_\varepsilon^M\right\| \le C$ easily follows from this. ∎

LEMMA 7. *Let ε_0 as in Lemma 6. Then*

$$\left\|\rho G_\varepsilon^M \rho\right\| \leq C\hbar^{-\beta}, \tag{18}$$

$$\left\|G_\varepsilon^M \rho\right\| \leq C\hbar^{-\beta}\varepsilon^{-1/2} \tag{19}$$

for $0 < \varepsilon \leq \varepsilon_0$, $0 < \hbar \leq 1$ *and* $z \in \Omega_\pm$.

PROOF: Let $F_\varepsilon^M = \rho G_\varepsilon^M \rho$. Substituting $\varphi = \rho\psi$ to (12) and using (14), we obtain

$$\begin{aligned}\left\|G_\varepsilon^M \rho\psi\right\| &\leq \left\|\widetilde{f} G_\varepsilon^M \rho\psi\right\| + \left\|f G_\varepsilon^M \rho\psi\right\| \\ &\leq C\left\|\psi\right\| + C\hbar^{-\beta/2}\varepsilon^{-1/2}\left|\langle\psi, \rho G_\varepsilon^M \rho\psi\rangle\right|^{1/2} \\ &\leq C\left(1 + \hbar^{-\beta/2}\varepsilon^{-1/2}\left\|F_\varepsilon^M\right\|^{1/2}\right)\left\|\psi\right\|.\end{aligned}$$

Thus

$$\left\|G_\varepsilon^M \rho\right\| \leq C\left(1 + \hbar^{-\beta/2}\varepsilon^{-1/2}\left\|F_\varepsilon^M\right\|^{1/2}\right). \tag{20}$$

On the other hand, as in the proof of Lemma 4.15 of [CFKS], we have

$$\begin{aligned}\frac{1}{i}\frac{d}{d\varepsilon}F_\varepsilon^M &= \rho G_\varepsilon^M M^2 G_\varepsilon^M \rho = Q_1 + Q_2 + Q_3, \\ Q_1 &= -\rho G_\varepsilon^M \widetilde{f} B_1 \widetilde{f} G_\varepsilon^M \rho, \\ Q_2 &= -\rho G_\varepsilon^M \widetilde{f} B_1 f G_\varepsilon^M \rho - \rho G_\varepsilon^M f B_1 \widetilde{f} G_\varepsilon^M \rho, \\ Q_3 &= \rho G_\varepsilon^M [H, iA] G_\varepsilon^M \rho.\end{aligned}$$

By (13), (14) and (20), Q_1 and Q_2 are estimated as follows:

$$\begin{aligned}\left\|Q_1\right\| &\leq \left\|G_\varepsilon^M \widetilde{f}\right\| \left\|B_1(H+i)^{-1}\right\| \left\|(H+i)\widetilde{f} G_\varepsilon^M\right\| \leq C\hbar, \\ \left\|Q_2\right\| &\leq 2\left\|G_\varepsilon^M \widetilde{f}\right\| \left\|B_1(H+i)^{-1}\right\| \left\|(H+i)f\right\| \left\|G_\varepsilon^M \rho\right\| \\ &\leq C\hbar\left(1 + \hbar^{-\beta/2}\varepsilon^{-1/2}\left\|F_\varepsilon^M\right\|^{1/2}\right).\end{aligned}$$

We decompose $Q_3 = Q_4 + Q_5$ where

$$\begin{aligned}Q_4 &= \rho G_\varepsilon^M \left[H - i\varepsilon M^2 - z, iA\right] G_\varepsilon^M \rho, \\ Q_5 &= \rho G_\varepsilon^M \left[i\varepsilon M^2, iA\right] G_\varepsilon^M \rho.\end{aligned}$$

Using (20) again, we have

$$\left\|Q_4\right\| \leq 2\left\|\rho G_\varepsilon^M A\rho\right\| \leq 2\left\|\rho G_\varepsilon^M\right\| \leq C\left(1 + \hbar^{-\beta/2}\varepsilon^{-1/2}\left\|F_\varepsilon^M\right\|\right).$$

Since

$$\| [M^2, iA] \| \leq 2 \| [f, iA] \| \, \| [H, iA] f \| + \| [[H, iA], iA] f \| \leq C\hbar^2,$$

Q_5 is estimated as

$$\| Q_5 \| \leq 2\varepsilon \left\| \rho G_\varepsilon^M \right\|^2 \cdot C\hbar^2 \leq C\hbar^{2-\beta} \left\| F_\varepsilon^M \right\| \leq C \left\| F_\varepsilon^M \right\|.$$

Combining these, we obtain

$$\left\| \frac{d}{d\varepsilon} F_\varepsilon^M \right\| \leq \left(1 + \hbar^{-\beta/2} \varepsilon^{-1/2} \left\| F_\varepsilon^M \right\|^{1/2} + \left\| F_\varepsilon^M \right\| \right). \tag{21}$$

By (13) and (14), we learn

$$\left\| F_\varepsilon^M \right\| \leq \left\| G_\varepsilon^M \right\| \leq C\hbar^{-\beta} \varepsilon^{-1}. \tag{22}$$

(21) and (22) imply $\| \frac{d}{d\varepsilon} F_\varepsilon^M \| \leq C \left(1 + \hbar^{-\beta} \varepsilon^{-1} \right)$. Integrating this, we obtain

$$\begin{aligned} \left\| F_\varepsilon^M \right\| &\leq C\hbar^{-\beta} \varepsilon_0^{-1} + C \int_\varepsilon^{\varepsilon_0} \left(1 + \hbar^{-\beta} \nu^{-1} \right) d\nu \\ &\leq C\hbar^{-\beta} (1 + |\log \varepsilon|). \end{aligned}$$

We substitute this to (21) and integrate again:

$$\left\| F_\varepsilon^M \right\| \leq C\hbar^{-\beta} + C\hbar^{-\beta} \int_0^{\varepsilon_0} (1 + |\log \varepsilon|) d\varepsilon \leq C\hbar^{-\beta}.$$

This proves (18) and (19) follows from (18) and (20). ∎

For $m \geq 2$ we set

$$C_m(\varepsilon) = \sum_{j=1}^{m} \frac{(-i\varepsilon)^j}{j!} B_j, \qquad \varepsilon > 0,$$

which is bounded from $D(H)$ to $\mathcal{H}$.

LEMMA 8. *There is $\varepsilon_0 > 0$ such that $(H + C_m(\varepsilon) - z)$ has a bounded inverse $G_\varepsilon(z)$ for $0 \leq \varepsilon \leq \varepsilon_0$ and $z \in \Omega_\pm$. $G_\varepsilon(z)$ is continuous in ε for $0 \leq \varepsilon \leq \varepsilon_0$ and smooth for $0 < \varepsilon \leq \varepsilon_0$. Moreover, it satisfies*

$$\| G_\varepsilon \| + \| H G_\varepsilon \| \leq C\hbar^{-\beta} \varepsilon^{-1}, \tag{23}$$

$$\| G_\varepsilon \rho \| + \| H G_\varepsilon \rho \| \leq C\hbar^{-\beta} \varepsilon^{-1/2}. \tag{24}$$

PROOF: We construct G_ε following [JMP]. (14) implies $\left\|\varepsilon B_1 f G_\varepsilon^M \tilde{f}\right\| \leq C\hbar\varepsilon$. Hence

$$G_\varepsilon^0(z) = G_\varepsilon^M - G_\varepsilon^M \tilde{f}\left(1 - i\varepsilon B_1 f G_\varepsilon^M \tilde{f}\right)^{-1}(-i\varepsilon B_1) f G_\varepsilon^M$$

is bounded, and it is an inverse to $(H - i\varepsilon B_1 f)$ if ε is sufficiently small. Moreover, by (13), (14) and (19), we learn that estimates (23)–(24) hold for G_ε^0 and

$$\left\|\tilde{f} G_\varepsilon^0\right\| + \left\|H\tilde{f}G_\varepsilon^0\right\| \leq C. \tag{25}$$

Now (25) implies $\left\|\varepsilon\tilde{f}G_\varepsilon^0 B_1\right\| \leq C\hbar\varepsilon$, and hence

$$G_\varepsilon^1 = G_\varepsilon^0 - G_\varepsilon^0(-i\varepsilon B_1)\left(1 + \tilde{f}G_\varepsilon^0(-i\varepsilon B_1)\right)^{-1}\tilde{f}G_\varepsilon^0$$

is bounded, and it is an inverse to $(H - i\varepsilon B_1 - z)$. Moreover, estimates (23)–(25) hold for G_ε^1.

At last, noting

$$\begin{aligned}\left\|(C_m(\varepsilon) - (-i\varepsilon)B_1)G_\varepsilon^1\right\| &\leq \left\|(C_m - (-i\varepsilon)B_1)(H+i)^{-1}\right\|\left\|(H+i)G_\varepsilon^1\right\| \\ &\leq C\hbar^2\varepsilon^2 \cdot C\hbar^{-\beta}\varepsilon^{-1} \leq C\hbar^{2-\beta}\varepsilon \leq C\varepsilon,\end{aligned}$$

we learn that

$$G_\varepsilon = G_\varepsilon^1 - G_\varepsilon^1\left(1 + (C_m - (-i\varepsilon)B_1)G_\varepsilon^1\right)^{-1}(C_m - (-i\varepsilon)B_1)G_\varepsilon^1$$

is bounded and it is an inverse to $(H + C_m - z)$. Now (23)–(24) follow easily from the corresponding estimates for G_ε^1. The smoothness in $\varepsilon > 0$ follows from the H-boundedness of B_j. ∎

LEMMA 9. *Let $G_\varepsilon(z)$ as in Lemma 8. Then*

$$\frac{d}{d\varepsilon}G_\varepsilon = (-i)[G_\varepsilon, iA] + i\frac{(-i\varepsilon)^m}{m!}G_\varepsilon B_{m+1}G_\varepsilon. \tag{26}$$

PROOF: We first note $\frac{d}{d\varepsilon}G_\varepsilon = -G_\varepsilon\left(\frac{d}{d\varepsilon}C_m(\varepsilon)\right)G_\varepsilon$, and

$$\begin{aligned}\frac{d}{d\varepsilon}C_m(\varepsilon) &= \frac{d}{d\varepsilon}\sum_{j=1}^m \frac{(-i\varepsilon)^j}{j!}B_j = (-i)\sum_{j=1}^m \frac{(-i\varepsilon)^{j-1}}{(j-1)!}B_j \\ &= -iB_1 + (-i)\sum_{j=1}^m \frac{(-i\varepsilon)^j}{j!}B_{j+1} - (-i)\frac{(-i\varepsilon)^m}{m!}B_{m+1} \\ &= (-i)[H + C_m - z, iA] + i\frac{(-i\varepsilon)^m}{m!}B_{m+1}.\end{aligned}$$

(23) follows from this and $[G_\varepsilon, iA] = -G_\varepsilon[H + C_m - z, iA]G_\varepsilon$. ∎

PROOF OF THEOREM 1: Since the case $n = 1$ is already known, we may suppose $n \geq 2$ and hence $s > n - 1/2 > 1$. Let $m \geq \beta(n+1) - 1$ and let $G_\varepsilon = (H - C_m - z)^{-1}$, $F_\varepsilon = \rho^s (G_\varepsilon)^n \rho^s$. We compute its derivative in ε:

$$\begin{aligned}
\frac{d}{d\varepsilon} F_\varepsilon &= \rho^s \frac{d}{d\varepsilon}(G_\varepsilon)^n \rho^s = \rho^s \sum_{j=0}^{n-1} {G_\varepsilon}^j \left(\frac{d}{d\varepsilon} G_\varepsilon\right) {G_\varepsilon}^{n-j-1} \rho^s \\
&= -i \sum_{j=0}^{n-1} \rho^s {G_\varepsilon}^j [G_\varepsilon, iA] {G_\varepsilon}^{n-1-j} \rho^s + i \frac{(-i\varepsilon)^m}{m!} \sum_{j=0}^{n-1} \rho^s {G_\varepsilon}^{j+1} B_{m+1} {G_\varepsilon}^{n-j} \rho^s \\
&= -i\rho^s \left[{G_\varepsilon}^n, iA\right] \rho^s + i \frac{(-i\varepsilon)^m}{m!} \sum_{j=0}^{n-1} \rho^s {G_\varepsilon}^{j+1} B_{m+1} {G_\varepsilon}^{n-j} \rho^s \\
&\equiv I + II.
\end{aligned}$$

We estimate II using Lemma 8:

$$\begin{aligned}
\|II\| &\leq C\varepsilon^m \sum_{j=0}^{n-1} \|\rho G_\varepsilon\| \left\|{G_\varepsilon}^j\right\| \left\|B_{m+1}(H+i)^{-1}\right\| \left\|(H+i){G_\varepsilon}^{n-j-1}\right\| \|G_\varepsilon \rho\| \\
&\leq C\varepsilon^m \sum_{j=1}^{n-1} \hbar^{-\beta}\varepsilon^{-1/2} \left(\hbar^{-\beta}\varepsilon^{-1}\right)^j \hbar^{m+1} \left(\hbar^{-\beta}\varepsilon^{-1}\right)^{n-j-1} \hbar^{-\beta}\varepsilon^{-1/2} \\
&\leq C\hbar^{(m+1)-(n+1)\beta}\varepsilon^{m-n} \leq C.
\end{aligned}$$

In the last step we have used the condition: $m + 1 \geq (n+1)\beta$. The other term is

$$\begin{aligned}
\|I\| &\leq 2\left\|\rho^s {G_\varepsilon}^n A \rho^s\right\| \leq 2\left\|\rho^{s-1} {G_\varepsilon}^n \rho^s\right\| \leq 2\left\|\rho^s {G_\varepsilon}^n \rho^s\right\|^{1-1/s} \left\|{G_\varepsilon}^n \rho^s\right\|^{1/s} \\
&\leq C\left\|F_\varepsilon\right\|^{1-1/s} \left(\left(\hbar^{-\beta}\varepsilon^{-1}\right)^{n-1} \left(\hbar^{-\beta}\varepsilon^{-1/2}\right)\right)^{1/s} \\
&\leq C\hbar^{-n\beta/s}\varepsilon^{-(n-1/2)/s} \left\|F_\varepsilon\right\|^{1-1/s}.
\end{aligned}$$

Combining these we have

$$\left\|\frac{dF_\varepsilon}{d\varepsilon}\right\| \leq C\left(1 + \hbar^{-n\beta/s}\varepsilon^{-(n-1/2)/s} \left\|F_\varepsilon\right\|^{1-1/s}\right). \tag{27}$$

On the other hand, Lemma 8 implies

$$\|F_\varepsilon\| \leq C\|\rho G_\varepsilon\| \|G_\varepsilon\|^{n-2} \|G_\varepsilon \rho\| \leq C\hbar^{-n\beta}\varepsilon^{-(n-1)}.$$

If we substitute $\|F_\varepsilon\| \le C\hbar^{-n\beta}\varepsilon^{-\gamma}$, $\gamma > 0$, to (27), by integration by parts we obtain

$$\|F_\varepsilon\| \le C\hbar^{-n\beta}\varepsilon^{-\gamma(1-1/s)-(n-1/2)/s+1} \le C\hbar^{-n\beta}\varepsilon^{-\gamma+(1-(n-1/2)/s)}.$$

Since $1 > (n-1/2)/s$, finitely many iterations give us $\|F_\varepsilon\| \le C\hbar^{-n\beta}$ for any $0 < \varepsilon \le \varepsilon_0$. Hence

$$\sup_{z\in\Omega_\pm} \left\|\rho^s(H-z)^{-n}\rho^s\right\| \le \sup_{z\in\Omega_\pm}\sup_{\varepsilon\in(0,\varepsilon_0]} \|\rho^s G_\varepsilon{}^n\rho^s\| \le C\hbar^{-n\beta}.$$

Since the existence of the boundary value is proved in [JMP], this completes the proof. ∎

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