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Scattering Theory for the Shape Resonance Model I. Non-Resonant Energies

by

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ABSTRACT. — We consider the semi-classical behavior of scattering matrix for the shape resonance model (cf. (3)), and we show that if the energy is non-resonant i.e. it is separated from the eigenvalues coming from the potential wells by some power of the Planck constant h , the effect of the wells on the scattering matrix is exponentially small in h^{-1} . The exponent is given by the Agmon distance between the wells and the exterior region. This implies, in particular, the quasi-classical expansion is valid for such energies (cf. [17], [18], [24], [25]).

RÉSUMÉ. — Nous étudions le comportement semi-classique de la matrice de diffusion pour le modèle de résonance de forme (voir (3)) et nous montrons que si l'énergie est non résonante, c'est-à-dire si elle est à une distance des valeurs propres du puits de potentiel au moins de l'ordre d'une puissance de la constante de Planck, l'effet des puits sur la matrice de diffusion est exponentiellement petit en h^{-1} . L'exposant est donné par la distance de Agmon entre les puits et la région extérieure. Ce résultat implique en particulier que le développement quasi-classique est valable pour de telles énergies.

§ 1. INTRODUCTION

We consider Schrödinger operators:

$$H = H_0 + V(x), \quad H_0 = -h^2 \Delta$$

on $\mathcal{H} = L^2(\mathbb{R}^n)$, $D(H_0) = H^2(\mathbb{R}^n)$, where h is the Planck constant. We assume for some $\alpha > 1$,

ASSUMPTION (A) $_{\alpha}$. — $V(x)$ is real-valued, continuous and satisfies

$$|V(x)| \leq C(1 + |x|)^{-\alpha} \quad (x \in \mathbb{R}^n).$$

We set $\Omega_{\text{int}} \subset \mathbb{R}^n$ so that $K = \partial\Omega_{\text{int}}$ is smooth and $\inf_{x \in K} V(x) > 0$. Let $\Omega_{\text{ext}} = \mathbb{R}^n \setminus \overline{\Omega_{\text{int}}}$ and $\lambda_0 = \inf_{x \in K} V(x)$. We shall consider energy λ in $(0, \lambda_0)$. For $\lambda \in (0, \lambda_0)$, we write

$$\mathcal{I}(\lambda) = \{x \in \mathbb{R}^n \mid V(x) > \lambda\},$$

then $\mathcal{I}(\lambda) \supset K$. Let Δ^D denote the Laplacian with Dirichlet boundary condition on K i. e.

$$D(\Delta^D) = H_0^1(\mathbb{R}^n \setminus K) \cap H^2(\mathbb{R}^n \setminus K)$$

and let

$$H^D = -h^2\Delta^D + V(x) = H_{\text{int}} \oplus H_{\text{ext}}$$

on $L^2(\mathbb{R}^n) = L^2(\Omega_{\text{int}}) \oplus L^2(\Omega_{\text{ext}})$, $D(H^D) = (H_0^1 \cap H^2)(\Omega_{\text{int}}) \oplus (H_0^1 \cap H^2)(\Omega_{\text{ext}})$. We write $L^{2,\beta}(\mathbb{R}^n)$ ($L^{2,\beta}(\Omega_{\text{ext}})$) for the weighted L^2 -space of order β en \mathbb{R}^n (Ω_{ext} respectively): $L^{2,\beta}(\mathbb{R}^n) = \{f \in \mathcal{S}' \mid (1 + |x|^2)^{\beta/2} f(x) \in L^2(\mathbb{R}^n)\}$. For $I \subset \subset (0, \lambda_0)$, we assume

ASSUMPTION (B) $_I$. — For any $h \in (0, 1)$, $\beta > 1/2$ and $\mu \in I$,

$$\lim_{\varepsilon \downarrow 0} (H_{\text{ext}} - (\mu \pm i\varepsilon))^{-1} = (H_{\text{ext}} - (\mu \pm i0))^{-1}$$

exists uniformly in μ as an operator from $L^{2,\beta}(\Omega_{\text{ext}})$ to $L^{2,-\beta}(\Omega_{\text{ext}})$. Moreover, for some $p > 0$

$$\|(H_{\text{ext}} - (\mu \pm i0))^{-1}\|_{B(L^{2,\beta}, L^{2,-\beta})} \leq Ch^{-p} \quad (\mu \in I). \quad (1.1)$$

This assumption can be considered as a variation of so-called « non-trapping condition ». In fact (B) $_I$ follows from the non-trapping conditions of Robert-Tamura [18] or Klein [13], [3], with $p = 1$ (see Appendix for the proof).

On the other hand, it is wellknown that H_{int} has discrete spectrum. For $a, q > 0$, we set $\mathcal{E}(a, q; h) = \{\mu \in \mathbb{R} \mid \exists v \in \sigma(H_{\text{int}}), |v - \mu| \leq ah^q\}$.

We consider two sets of wave operators:

$$W_{\pm}(H, H_0) = s\text{-}\lim_{t \rightarrow \pm\infty} e^{itH} e^{-itH_0} \quad ;$$

$$W_{\pm}(H^D, H_0) = s\text{-}\lim_{t \rightarrow \pm\infty} e^{itH^D} e^{-itH_0} \quad ,$$

and scattering operators:

$$S(H, H_0) = W_+(H, H_0) * W_-(H, H_0); \quad S(H^D, H_0) = W_+(H^D, H_0) * W_-(H^D, H_0).$$

Let $\Sigma = L^2(S^{n-1})$, $\mathbb{R}_+ = (0, \infty)$ and let $F_0: L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}_+, dx; \Sigma)$ be defined by

$$(F_0 f)(\lambda)(\omega) = 2^{-1/2} \lambda^{(n-2)/4} (\mathcal{F}^h f)(\lambda^{1/2} \omega) \quad (\lambda \in \mathbb{R}_+, \omega \in S^{n-1}), \quad (1.2)$$

where \mathcal{F}^h is the Fourier transform:

$$(\mathcal{F}^h f)(\xi) = (2\pi h)^{-n/2} \int e^{-ix\xi/h} f(x) dx.$$

Then F_0 is unitary and $(F_0, L^2(\mathbb{R}_+, dx; \Sigma))$ gives a spectral representation of H . Since $S(H, H_0)$ commutes with H_0 , scattering matrix $S(H, H_0; \lambda) \in \mathbf{B}(\Sigma)$ can be defined by the following equation:

$$S(H, H_0; \lambda)(F_0 f)(\lambda) = (F_0 S(H, H_0) f)(\lambda) \quad (1.3)$$

for almost all $\lambda \in \mathbb{R}_+$. $S(H^D, H_0; \lambda) \in \mathbf{B}(\Sigma)$ is defined analogously.

The main result in this paper is stated as follows:

THEOREM 1. — Suppose $(A)_\alpha$ ($\alpha > 1$) and $(B)_I$ for $I \subset\subset (0, \lambda_0)$. Then for any $\alpha > 0$, $q > 0$ and $\varepsilon > 0$, there is $C > 0$ such that if h is sufficiently small and $\lambda \in I \setminus \mathcal{E}(a, q; h)$,

$$\|S(H, H_0; \lambda) - S(H^D, H_0; \lambda)\| \leq C \exp \{ -2(\mathbf{d}_\lambda(K, \Omega_{\text{ext}} \setminus \mathcal{I}(\lambda)) - \varepsilon)/h \} \quad (1.4)$$

where $\mathbf{d}_\lambda(\cdot, \cdot)$ is the pseudo-distance associated with the Agmon metric $ds^2 = \max(0, V(x) - \lambda) \cdot dx^2$.

If $(A)_\alpha$ holds for $\alpha > (n+1)/2$, it is well-known that $S(H, H_0; \lambda)$ ($S(H^D, H_0; \lambda)$) has integral kernel: $S(H, H_0; \lambda, \omega, \omega')$ ($S(H^D, H_0; \lambda, \omega, \omega')$ respectively) ($\omega, \omega' \in S^{n-1}$), and Theorem 1 can be improved:

THEOREM 2. — Suppose $(A)_\alpha$ with $\alpha > (n+1)/2$ and $(B)_I$ for $I \subset\subset (0, \lambda_0)$. Then for any $a > 0$, $q > 0$ and $\varepsilon > 0$, there is $C > 0$ such that if h is sufficiently small and $\lambda \in I \setminus \mathcal{E}(a, q; h)$,

$$\begin{aligned} |S(H, H_0; \lambda, \omega, \omega') - S(H^D, H_0; \lambda, \omega, \omega')| \\ \leq C \exp \{ -2(\mathbf{d}_\lambda(K, \Omega_{\text{ext}} \setminus \mathcal{I}(\lambda)) - \varepsilon)/h \} \end{aligned} \quad (1.5)$$

uniformly in $\omega, \omega' \in S^{n-1}$.

REMARK 1.1. — Let us consider two potential functions V_1 and V_2 such that they satisfy $(A)_\alpha$ and $(B)_I$, and they coincide in Ω_{ext} . Theorem 1 implies

$$\|S(H_0 + V_1; \lambda) - S(H_0 + V_2; \lambda)\| \leq C \exp \{ -2(\mathbf{d}_\lambda(K, \Omega_{\text{ext}} \setminus \mathcal{I}(\lambda)) - \varepsilon)/h \}$$

if for some $a, q > 0$, $\text{dist}(\lambda, \sigma((H_0 + V_1)_{\text{int}}) \cup \sigma((H_0 + V_2)_{\text{int}})) \geq ah^q$ ($\lambda \in I$). Moreover, if $\inf_{x \in \Omega_{\text{int}}} V_2(x) > \sup I$ and I is non-trapping in the sense of Robert-Tamura [18], $\sigma((H_0 + V_2)_{\text{int}}) \cap I = \emptyset$ and the semi-classical asymptotics of several quantities related to $S(H_0 + V_2, H_0; \lambda)$ can be computed

([17], [18], [26]). Hence we can obtain the asymptotics of these quantities for $S(H_0 + V_1, H_0; \lambda)$ if λ is non-resonant i. e. $\text{dist}(\lambda, \sigma((H_0 + V_1)_{\text{int}})) > ah^q$.

If we can deform K to be very close to $\Omega_{\text{int}} \setminus \mathcal{J}(\lambda)$ for fixed energy λ , we can elaborate on Theorem 1. For example, if $\partial\mathcal{J}(\lambda) \cap \Omega_{\text{int}}$ is smooth and $|\nabla V(x)| \neq 0$ on $\partial\mathcal{J}(\lambda) \cap \Omega_{\text{int}}$, then $\partial\mathcal{J}(\lambda + \delta) \cap \Omega_{\text{int}}$ is also smooth for small $\delta > 0$ (in fact, they are diffeomorphic by the implicit function theorem) Moreover, we have

$$\mathbf{d}_\lambda(\Omega_{\text{int}} \setminus \mathcal{J}(\lambda), \partial\mathcal{J}(\lambda + \delta) \cap \Omega_{\text{int}}) = \mathbf{d}_\lambda(\partial\mathcal{J}(\lambda) \cap \Omega_{\text{int}}, \partial\mathcal{J}(\lambda + \delta) \cap \Omega_{\text{int}}) = O(\delta^2).$$

If we take δ to be sufficiently small relative to ε , this implies

$$\begin{aligned} \mathbf{d}_\lambda(\partial\mathcal{J}(\lambda + \delta) \cap \Omega_{\text{int}}, \Omega_{\text{ext}} \setminus \mathcal{J}(\lambda)) & \\ & \geq \mathbf{d}_\lambda(\Omega_{\text{int}} \setminus \mathcal{J}(\lambda), \Omega_{\text{ext}} \setminus \mathcal{J}(\lambda)) - \mathbf{d}_\lambda(\partial\mathcal{J}(\lambda + \delta) \cap \Omega_{\text{int}}, \Omega_{\text{int}} \setminus \mathcal{J}(\lambda)) \\ & \geq \mathbf{d}_\lambda(\Omega_{\text{int}} \setminus \mathcal{J}(\lambda), \Omega_{\text{ext}} \setminus \mathcal{J}(\lambda)) - \varepsilon/2. \end{aligned}$$

We set $\tilde{\Omega}_{\text{int}} = \Omega_{\text{int}} \setminus \mathcal{J}(\lambda + \delta)$, $\tilde{\Omega}_{\text{ext}} = \mathbb{R}^n \setminus \tilde{\Omega}_{\text{int}}$, and $\tilde{K} = \partial\tilde{\Omega}_{\text{int}}$ (note that they depends on λ and δ). Let $\tilde{H}^D = \tilde{H}^D(\lambda, \delta) = \tilde{H}_{\text{int}} \oplus \tilde{H}_{\text{ext}}$ be the Hamiltonian with Dirichlet condition on \tilde{K} . Now, combining the above argument with Theorem 1, we obtain the following corollary:

COROLLARY 1.2. — *Suppose the assumptions of Theorem 1 and let $\lambda \in I$ be fixed. Suppose moreover that $\partial\mathcal{J}(\lambda) \cap \Omega_{\text{int}}$ is smooth and $\nabla V(x) \neq 0$ on $\partial\mathcal{J}(\lambda) \cap \Omega_{\text{int}}$. Then for any a, q and $\varepsilon > 0$, there are $\delta, C > 0$ and a neighborhood I' of λ such that if h is sufficiently small and $\mu \in I' \setminus \mathcal{E}'(a, q; h) := I' \setminus \{ \mu \in \mathbb{R} \mid \exists v \in \sigma(\tilde{H}_{\text{int}}), |\mu - v| < ah^q \}$,*

$$\begin{aligned} \| S(H, H_0; \mu) - S(\tilde{H}^D, H_0; \mu) \| & \\ & \leq C \exp \{ - 2(\mathbf{d}_\lambda(\Omega_{\text{int}} \setminus \mathcal{J}(\mu), \Omega_{\text{ext}} \setminus \mathcal{J}(\mu)) - \varepsilon)/h \}. \end{aligned}$$

Note that since the change of $\sigma(H_{\text{int}}) \cap (-\infty, \lambda + \delta/2)$ is exponentially small in h^{-1} if one deform K in $\mathcal{J}(\lambda + \delta)$ (cf. e. g. [9]), $\mathcal{E}'(a, q; h)$ is essentially the same as $\mathcal{E}(a, q; h)$ on I' .

Of course, Theorem 2 can be elaborated on similarly.

On the shape resonance problem, we mention a work by Ashbaugh and Harrell [2] for one-dimensional case. Higher dimensional problem was treated by Combes, Duclos, Klein and Seiler [3] (see also [5], [13]), and by Helffer and Sjöstrand [10]. Combes and others considered the location of resonance eigenvalues for exterior-dilatation analytic potentials, and this work has been inspired by their paper. Shape resonance problem is closely related to the tunneling effect problem for eigenvalues, and it was studied by Harrell [7], Combes, Duclos and Seiler [4] for one-dimensional case, and by Simon [20], Helffer and Sjöstrand [9] for higher dimensional case (see also [8], [21]).

Semi-classical limit of scattering matrix has been studied by many authors, and we only mention some recent results for non-trapping energies. Robert

and Tamura obtained the asymptotics of total cross-sections using their semi-classical resolvent estimate ([17], [18]), and Yajima obtained the asymptotics for off-diagonal elements of scattering matrix under certain conditions ([26]). We also refer to [6], [19], [22], [23], [24] and [25].

In Sect. 2, we prepare some results concerning Krein's formula and two space scattering theory. We study $W_{\pm}(H^D, H_0)$ and $W_{\pm}(H, H^D)$ in Sect. 3 and Sect. 4 respectively. In particular, exponential decay of generalized eigenfunction for H^D is proved in Sect. 3 and a representation formula for $S(H, H^D)$ is given in Sect. 4. Then we prove Theorems 1 and 2 in Sect. 5. Sufficient conditions for $(B)_1$ are given in Appendix.

In part II of this series, we shall consider the asymptotic behavior of scattering matrix near resonance eigenvalues combining the methods of [3] and this paper.

§ 2. PRELIMINARIES

2.1. Krein's formula.

$T_{\text{int}}(T_{\text{ext}})$ denotes the trace operator from $H^{\gamma}(\Omega_{\text{int}})(H^{\gamma}(\Omega_{\text{ext}}))$ respectively with $\gamma > 1/2$, to $L^2(K)$; $T_{\text{int/ext}}f(x) = f(x)$ ($x \in K$). In the case $T_{\text{int}}f = T_{\text{ext}}f$ for $f \in H^{\gamma}(\Omega_{\text{int}}) \in H^{\gamma}(\Omega_{\text{ext}})$, we write $Tf = T_{\text{int}}f = T_{\text{ext}}f$.

Following [3], we introduce $A(z)$ and $B(z)$ ($z \in \mathbb{C} \setminus \mathbb{R}$):

$$\begin{aligned} A(z) &= T(H - z)^{-1} : L^2(\mathbb{R}^n) \rightarrow L^2(K), \\ B(z) &= B_{\text{int}}(z) + B_{\text{ext}}(z) : L^2(\mathbb{R}^n) = L^2(\Omega_{\text{int}}) \oplus L^2(\Omega_{\text{ext}}) \rightarrow L^2(K), \\ B_{\text{int}}(z) &= -T_{\text{int}}\nabla_n(H_{\text{int}} - z)^{-1} : L^2(\Omega_{\text{int}}) \rightarrow L^2(K), \\ B_{\text{ext}}(z) &= T_{\text{ext}}\nabla_n(H_{\text{ext}} - z)^{-1} : L^2(\Omega_{\text{ext}}) \rightarrow L^2(K) \end{aligned}$$

where ∇_n denotes the derivative with respect to the outer normal unit vector of $K = \partial\Omega_{\text{int}}$. We write $R(z) = (H - z)^{-1}$, $R^D(z) = (H^D - z)^{-1}$ and $W(z) = R(z) - R^D(z)$.

PROPOSITION 2.1 (Krein's formula, [3]). — For $z \in \mathbb{C} \setminus \mathbb{R}$

$$W(z) = h^2 A(\bar{z}) * B(z) \quad (2.1)$$

$$= h^4 B(\bar{z}) * TR(z) T * B(z). \quad (2.2)$$

Proof (cf. [3], Appendix II). — We set $\hat{u} = R(\bar{a})u$, $\hat{v} = R^D(a)v$ for $u, v \in L^2(\mathbb{R}^n)$, Then

$$(u, (R(a) - R^D(a))v) = -h^2 \{ (\hat{u}, \Delta^D \hat{v}) - (\Delta \hat{u}, \hat{v}) \}$$

and Green's formula gives (2.1) since $T_{\text{int}} \hat{v} = T_{\text{ext}} \hat{v} = 0$. Iterating (2.1) and using $T_{\text{int}} R^D(a) = T_{\text{ext}} R^D(a) = 0$, we obtain (2.2). \square

PROPOSITION 2.2. — Suppose $(A)_\alpha$ ($\alpha > 1$) and $(B)_I$ ($I \subset \subset (0, \lambda_0)$). Let $a(h)$ be a complex-valued function of h such that $\text{Im } a(h) > 0$; $\text{Re } a(h) \rightarrow \lambda \in I$; $(\text{Im } a(h))^{-1} = O(h^{-r})$ ($h \downarrow 0$) for some $r > 0$. Then for any $\beta > 0$

$$\|W(z)\|_{B(L^{2,-\beta}(\mathbb{R}^n), L^{2,\beta}(\mathbb{R}^n))} \leq C_\beta \quad (h \in (0, 1)). \quad (2.3)$$

Proof. — The outline of the proof is the same as that of Theorem III-3 of [3] and we only sketch it.

1) Instead of Lemma III-4 of [3], we employ

$$\|T_{\text{int/ext}} f\|^2 \leq C \|\chi f\| \|\nabla \chi f\| \quad (2.4)$$

where χ is a C_0^∞ -function so that $\chi = 1$ on K .

2) We choose χ so that $\chi = 1$ on K and for some $\delta > 0$, $V(x) \geq \lambda + 2\delta$ if $x \in \text{supp } (\chi)$.

3) The next estimate can be proved by the standard argument using commutators (cf. Lemma 1 of § XIII-8 [16]): for any $\beta > 0$,

$$\|(H^D - z)^{-1}\|_{B(L^{2,-\beta}, L^{2,-\beta})} \leq C(1 + |\text{Im } z|^{-N}) \quad (2.5)$$

with some C and N . Hence we have

$$\|f(H^D - a(h))^{-1}u\| \leq Ch^{-rN} \|u\|_{L^{2,-\beta}}. \quad (2.6)$$

for any $f \in C_0^\infty(\mathbb{R}^n)$.

4) We note a quadratic estimate:

$$\delta \|\chi \hat{u}\|^2 + h^2 \|\nabla \chi \hat{u}\|^2 \leq \text{Re}(\chi \hat{u}, \chi u) + h^2 \|\nabla \chi \hat{u}\|^2$$

($\hat{u} = R^D(a)u$) which follows from the identity: $\text{Re } \chi(H^D - a)^D = \chi(H^D - \text{Re } a)\chi - h^2(\nabla \chi)^2$ (cf. (3.8) of [3]). Then combining the estimate with (2.6), we have $\|\chi \hat{u}\| \leq C_1(1 + h^{-rN+1}) \|u\|_{L^{2,-\beta}}$. Iterating this procedure, we obtain

$$\|\chi R^D(a)u\| \leq C_2 \|u\|_{L^{2,-\beta}}.$$

Similarly, we can prove

$$\begin{aligned} \|\nabla \chi R^D(a)u\| &\leq C_3 h^{-1} \|u\|_{L^{2,-\beta}}; \\ \|\nabla \chi V R^D(a)u\| &\leq C_4 h^{-1} \|u\|_{L^{2,-\beta}}. \end{aligned}$$

These estimates and (2.4) yield

$$\|B(a)u\| \leq C_5 h^{-3/2} \|u\|_{L^{2,-\beta}}. \quad (2.7)$$

5) An analogous argument can be applied to $R(a)$ to conclude

$$\|TR(a)T^*\|_{B(L^2(K))} \leq C_6 h^{-1}. \quad (2.8)$$

(2.3) follows from (2.2), (2.7) and (2.8).

2.2. Two Hilbert space scattering theory.

Here we give some notations and propositions on two Hilbert space scattering theory (cf. [11]).

Let H_i be a self-adjoint operator on a Hilbert space \mathcal{H}_i ($i = 1, 2$), and

let J be a bounded operator from \mathcal{H}_1 to \mathcal{H}_2 . The wave operator $W_{\pm}(H_1, H_2, J) \in \mathcal{B}(\mathcal{H}_1, H_2)$ is defined by

$$W_{\pm}(H_1, H_2, J) = s\text{-}\lim_{t \rightarrow \pm\infty} e^{itH_2} J e^{-itH_1} E_{ac}(H_1) \quad (2.9)$$

where $E_{ac}(H_i)$ is the orthogonal projection into the absolutely continuous subspace for H_i . Scattering operator $S(H_2, H_1, J) \in \mathcal{B}(\mathcal{H}_1)$ is defined by

$$S(H_2, H_1, J) = W_+(H_2, H_1, J) * W_-(H_2, H_1, J).$$

If $J_1, J_2 \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$ and $J_2 - J_1$ is H_1 -compact, then it is easy to see

$$W_{\pm}(H_2, H_1, J_1) = W_{\pm}(H_2, H_1, J_2). \quad (2.10)$$

For example, if $H_1 = H_2 = L^2(\mathbb{R}^n)$, $H_1 = -h^2\Delta$, $J_1 = 1$ and $J_2 - 1$ is a multiplication operator by a C_0^∞ -function, then (2.10) holds.

If J and H_1 satisfy

$$\lim_{t \rightarrow \pm\infty} \| J e^{-itH_1} E_{ac}(1) \varphi \| = \| E_{ac}(H_1) \varphi \| \quad (\forall \varphi \in \mathcal{H}_1), \quad (2.11)$$

then $W_{\pm}(H_1, H_2, J)$ is partially isometric.

Let H_i be a self-adjoint operator on \mathcal{H}_i for $i = 1, 2, 3$, and let $J_i \in \mathcal{B}(\mathcal{H}_i, \mathcal{H}_{i+1})$ for $i = 1, 2$. Then it is easy to verify the chain rule (if they exist):

$$W_{\pm}(H_3, H_2, J_2 J_1) = W_{\pm}(H_3, H_2, J_2) W_{\pm}(H_2, H_1, J_1); \quad (2.12)$$

$$S(H_3, H_1, J_2 J_1) = W_+(H_2, H_1, J_1) * S(H_3, H_2, J_2) W_-(H_2, H_1, J_1). \quad (2.13)$$

At last we give a two space analogue of the well-known Lippman-Schwinger equation: we suppose

ASSUMPTION (D1). — X_i is a Banach space and it is densely embedded in \mathcal{H}_i ($i = 1, 2$).

We will consider \mathcal{H}_i as a subspace of X_i^* .

ASSUMPTION (D2)_I. — For an open interval $I \subset \mathbb{R}$, there exist a Hilbert space S and an operator $F: \mathcal{H}_1 \rightarrow L^2(I, dx; S)$ (S -valued L^2 -space on I) such that F is a spectral representation of H_1 on I . Moreover, for $f \in X_1$, $(Ff)(\lambda) = F(\lambda)f$ with $F(\lambda) \in \mathcal{B}(X_1, S)$ ($\lambda \in I$), and $\|F(\lambda)\|_{\mathcal{B}(X_1, S)}$ is uniformly bounded on I .

Remark that (D2)_I implies *i*) $F(\lambda)^* \in \mathcal{B}(S, X_1^*)$; *ii*) the absolute continuity of H_1 on I .

ASSUMPTION (D3). — $J \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$ satisfies *i*) $JD(H_1) \subset D(H_2)$; *ii*) J is extended to a bounded operator from X_1^* to X_2^* ; *iii*) if we set

$$T = H_2 J - J H_1 : D(H_1) \rightarrow \mathcal{H}_2, \quad (2.14)$$

$T(H_1 - i)^{-1}$ is extended to a bounded operator from X_1^* into X_2 .

ASSUMPTION (D4). — $W_{\pm}(H_2, H_1, J)$ exists.

ASSUMPTION (D5)_I. — On an open interval $I \subset \mathbb{R}$,

$$\lim_{\varepsilon \downarrow 0} (H_2 - (\lambda \pm i\varepsilon))^{-1} = (H_2 - (\lambda \pm i0))^{-1}$$

exists uniformly in $\lambda \in I$ as an operator from X_1 to X_2^* .

THEOREM 2.3. — Suppose (D1), (D2)_I, (D3), (D4) and (D5)_I for some open interval $I \subset \mathbb{R}$. Then for $\varphi \in X_1$,

$$W_{\pm}(H_2, H_1, J)E_I(H_1)\varphi = \int_I d\lambda \{ J_{\mp}(H_2 - (\lambda_{\pm} - i0))^{-1}T \} F(\lambda)^* F(\lambda)\varphi \quad (2.15)$$

where the integral is the Riemann integral in X_2^* . Moreover, if (2.11) holds, the scattering matrix $S(H_2, H_1, J; \lambda)$ is given by

$$S(H_2, H_1, J; \lambda) = 1 - 2\pi i F(\lambda) \{ T^*J - T^*(H_2 - (\lambda + i0))^{-1}T \} F(\lambda)^* \quad (2.16)$$

for $\lambda \in I$.

Of course, the scattering matrix is defined by (1.3) similarly. The proof is analogous to the standard argument of the abstract stationary scattering theory (cf. [12], [14]), and we omit it.

§ 3. $W_{\pm}(H^D, H_0)$ AND GENERALIZED EIGENFUNCTION EXPANSION FOR H_{ext} .

In order to apply Theorem 2.3 to $W_{\pm}(H^D, H_0)$, we introduce some notations. We have already defined $\Sigma = L^2(S^{n-1})$ and $F_0: L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}_+, dx; \Sigma)$ in Sect. 1. We set $\mathcal{X}_0 = L^{2, \alpha/2}(\mathbb{R}^n)$ where α is that in $(A)_{\alpha}$. Then they satisfy (D1) and (D2)_I for any $I \subset \subset \mathbb{R}_+$, $S = \Sigma$, $F = F_0$, $H_1 = H_0$ and $X_1 = \mathcal{X}_0$. Remark that $\mathcal{X}_0^* = L^{2, -\alpha/2}(\mathbb{R}^n)$ and V maps \mathcal{X}_0^* into \mathcal{X}_0 .

We choose $\tilde{J} \in C_0^{\infty}(\mathbb{R}^n)$ so that $\tilde{J} = 1$ on a neighborhood of $\overline{\Omega_{\text{int}}}$ and define $J = (1 - \tilde{J}(x)): L^2(\mathbb{R}^n) \rightarrow L^2(\Omega_{\text{ext}}) \subset L^2(\mathbb{R}^n)$. Since $\tilde{J}(x)$ is H_0 -compact, (2.10) implies $W_{\pm}(H^D, H_0) = W_{\pm}(H^D, H_0, J)$. By this representation, it is clear that $\text{Ran } W_{\pm}(H^D, H_0)$ is contained in $L^2(\Omega_{\text{ext}})$ and that

$$W_{\pm}(H^D, H_0) = O \oplus W_{\pm}(H_{\text{ext}}, H_0, J) \in B(L^2(\mathbb{R}^n), L^2(\Omega_{\text{int}}) \oplus L^2(\Omega_{\text{ext}})). \quad (3.1)$$

So we set $H_2 = L^2(\Omega_{\text{ext}})$, $X_2 = X_1 = L^{2, \alpha/2}(\Omega_{\text{ext}}) = L^{2, \alpha/2}(\mathbb{R}^n) \cap L^2(\Omega_{\text{ext}})$ and $H_2 = H_{\text{ext}}$. Then

$$T = H_{\text{ext}}J - JH_0 = [H_0, J] + JV.$$

If V satisfies $(A)_{\alpha}$ ($\alpha > 1$), $T(H_0 - i)^{-1}$ is bounded from \mathcal{X}_0^* to \mathcal{X}_1 . Thus (D3) follows from $(A)_{\alpha}$. (D4) also follows from $(A)_{\alpha}$, and $(B)_I$ implies (D5)_I.

PROPOSITION 3.1. — Suppose $(A)_\alpha$ ($\alpha > 1$) and $(D5)_1$ ($I \subset \subset \mathbb{R}_+$) with $H_2 = H_{\text{ext}}$ and $X_2 = L^{2,\alpha/2}(\Omega_{\text{ext}})$ as above. Then for $\varphi \in \mathcal{X}_0$,

$$W_\pm(H_{\text{ext}}, H_0, J)E_I(H_0)\varphi = \int_I d\mu \{ J - (H_{\text{ext}} - (\mu \mp i0))^{-1}T \} F_0(\mu)^* F_0(\mu)\varphi. \quad (3.2)$$

If we define

$$\Phi_\pm(\mu)\varphi = \{ J - (H_{\text{ext}} - (\mu \mp i0))^{-1}T \} F_0(\mu)^*\varphi \quad (3.3)$$

for $\varphi \in \Sigma$, we have

COROLLARY 3.2. — For $\varphi \in L^2(I, \Sigma)$,

$$W_\pm(H^D, H_0)F_0^*\varphi = \int_I d\mu \Phi_\pm(\mu)\varphi(\mu). \quad (3.4)$$

PROPOSITION 3.3. — Suppose $(A)_\alpha$ ($\alpha > 1$) and $(B)_1$ ($I \subset \subset (0, \lambda_0)$). Then for $\varphi \in \Sigma$ and $\lambda \in I$, $\Phi_\pm(\lambda)\varphi$ is a generalized eigenfunction of H_{ext} i. e. it is a λ -eigenfunction in distribution sense on Ω_{ext} , and satisfies Dirichlet boundary condition on K . Moreover, for any $\varepsilon > 0$, there is $C > 0$ such that

$$\| \Phi_\pm(\lambda)\varphi(x) \| \leq C \cdot e^{-\{\mathbf{d}_\lambda(x, \Omega_{\text{ext}} \setminus \mathcal{J}(\lambda)) - \varepsilon\}/h} \| \varphi \|_\Sigma \quad (3.5)$$

for $\lambda \in I$, $x \in \Omega_{\text{ext}} \cap \mathcal{J}(\lambda + \varepsilon)$ and $\varphi \in \Sigma$, where $\mathbf{d}_\lambda(\cdot, \cdot)$ is the pseudo-distance associated with the Agmon metric $ds^2 = \max(V(x) - \lambda, 0)dx^2$.

Proof. — Since $(H_0 - \lambda)F_0(\lambda)^*\varphi = 0$, the first statement follows easily from (3.3). The proof of (3.5) is essentially the same as that of the exponential decay of eigenfunctions by the Agmon method (Theorem 2.3 of [20], see also [1]), and we only sketch the idea.

1) $(B)_1$ implies

$$\begin{aligned} \| \Phi_\pm(\lambda)\varphi \|_{L^2(\Omega_{\text{ext}} \cap \mathcal{J}(\lambda))} &\leq C_1 \| \Phi_\pm(\lambda)\varphi \|_{L^{2, -\alpha/2}(\Omega_{\text{ext}})} \\ &\leq C_2 h^{-p} \| F_0(\lambda)^*\varphi \|_{L^{2, -\alpha/2}(\Omega_{\text{ext}})} \\ &\leq C_3 h^{-p} h^{-\alpha/2} \| \varphi \|_\Sigma. \end{aligned} \quad (3.6)$$

2) We can find a smooth function τ on $\Omega_{\text{ext}} \cap \mathcal{J}(\lambda)$ such that τ is very close to $\mathbf{d}_\lambda(x, \Omega_{\text{ext}} \setminus \mathcal{J}(\lambda))$ i. e. it satisfies

$$\begin{aligned} \mathbf{d}_\lambda(x, \Omega_{\text{ext}} \setminus \mathcal{J}(\lambda)) - \varepsilon &\leq \tau(x) \leq \mathbf{d}_\lambda(x, \Omega_{\text{ext}} \setminus \mathcal{J}(\lambda)) + \varepsilon; \\ | \nabla \tau(x) | &\leq (1 - \delta_1) (\max(V(x) - \lambda, 0))^{1/2}, \end{aligned}$$

for some $\delta_1 > 0$. Let η be a smooth cut-off function such that $\text{supp}(\eta) \subset \mathcal{J}(\lambda + \delta_2)$ for some δ_2 , and $\eta(x) = 1$ if $| \tau(x) | \geq 2\varepsilon$ or $x \in \mathcal{J}(\lambda + \varepsilon)$. Let $\psi = e^{\tau/h} \eta \Phi_\pm(\lambda)\varphi$, then $\psi \in L^2(\mathbb{R}^n)$.

3) By easy computations, we have

$$\begin{aligned} \text{Re}(e^{\tau/h}\psi, (H - \lambda)e^{-\tau/h}\psi) &= \text{Re}(\psi, \{ -(h\nabla - \nabla\tau)^2 + (V - \lambda) \} \psi) \\ &\geq (\psi, (V - \lambda - (\nabla\tau)^2)\psi) \geq \delta_1 \delta_2 \| \psi \|^2. \end{aligned}$$

Here we have used $\operatorname{Re}(\psi, \{(\nabla\tau)\nabla + \nabla(\nabla\tau)\}\psi) = 0$. Since $\Phi_{\pm}(\lambda)\varphi$ is a λ -generalized eigenfunction of H_{ext} , this implies

$$\operatorname{Re}(e^{2\tau/h}\eta\Phi_{\pm}(\lambda)\varphi, -h^2(\nabla\eta)(\nabla\Phi_{\pm}(\lambda)\varphi) - h^2(\Delta\eta)\Phi_{\pm}(\lambda)\varphi) \geq \delta_1\delta_2 \|e^{\tau/h}\eta\Phi_{\pm}(\lambda)\varphi\|^2, \quad (3.7)$$

but the left hand side term is bounded by $C \cdot h^{-p-\alpha/2+2} \cdot e^{4\varepsilon/h} \cdot \|\varphi\|_{\Sigma}^2$. Since $\Phi_{\pm}(\lambda)\varphi$ is subharmonic in $\mathcal{I}(\lambda)$, we conclude by (3.7).

$$|\Phi_{\pm}(\lambda)\varphi(x)| \leq Ce^{-\tau(x)-3\varepsilon/h} \|\varphi\|_{\Sigma} \leq C \exp\{-\langle \mathbf{d}_{\lambda}(x, \Omega_{\text{ext}} \setminus \mathcal{I}(\lambda)) - 4\varepsilon \rangle / h\}$$

on $\mathcal{I}(\lambda + \varepsilon)$. \square

COROLLARY 3.4. — *Under the same assumptions as in Proposition 3.3, for any $\varepsilon > 0$, there is $C > 0$ such that*

$$\|T_{\text{ext}}\nabla\Phi_{\pm}(\lambda)\varphi\|_{L^2(K)} \leq Ce^{-\langle \mathbf{d}_{\lambda}(K, \Omega_{\text{ext}} \setminus \mathcal{I}(\lambda)) - \varepsilon \rangle / h} \|\varphi\|_{\Sigma}. \quad (3.8)$$

Proof. — By Proposition 3.3, we see

$$\|\chi\Phi_{\pm}(\lambda)\varphi\| \leq Ce^{-\langle \mathbf{d}_{\lambda}(K, \Omega_{\text{ext}} \setminus \mathcal{I}(\lambda)) - \varepsilon \rangle / h} \|\varphi\|_{\Sigma}$$

if χ is supported in a sufficiently small neighborhood of K . Since $\Phi_{\pm}\varphi$ is a generalized eigenfunction of $H^{\mathbb{D}}$,

$$\|\chi\Delta\Phi_{\pm}(\lambda)\varphi\| = \|\chi h^{-2}(\lambda - V)\Phi_{\pm}(\lambda)\varphi\| \leq Ch^{-2}e^{-\langle \mathbf{d}_{\lambda}(K, \Omega_{\text{ext}} \setminus \mathcal{I}(\lambda)) - \varepsilon \rangle / h} \|\varphi\|_{\Sigma} \leq C'e^{-\langle \mathbf{d}_{\lambda}(K, \Omega_{\text{ext}} \setminus \mathcal{I}(\lambda)) - 2\varepsilon \rangle / h} \|\varphi\|_{\Sigma}.$$

This implies that the analogous estimates hold for $\|\nabla\chi\nabla\Phi_{\pm}(\lambda)\varphi\|$ and $\|\chi\nabla\Phi_{\pm}(\lambda)\varphi\|$. (3.8) then follows from (2.4) and these estimates. \square

Next we consider the case $\alpha > (n+1)/2$. We choose γ and δ so that $\alpha = \gamma + \delta$, $\gamma > n/2$ and $\delta > 1/2$. Let $\mathcal{X}_0 = L^{2,\gamma}(\mathbb{R}^n)$ and $\mathcal{X}_1 = L^{2,\delta}(\mathbb{R}^n)$, then the above arguments are also valid. Furthermore, $(F_0(\lambda)^*\delta_{\omega})(x) = 2^{1/2}(2\pi h)^{-n/2}\lambda^{-n/4}e^{i\lambda\omega \cdot x/4}$ is in $\mathcal{X}_0^* = L^{2,-\gamma}(\mathbb{R}^n)$ where δ_{ω} is the unit point measure at $\omega \in S^{n-1}$. Hence we can define

$$\Psi_{\pm}(\lambda, \omega) = \Phi_{\pm}(\lambda)\delta_{\omega} = \{J - (H_{\text{ext}} - (\lambda \mp i0))^{-1}T\} F_0(\lambda)^*\delta_{\omega} \in \mathcal{X}_0^*. \quad (3.9)$$

PROPOSITION 3.5. — *Suppose $(A)_{\alpha}$ with $\alpha > (n+1)/2$ and $(D5)_I$ ($I \subset \subset \mathbb{R}_+$) with $H_2 = H_{\text{ext}}$ on $L^2(\Omega_{\text{ext}})$. Then for $\varphi \in L^2(I; \Sigma)$,*

$$W_{\pm}(H_{\text{ext}}, H_0, J)F_0^*\varphi = \int_I d\mu \int_{S^{n-1}} d\omega \Psi_{\pm}(\mu, \omega)\varphi(\mu, \omega). \quad (3.10)$$

where the integral is the Riemann integral in \mathcal{X}_0^* .

PROPOSITION 3.6. — *Under the same assumptions as in Proposition 3.5, the scattering matrix $S(H^{\mathbb{D}}, H_0; \lambda)$ is Hilbert-Schmidt type and has an integral kernel $S(H^{\mathbb{D}}, H_0; \lambda, \omega, \omega')$.*

Since $S(H^{\mathbb{D}}, H_0) = S(H_{\text{ext}}, H_0, J)$, Propositions 3.5 and 3.6 follow from Theorem 2.3 and the standard technics in scattering theory (cf. § XI-6 of [16]). Analogous to Proposition 3.3 and Corollary 3.4, we have

PROPOSITION 3.7. — Suppose $(A)_\alpha$ with $\alpha > (n+1)/2$ and $(B)_I$ ($I \subset \subset (0, \lambda_0)$), then $\Psi_\pm(\lambda, \omega)$ is a generalized eigenfunctions of H_{ext} . Moreover for any $\varepsilon > 0$, there is $C > 0$ such that

$$|\Psi_\pm(\lambda, \omega; x)| \leq C e^{-\{d_\lambda(x, \Omega_{\text{ext}} \setminus \mathcal{J}(\lambda)) - \varepsilon\}/h} \quad (3.11)$$

for $\lambda \in I$, $\omega \in S^{n-1}$ and $x \in \Omega_{\text{ext}} \cap \mathcal{J}(\lambda + \varepsilon)$.

COROLLARY 3.8. — Under the same assumptions as in Proposition 3.7, for any $\varepsilon > 0$ there is $C > 0$ such that

$$\|T_{\text{ext}} \nabla_n \Psi_\pm(\lambda, \omega)\|_{L^2(K)} \leq C e^{-\{d_\lambda(K, \Omega_{\text{ext}} \setminus \mathcal{J}(\lambda)) - \varepsilon\}/h} \quad (3.12)$$

for $\lambda \in I$ and $\omega \in S^{n-1}$.

§ 4. A REPRESENTATION OF $S(H, H^D)$

PROPOSITION 4.1. — Suppose $(A)_\alpha$ ($\alpha > 1$), and suppose that $(B)_\Lambda$ holds on a neighborhood Λ of $I \subset \subset \mathbb{R}_+$. Then for any $a > 0$ and $q > 0$, if h is sufficiently small, $(H - (\mu \pm i0))^{-1} = \lim_{\varepsilon \downarrow 0} (H - (\mu + i\varepsilon))^{-1}$ exists in $B(L^{2,\beta}(\mathbb{R}^n), L^{2,-\beta}(\mathbb{R}^n))$ for any $\beta > 1/2$ and $\mu \in I \setminus \mathcal{E}(a, q; h)$. Moreover

$$\|(H - (\mu \pm i0))^{-1}\|_{B(L^{2,\beta}, L^{2,-\beta})} \leq Ch^{-r} \quad (4.1)$$

for $\mu \in I \setminus \mathcal{E}(a, q; h)$, where $r = \max(p, q)$ (p is the constant in $(B)_I$).

Proof. — For $\mu \in I \setminus \mathcal{E}(a, q; h)$,

$$\|(H^D - (\mu \pm i\varepsilon))^{-1}\|_{B(L^{2,\beta}, L^{2,-\beta})} \leq C \max(h^{-p}, h^{-q}) = Ch^{-r}. \quad (4.2)$$

If we set $a = \mu + ih^r$ and $z = \mu + i\varepsilon$ ($|\varepsilon| \in (0, h^r)$),

$$(R^D(a) - (z - a)^{-1})^{-1} = -(z - a) - (z - a)^2 R^D(z) = O(h^r). \quad (4.3)$$

in $B(L^{2,\beta}, L^{2,-\beta})$. From Proposition 2.2 and (4.3), it follows that the following series:

$$(R(a) - (z - a)^{-1})^{-1} = (R^D(a) - (z - a)^{-1}) \sum_{m=0}^{\infty} \{W(a)(R^D(a) - (z - a)^{-1})^{-1}\}^m$$

is absolutely convergent in $B(L^{2,\beta}, L^{2,-\beta})$ if h is sufficiently small, and

$$\|(R(a) - (z - a)^{-1})^{-1}\|_{B(L^{2,\beta}, L^{2,-\beta})} \leq O(h^r) \sum_{m=0}^{\infty} \{CO(h^r)\}^m = O(h^r). \quad (4.4)$$

Furthermore, since $(R^D(a) - (\mu \pm i0 - a)^{-1})^{-1}$ exists, $(R(a) - (\mu \pm i0 - a)^{-1})^{-1}$ also exists in $B(L^{2,\beta}, L^{2,-\beta})$. Thus (4.4) and

$$R(z) = -(z - a)^{-1} - (z - a)^{-2}(R(a) - (z - a)^{-1})^{-1}$$

with $z = \mu \pm i0$ prove the proposition. \square

COROLLARY 4.2. — *Under the same assumptions as in Proposition 4.1,*

$$\|T(H - (\mu \pm i0))^{-1}T^*\|_{\mathcal{B}(L^2(K))} \leq Ch^{-(r+2)} \tag{4.5}$$

if h is sufficiently small and $\mu \in I \setminus \mathcal{E}(a, q; h)$.

Proof. — Since

$$(H - \mu \mp i0)^{-1}H = H(H - \mu \mp i0)^{-1} = 1 + \mu(H - \mu \mp i0)^{-1},$$

$(H - \mu \mp i0)^{-1}$ maps the weighted sobolev space

$$H^{s,\beta}(\mathbb{R}^n) = \{ f \in \mathcal{F}' \mid (1 + |x|^2)^{\beta/2} f(x) \in H^s(\mathbb{R}^n) \} \quad \text{into} \quad H^{s+2,-\beta}(\mathbb{R}^n)$$

with $s = 2$ or 0 , and its norms are $O(h^{-r-2})$. Interpolating these estimates, we see that the above estimate holds for $s = 1$. From this the corollary follows immediately.

We remark that since $W_{\pm}(H^D, H_0)$ is complete, if we set $F_{\pm}^D = F_0 W_{\pm}(H^D, H_0)^*$, F_{\pm}^D is a spectral representation of H^D on $\mathcal{H}^{ac}(H^D) = \mathcal{H}^{ac}(H_{\text{ext}})$. By Proposition 3.1, $W_{\pm}(H^D, H_0)F_0(\lambda)^*$ maps $\Sigma = L^2(S^{n-1})$ into $\mathcal{X}_1^* = L^{2,-\alpha/2}(\Omega_{\text{ext}})$, and $F_{\pm}^D(\lambda) = F_0(\lambda)W_{\pm}(H^D, H_0)^*$ maps $\mathcal{X}_1 = L^{2,\alpha/2}(\Omega_{\text{ext}})$ into Σ . Using F_{\pm}^D , we can define scattering matrix for H and H^D : since $(H^D, S(H, H^D)) = 0$ on $D(H^D)$, there is $S_{\pm}(H, H^D; \lambda) \in \mathcal{B}(\Sigma)$ such that

$$F_{\pm}^D(\lambda)S(H, H^D)\varphi = S_{\pm}(H, H^D; \lambda)F_{\pm}^D(\lambda)\varphi \quad (\varphi \in \mathcal{X}_1)$$

for almost all $\lambda \in (0, \infty)$.

THEOREM 4.3. — *Suppose $(A)_{\alpha}$ ($\alpha > 1$) and that $(H - (\mu + i0))^{-1}$ and $(H^D - (\mu \pm i0))^{-1}$ exist in $\mathcal{B}(L^{2,\alpha/2}, L^{2,-\alpha/2})$ for $\mu \in I \subset \subset \mathbb{R}_+$ uniformly. We write $F = F_+^D$ or F_-^D and $S(H, H^D; \lambda) = S_+(H, H^D; \lambda)$ or $S_-(H, H^D; \lambda)$ respectively. Then for $\lambda \in I$,*

$$S(H, H^D; \lambda) = 1 + 2\pi i h^4 F(\lambda)(T^*T_{\text{ext}}\nabla_n)^*(H - (\lambda + i0))^{-1}(T^*T_{\text{ext}}\nabla_n)F(\lambda)^*. \tag{4.6}$$

Proof. — Using Krein's formula (Proposition 2.1), we will mimic the standard procedure of scattering theory. Let $\varphi \in C(I; \Sigma)$, then

$$\begin{aligned} W_-(H, H^D)F^*\varphi &= s\text{-}\lim_{t \rightarrow -\infty} e^{itH}e^{-itH^D}F^*\varphi \\ &= s\text{-}\lim_{t \rightarrow -\infty} (H+i)e^{itH}(H+i)^{-1}(H^D+i)^{-1}e^{-itH^D}(H^D+i)F^*\varphi \\ &= F^*\varphi + i s\text{-}\lim_{t \rightarrow -\infty} (H+i) \int_t^0 e^{itH} \{ (H+i)^{-1} - (H^D+i)^{-1} \} e^{-itH^D} dt (H^D+i)F^*\varphi \\ &= F^*\varphi + i s\text{-}\lim_{\varepsilon \downarrow 0} (H+i) \int_{-\infty}^0 (H+i)^{-1} h^2 T^*T_{\text{ext}}\nabla_n(H_{\text{ext}}+i)^{-1} e^{-itH^D} e^{\varepsilon t} dt \times \\ & \hspace{20em} \times (H^D+i)^{-1} F^*\varphi \\ &= F^*\varphi + i s\text{-}\lim_{\varepsilon \downarrow 0} \int_{-\infty}^0 e^{itH} h^2 T^*T_{\text{ext}}\nabla_n F^*(e^{-it\lambda}\varphi)\varepsilon^{\varepsilon t} dt. \end{aligned} \tag{4.7}$$

Since $F(\lambda)^*$ maps $L^2(K)$ into $H^{2, -\alpha/2}(\Omega_{\text{ext}})$ and $T^*T_{\text{ext}}\nabla_n$ maps $H^{2, -\alpha/2}(\Omega_{\text{ext}})$ into $H^{-1}(\mathbb{R}^n) \subset D(H)^* = H^{-2}(\mathbb{R}^n)$, we can write (4.7) as

$$\begin{aligned} F^*\varphi + ih^2 \underset{\varepsilon \downarrow 0}{s\text{-}\lim} \int_{-\infty}^0 dt \int_I d\lambda e^{it(H-\lambda-i\varepsilon)} T^*T_{\text{ext}}\nabla_n F(\lambda)^*\varphi \\ = F^*\varphi + h^2 \underset{\varepsilon \downarrow 0}{s\text{-}\lim} \int_I d\lambda (H-\lambda-i\varepsilon)^{-1} T^*T_{\text{ext}}\nabla_n F(\lambda)^*\varphi. \end{aligned} \quad (4.8)$$

By the assumption, we can take limit in the integral and (4.8) equals

$$\begin{aligned} F^*\varphi + h^2 \int_I d\lambda (H-(\lambda+i0))^{-1} T^*T_{\text{ext}}\nabla_n F(\lambda)^*\varphi \\ = \int_I d\lambda \{1 + h^2(H-(\lambda+i0))^{-1} T^*T_{\text{ext}}\nabla_n\} F(\lambda)^*\varphi. \end{aligned}$$

Clearly $\{1 + h^2(H-(\lambda+i0))^{-1} T^*T_{\text{ext}}\nabla_n\} F(\lambda)^*\varphi$ is a generalized eigenfunction of H , and is in $H^{2, -\alpha/2}(\mathbb{R}^n)$.

Let $\varphi, \psi \in C^1(I; \Sigma)$, then by arguments similar to the above, we have

$$\begin{aligned} (F^*\varphi, (S(H, H^D) - 1)F^*\psi) &= ((W_+(H, H^D) - W_-(H, H^D))F^*\varphi, W_-(H, H^D)F^*\psi) \\ &= \underset{\varepsilon \downarrow 0}{s\text{-}\lim} ih^2 \int_{-\infty}^{\infty} (T^*T_{\text{ext}}\nabla_n e^{-itH} F^*\varphi, e^{-itH} W_-(H, H^D)F^*\psi) e^{-\varepsilon|t|} dt \\ &= \underset{\varepsilon \downarrow 0}{s\text{-}\lim} ih^2 \int_I \int_I \int_{-\infty}^{\infty} (T^*T_{\text{ext}}\nabla_n F(\lambda)^*\varphi, W_-(H, H^D)F(\mu)^*\psi) e^{-it(\lambda-\mu)-\varepsilon|t|} dt \\ &= 2\pi ih^4 \int_I (T^*T_{\text{ext}}\nabla_n F(\lambda)^*\varphi, \{1 + (H-(\lambda+i0))^{-1} T^*T_{\text{ext}}\nabla_n\} F(\lambda)^*\psi) dt. \end{aligned} \quad (4.9)$$

Since $F(\lambda)^*\psi$ is a generalized eigenfunction of H^D , we have

$$(T^*T_{\text{ext}}\nabla_n)^* F(\lambda)^*\psi = (T_{\text{ext}}\nabla_n)^*(TF(\lambda)^*\psi) = 0$$

and hence (4.9) equals

$$2\pi ih^2 \int_I (\varphi, F(\lambda)(T^*T_{\text{ext}}\nabla_n)^*(H-(\lambda+i0))^{-1}(T^*T_{\text{ext}}\nabla_n)F(\lambda)^*\psi) d\lambda.$$

This implies (4.6). \square

REMARK 4.4. — Although we have used specific spectral representation F_{\pm}^D , (4.6) is independent of the choice of the spectral representation. It is apparent from the proof since the only one property we need is $F(\lambda)^*\varphi \in \mathcal{X}_1^*$.

§ 5. PROOF OF THEOREMS 1 AND 2

PROPOSITION 5.1. — Suppose $(A)_\alpha$ ($\alpha > 1$) and $(B)_I$ ($I \subset \subset \mathbb{R}_+$). Suppose moreover that $(H - (\lambda \pm i0))^{-1}$ exists in $B(L^{2,\alpha/2}, L^{2,-\alpha/2})$ for $\lambda \in I$. Then

$$(\varphi, \{ S(H, H_0; \lambda) - S(H^D, H_0; \lambda) \} \psi) \\ = 2\pi i h^4 (T_{\text{ext}} \nabla_n \Phi_+(\lambda) \varphi, (T(H - (\lambda + i0))^{-1} T^*) T_{\text{ext}} \nabla_n \Phi_-(\lambda) \psi) \quad (5.1)$$

for $\lambda \in I$, φ and $\psi \in \Sigma$.

Proof. — We write $W_\pm^D = W_\pm(H^D, H_0)$. Then

$$F_0 S(H, H_0) F_0^* = F_0 W_+^{D*} S(H, H^D) W_-^D F_0^* \\ = F_0 W_+^{D*} S(H, H^D) W_+^D F_0^* F_0 W_+^{D*} W_-^D F_0^* = (F_+^D S(H, H^D) F_+^{D*}) (F_0 S(H^D, H_0) F_0^*).$$

Hence for φ and $\psi \in \Sigma$, we have

$$(\varphi, S(H, H_0; \lambda) \psi) = (\varphi, S_+(H, H^D; \lambda) S(H^D, H_0; \lambda) \psi) = (\varphi, S(H^D, H_0; \lambda) \psi) \\ + 2\pi i h^4 (T^* T_{\text{ext}} \nabla_n W_+^D F_0(\lambda)^* \varphi, (H - (\lambda + i0))^{-1} T^* T_{\text{ext}} \nabla_n W_+^D F_0(\lambda)^* S(H^D, H_0; \lambda) \psi)$$

by Theorem 4.3. Since

$$W_+^D F_0(\lambda)^* S(H^D, H_0; \lambda) \\ = (W_+^D W_+^{D*}) W_-^D F_0(\lambda)^* = W_-^D F_0(\lambda)^*,$$

we see

$$(\varphi, \{ S(H, H_0; \lambda) - S(H^D, H_0; \lambda) \} \psi) \\ = (2\pi i h^4 (T^* T_{\text{ext}} \nabla_n W_+^D F_0(\lambda)^* \varphi, (H - (\lambda + i0))^{-1} T^* T_{\text{ext}} \nabla_n W_-^D F_0(\lambda)^* \psi)). \quad (5.2)$$

(5.2) and Corollary 3.2 prove the proposition. \square

COROLLARY 5.2. — Suppose the assumptions of Proposition 5.1. Suppose moreover $\alpha > (n + 1)/2$. Then

$$S(H, H_0; \lambda, \omega, \omega') - S(H^D, H_0; \lambda, \omega, \omega') \\ = 2\pi i (T_{\text{ext}} \nabla_n \Psi_+(\lambda, \omega), (T(H - (\lambda + i0))^{-1} T^*) T_{\text{ext}} \nabla_n \Psi_-(\lambda, \omega')) \quad (5.3)$$

for $\omega, \omega' \in S^{n-1}$.

Proof of Theorems 1 and 2. — By Proposition 5.1,

$$\| S(H, H_0; \lambda) - S(H^D, H_0; \lambda) \| \\ \leq 2\pi h^4 \| T_{\text{ext}} \nabla_n \Phi_+ \|_{B(\Sigma, L^2(K))} \| T(H - (\lambda + i0))^{-1} \|_{B(L^2(K))} \times \| T_{\text{ext}} \nabla_n \Phi_- \|_{B(\Sigma, L^2(K))} \\ \leq C_\varepsilon h^{-r+2} \exp \{ -2(\mathbf{d}_\lambda(K, \Omega_{\text{ext}} \setminus \mathcal{J}(\lambda)) - \varepsilon)/h \} \\ \leq C'_\varepsilon \exp \{ -2(\mathbf{d}_\lambda(K, \Omega_{\text{ext}} \setminus \mathcal{J}(\lambda)) - 2\varepsilon)/h \}$$

for any $\varepsilon > 0$. Here we have used Corollaries 3.4 and 4.2. Similarly, Theorem 2 follows from Corollaries 3.7, 4.2 and 5.2. \square

APPENDIX

SEMI-CLASSICAL RESOLVENT ESTIMATES

In this appendix, we give two sufficient conditions for $(B)_1$. The former one is essentially due to Lavine [15], and the latter to Robert and Tamura [17], [18].

PROPOSITION A.1. — *Suppose $V \in C^1(\mathbb{R}^n)$, $\lim_{|x| \rightarrow \infty} V(x) = 0$ and $|x \cdot \nabla V(x)| \leq C(1 + |x|)^{(1-\gamma)}$ for some $\gamma > 0$. Let $\lambda \in (0, \lambda_0)$ and suppose moreover that*

$$V(x) + \frac{1}{2} x \cdot \nabla V(x) \leq \lambda - \varepsilon. \quad (\text{A.1})$$

for some $\varepsilon > 0$ if $x \in \Omega_{\text{ext}} \setminus \mathcal{S}(\lambda)$. Then $(B)_1$ holds in a neighborhood I of λ with $p = 1$.

Proof. — 1) If (A.1) holds for all $x \in \Omega_{\text{ext}}$, $(B)_1$ follows from the argument of § 3 in [15]. We sketch the idea: we set

$$A = -ih \left\{ g_{\mathbb{R}}(|x|) \frac{x}{|x|} \cdot \nabla + \nabla \cdot \frac{x}{|x|} g_{\mathbb{R}}(|x|) \right\},$$

$$g^{\mathbb{R}}(r) = \int_0^r \left(1 + \left(\frac{s}{\mathbb{R}} \right)^2 \right)^{-\beta/2} ds \quad (1 < \beta < \min(\gamma, 2)).$$

Then there is $\delta > 0$ such that for $\varphi \in D(H)$,

$$2 \operatorname{Re} \left((H^{\mathbb{D}} - \lambda - \delta) \varphi, \left(1 + \left(\frac{|x|}{\mathbb{R}} \right)^2 \right)^{-\beta/2} \varphi \right) \leq h^{-1} \operatorname{Im} (A \varphi, H^{\mathbb{D}} \varphi)$$

if \mathbb{R} is sufficiently large (cf. Lemma 3.2 of [15]). This implies the local $H^{\mathbb{D}}$ -smoothness of $(1 + (|x|/\mathbb{R})^2)^{-\beta/4}$ near λ , and its $H^{\mathbb{D}}$ -smooth bound is of $O(h^{-1})$ (cf. Theorem 3 of [15]). Hence $(B)_1$ follows by the theory of smooth operators (see § XIII-7 of [16]).

2) Under our assumptions, (A.1) holds for $x \in Q_{\text{ext}} \setminus \mathcal{S}(\lambda + \delta)$ with some $\delta > 0$ if ε is replaced by $\varepsilon/2$. So the proof of 1) applies to $\tilde{H}^{\mathbb{D}} = H_0 + V$, $D(\tilde{H}^{\mathbb{D}}) = (H^2 \cap H_0^1)(\Omega_{\text{ext}} \setminus \mathcal{S}(\lambda + \delta))$. We can apply Krein's formula (Propositions 2.1, 2.2) to the pair $(H^{\mathbb{D}}, \tilde{H}^{\mathbb{D}})$. Setting $\tilde{H}_{\text{int}} : D(\tilde{H}_{\text{int}}) = (H^2 \cap H_0^1)(\Omega_{\text{ext}} \cap \mathcal{S}(\lambda + \delta))$, we have $\sigma(\tilde{H}_{\text{int}}) \subset (\lambda + \delta, \infty)$. Hence the proof of Proposition 4.1 is valid to conclude $(B)_1$ if H , $H^{\mathbb{D}}$ and H_{int} are replaced by $H^{\mathbb{D}}$, $\tilde{H}^{\mathbb{D}}$ and \tilde{H}_{int} respectively. \square

PROPOSITION A.2. — *Suppose $V \in C^\infty(\mathbb{R}^n)$ and V satisfies*

$$|\partial_x^\alpha V(x)| \leq C_\alpha (1 + |x|)^{-\rho - |\alpha|}$$

for some $\rho > 0$ and any α . Suppose moreover that $\lambda \in (0, \lambda_0)$ is non-trapping in the following sense (cf. [18]):

(NT): Let $\{x(t; y, \eta), \xi(t; y, \eta)\}$ be the solution of the Hamilton system $\dot{x} = 2\xi$, $\dot{\xi} = -\nabla V(x)$ with initial state (y, η) . We say $\lambda \in (0, \lambda_0)$ is non-trapping if for any $\mathbb{R} \gg 1$, there exists $T = T(\mathbb{R})$ such that $|x(t; y, \xi)| > \mathbb{R}$ for $|y| < \mathbb{R}$, $y \in \Omega_{\text{ext}}$ and $\lambda = |\eta|^2 + V(y)$.

Then $(B)_1$ holds in a neighborhood I of λ with $p = 1$.

Proof. — We can find $\tilde{V} \in C^\infty(\mathbb{R}^n)$ so that $\tilde{V} = V$ on Ω_{ext} , $\tilde{V}(x) \geq \lambda + \delta$ in Ω_{int} with some $\delta > 0$. Then Theorem 2 of [18] implies the property for $\tilde{H} = H_0 + \tilde{V}$. Obviously, $\sigma(\tilde{H}_{\text{int}}) \subset (\lambda + \delta, \infty)$ and we can apply the proof of Proposition 4.1 with reversing the roles of H and H^D to conclude $(B)_1$. \square

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