Quantum resonances and related topic
In honor of 60th birthday of André Martinez
Institut Henri Poincaré, Paris, France
June 11 – 13, 2019

Long-range scattering matrix for Schrödinger-type operators

Shu Nakamura

Gakushuin University

(Long) Foreword : A very short introduction to Martinez' theory on phase space tunneling estimates

▷ 1980∼ Tunneling estimates

- Agmon distance/estimates (in x-space).

▷ What is tunneling in phase space?

- Helffer-Sjöstrand : Harper operators
- tunneling estimates in momentum space (Agmon estimates for pseudodifferential operators)

Break through: A. Martinez: *Estimates on complex interactions in phase space* Math. Nachr. **167** (1994), 203–254 (Preprint 1992)

▷ Purely phase space formulation of tunneling estimates/exponential decay estimates.

Math. Nachr. **167** (1994) 203–254

Estimates on Complex Interactions in Phase Space

By André Martinez of Villetaneuse

(Received May 14, 1993)

Abstract. We propose a method to study the complex interactions (or microlocal tunneling) between electronic levels that do not intersect in the real domain. The method consists in using a special kind of Fourier-Bros-Iagolnitzer transformation, and in adjoining an exponential weight to the L^2-type Hilbert spaces which are associated to a complex Lagrangian manifold and have been introduced by Helffer and Sjöstrand for the study of resonances.

0. Introduction

This paper is an attempt to understand better the complex interaction between wells in phase space, in rather general situations. A very simple example where the usual techniques don't work is the following one:

Consider the matrix operator P on $L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n)$

$$P = \begin{pmatrix} -h^2\triangle - x_n - 1 & 0 \\ 0 & -h^2\triangle + x^2 \end{pmatrix} + hR(x, hD_x), \tag{0.1}$$

where R is a symmetric 2×2 matrix of differential operators of order less than two. This is typically the kind of operator one can expect to obtain (at least approximately) by the Feshbach reduction for a polyatomic molecule, in the Born-Oppenheimer approximation. (In this case, $h > 0$ will tend to zero as the masses of the nuclei tend to infinity: see e.g. [KMSW] and references there.)

When h tends to 0_+, the principal part of P is

▷ When Nakamura was invited to Paris 13 (1992, 1993?), André Martinez kindly explained me the main idea:

▷ FBI transform (Bargman transform, Gaussian wave (coherent state) expansion, Gabor transform, ...)

$$Tu(x,\xi) = c_n \int e^{i(x-y)\cdot\xi/h - |x-y|^2/2h} u(y)dy, \quad c_n = 2^{-n/2}(\pi h)^{-3n/4},$$

for $u \in L^2(\mathbb{R}^n)$. T is isometry from $L^2(\mathbb{R}^n)$ into $L^2(\mathbb{R}^n \times \mathbb{R}^n)$.

▷ Basic properties:

$$T[xu] = (x - hD_\xi)(Tu), \quad T[hD_x u] = hD_x(Tu),$$

and hence $T[p(x, hD_x)u] = p(x - hD_\xi, hD_x)(Tu)$.

$$(hD_x - \xi - ihD_\xi)(Tu) = 0 \quad \text{(Cauchy-Riemann equation)}.$$

Hence we have $\langle Tu, (hD_x - \xi - ihD_\xi)(Tu)\rangle = 0$, and then

$$\langle Tu, (hD_x - \xi)(Tu)\rangle = 0, \quad \langle Tu, hD_\xi(Tu)\rangle = 0.$$

i.e., $hD_x \sim \xi$, $hD_\xi \sim 0$ as quadratic forms on $\mathrm{Ran}[T]$. Hence we have

$$\langle Tu, T[p(x, hD_x)u]\rangle \sim \langle Tu, p(x,\xi)Tu\rangle.$$

▷ Put an exponential weight $e^{\psi(x,\xi)/h}$ on Tu.

$$e^{\psi/h}T[p(x, hD_x)u] = e^{\psi/h}p(x - hD_\xi, hD_x)(Tu)$$
$$\sim p(x - hD_\xi - i\partial_\xi\psi, hD_x + i\partial_x\psi)e^{\psi/h}(Tu).$$

The Cauchy-Riemann equation becomes

$$(hD_x - \xi + \partial_\xi\psi - i(hD_\xi - \partial_x\psi))e^{\psi/h}(Tu) = 0.$$

This implies

$$hD_x \sim \xi + \partial_\xi\psi, \quad hD_\xi \sim \partial_x\psi$$

as quadratic forms on $\mathrm{Ran}[e^{\psi/h}T]$. Combining them, we have

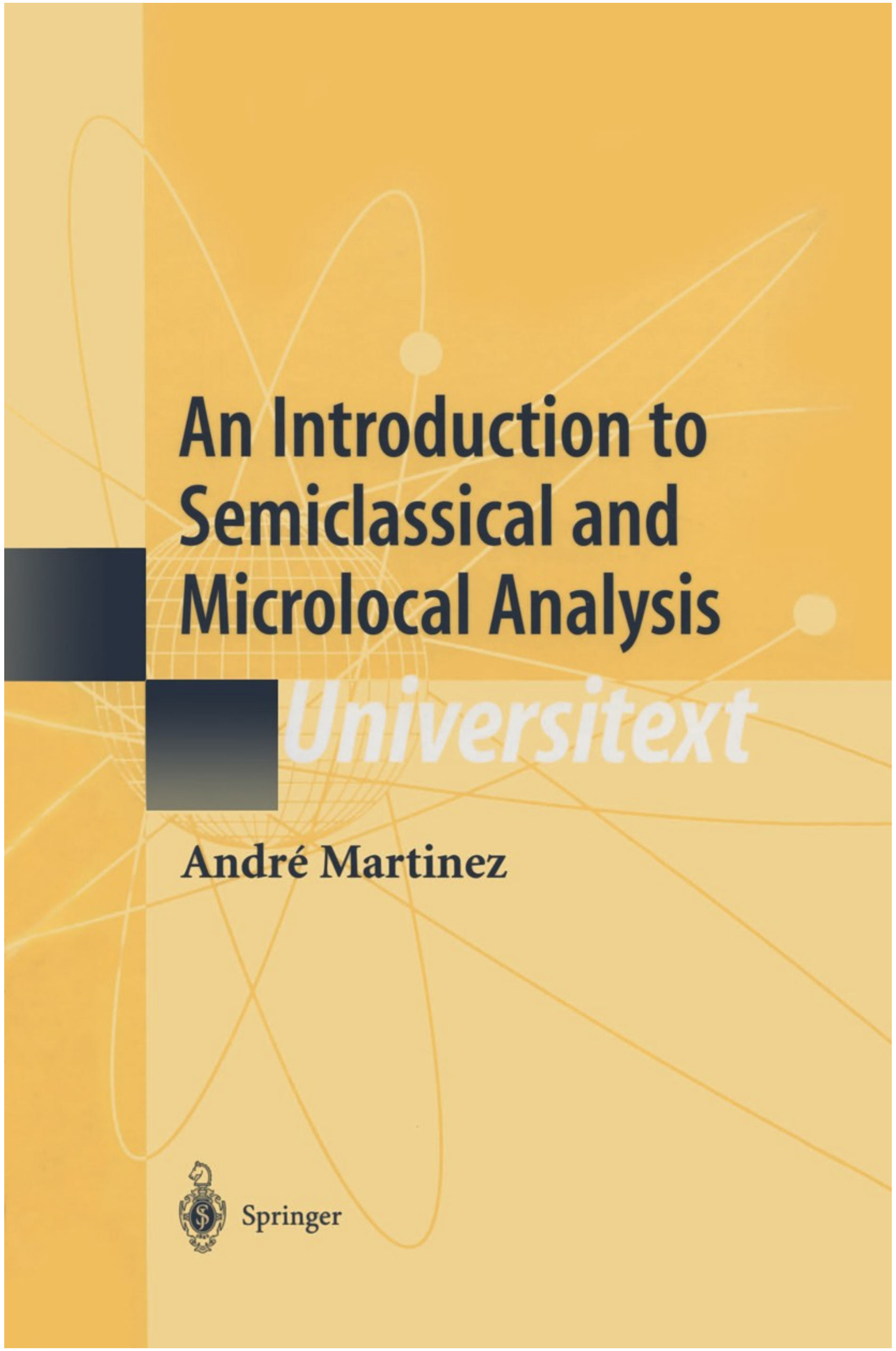
$$\langle e^{\psi/h}Tu, e^{\psi/h}T[p(x, hD_x)u]\rangle \sim \langle e^{\psi/h}Tu, p(x - \bar{\partial}\psi, \xi + i\bar{\partial}\psi)e^{\psi/h}Tu\rangle,$$

where $\bar{\partial}\psi = \partial_x\psi + i\partial_\xi\psi$.

▷ Martinez carried out this analysis for differential operators $p(x, hD_x)$ using the Sjöstrand theory of analytic singularities.

▷ Nakamura found a way to prove it by elementary pseudodifferential operator calculus to show this for pseudodifferential operators. (*On Martinez' method of phase space tunneling*, Rev. Math. Phys. 1995)

▷ Then Martinez wrote a textbook (2002) on microlocal analysis / semiclassical analysis and he used this method to prove various theorems, including propagation theorem of analytic singularities, Kawai-Kashiwara theorem, ...



▷ Then we start collaboration based on this method:

- Martinez, A., Nakamura, S., Sordoni, V.: Phase space tunneling in multistate scattering. J. Funct. Anal. **191** (2002), no. 2, 297–317.
- Martinez, A., Nakamura, S., Sordoni, V.: Analytic smoothing effect for the Schrödinger equation with long-range perturbation. Comm. Pure Appl. Math. **59** (2006), no. 9, 1330–1351.
- Martinez, A., Nakamura, S., Sordoni, V.: Analytic singularities for long range Schrödinger equations. C. R. Math. Acad. Sci. Paris **346** (2008), no. 15-16, 849–852.
- Martinez, A., Nakamura, S., Sordoni, V.: Analytic wave front set for solutions to Schrödinger equations. Adv. Math. **222** (2009), no. 4, 1277–1307.
- Martinez, A., Nakamura, S., Sordoni, V.: Analytic wave front set for solutions to Schrödinger equations II — long range perturbations. Comm. Partial Differential Equations **35** (2010), no. 12, 2279–2309.

▷ Still there are many questions to be solved, or understood, e.g.,
"Why do we need *global* analyticity?"

1 Schrödinger operators with long-range potentials

(1) Schrödinger operators on $\mathbb{R}^d$, $d \geq 1$:

$$H = -\frac{1}{2}\triangle + V(x) \quad \text{on } \mathcal{H} = L^2(\mathbb{R}^d),$$

where $V(x)$ is a real-valued bounded function. H is self-adjoint on $H^2(\mathbb{R}^d)$.

Assumption A. Suppose $V \in C^\infty(\mathbb{R}^d; \mathbb{R})$; there is $\mu > 0$ and for any $\alpha \in \mathbb{Z}_+^d$,

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

We call V is *short-range* if $\mu > 1$, and *long-range* if $0 < \mu \leq 1$.

▷ If V is short-range, then it is well-known that the wave operators

$$W_\pm = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH} e^{-itH_0}, \quad H_0 = -\frac{1}{2}\triangle,$$

exist and are complete: $\mathrm{Ran}[W_\pm] = \mathcal{H}_{ac}(H)$. Namely, for any $\varphi_0 \in \mathcal{H}_{ac}(H)$,

$$e^{-itH}\varphi_0 \sim e^{-itH_0}\varphi_\pm \quad \text{as } t \to \pm\infty$$

where $\varphi_\pm = (W_\pm)^*\varphi_0$.

(2) Long-range scattering:

▷ If V is long-range, then it is also well-known that the wave operators do not converge in general. The **modified** wave operators are defined by

$$W_\pm^{\mathrm{D}} = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH} e^{-i\phi(t,D_x)}$$

where $\phi(t,\xi)$ is a solution to Hamilton-Jacobi equation in the Fourier space, and they are complete: $\mathrm{Ran}[W_\pm^{\mathrm{D}}] = \mathcal{H}_{ac}(H)$. Namely, for any $\varphi_0 \in \mathcal{H}_{ac}(H)$,

$$e^{-itH}\varphi_0 \sim e^{-i\phi(t,D_x)}\varphi_\pm \quad \text{as } t \to \pm\infty$$

where $\varphi_\pm = (W_\pm^D)^*\varphi_0$. (Dollard, Hörmander, Saito, Isozaki, Kitada, Enss, Kitada-Yajima, Yafaev, Derezinski-Gérard. . .).

Remark 1. If $1/2 < \mu \le 1$, we can use **Dollard-type** modifier:

$$\phi^{\mathrm{D}}(t,\xi) = \frac{t}{2}|\xi|^2 + \int_0^t V(s\xi)ds, \quad t \in \mathbb{R}, \xi \in \mathbb{R}^d, \xi \neq 0,$$

to define the modified wave operators.

▷ There is another approach due to Isozaki and Kitada: We use suitable Fourier integral operators:

$$J_{\pm}u(x) = (2\pi)^{-d/2} \int e^{i\psi_{\pm}(x,\xi)} \hat{u}(\xi) d\xi, \quad x \in \mathbb{R}^d, u \in \mathcal{S}(\mathbb{R}^d),$$

called the **time-independent modifiers**, where $\psi_{\pm}(x,\xi)$ on $\mathbb{R}^{2d}$ are solutions to the eikonal equation. Then the modified wave operators

$$W_{\pm}^{\mathrm{IK}} = \operatorname*{s-lim}_{t \to \pm\infty} e^{itH} J_{\pm} e^{-itH_0}$$

exists and are complete.

Remark 2. If $1/2 < \mu \leq 1$, we can use approximate solutions to the eikonal equation (due to D. Yafaev):

$$\psi_{\pm}^{\mathrm{D}}(x,\xi) = x \cdot \xi + \int_0^{\pm\infty} (V(x + t\xi) - V(t\xi)) dt.$$

Remark 3. With suitable constructions of ϕ and $\psi_{\pm}$, it is known $W_{\pm}^{\mathrm{D}} = W_{\pm}^{\mathrm{IK}}$ (see the textbook by Dereziński-Gérard).

2 Scattering matrix

▷ In the following, we simply write the modified wave operators by $W_\pm = W_\pm^{\mathsf{D}}$, or $W_\pm = W_\pm^{\mathsf{IK}}$.

▷ **The scattering operator** is $S = W_+^* W_-$, $\mathcal{H} \to \mathcal{H}$, unitary, and by the definition, we have the intertwining property: (formally), $SH_0 = W_+^* H W_- = H_0 S$ on $\mathcal{D}(H_0)$. Hence,

$$(\mathcal{F}S\mathcal{F}^*)|\xi|^2 = |\xi|^2(\mathcal{F}S\mathcal{F}^*) \quad \text{on } L^2(\mathbb{R}^d_\xi),$$

where $\mathcal{F}$ is the Fourier transform. If we decompose $L^2(\mathbb{R}^d_\xi) = \mathcal{F}\mathcal{H}$ as

$$L^2(\mathbb{R}^d_\xi) \simeq \int_{(0,\infty)}^{\oplus} L^2(\Sigma_\lambda, m_\lambda)d\lambda, \quad \Sigma_\lambda = \sqrt{2\lambda}S^{d-1}, m_\lambda = dS/\sqrt{2\lambda},$$

then the scattering operator is decomposed as

$$(\mathcal{F}S\mathcal{F}^*)\varphi(\lambda,\omega) = (S(\lambda)\varphi(\lambda,\cdot))(\omega)$$

for $\varphi \in \int^\oplus L^2(\Sigma_\lambda, m_\lambda)d\lambda$, where $S(\lambda)$, $L^2(\Sigma_\lambda, m_\lambda) \to L^2(\Sigma_\lambda, m_\lambda)$. $S(\lambda)$ is unitary for a.e. $\lambda > 0$, and called **the scattering matrix**.

▷ By scaling, we may consider $S(\lambda)$ as an operator on $L^2(S^{d-1}, dS)$.

Notation: We consider operators and symbol classes on $\Sigma_\lambda = \sqrt{2\lambda}S^{d-1}$. We denote $a(y,\eta) \in S^\ell_{\rho,\delta}$ for $a \in C^\infty(T^*\Sigma_\lambda)$ ($\eta \in \Sigma_\lambda$, $y \in T^*_\eta\Sigma_\lambda$) if $\forall\alpha, \beta \in \mathbb{Z}^d_+$, $\exists C_{\alpha\beta} > 0$ s.t.

$$\left|\partial_y^\alpha \partial_\eta^\beta a(y,\eta)\right| \le C_{\alpha\beta}\langle y\rangle^{\ell-\rho|\alpha|+\delta|\beta|}, \quad (\eta, y) \in T^*\Sigma_\lambda,$$

in each local coordinate system.

Theorem 1. *Suppose Assumption A with $0 < \mu < 1$, and let $\lambda > 0$. Then $S(\lambda)$ has the following Fourier integral operator representation:*

$$S(\lambda)f(\eta) = (2\pi)^{-(d-1)} \iint e^{-i\psi(y,\eta)+iy\cdot\zeta}\Theta(y,\eta)a(y,\eta)f(\zeta)d\zeta dy$$

for $f \in C^\infty(\Sigma_\lambda)$ in a local coordinate of Σ_λ, where $\psi \in S^1_{1,0}(\Sigma_\lambda)$, $a \in S^0_{1,0}(\Sigma_\lambda)$, and $\Theta(y,\eta) = \left|\det(\partial_y\partial_\eta\psi(y,\eta))\right|^{1/2}$. Moreover, $\psi(y,\eta) - y\cdot\eta \in S^{1-\mu}_{1,0}(\Sigma_\lambda)$ and $a(y,\eta) - 1 \in S^{-1}_{1,0}(\Sigma_\lambda)$.

Remark 4. For sort-range case, i.e., $\mu > 1$, $S(\lambda)$ is a pseudo-differential operator [Nakamura 2016]. For the long-range case, $S(\lambda)$ is not necessarily a pseudo-differential operator, but still it has the *pseudo-local property*, i.e, $\mathrm{Sing}[S(\lambda)\varphi] \subset \mathrm{Sing}[\varphi]$, which follows from the claim $\psi(y,\eta) - y\cdot\eta \in S^{1-\mu}_{1,0}$ with $\mu < 1$. This also implies the off-diagonal smoothness of the integral kernel [Isozaki-Kitada 1985].

Remark 5. The phase function ψ is the generating function of the (modified) classical scattering map. $\Theta(y, \eta)$ is the corresponding volume factor, which makes the operator asymptotically unitary. Thus we may consider that $S(\lambda)$ is a natural quantization of the classical scattering map.

Remark 6. For $1/2 < \mu < 1$, D. Yafaev [1998, CMP] proved closely related result with

$$\psi^D(y, \eta) = y \cdot \eta + (2\lambda)^{-1/2} \int_{-\infty}^{\infty} (V(y + t\eta) - V(t\eta)) dt, \quad \eta \in S^{d-1}, y \in \eta^\perp \simeq T^*_\eta S^{d-1}.$$

Yafaev considered $S(\lambda)$ as a pseudo-differential operator with a symbol in $S^0_{1-\mu,\mu}$, and used calculus in the symbol class. We construct ψ using exact solutions to an eikonal equation, and we use the Fourier integral operator calculus. Our method also applies to more general models.

Remark 7. For Schrödinger operators (with short-range perturbations) on scattering manifolds, it is known that $S(\lambda)$ is an FIO (Melrose-Zworski, Ito-N)

Remark 8. The theorem is proved for more general operators, i.e., $H_0 = p_0(D_x)$, λ in the non-critical values of $p_0(\xi)$, and $V = V(x, D_x)$ pseudodifferential operators (with the long-range condition). The method also applies to discrete Schrödinger operators.

3 Critical decay case, and the spectrum of scattering matrix

▷ Here we consider the case $\mu = 1$. Here we set

$$\Psi(y,\eta) = \int_{-\infty}^{\infty} (V(y+t\eta) - V(t\eta))dt, \quad \eta \in S^{d-1}, y \in \eta^\perp \simeq T_\eta^* S^{d-1}.$$

We note that for any $\alpha, \beta \in \mathbb{Z}_+^{d-1}$, there is $C_{\alpha\beta} > 0$ s.t.

$$\left|\partial_y^\alpha \partial_\eta^\beta \Psi(y,\eta)\right| \le C_{\alpha\beta} \langle y \rangle^{-|\alpha|} \langle \log\langle y \rangle \rangle, \quad (\eta, y) \in T^* S^{d-1}.$$

Then we have slightly stronger results than the case $\mu < 1$.

Theorem 2. *Suppose Assumption A with $\mu = 1$, and let $\Psi(x,\xi)$ be given above. Then $S(\lambda)$ on $L^2(S^{d-1})$ is a pseudo-differential operator on S^{d-1}. Let $s(y,\eta)$ be the symbol of the operator in a local coordinate, i.e.,*

$$S(\lambda)f(\eta) = (2\pi)^{-(d-1)} \iint e^{-i(\eta-\zeta)\cdot y} s(y,\eta) f(\zeta) d\zeta dy,$$

for $f \in C^\infty(S^{d-1})$ supported in the local patch. The principal symbol of $S(\lambda)$ is given by $\exp(-i\sqrt{2\lambda}\Psi(y,\eta))$, i.e., if we set $s_1(y,\eta) = s(y,\eta) - \exp(-i\sqrt{2\lambda}\Psi(y,\eta))$, then s_1 satisfies, for $\forall \alpha, \beta \in \mathbb{Z}_+^{d-1}$,

$$\left|\partial_y^\alpha \partial_\eta^\beta s_1(y,\eta)\right| \le C_{\alpha\beta} \langle y \rangle^{-1-|\alpha|} \langle \log\langle y \rangle \rangle^{1+|\beta|}, \quad \eta \in S^{d-1}, y \in \eta^\perp \simeq T_\eta^* S^{d-1}.$$

▷ In the case $\mu = 1$, we can use the pseudo-differential operator calculus extensively, and we can determine spectrum in several cases.

Proposition 3 (Yafaev). *Suppose Assumption A with $\mu = 1$, and suppose $V(x)$ is rotation symmetric. Moreover, suppose there are $c, R > 0$ such that*

$$|x \cdot \partial_x V(x)| \geq c|x|^{-1}, \quad \textit{if } |x| \geq R.$$

Then, for $\lambda > 0$, the scattering matrix has dense point spectrum on $S^1 = \{z \in \mathbb{C} \mid |z| = 1\}$.

▷ If the potential is not rotation symmetric, we have somewhat weaker result. We write

$$x = r\hat{x}, \quad r = |x|, \quad \hat{x} = x/|x|, \quad \partial_r f(x) = \hat{x} \cdot \partial_x f(x),$$

$$\partial_r^\perp f(x) = (E - \hat{x} \otimes \hat{x})\partial_x f(x) = \partial_x f(x) - \partial_r f(x)\hat{x}.$$

Proposition 4. *Suppose Assumption A with $\mu = 1$, and suppose there are constants $c_1, c_2, R > 0$ such that $c_1 > c_2$ and*

$$|\partial_r V(x)| \geq \frac{c_1}{|x|^2}, \quad |\partial_r^\perp V(x)| \leq \frac{c_2}{|x|^2}, \quad \textit{if } |x| \geq R.$$

Then, for $\lambda > 0$, $\sigma(S(\lambda)) = S^1$, and $S(\lambda)$ has no absolutely continuous spectrum.

Remark 9. We use perturbation theory (or scattering theory) to prove Proposition 4. We cannot exclude the existence of singular continuous spectrum, since the singular continuous spectrum is very unstable under weak perturbations, whereas the absolutely continuous spectrum is stable.

▷ If the potential change sign, the scattering matrix may have absolutely continuous spectrum.

Proposition 5. *Suppose $d = 2$, and let*

$$V(x) = a\frac{x_1}{\langle x\rangle^2}, \quad x = (x_1, x_2) \in \mathbb{R}^2.$$

with $a \neq 0$. Then $S(\lambda)$ has absolutely continuous spectrum on $S^1 \setminus \{e^{\pm ia\pi(2\lambda)^{-1/2}}\}$, except for possibly discrete eigenvalues. The eigenvalues may accumulate only at $\{e^{\pm ia\pi(2\lambda)^{-1/2}}\}$.

Remark 10. If $|a|(2\lambda)^{-1/2} \geq 1$, i.e., $|a| \geq \sqrt{2\lambda}$, then $\sigma(S(\lambda)) = S^1$. On the other hand, if $|a| < \sqrt{2\lambda}$ then $\sigma_{ess}(S(\lambda)) = \{e^{i\theta} \,|\, |\theta| \leq |a|\pi(2\lambda)^{-1/2}\}$.

4 Proof of Theorem 1, outline

4.1 Classical mechanics with space cut-off

▷ We choose $\chi \in C^\infty(\mathbb{R})$ such that $\chi(r) = 1$ if $r \geq 2$; $\chi(r) = 0$ if $r \leq 1$.

▷ We fix an energy interval $I = [E_0, E_1] \Subset (0, \infty)$.

▷ For sufficiently large $R > 0$, we set

$$V_R(x) = \chi(|x|/R)V(x), \quad x \in \mathbb{R}^d,$$

and then

$$p(x, \xi) = \frac{1}{2}|\xi|^2 + V_R(x), \quad p_0(\xi) = \frac{1}{2}|\xi|^2.$$

We consider the classical mechanics with the Hamiltonian $p(x, \xi)$. We write

$$(x(t), \xi(t)) = (x(x_0, \xi_0; t), \xi(x_0, \xi_0; t)) = \exp tH_p(x_0, \xi_0), \quad (x_0, \xi_0) \in \mathbb{R}^{2d}.$$

▷ We may suppose $|V_R(x)| \leq E_0/2$, and hence if $p(x, \xi) = \lambda \in I$ then $|\xi| \geq \sqrt{E_0}$. Moreover, provided R is sufficiently large, $\frac{d^2}{dt^2}|x(t)|^2 \geq c_3 > 0$, and the trajectories are nontrapping.

▷ We can also show $\left\| \frac{\partial \xi(t)}{\partial \xi_0} \right\| = O(R^{-\mu})$, and by choosing R large, we may assume $\xi_0 \mapsto \xi(t)$ is diffeomorphic with the determinant close to 1, uniformly.

4.2 Solution to the Hamilton-Jacobi equation

▷ We consider the solution to

$$\frac{\partial}{\partial t}\phi(t,\xi) = p(\partial_\xi \phi(t,\xi),\xi), \quad \phi(0,\xi) = 0,$$

with $p_0(\xi) \in I$. By the above observations,

$$\Lambda_t \ : \ \eta \mapsto \xi(0,\eta;t)$$

is diffeomorphic for all $t \in \mathbb{R}$. We set

$$u(t,\xi) = \int_0^t \Big\{p(x(0,\eta:s),\xi(0,\eta;s)) - x(0,\eta;s)\cdot\partial_x V_R(x(0,\eta;s))\Big\}ds.$$

Then by the characteristic curve method, we learn

$$\phi(t,\xi) = u(t,\Lambda_t^{-1}(\xi))$$

is the solution to the Hamilton-Jacobi equation.

▷ We can show

$$\partial_\xi^\alpha(\phi(t,\xi) - tp_0(\xi)) = O(\langle t\rangle^{1-\mu}), \quad t \in \mathbb{R},$$

for any $\alpha \in \mathbb{Z}_+^d$.

4.3 Classical wave map and the interaction picture

▷ We note

$$\partial_\xi \phi(t,\xi) = x(0,\xi(0,\eta),t), \quad \text{where } \xi(t,\eta)=\xi.$$

We may consider

$$t \mapsto (\partial_\xi \phi(t,\xi),\xi) = (t\xi + O(\langle t\rangle^{1-\mu}),\xi)$$

be the **modified free motion**, starting from $x=0$ at $t=0$. We subtract the modified free motion from the Hamilton flow:

$$y(x_0,\xi_0;t) = x(x_0,\xi_0;t) - \partial_\xi \phi(t,\xi(x_0,\xi_0;t)).$$

▷ The **classical (inverse) wave map** is defined by the limit of this flow:

$$x_\pm(x_0,\xi_0) = \lim_{t\to\pm\infty} y(x_0,\xi_0;t), \quad \xi_\pm(x_0,\xi_0) = \lim_{t\to\pm\infty} \xi(x_0,\xi_0;t).$$

▷ We denote these maps by w_t and $w_\pm$, respectively:

$$w_t : (x_0,\xi_0) \mapsto (y(t),\xi(t)), \quad w_\pm : (x_0,\xi_0) \mapsto (x_\pm,\xi_\pm).$$

The convergence $w_t \to w_\pm$ $(t \to \pm\infty)$ is locally uniform, including the derivatives.

▷ We note the flow: $t \mapsto (y(t), \xi(t))$ is generated by the Hamiltonian:

$$\begin{aligned} q(t, y, \xi) &= p(y + \partial_\xi \phi(t, \xi), \xi) - p(\partial_\xi \phi(t, \xi), \xi) \\ &= V_R(y + \partial_\xi \phi(t, \xi)) - V_R(\partial_\xi \phi(t, \xi)). \end{aligned}$$

▷ We solve a Hamilton-Jacobi equation to construct the generating function of w_t:

$$\frac{\partial}{\partial t} \psi(t, x_0, \xi) = q(t, \partial_\xi \psi(t, x_0, \xi), \xi), \quad \psi(0, x_0, \xi) = x_0 \cdot \xi.$$

The solution can be constructed by the characteristic curve method, globally in time t (as well as $\phi(t, \xi)$). Then, as in the usual classical mechanics, $\psi(t, x, \xi)$ is the generating function of w_t:

$$w_t : \begin{pmatrix} x \\ \partial_x \psi(t, x, \xi) \end{pmatrix} \mapsto \begin{pmatrix} \partial_\xi \psi(t, x, \xi) \\ \xi \end{pmatrix}.$$

▷ We take limit $t \to \pm\infty$, and we obtain generating functions of the wave maps $w_\pm$:

$$w_\pm : \begin{pmatrix} x \\ \partial_x \psi_\pm(x, \xi) \end{pmatrix} \mapsto \begin{pmatrix} \partial_\xi \psi_\pm(x, \xi) \\ \xi \end{pmatrix}, \quad \psi_\pm(x, \xi) = \lim_{t \to \pm\infty} \psi(t, x, \xi).$$

The corresponding energy conservation law is the eikonal equation:

$$p(x, \partial_x \psi_\pm(x, \xi)) = p_0(\xi).$$

4.4 Quantum long-range scattering

▷ Using the solution to the Hamilton-Jacobi equation, we can define modified wave operators:

$$W_\pm^{\mathrm{D}} E_I(H_0) = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH} e^{-i\phi(t,D_x)} E_I(H_0).$$

on the energy interval $I = [E_0, E_1] \Subset (0,\infty)$ with the modified free motion $e^{-i\phi(t,D_x)}$.

▷ Similarly, using $\psi_\pm(x,\xi)$, we can define the Isozaki-Kitada modifiers by

$$J_\pm u(x) = (2\pi)^{-d/2} \int e^{i\psi_\pm(x,\xi)} \chi_\pm(x,\xi)\hat{u}(\xi)d\xi, \quad \hat{u} = \mathcal{F}u, u \in \mathcal{S}(\mathbb{R}^d),$$

with suitable cut-off $\chi_\pm(x,\xi)$ in the phase space so that the definition make sense. Then the modified wave operators with Isozaki-Kitada type is defined as

$$W_\pm^{\mathrm{IK}} E_I(H_0) = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH} J_\pm e^{-itH_0} E_I(H_0).$$

Remark 11. We note $J_\pm$ can be considered as a quantization of the classical wave maps $w_\pm^{-1}$. Even tough $\psi_\pm$ corresponds to the inverse wave maps, the stationary phase points of $J_\pm$ corresponds to the wave maps $w_\pm^{-1}$.

4.5 Improved Isozaki-Kitada modifiers

▷ The idea of the proof of the existence of Isozaki-Kitada modifier is that, by the Cook-Kuroda method,

$$W_\pm^{\mathrm{IK}} - J_\pm = i \int_0^{\pm\infty} e^{itH} G_\pm e^{-itH_0} dt,$$

where

$$G_\pm = HJ_\pm - J_\pm H_0 = O(\langle x \rangle^{-1-\mu}) \quad \text{in some sense.}$$

▷ We replace $J_\pm$ with $\tilde{J}_\pm$:

$$\tilde{J}_\pm u(x) = (2\pi)^{-d/2} \int e^{i\psi_\pm(x,\xi)} \Theta_\pm(x,\xi) a_\pm(x,\xi) \chi(x,\xi) \hat{u}(\xi) d\xi,$$

where

$$\Theta_\pm(x,\xi) = (\det(\partial_x \partial_\xi \psi_\pm))^{1/2},$$

and suitable $a_\pm \in S^0_{1,0}$ with $a_\pm - 1 \in S^{-1}_{1,0}$. Then the wave operators defined using $\tilde{J}_\pm$ are the same, but we have improved estimates:

$$\tilde{G}_\pm = H\tilde{J}_\pm - \tilde{J}_\pm H_0 = O(\langle x \rangle^{-N}), \quad \forall N,$$

i.e., $\tilde{G}_\pm$ is rapidly decreasing in $|x|$. In the following, we replace $J_\pm$ by $\tilde{J}_\pm$.

4.6 Scattering matrix and the proof of Theorem 1

▷ We use the stationary representation of the scattering matrix. We write

$$T(\lambda):\ f\in L^{2,s}(\mathbb{R}^d)\mapsto \hat{f}|_{\Sigma_\lambda}\in L^2(\Sigma_\lambda),\quad \lambda>0.$$

The scattering matrix has the representation:

$$S(\lambda)=-2\pi i T(\lambda)\big(J_+^*G_- - G_+^*(H-\lambda-i0)^{-1}G_-\big)T(\lambda)^*$$

(due to Isozaki-Kitada and Yafaev). The second term is a smoothing operator by the micro-local resolvent estimate of Isozaki-Kitada, and the first term is a composition of Fourier integral operators.

▷ We can compute (analogously to [Nakamura 2016, CPDE]) the first term and we have the formula of Theorem 1. The argument is rather technical, and we omit the detail.

5 Scattering matrix with discrete or singular spectrum

▷ Here we show the scattering matrix are often expected to have discrete spectrum.

▷ We suppose $\mu = 1$ here. Then we may consider the scattering matrix is approximated by pseudo-differential operator with the symbol

$$\exp(-i\sqrt{2\lambda}\Psi(y,\eta)), \quad \Psi(y,\eta) = \int_{-\infty}^{\infty} (V(y+t\eta) - V(t\eta))dt,$$

where $\eta \in S^{d-1}$, $y \in T^*_\eta S^{d-1} \simeq \eta^\perp$.

▷ In general, if the potential is rotation symmetric, then the scattering matrix is also rotation symmetric, and hence it is a function of the Laplacian on S^{d-1}. Thus the spectrum is always pure point.

▷ If $V(x)$ satisfies the condition $x \cdot \partial_x V(x) \geq c|x|^{-1}$, $|x| \gg 0$, then we use the representation:

$$\Psi(y,\eta) = \int_0^1 \int_{-\infty}^{\infty} y \cdot (\partial_x V)(sy+t\eta)dtds \tag{*}$$

to obtain $c_1\langle\log\langle y\rangle\rangle \leq \Psi(y,\eta) \leq c_2\langle\log\langle y\rangle\rangle$ with $0 < c_1 < c_2$, $|y| \gg 0$.
By Weyl's theorem on the essential spectrum, we have $\sigma(S(\lambda)) = S^1$.

▷ If V is not necessarily rotation symmetric, but satisfies the conditions:

$$|\partial_r V(x)| \geq \frac{c_1}{|x|^2}, \quad |\partial_r^\perp V(x)| \leq \frac{c_2}{|x|^2}, \quad \text{if } |x| \geq R.$$

with $c_1 > c_2 > 0$, then we still have

$$c_1' \langle \log\langle y\rangle\rangle \leq |\Psi(y,\eta)| \leq c_2'\langle \log\langle y\rangle\rangle \quad \text{with } 0 < c_1' < c_2', |y| \gg 0.$$

Hence we have $\sigma(S(\lambda)) = S^1$.

▷ We can show that there is $\Phi(y,\eta)$ such that $\Phi - \Psi \in S_{1,0}^{-1+\delta}(\Sigma_\lambda)$ with any $\delta > 0$ such that

$$S(\lambda) - e^{-i\sqrt{2\lambda}\Phi(-D_\eta,\eta)} \in \mathrm{Op}(S_{1,0}^{-N}(\Sigma_\lambda)), \quad \forall N.$$

On the other hand, $\Phi(-D_\eta, \eta)$ has compact resolvent, and hence has discrete spectrum. Thus by the trace-class scattering theory (the Birman-Kuroda theorem), we learn

$$\sigma_{\mathrm{ac}}(S(\lambda)) = \sigma_{\mathrm{ac}}(e^{-i\sqrt{2\lambda}\Phi(-D_\eta,\eta)}) = \emptyset.$$

Remark 12. For the moment, it is not known how to show the absence of singular continuous spectrum.

Remark 13. Probably similar argument can be carried out for $0 < \mu < 1$, though it would be technically more complicated.

6 Scattering matrix with absolutely continuous spectrum

▷ Here we suppose $d = 2$, $\mu = 1$. We set

$$V(x) = a\frac{x_1}{\langle x\rangle^2}, \quad x = (x_1, x_2) \in \mathbb{R}^2.$$

We use the coordinate $(\theta, \omega) \in (\mathbb{R}/(2\pi\mathbb{Z})) \times \mathbb{R}$ of T^*S^1 so that

$$\eta = (\cos\theta, \sin\theta), \quad y = (-\omega\sin\theta, \omega\cos\theta).$$

▷ Then by direct computations, we can compute $\Psi(y, \eta)$ explicitly using (*):

$$\Psi(\theta, \omega) = -a\pi\sin\theta(\omega/\langle\omega\rangle).$$

▷ We set $L = \mathrm{Op}(\ell)$, $\ell(\theta, \omega) = \mathrm{sgn}(a)\cos\theta\langle\omega\rangle$, $\mathrm{Op}(\cdot)$ denotes the Weyl quantization. Let $J \subset S^1$ is an interval such that $J \cap \{e^{\pm ia\pi\sqrt{2\lambda}}\} = \emptyset$. Then there is $c > 0$ and a compact operator K such that the Mourre inequality holds:

$$E_J(S(\lambda))S(\lambda)^*[L, S(\lambda)]E_J(S(\lambda)) \geq cE_J(S(\lambda)) + K.$$

Thus we can apply the Mourre theory for unitary operators (e.g., [Fernandez, Richard, Tieda de Aldecoa 2013, JST]), we learn the claim of Proposition 5, i.e., the spectrum is absolutely continuous except for possibly discrete point spectrum.

▷ The key of the above argument is the Hamilton flow generated by $\Psi(\theta,\omega) = -a\pi \sin\theta(\omega/\langle\omega\rangle)$ on T^*S^1. We note

$$\{\Psi(\theta,\omega), \langle\omega\rangle^2\} = -a\pi\cos\theta(\omega^2/\langle\omega\rangle) = -a\pi\cos\theta\langle\omega\rangle + O(\langle\omega\rangle^{-1}),$$

and

$$-\{\Psi(\theta,\omega), \mathrm{sgn}(a)\cos\theta\langle\omega\rangle\} = |a|\pi\left(\frac{\sin^2\theta}{\langle\omega\rangle^2} + \cos^2\theta\frac{\omega^2}{\langle\omega\rangle^2}\right) \geq |a|\pi\cos^2\theta\frac{\omega^2}{\langle\omega\rangle^2}.$$

These imply we may consider $\ell(\theta,\omega) = \mathrm{sgn}(a)\cos\theta\langle\omega\rangle$ as an escaping function of the Hamilton flow generated by $\Psi(\theta,\omega)$. From these observation, the Mourre estimates follows naturally.

Remark 14. There are other cases when we can compute $\Psi(y,\eta)$ (almost) explicitly, but for the moment, we do not have good general formulation.

Remark 15. In general $\Psi(\theta,\omega)$ is not bounded (even if $\mu = 1$), and then we cannot use the Mourre theory for unitary operators directly. We need different argument to determine the spectral properties of $S(\lambda)$. One possibility may be construct Enss-type scattering theory for the pair of unitary operators $S(\lambda)$ and $e^{i\mathrm{Op}(\Psi)}$.

References

1. S. Nakamura: Long-range scattering matrix for Schrödinger-type operators, Preprint 2018, (arXiv:1804.05488).
2. S. Nakamura: Remarks on scattering matrices for Schrödinger operators with critically long-range perturbations, Preprint 2018 (arXiv:1804.05489).