Remarks on scattering theory for Schrödinger operators on scattering manifolds

(or 2-body scattering theory in the polar coordinate system)

Kenichi Ito (Tsukuba U) and Shu Nakamura (U Tokyo)

ICM Satellite Conference on “Quantum Systems”

Chennai, 2010, August 15

Contents:

1. Schrödinger operators on scattering manifolds (Model)

Suppose $M = M_c \cup M_\infty$, where M_c is relatively compact, $M_\infty \cong (0,\infty) \times \partial M$, ∂M: a closed manifold. We consider a formally self-adjoint operator on M such that P is expressed as

$$P = -\frac{1}{2} G^{-1} (\partial_r, \partial_\theta / r) G \begin{pmatrix} a_1 & a_2 \\ {}^t a_2 & a_3 \end{pmatrix} \Big(\partial_r, \partial_\theta / r \Big) + V, \qquad (r,\theta) \in \mathbb{R}_+ \times \partial M,$$

on M_∞. We consider P as an operator on $\mathcal{H} = L^2(M, G dx)$, where $a_k, V \in C^\infty(M)$ such that for any ℓ, α,

$$|\partial_r^\ell \partial_\theta^\alpha (a_1 - 1)| \le C r^{-1-\mu-\ell}, \quad |\partial_r^\ell \partial_\theta^\alpha a_2| \le C r^{-\mu-\ell},$$

$$|\partial_r^\ell \partial_\theta^\alpha (a_3 - \hat{h})| \le C r^{-\mu-\ell}, \quad |\partial_r^\ell \partial_\theta^\alpha V| \le C r^{-1-\mu-\ell}.$$

Here $G(r,\theta) = r^{n-1} H(\theta)$ with $H(\theta)$: some density on ∂M, $\hat{h}$ is a positive 2-tensor on ∂M. We suppose $\mu > 0$.

Example: $M=\mathbb{R}^n$, $H=-\triangle+V$. In this case, we set $\partial M=S^{n-1}$, $\hat{h}$ is the standard (co)metric on S^{n-1}, $a_1=1$, $a_2=0$, $a_3=\hat{h}$, and V satisfies the short-range condition of the usual scattering theory. Even if $M=\mathbb{R}^n$, our assumption is weaker than the usual short-range condition (with respect to a_2, a_3).

Remark: Our model is somewhat more general than the *scattering metric* in the sense of Melrose. In his setting, $\mu=1$ and all coefficients (a_1, a_2, a_3, V) have asymptotic expansions in r^{-1} as $r\to\infty$.

2. Spectral propertirs of the operator

(cf. e.g. Froese-Hislop-Perry 1989, etc.)

Theorem 0: (1) P is essentially self-adjoint on $C_0^\infty(M)$.
(2) $\sigma_{ess}(P) = [0, \infty)$ and $\sigma_d(P) \subset (-\infty, 0]$ is bounded.
(3) $\sigma_{pp}(P)$ is discrete except for 0, $\sigma_{ac}(P) = [0, \infty)$,
and $\sigma_{sc}(P) = \emptyset$.

Proof: Use the Weyl sequence, the Mourre estimate. $\square$

3. Construction of the scattering theory

Reference system: We set

$$M_f = \mathbb{R} \times \partial M, \quad \mathcal{H}_f = L^2(M_f, H(\theta)drd\theta), \quad P_f = -\frac{1}{2}\frac{\partial^2}{\partial r^2}$$

as the "free" system. We let $j(r) \in C^\infty(\mathbb{R})$ such that $j(r) = \begin{cases} 1, & (r \geq 1) \\ 0, & (r \leq 0) \end{cases}$. We set $\mathcal{J}$: $\mathcal{H}_f \to \mathcal{H}$ by

$$\mathcal{J}\phi(r,\theta) = r^{-(n-1)/2} j(r)\phi(r,\theta) \qquad \text{if } (r,\theta) \in M_\infty$$

for $\phi \in \mathcal{H}_f$. Then we define the wave operators by

$$W_\pm = W_\pm(P, P_f, \mathcal{J}) = \operatorname*{s-lim}_{t\to\pm\infty} e^{itP}\mathcal{J}e^{-itP_f}.$$

We can easily show $W_\pm$ exist, but it is *not* isometry.

We write

$\mathcal{F}$: Fourier transform in r,

We decompose $\mathcal{H}_0 = \mathcal{H}_{0,+} \oplus \mathcal{H}_{0,-}$ where

$$\mathcal{H}_{0,\pm} = \{\phi \in \mathcal{H}_0 \,|\, \mathrm{supp}(\mathcal{F}\phi) \subset \overline{\mathbb{R}_\pm} \times \partial M\}.$$

Theorem 1: (1) The wave operators $W_\pm$ exist. Moreover, $W_\pm \mathcal{H}_{0,\mp} = 0$ and $W_\pm$ are isometry from $\mathcal{H}_{0,\pm}$ into $\mathcal{H}$.
(2) $W_\pm$ are complete, i.e., Ran $W_\pm = \mathcal{H}_c(P)$.

Thus we can approximate the solution $\psi(t) = e^{-itP}\psi_0$ $(\psi_0 \in \mathcal{H}_c(P))$ by

$$\psi(t) \sim \mathcal{J}\, e^{-itP_f}\varphi_\pm \quad \text{as } t \to \pm\infty$$

where P_f is the 1-dim Laplacian, and $\varphi_\pm = W_\pm^* \psi_0$.

Remarks: (1) Even for $P = -\triangle + V$ on $\mathbb{R}^n$, the wave operators $W_\pm$ are <u>not</u> the same as the standard wave operators, since P_f is not the same as the free Laplacian.

(2) Scattering theory for such manifolds were studied by, e.g., De Biévre-Hislop-Sigal (1992), but the construction and hence the wave operators are quite different.

(3) P is <u>not</u> a small perturbation of P_f. In fact, $P - P_f$ is not P_f-bounded, and not even P-bounded. So, standard theorems of the scattering theory do not directly apply.

(4) Still, the idea is functional analytic, and we follow the essential ideas of the scattering theory very closely (Birman, Kato, Kuroda, etc.). We use a generalized formalism of the abstract 2-space stationary scattering theory.

Scattering matrix: By the asymptotic completeness, the scattering operator:

$$S = W_+^* W_- \ : \ \mathcal{H}_{0,-} \to \mathcal{H}_{0,+}$$

is a unitary operator. We set

$$(F_{0,\pm}(\lambda)\phi)(\theta) = (2\lambda)^{-1/4}(\mathcal{F}\phi)(\pm\sqrt{2\lambda}, \theta)$$

for $\phi \in \mathcal{H}_{0,\pm}$. Then there exists the scattering matrix: $\{S(\lambda) \in \mathcal{L}(\mathcal{H}_b) \,|\, \lambda > 0\}$ (where $\mathcal{H}_b = L^2(\partial M, H d\theta)$) such that

$$F_{0,+}(\lambda) S\phi = S(\lambda) F_{0,-}(\lambda)\phi$$

for $\phi \in \mathcal{H}_0^-$. ($S(\lambda)$ is unitary for a.e. λ.)

Theorem 2: For $\phi \in H^2(\partial M)$ and $\lambda > 0$, there exists a λ-generalized eigenfunction Ψ such that

$$\left\| \Psi(r, \cdot) - r^{-(n-1)/2}(e^{-ikr}\phi + e^{ikr}(S(\lambda)\phi)) \right\|_{\mathcal{H}_b} = O(r^{-(n-1)/2-\delta})$$

as $r \to \infty$ with some $\delta > 0$, where $k = \sqrt{2\lambda}$.

Thus $S(\lambda)$ is the same scattering matrix as defined using asymptotic expansion of generalized eigenfunctions (*the absolute scattering matrix* due to Melrose).

4. Microlocal properties of the scattering matrix

We write $q(\theta,\omega) = \dfrac{1}{2}\sum_{j,k} \widehat{h}^{jk}(\theta)\omega_j\omega_k$ be the symbol of the Laplace operator on ∂M. We denote the Hamilton flow generated by a symbol b by $\exp(tH_b)$, $t \in \mathbb{R}$.

Theorem 3.(Melrose-Zworski) Suppose P and S as above with $\mu = 1$. Then $S(\lambda)$ is an FIO (Fourier integral operator) associated to $\exp(\pi H_{\sqrt{2q}})$.

Remark: (1) $\exp(tH_{\sqrt{2q}})$ is the geodesic flow on ∂M corresponding to the (co)metric $\widehat{h}$.
(2) The above result is true for $\mu > 0$ if we generalize the definition of FIOs.

Theorem 3 implies

$$(*) \qquad WF(S(\lambda)\phi) = \exp(\pi H_{\sqrt{2q}})(WF(\phi))$$

for $\phi \in L^2(\partial M, H d\theta)$. This holds more generally:

Theorem 4. $(*)$ holds under the assumption $\mu > 0$.

Example: If $M = \mathbb{R}^n$, and if $\widehat{h}$ is the standard metric on S^{n-1}, then $\exp(\pi H_{\sqrt{2q}})$ is the antipodal map. This result is a generalization and refinement of the well-known result: the integral kernel of $S(\lambda)$ is smooth except for the diagonal set.

5. Idea of proof

(1) The classical mechanical scattering for conic manifolds

We set

$$p_c(r,\rho,\theta,\omega) = \frac{1}{2}\Big(\rho^2 + \frac{q(\theta,\omega)}{r^2}\Big), \quad r > 0, \rho \in \mathbb{R}, (\theta,\omega) \in T^*\partial M,$$

be the classical hamilton function corresponding to the *conic* metric, and we consider the scattering for the classical mechanics. If we set

$$(r(t),\rho(t),\theta(t),\omega(t)) = \exp(tH_{p_c})(r_0,\rho_0,\theta_0,\omega_0), \quad t \in \mathbb{R}.$$

We can solve the Hamilton equation explicitly, and

$$r(t) = \sqrt{2E_0t^2 + 2r_0\rho_0 + r_0^2}, \quad \rho(t) = \frac{2E_0t + r_0\rho_0}{\sqrt{2E_0t^2 + 2r_0\rho_0 + r_0^2}},$$

where $E_0 = p_c(r_0,\rho_0,\theta_0,\omega_0) = p_c(r(t),\rho(t),\theta(t),\omega(t))$, and

$$(\theta(t), \omega(t)) = \mathsf{exp}(\tau(t) H_q)(\theta_0, \omega_0),$$

where

$$\tau(t) = \int_0^t \frac{ds}{r(s)^2} = \frac{1}{\sqrt{2q_0}}\Big\{\mathsf{tan}^{-1}\Big(\frac{2E_0 t + \rho_0 r_0}{\sqrt{2q_0}}\Big) - \mathsf{tan}^{-1}\Big(\frac{\rho_0 r_0}{\sqrt{2q_0}}\Big)\Big\}$$

with $q_0 = q(\theta_0, \omega_0) = q(\theta(t), \omega(t))$. Noting

$$\frac{1}{\sqrt{2q}} H_q = H_{\sqrt{2q}},$$

we can also write

$$(\theta(t), \omega(t)) = \mathsf{exp}(\sigma(t) H_{\sqrt{2q}})(\theta_0, \omega_0),$$

where $\sigma(t) = \mathsf{tan}^{-1}\Big(\frac{2E_0 t + \rho_0 r_0}{\sqrt{2q_0}}\Big) - \mathsf{tan}^{-1}\Big(\frac{\rho_0 r_0}{\sqrt{2q_0}}\Big).$

Now we consider the behavior as $t \to \pm\infty$. Then

$$r_\pm = \lim_{t\to\pm\infty}(r(t) - t\rho(t)) = \pm\frac{r_0\rho_0}{\sqrt{2E_0}},$$

$$\rho_\pm = \lim_{t\to\pm\infty}\rho(t) = \pm\sqrt{2E_0},$$

$$(\theta_\pm, \omega_\pm) = \lim_{t\to\pm\infty}(\theta(t), \omega(t)) = \exp(\sigma_\pm H_{\sqrt{2q}})(\theta_0, \omega_0)$$

where $\sigma_\pm = \pm\frac{\pi}{2} - \tan^{-1}\left(\frac{\rho_0 r_0}{\sqrt{2q_0}}\right)$.

We write this map (the classical wave operator) by

$$w_\pm : (r_0, \rho_0, \theta_0, \omega_0) \mapsto (r_\pm, \rho_\pm, \theta_\pm, \omega_\pm)$$

and $w_\pm$ are diffeomorphism from $\mathbb{R}_+ \times \mathbb{R} \times (T^*\partial M \setminus 0)$ to $\mathbb{R} \times \mathbb{R}_\pm \times (T^*\partial M \setminus 0)$. ($w_\pm^{-1}$ is also easily computed.)

If we write $p_f = \frac{1}{2}\rho^2$, then we may write

$$w_\pm(r_0, \rho_0, \theta_0, \omega_0) = \lim_{t \to \pm\infty} \exp(-tH_{p_f}) \circ \exp(tH_{p_c})(r_0, \rho_0, \theta_0, \omega_0)$$

Then the classical scattering operator:

$$s_c = w_+ \circ w_-^{-1} : \mathbb{R} \times \mathbb{R}_- \times (T^*\partial M \setminus 0) \ \to \ \mathbb{R} \times \mathbb{R}_+ \times (T^*\partial M \setminus 0)$$

is a diffeomorphism and easily computed:

$$s_c : (r, \rho, \theta, \omega) \mapsto (-r, -\rho, \exp(\pi H_{\sqrt{2q_0}}(\theta, \omega)).$$

This is the quantity we saw in Theorems 3 and 4.

(2) Scaling (or semiclassical formalism)

— How the classical mechanical scattering for the conic case is related to our scattering matrix?

— We fix an energy:

$$E = \frac{1}{2}\Big(\rho^2 + \frac{q(\theta,\omega)}{r^2}\Big) + O(\rho^2 r^{-1-\mu}) + O(\rho r^{-1-\mu}|\omega|) + O(r^{-2-\mu}|\omega|^2).$$

The singularities of $S(E)$ is related to the behavior of the scattering as $|\omega| \to \infty$. If $|\omega| = O(h^{-1})$, then have to have $r = O(h^{-1})$. So we consider the scaling:

$$(r,\rho,\theta,\omega) \ \mapsto \ (h^{-1}r, \rho, \theta, h^{-1}\omega)$$

and take $h \to 0$. Then

$$p(h^{-1}r, \rho, \theta, h^{-1}\omega) = p_c(r,\rho,\theta,\omega) + O(h^\mu).$$

Thus we may approximate the Hamiltonian by p_c.

(3) (Semiclassical) Egorov type theorem

Let $a = a(r, \rho, \theta, \omega) \in C_0^\infty(T^*M_\infty)$ (or $\in C_0^\infty(T^*M_f)$), and we denote the quntization of a by $Op(a)$:

$$Op(a) = a(r, D_r, \theta, D_\theta).$$

We consider the corresponding scaling:

$$a^h(r, \rho, \theta, \omega) = a(hr, \rho, \theta, h\omega),$$

and hence the corresponding (semiclassical) quantization is

$$Op(a^h) = a(hr, D_r, \theta, hD_\theta).$$

It satisfies for any indices $\alpha, \beta, \gamma, \delta$,

$$\left|\partial_r^\alpha \partial_\rho^\beta \partial_\theta^\gamma \partial_\omega^\delta a^h(r, \rho, \theta, \omega)\right| = O(h^{-|\alpha|-|\delta|}).$$

— We fix $(r_0, \rho_0, \theta_0, \omega_0) \in T^*M_\infty$ with $r > 0$, $\omega_0 \neq 0$, and we suppose $a \in C_0^\infty(T^*M_\infty)$ is supported in a small neighborhood of $(r_0, \rho_0, \theta_0, \omega_0)$. we set

$$A_0 = Op(a^h), \quad \text{(where } a^h(r, \rho, \theta, \omega) = a(hr, \rho, \theta, h\omega))$$

and study $A_\pm = W_\pm^* A_0 W_\pm$.

— We set $\eta(r) \in C^\infty(\mathbb{R})$ so that $\eta(r) = 1$ if $r \geq 1$ and $= 0$ if $r \leq 1/2$; we set: $Y = \eta(hr/\varepsilon\langle t\rangle)$ with sufficiently small $\varepsilon > 0$.

Step 1. Let $Z = \eta(P_f/\delta)$ with small $\delta > \varepsilon^2 > 0$. Then

$$ZW_\pm^* A_0 W_\pm Z = \lim_{t\to\pm\infty} Z(e^{itP_f/h}\mathcal{J}^* Y e^{-itP/h}) A_0 (e^{itP/h} Y \mathcal{J} e^{-itP_f}/h) Z.$$

— So we study: $A(t) = (e^{itP_f/h}\mathcal{J}^* Y e^{-itP/h}) A_0 (e^{itP/h} Y \mathcal{J} e^{-itP_f/h})$.

Step 2. We compute:

$$\frac{d}{dt}(e^{itP/h}Y\mathcal{J}e^{-itP_f/h}) = \frac{i}{h}e^{itP/h}T(t)e^{-itP_f/h}$$

with $T(t) = PY\mathcal{J} - Y\mathcal{J}P_f + \frac{h(hr)t}{i\varepsilon\langle t\rangle^3}\eta'(\frac{hr}{\varepsilon\langle t\rangle})\mathcal{J}$. This can be further rewritten to obtain:

$$\frac{d}{dt}(e^{itP/h}Y\mathcal{J}e^{-itP_f/h}) = \frac{i}{h}(e^{itP/h}Y\mathcal{J}e^{-itP_f/h})L(t) + R_1(t)$$

with $L(t) = e^{itP_f/h}\mathcal{J}^*T(t)e^{-itP_f/h}$, and a remainder term $R_1(t)$. Thus we expect that $A(t)$ satisfies a Heisenberg equation:

$$\frac{d}{dt}A(t) \sim -\frac{i}{h}[L(t), A(t)], \quad A(0) \sim \mathcal{J}^*A_0\mathcal{J}.$$

Step 3. We can construct an asymptotic solution to the Heisenberg equation: $A(t) = Op(b^h(t))$, where $b^h \in C_0^\infty(T^*M_f)$ such that

$$\text{supp } b^h(t) = w_c^{-1}[\text{supp } a^h], \quad b^h(t) - a^h \circ w_c(t) = O(h^\mu)$$

uniformly in t, where $w_c(t) = \exp(-tH_{p_c}) \circ \exp(tH_{p_f})$. Moreover,

$$b_\pm^h = \lim_{t\to\pm\infty} b^h(t), \quad \text{exists and} \quad b_\pm^h - a^h \circ w_\pm = O(h^\mu).$$

Hence we have

$$W_\pm^* A_0 W_\pm = Op(b^h), \quad \text{supp } [b_\pm^h] = w_\pm[\text{supp } a^h].$$

Similarly, we can show for $a \in C_0^\infty(T^*M_f)$ with small support, there is b such that $W_\pm Op(a^h) W_\pm^* = Op(b^h)$,

$$b^h - a^h \circ w_\pm^{-1} = O(h^\mu), \quad \text{supp } b^h = w_\pm[\text{supp } a^h].$$

Step 4. Combining above results: for any $a \in C_0^\infty(T^*M_f)$, supported in a small neighborhood of $(r_-, \rho_-, \theta_-, \omega_-)$ with $\omega_- \neq 0$, there is $b \in C_0^\infty(T^*M_f)$ such that

$$SOp(a^h)S^* = Op(b^h),$$

and supp $b^h = s_c[\text{supp } a^h]$, $b^h - a^h \circ s_c^{-1} = O(h^\mu)$.

Step 5. Let $\lambda > \delta > 0$ and $a(\theta, \omega) \in C_0^\infty(T^*\partial M)$. We set $a^h(\theta, \omega) = a(\theta, h\omega)$. Then there is $b^h \in C_0^\infty(T^*\partial M)$ such that

$$S(\lambda)Op(a^h)S(\lambda)^* = Op(b^h).$$

Moreover, $b^h - a^h \circ (\exp(\pi H_{\sqrt{2q}}))^{-1} = O(h^\mu)$, and b^h is supported in $\exp(\pi H_{\sqrt{2q}})(\text{supp } a^h)$.

(4) Proof of Theorems 3 and 4:

— If $\mu = 1$, then by a Beals type characterization of FIOs (cf. Ref.4.), we have Theorem 3, i.e., $S(E)$ are FIOs associated to $\exp(\pi H_{\sqrt{2q}})$.

— If $\mu < 1$, we can use the the usual characterization of the wave front sets using (semiclassical) h-pseudodifferential operators to show Theorem 4, i.e., $WF(S(E)\phi) = \exp(\pi H_{\sqrt{2q}})[WF(\phi)]$ for $\phi \in L^2(\partial M)$.

References:

1. Melrose, R: Spectral and scattering theory for the Laplacian on asymptotically Euclidian spaces. In Spectral and Scattering Theory (M. Ikawa, ed.), 85–130, Marcel Decker, 1994.
2. Melrose, R. B., Zworski, M.: Scattering metrics and geodesic flow at infinity. Inventiones Mathematicae **124**, 389–436 (1996).
3. Ito, K., Nakamura, S.: Time-dependent scattering theory for Schrödinger operators on scattering manifolds, J. London Math. Soc. **81**, 774-792 (2010).
4. Ito, K., Nakamura, S.: Remarks on the fundamental solution to Schrödinger equation with variable coefficients. Preprint 2009 Dec. (submitted)

5. Ito, K., Nakamura, S.: Microlocal properties of scattering matrices for Schrödinger equations on scattering manifolds. In preparation.