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Asymptotic Properties of Solutions to 3-particle Schrödinger Equations

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Abstract

We construct a generalized Fourier transformation $\mathcal{F}(\lambda)$ associated with the 3-body Schrödinger operator $H=-\Delta+\sum_a V_a(x^a)$ and characterize all solutions of $(H-\lambda)u=0$ in the Agmon-Hörmander space $\mathcal{B}^*$ as the image of $\mathcal{F}(\lambda)^*$. These stationary solutions admit asymptotic expansions in $\mathcal{B}^*$ in terms of spherical waves associated with scattering channels.

1 Introduction

1.1 *Helmholtz equation.* Consider the Helmholtz equation in $\mathbf{R}^n$

$$(-\Delta-\lambda)u=0, \quad \lambda>0. \tag{1.1}$$

According to a classical theorem of Sommerfeld-Rellich, $u=0$ if u satisfies (1.1) and $u=O(|x|^{-s})$ as $|x|\to\infty$ for $s>(n-1)/2$. Non-trivial solutions arise from the decay rate $s\leq(n-1)/2$, and the border line case $s=(n-1)/2$ was characterized by Agmon-Hörmander [2] : Let u be a solution to (1.1). Then u satisfies

$$\sup_{R>1}\frac{1}{R}\int_{|x|<R}|u(x)|^2dx<\infty \tag{1.2}$$

if and only if u is written as

$$u(x)=\int_{S^{n-1}}e^{i\sqrt{\lambda}\omega\cdot x}\varphi(\omega)d\omega \tag{1.3}$$

for some $\varphi\in L^2(S^{n-1})$. This, combined with the stationary phase method on the sphere, implies that all the solution u of (1.1) satisfying (1.2) admits an asymptotic expansion

$$u\simeq C(\lambda)r^{-(n-1)/2}e^{i\sqrt{\lambda}r}\varphi(\hat{x})+\overline{C(\lambda)}r^{-(n-1)/2}e^{-i\sqrt{\lambda}r}\varphi(-\hat{x}), \tag{1.4}$$

where $r=|x|,\hat{x}=x/r$, and the asymptotic relation $u\simeq v$ means that

$$\lim_{R\to\infty}\frac{1}{R}\int_{|x|<R}|u(x)-v(x)|^2dx=0. \tag{1.5}$$

The intention of Agmon-Hörmander is to characterize the restriction of Fourier transforms on submanifolds in $\mathbf{R}^n$ and they introduced the following Besov type space : It is the Banach space $\mathcal{B}$ equipped with the norm

$$\|u\|_{\mathcal{B}} = \left(\int_{\Omega_0} |u(x)|^2 dx\right)^{1/2} + \sum_{j=1}^{\infty} \left(2^{j-1} \int_{\Omega_j} |u(x)|^2 dx\right)^{1/2} < \infty,$$

where $\Omega_0 = \{x \in \mathbf{R}^n; |x| < 1\}$, $\Omega_j = \{x \in \mathbf{R}^n; 2^{j-1} < |x| < 2^j\}$ for $j \geq 1$. The norm of the dual space $\mathcal{B}^*$ is equivalent to the following one

$$\|u\|_{\mathcal{B}^*} = \sup_{R>0} \left(\frac{1}{R} \int_{|x|<R} |u(x)|^2 dx\right)^{1/2}.$$

Let for $s \in \mathbf{R}$

$$u \in L^{2,s} \iff \|u\|_s = \|(1 + |x|)^s u(x)\|_{L^2(\mathbf{R}^n)} < \infty.$$

For $s > 1/2$ we have the following inclusion relations

$$L^{2,s} \subset \mathcal{B} \subset L^{2,1/2} \subset L^2 \subset L^{2,-1/2} \subset \mathcal{B}^* \subset L^{2,-s}.$$

We also have

$$|(u, v)| \leq C\|u\|_{\mathcal{B}}\|v\|_{\mathcal{B}^*}.$$

1.2 *2-body Schrödinger equation.* There are two directions for generalization of the above facts. One is the extension to Laplacians on non-compact Riemannian manifolds. This is actually a classical problem and had been studied by Helgason [12], [13] for example. The general case was studied by Agmon [1], Melrose [24], Melrose-Zworski [25]. Another is the extension to Schrödinger equations. Kato [23] proved that the solution of the 2-body Schrödinger equation

$$(-\Delta + V(x) - \lambda)u(x) = 0, \quad \lambda > 0$$

satisfying $u \in L^{2,-\alpha}, \alpha < 1/2$, vanishes identically. Non-trivial solutions to the critical case were charactrerized by Yafaev [31], Gâtel-Yafaev [6].

For the sake of simplicity, let us mention the 2-body Schrödinger operator with short-range potential $H = -\Delta + V(x)$, $V(x) = O(|x|^{-1-\epsilon})$ $(\epsilon > 0)$. Suppose u is a solution to the equation

$$(H - \lambda)u = 0, \quad \lambda > 0. \tag{1.6}$$

Then u satisfies (1.2) if and only if u is written as

$$u = \mathcal{F}(\lambda)^*\varphi, \quad \varphi \in L^2(S^{n-1}), \tag{1.7}$$

where $\mathcal{F}(\lambda)$ is the operator defined by

$$\mathcal{F}(\lambda)f = \int_{\mathbf{R}^n} e^{-i\sqrt{\lambda}\omega\cdot x} f(x)dx - \int_{\mathbf{R}^n} e^{-i\sqrt{\lambda}\omega\cdot x} V(x)R(\lambda + i0)f dx, \tag{1.8}$$

with $R(z) = (H - z)^{-1}$. The solution u of (1.6) satisfying (1.2) admits an asymptotic expansion

$$u \simeq C(\lambda)r^{-(n-1)/2}e^{i\sqrt{\lambda}r}\varphi_+(\hat{x}) + \overline{C(\lambda)}r^{-(n-1)/2}e^{-i\sqrt{\lambda}r}\varphi_-(\hat{x}), \tag{1.9}$$

and $\varphi_\pm$ are related as follows

$$\varphi_+ = \hat{S}(\lambda)J\varphi_-, \tag{1.10}$$

where $(J\varphi)(\omega) = \varphi(-\omega)$ and $\hat{S}(\lambda)$ is the scattering matrix for H. The operator $\mathcal{F}(\lambda)$ is a spectral representation (generalized Fourier transformation) for H. In fact there are two types of generalized Fourier transformation $\mathcal{F}_\pm(\lambda)$, which are related to the spatial asymptotics of the resolvent in the following way :

$$\mathcal{F}_\pm(\lambda)f = \lim_{r\to\infty} C_\pm(\lambda)r^{(n-1)/2}e^{\mp i\sqrt{\lambda}r}(R(\lambda \pm i0)f)(r\cdot).$$

Moreover

$$\mathcal{F}(\lambda)f = \mathcal{F}_+(\lambda)f = \overline{J\mathcal{F}_-(\lambda)\overline{f}}.$$

The above facts (1.7), (1.9) and (1.10) are thus closely related each other and arise from fundamental properties of the generalized Fourier transformation associated with H.

1.3 *3-body Schrödinger equation.* To extend the above results to many-body Schrödinger equations is a very difficult problem. It was shown in [18] that a solution u of the N-body Schrödinger equation $(H-\lambda)u = 0$ vanishes identically if $u \in L^{2,-\alpha}$ for some $\alpha < 1/2$ and if λ is neither the eigenvalue nor in the set of thresholds of H. This is a generalization of Sommerfeld-Rellich's classical result to the many-body problem. To charcterize the solutions of the border line case is much harder, since it requires a detailed knowledge of the N-body stationary Schrödinger equation, which remains unknown in spite of the success of the proof of asymptotic completeness by the time-dependent method [4], [26], [8], [3].

In this paper, we shall study this problem in the case of 3-particle systems in $\mathbf{R}^3$. We consider 3 particles with mass $m_i > 0$ and position $q_i \in \mathbf{R}^3$. To remove the motion of the center of mass, our Hamiltonian is defined over the space

$$\mathcal{X} = \{(q_1, q_2, q_3); \sum_{i=1}^{3} m_i q_i = 0\} \simeq \mathbf{R}^6.$$

Let $a = (i, j)$ be a pair of particles i and j, and k be the 3rd partcle. The reduced masses m_a, n_a and the Jacobi-coordinates are defined by

$$\frac{1}{m_a} = \frac{1}{m_i} + \frac{1}{m_j}, \quad \frac{1}{n_a} = \frac{1}{m_i + m_j} + \frac{1}{m_k},$$

$$x^a = \sqrt{2m_a}(q_i - q_j), \quad x_a = \sqrt{2n_a}(q_k - \frac{m_i q_i + m_j q_j}{m_i + m_j}).$$

The 3-particle Hamiltonians H_0, H are defined by

$$H_0 = -\triangle_{x_a} - \triangle_{x^a}, \quad H = H_0 + \sum_a V_a(x^a),$$

where $\triangle_{x_a}$ $(\triangle_{x^a})$ denotes the Laplacian with respect to the variable x_a (x^a). We put

$$T_a = -\triangle_{x_a}, \quad H^a = -\triangle_{x^a} + V_a(x^a),$$

$$H_a = T_a + H^a = H_0 + V_a(x^a).$$

Let

$$R(z) = (H - z)^{-1}, \quad R_a(z) = (H_a - z)^{-1}, \quad R^a(z) = (H^a - z)^{-1}.$$

Let $\mathcal{T}$ be the set of thresholds of H, namely

$$\mathcal{T} = \{0\} \cup \cup_a \sigma_p(H^a),$$

where $\sigma_p(H^a)$ is the set of eigenvalues of H^a. Let $\mathcal{T}' = \mathcal{T} \cup \sigma_p(H)$. We define

$$a(\lambda) = \inf\{\lambda - t; t \in \mathcal{T}', t < \lambda\}.$$

$a(\lambda) = \lambda$ if $\lambda > 0$.

To get the complete result, we assume that each pair potential decays rapidly. More precisely, each pair potential $V_{ij}(y)$ is assumed to be a real C^∞-function on $\mathbf{R}^3$ and to satisfy

Assumption $$\partial_y^m V_{ij}(y) = O(|y|^{-m-\rho}), \quad \forall m \geq 0 \tag{1.11}$$

for some $\rho > 5$. Here ∂_y^m stands for any differentiaition of order m.

Let us stress that this is the only assumption we impose on our 3-particle systems. We assume no extra assumptions such as nonexistence of zero-eigenvlue or zero-resonances.

One can allow Coulombic singularities for V_{ij}. Namely our results below also hold if $V_{ij} = V_{ij}^{(1)} + V_{ij}^{(2)}$, where $V_{ij}^{(1)}$ is a smooth function satisfying (1.11), $V_{ij}^{(2)}$ is a compactly supported function satisfying $|V_{ij}^{(2)}(y)| \leq C|y|^{-1}$, and all the multiple commutators of $V_{ij}^{(2)}$ and $A = \frac{1}{2i}(x \cdot \nabla + \nabla \cdot x)$ extend to bounded operators.

1.4 *Main results.* Let us summarize our main results in this paper. Let $H = H_0 + \sum_a V_a(x^a)$ be the 3-body Schrödinger operator with center of mass removed. Each pair potential is assumed to satisfy (1.11). Let $\mathcal{T}$ be the set of thresholds for H and $\mathcal{T}' = \mathcal{T} \cup \sigma_p(H)$. In the following, $\sum_{a,n} = \sum_a \sum_n$ denotes the sum ranging over all pairs of particles and over the eigenvalues of the subsystem $H^a = -\Delta_{x^a} + V_a(x^a)$. The meaning of the notation $\oplus_{a,n}$ is similar to this.

THEOREM 1. *For $\lambda \in \sigma_{cont}(H) \setminus \mathcal{T}'$, there exists a bounded operator*

$$\mathcal{F}(\lambda) : \mathcal{B} \to L^2(S^5) \oplus \oplus_{a,n} L^2(S^2)$$

having the following properties :
(1) $\mathcal{F}(\lambda)$ diagonalizes H :

$$\mathcal{F}(\lambda) H f = \lambda \mathcal{F}(\lambda) f.$$

(2) Define $(\mathcal{F}f)(\lambda)$ by $\mathcal{F}(\lambda)f$. Then the operator $\mathcal{F}$ is uniquely extended to a partial isometry with initial set $\mathcal{H}_{ac}(H)$ = the absolutely continuous subspace for H, and final set

$$L^2((0,\infty); L^2(S^5); \rho_0(\lambda)d\lambda) \oplus \oplus_{a,n} L^2((\lambda^{a,n},\infty); L^2(S^2); \rho_{a,n}(\lambda)d\lambda),$$

$$\rho_0(\lambda) = \frac{\lambda^2}{2}, \quad \rho_{a,n}(\lambda) = \frac{1}{2}\sqrt{\lambda - \lambda^{a,n}},$$

where $\lambda^{a,n} \in \sigma_p(H^a)$.
(3) Let $\mathcal{F}_0(\lambda), \mathcal{F}_{a,1}(\lambda), \cdots$ *be the components of* $\mathcal{F}(\lambda)$. *They are eigenoperators of* H *in the sense that*

$$(H-\lambda)\mathcal{F}_0(\lambda)^*\varphi_0 = 0, \quad (H-\lambda)\mathcal{F}_{a,n}(\lambda)^*\varphi_{a,n} = 0$$

hold for $\varphi_0 \in L^2(S^5), \varphi_{a,n} \in L^2(S^2)$.
(4) For $f \in \mathcal{H}_{ac}(H)$, *the following inversion formula holds :*

$$f = \int_0^\infty \mathcal{F}_0(\lambda)^*(\mathcal{F}_0 f)(\lambda)\rho_0(\lambda)d\lambda + \sum_{a,n}\int_{\lambda^{a,n}}^\infty \mathcal{F}_{a,n}(\lambda)^*(\mathcal{F}_{a,n}f)(\lambda)\rho_{a,n}(\lambda)d\lambda.$$

THEOREM 2. *For* $f \in \mathcal{B}$ *and* $\lambda \in \sigma_{cont}(H)\setminus\mathcal{T}'$, *the boundary value of the resolvent of* H *admits the following asymptotic expansion in the sense of (1.5)*

$$\begin{aligned} R(\lambda+i0)f &\simeq C(\lambda)\frac{e^{i\sqrt{\lambda}r}}{r^{5/2}}\mathcal{F}_0(\lambda)f \\ &+ \sum_{a,n} C_{a,n}(\lambda)\frac{e^{i\sqrt{\lambda-\lambda^{a,n}}r_a}}{r_a}\mathcal{F}_{a,n}(\lambda)f(\omega_a)\otimes\varphi^{a,n}(x^a), \end{aligned}$$

$$C(\lambda) = \sqrt{\frac{\pi}{2}}e^{-3\pi i/4}(\lambda_+)^{3/4}, \quad C_{a,n}(\lambda) = \sqrt{\frac{\pi}{2}}h(\lambda-\lambda^{a,n}),$$

where $k_+ = \max\{k, 0\}$ *and* $h(t) = 1$ *if* $t \geq 0$, $h(t) = 0$ *if* $t < 0$, *and* $\varphi^{a,n}$ *is the eigenvector of* H^a *associated with the eigenvalue* $\lambda^{a,n}$.

THEOREM 3. *Let* $\lambda \in \sigma_{cont}(H)\setminus\mathcal{T}'$. *Let* u *satisfy* $(H-\lambda)u = 0$. *Then* $u \in \mathcal{B}^*$ *if and only if* u *is written as*

$$u = \mathcal{F}(\lambda)^*\varphi$$

for some $\varphi \in L^2(S^5)\oplus\oplus_{a,n}L^2(S^2)$.

THEOREM 4 *Let* $\lambda \in \sigma_{cont}(H)\setminus\mathcal{T}'$. *Let* $u \in \mathcal{B}^*$ *satisfy* $(H-\lambda)u = 0$. *Then* u *admits the asymptotic expansion*

$$\begin{aligned} u &\simeq C(\lambda)r^{-5/2}e^{i\sqrt{\lambda}r}\varphi_0^{(+)}(\hat{x}) + \overline{C(\lambda)}r^{-5/2}e^{-i\sqrt{\lambda}r}\varphi_0^{(-)}(\hat{x}) \\ &+\sum_{a,n}\Big[C_{a,n}(\lambda)r_a^{-1}e^{i\sqrt{\lambda-\lambda^{a,n}}r_a}\varphi_{a,n}^{(+)}(\omega_a)\otimes\varphi^{a,n}(x^a) \\ &+ \overline{C_{a,n}(\lambda)}r_a^{-1}e^{-i\sqrt{\lambda-\lambda^{a,n}}r_a}\varphi_{a,n}^{(-)}(\omega_a)\otimes\varphi^{a,n}(x^a)\Big] \end{aligned} \tag{1.12}$$

in the sense of (1.5), where

$$C(\lambda) = (2\pi)^{-1/2}e^{-5\pi i/4}(\lambda_+)^{-5/4},$$

$$C_{a,n}(\lambda) = (2\pi)^{-1/2}e^{-\pi i/2}((\lambda-\lambda^{a,n})_+)^{-1/2}.$$

Let $\varphi^{(\pm)} = {}^t(\varphi_0^{(\pm)}, \varphi_{a,1}^{(\pm)}, \cdots)$. *Then*

$$\varphi^{(+)} = \hat{\mathbf{S}}(\lambda)\mathbf{J}\varphi^{(-)}, \tag{1.13}$$

where $\hat{\mathbf{S}}(\lambda)$ *is the S-matrix and* $\mathbf{J}$ *is the reflection*

$$\mathbf{J} : (\varphi_0(\theta), \varphi_{a,1}(\omega_a), \cdots) \to (\varphi_0(-\theta), \varphi_{a,1}(-\omega_a), \cdots). \tag{1.14}$$

For any $\varphi^{(-)}$*, there exist a unique solution* u *of* $(H - \lambda)u = 0$ *and* $\varphi^{(+)}$ *for which the expansion (1.12) is valid.*

Theorem 2 is a fundamental result concerning the behavior at infinity of solutions to stationary Schrödinger equations. We shall discuss its other applications elsewhere.

1.5 *Related works.* Let us consider the N-body Schrödinger operator $H = H_0 + \sum_{1 \leq i < j \leq N} V_{ij}(q_i - q_j)$. As is inferred from the 2-body case, the above problem boils down to the asymptotic expansion of the resolvent $(H - \lambda \mp i0)^{-1}$ at infinity, which leads to the construction of generalized eigenfunctions for H and to the properties of S-matrices. All the difficulties of the N-body problem arise from the directions $\{q_i = q_j\}$, along which the pair potential $V_{ij}(q_i - q_j)$ does not decay. Let us call them *singular directions* in this paper.

Most of the study of the stationary N-particle Schrödinger equation has been done outside the singular directions. The asymptotic expansion of the resolvent outside the singular directions (*free region*) was obtained by Herbst-Skibsted [14].

In a series of papers [9], [10], [11], [27], [28] Hassell and Vasy continued the study of generalized eigenfunction for H and S-matrices in the free region. As for the behavior around the singular directions, Vasy [29] studied it by projecting the solution of $(H-\lambda)u = 0$ onto the bound states of subsystems and investigating the spatial asymptotics in the free region for the subsystem. Let us also mention the work of Vasy [30] on the propagation of singularirties for the S-matrix, the underlying idea of which is to look at the micro-local behavior of the resolvent at infinity.

The works [15], [16] studied directly the scattering matrix and generalized eigenfunctions around the singular directions. Since they lean heavily upon the spectral property near the zero energy of subsystems, they are restricted to the 3-body case.

1.6 *Methods.* The present paper is essentially a continuation of our previous works [15], [16], which are based on the micro-local resolvent estimates for N-body Schrödinger operators. The germ of the idea of the generalized Fourier transformation for 3-particle system has already been given in [16]. However we need two optimal results to overcome new difficulties in the many-body problem.

The first one is the Agmon-Hörmander space $\mathcal{B}, \mathcal{B}^*$, which is not only optimal for the restriction of the Fourier transform on the sphere, but also appropriate to deal with the multi-channel property of the many-body problem. We encounter two types of spherical scattering waves, $r^{-5/2}e^{i\sqrt{\lambda}r}$ and $r_a^{-1}e^{i\sqrt{\lambda - \lambda^{a,n}}r_a}$. The former is dominant in the free region, while the latter is dominant near the singular direction $\{x^a = 0\}$. The space $\mathcal{B}^*$ enables us to show the orthogonality of these two waves and hence the expansion of the resolvent.

The second new tool employed in this paper is a micro-local version of Yafaev's resolvent estimates concerning the spherical part of the radiation condition [32]. Our Theorem 3.5 is a many-body counter part of Agmon-Hörmander's result [2], Theorem 7.4, and is crucial to construct the generalized Fourier transformation near the singular directions.

1.6 *Generalized eigenfunctions with 2-cluster incoming state.* Finally, we shall discuss the asymptotic expansion of generalized eigenfunction for H. From the practical point of view, in the real scattering experiment, the most important case is the one in which the initial state is of 2-cluster. Suppose in the remote past the pair $a = (i, j)$ forms a bound state with energy $\lambda^{a,n} < 0$ and eigenstate $\varphi^{a,n}(x^a)$. Then the generalized eigenfunction $\Psi(x, \lambda, \omega_a)$ is written as

$$\Psi(x, \lambda, \omega_a) = e^{i\sqrt{\lambda - \lambda^{a,n}}\omega_a \cdot x_a}\varphi^{a,n}(x^a) - v, \tag{1.15}$$

$$v = R(\lambda + i0)f, \tag{1.16}$$

$$f = \sum_{c \neq a} V_c(x^c)\varphi^{a,n}(x^a)e^{i\sqrt{\lambda - \lambda^{a,n}}\omega_a \cdot x_a}. \tag{1.17}$$

In our previous work [16], we derived asymptotic expansions of v at infinity. However, the results were not satisfactory in that we have separated 3-cluster scattering and 2-cluster scattering. Moreover in Theorem 1.3 of [16], we multiplied a technical localization factor $\psi_b(D_{x_b})$ to v (we wrote it as $\psi_\beta(D_{x_\beta})$), although it was removed in [17], Theorem 6.6. By virtue of the analysis of the present paper, we can derive a more transparent asymptotic expansion.

THEOREM 5 *Let v be as in (1.16) and $\alpha = (a, \lambda^{a,n}, \varphi^{a,n})$. Then in the sense of (1.5)*

$$\begin{aligned} v \;\simeq\; & C_0(\lambda)r^{-5/2}e^{i\sqrt{\lambda}r}\hat{S}_{0\alpha}(\lambda; \hat{x}, \omega_a) \\ + & \sum_\beta C_\beta(\lambda)r_b^{-1}e^{i\sqrt{\lambda - \lambda^{b,m}}r_b}A_{\beta\alpha}(\lambda; \theta_b, \omega_a) \otimes \varphi^{a,n}(x^a), \end{aligned}$$

where $r = |x|, \hat{x} = x/r, r_b = |x_b|, \theta_b = x_b/r_b$,

$$C_0(\lambda) = e^{-\pi i/4}2\pi\lambda^{-1/4}(\lambda - \lambda^{a,n})^{-1/4},$$

$$C_\beta(\lambda) = 2\pi i(\lambda - \lambda^{a,n})^{-1/4}(\lambda - \lambda^{b,m})^{-1/4},$$

and $A_{\beta\alpha}(\lambda, \theta_b, \omega_a)$ is the scattering amplitude associated with the scattering process, in which after the collision the pair b takes the bound state $\varphi^{b,m}(x^b)$ with eigenvalue $\lambda^{b,m}$.

If the initial state is of 3-cluster, the behavior of the generalized eigenfunction is much more complicated. In fact, Hassell [9] derived an asymptotic expansion of $\Psi(x, \lambda, \theta) - e^{i\sqrt{\lambda}\theta \cdot x}$ away from singular directions, which contains in addition to the expected term $r^{-5/2}e^{i\sqrt{\lambda}r}a_0(\hat{x})$ extra terms like $r^{-p}e^{i\phi(\hat{x})r}a(\hat{x})$ with $0 < p < 5/2$.

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