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**Some new results in spectral and scattering theory of
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SOME NEW RESULTS IN SPECTRAL AND SCATTERING
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THEORY OF DIFFERENTIAL OPERATORS ON \mathbb{R}^n
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par S. AGMON

§ 1. INTRODUCTION

We shall consider in this lecture Schrödinger type second order elliptic differential operators on \mathbf{R}^n of the form :

$$P(x, D) = -\Delta + V(x, D),$$

where $V(x, D) = \sum_{|\alpha| \leq 2} V_\alpha(x) D^\alpha$ is a second order differential operator

with continuous coefficients on \mathbf{R}^n such that $V_\alpha(x) \rightarrow 0$ as $|x| \rightarrow \infty$. It is also assumed that V (and hence also that P) is symmetric when considered as an operator in L^2 with domain of definition $C_0^\infty(\mathbf{R}^n)$.

We shall call $V(x, D)$ as short range perturbation if

$$(1) \quad V_\alpha(x) \leq C(1 + |x|)^{-1-\varepsilon} \quad \text{for } |\alpha| \leq 2$$

and some $\varepsilon > 0$. ■

We shall call V an admissible long range perturbation if $V(x, D) = V^S(x, D) + V^L(x, D)$ where V^S and V^L are second operators such that the coefficients of V^S satisfy (1) whereas the coefficients $V_\alpha^L(x)$ of V^L are real C^1 functions satisfying :

$$(2) \quad |V_\alpha^L(x)| \leq C(1 + |x|)^{-\varepsilon}, \quad |\text{grad } V_\alpha^L(x)| \leq C(1 + |x|)^{-1-\varepsilon}$$

for $|\alpha| \leq 2$ and some $\varepsilon > 0$.

It is well known that under the general assumption $V_\alpha(x) \rightarrow 0$ P admits a unique self-adjoint realization which we denote by H . We denote by H_0 the self-adjoint realization of $P_0 = -\Delta$. The essential spectrum of H consists of the non-negative real axis. If V is an admissible long range perturbation then it is probable that there are no positive eigenvalues. (This result is proved in the literature for a more restrictive class of perturbations). In any case one can prove the following result.

Theorem : If V is an admissible long range perturbation then the positive eigenvalues of H are isolated and have a finite multiplicity.

Before proceeding with the discussion of the main problems let us mention that the results we shall describe can be extended to higher order elliptic operators. Also the smoothness assumption on the coefficients of V can be relaxed considerably (for instance one can allow general singularities in the coefficients of V in any bounded part of \mathbf{R}^n). For higher order operators one cannot exclude the possibility of imbedded eigenvalues in the continuous spectrum. Thus given $\lambda > 0$ one can find an infinitely differentiable function $V(x)$ with compact support such that $\Delta^2 + V(x)$ has an eigenvalue at the point λ .

§ 2. SHORT RANGE PERTURBATIONS

Let us first assume that V is a short range perturbation. In scattering theory one considers the limits

$$(3) \quad W_{\pm} = s - \lim_{t \rightarrow \pm \infty} \exp(itH) \exp(-itH_0) .$$

These limits exist and define two isometric operators W_{\pm} which are called the wave operators of (H, H_0) . It is easy to see that the wave operators intertwine H and H_0 : $HW_{\pm} = W_{\pm}H_0$. A basic property of wave operators is that they are asymptotically complete, i.e. that

$$(4) \quad \text{range } W_{+} = \text{range } W_{-} = L_{ac}^2$$

where L_{ac}^2 denotes the subspace of absolute continuity of L^2 relative to H . (In our situation L_{ac}^2 is the orthogonal complement of L_p^2 where L_p^2 denotes the closed subspace spanned by the eigenfunctions of H).

It follows from the above that H_0 is unitarily equivalent to $H_{ac} = H|_{L_{ac}^2}$.

The scattering operator is the unitary operator $S : L^2 \rightarrow L^2$ defined by $S = W_{+}^{-1} W_{-} = W_{+}^{*} W_{-}$. It commutes with H_0 . Set $\hat{S} = \mathfrak{F} S \mathfrak{F}^{-1}$ where \mathfrak{F} is the unitary Fourier map. Then \hat{S} is a unitary operator in $L^2(\mathbf{R}^n)$ which commutes with multiplication by the characteristic functions of the sets $\{\xi : a < |\xi| < b\}$. From this it follows that \hat{S} can be restricted to the shell $\Sigma_k = \{\xi : |\xi| = k\}$ and define a unitary map $\mathcal{S}(k) : L^2(\Sigma_k) \rightarrow L^2(\Sigma_k)$.

In an obvious way one considers $\mathcal{S}(k)$ as a unitary map : $L^2(S^{n-1}) \rightarrow L^2(S^{n-1})$. One refers to $\mathbf{R}_+ \ni k \rightarrow \mathcal{S}(k)$ as the scattering matrix. It is a non trivial fact that the operator valued function $\mathcal{S}(k)$ is defined for all $k > 0$ and not only for almost all k . ($\mathcal{S}(k)$ is defined even if $k > 0$ happens to be an eigenvalue of $H!$).

For each fixed $k > 0$ set : $T(k) = I - \mathcal{S}(k)$ where I is the identity operator on $L^2(S^{n-1})$. $T(k)$ is called the scattering amplitude. It is known (essentially) that $T(k)$ is a compact operator of a certain C_p class. For each k denote by $T(k; \omega, \omega')$ the distributional kernel of $T(k)$, $(\omega, \omega') \in S^{n-1} \times S^{n-1}$. If $T(k; \omega, \omega')$ is a function one refers to the quantity $|T(k; \omega, \omega')|^2$ as the scattering differential cross section. One of the problems we wish to discuss here is the following.

Problem I : Give general conditions which ensure that $T(k; \omega, \omega')$ is a smooth function on $S^{n-1} \times S^{n-1}$ off the diagonal set $\{(\omega, \omega') : \omega = \omega'\}$.

Now there is another way to define the scattering matrix which is used (formally) in physics text books. Suppose that the perturbation V is very short range. Then there exist two families of generalized eigenfunctions (distorted plane waves) $\Phi_{\pm}(x, \xi)$ for $(x, \xi) \in \mathbf{R}^n \times \mathbf{R}^n \setminus \{0\}$, given by the formula

$$(5) \quad \Phi_{\pm}(x, \xi) = e^{i\langle x, \xi \rangle} - \lim_{\varepsilon \downarrow 0} R(|\xi|^2 \pm i\varepsilon)(V(\cdot, \xi)e^{i\langle \cdot, \xi \rangle})(x, \xi)$$

where $R(z) = (H - z)^{-1}$ is the resolvent operator and where the limit in (5) is taken in some generalized sense (see Th. 3 later on). Introducing polar coordinates $r = |x|$, $\omega = x/r$ and $k = |\xi|$, $\omega' = \xi/k$, one derives under some strong conditions on V the asymptotic formula :

$$(6) \quad \Phi_{\pm}(x, \xi) = e^{i\langle x, \xi \rangle} + (kr)^{-\frac{n-1}{2}} e^{\pm ikr} a_{\pm}(k; \omega, \omega') + o(r^{-\frac{n-1}{2}}) \text{ as } r \rightarrow \infty .$$

It turns out that up to a constant factor $a_{\pm}(k; \omega, \omega')$ coincides with the scattering amplitude kernel,

$$(6') \quad a_{\pm}(k; \omega, \omega') = \gamma_n T(k; \omega, \omega')$$

where γ_n is some constant depending only on n . In view of the last remarks the following problems are of interest.

Problem II : Give general conditions on V which ensure that the proper generalized eigenfunctions $\Phi_{\pm}(x, \xi)$ exist as smooth functions of x and ξ on $\mathbb{R}^n \times \mathbb{R}^n \setminus \{0\}$.

Problem III : Give general conditions on V which ensure the validity of formulas of the type (6) - (6'), relating the scattering matrix and the asymptotic behavior of the generalized eigenfunctions.

The emphasize in the problems raised is on solutions under general conditions which would not require the coefficients $V_{\alpha}(x)$ to decay very rapidly at infinity. An answer of this type is given in the following.

Theorem 1 : Suppose that V is a short range perturbation of the form $V(x, D) = V^1(x, D) + V^{\infty}(x, D)$ where the coefficients of the second order operator V^1 are C^{∞} functions satisfying

$$(7) \quad |D^{\beta} V^1_{\alpha}(x)| \leq C_{\beta} (1 + |x|)^{-1-\epsilon-|\beta|}$$

for $\forall \beta$, $|\alpha| \leq 2$ and some $\epsilon > 0$, while the coefficients of V^{∞} are C^{∞} functions \diamond which decay more rapidly than any power of $|x|$ as $|x| \rightarrow \infty$.

Then the following results hold.

(i) The generalized eigenfunctions $\Phi_{\pm}(x, \xi)$ exist and are C^{∞} functions on $\mathbb{R}^n \times \mathbb{R}^n \setminus \{0\}$. Also,

$$(8) \quad |\Phi_{\pm}(x, \xi)| \leq C(1 + |x|)^m$$

uniformly in ξ in any compact set in $\mathbb{R}^n \setminus \{0\}$ where m is a number depending only on n .

(ii) The scattering amplitude has a kernel $T(k; \omega, \omega')$ which is C^{∞} on $S^{n-1} \times S^{n-1}$ for $\omega \neq \omega'$ (it is also C^{∞} in $k > 0$).

(iii) The formulas (6)-(6)' hold except in the forward direction $\omega = \omega'$ in the following generalized sense. Let $\chi(\xi)$ be any C^{∞} function vanishing in a neighborhood of the point $k\omega'$, $\chi \equiv \text{Const.}$ in some neighborhood of ∞ .

The following limit relation holds :

$$(9) \quad \lim_{r \rightarrow \infty} (kr)^{\frac{n-1}{2}} e^{-ikr} [\chi(D_x) \Phi_{\pm}(\cdot, k\omega')] (r\omega) = \gamma_n \chi(k\omega) T(k; \omega, \omega')$$

\diamond This smoothness assumption can be relaxed considerably. If, for instance, the coefficients of V^{∞} are only continuous functions which decay rapidly, then conclusions (ii) and (iii) of the theorem hold without any change.

where γ_n is a constant depending only on n . (For Φ_- a similar formula holds with $T(k; \omega, \omega')$ replaced by $\overline{T(k; -\omega', \omega)}$.)

The proof of Theorem 1 is rather technical. We shall make some comments related to its proof later on. We first, however, discuss a more general situation.

§ 3. LONG RANGE PERTURBATIONS

We consider the same problems in the more general case when V is an admissible long range perturbation. Here one encounters right at the beginning a serious difficulty which concerns the definition of the scattering matrix. Indeed, it is well known that for long range perturbations the wave operators defined by (3) need not exist. This was observed by Dollard [6,7] in the case of the Schrödinger operator with Coulomb potential $V = C/|x|$. Dollard has shown that in this case one could remedy the situation by introducing modified wave operators of the form :

$$(10) \quad \tilde{W}_{\pm} = s - \lim_{t \rightarrow \pm\infty} \exp(itH) \exp(-itH_0 - R_t)$$

where $R_t(D)$ is a suitably chosen pseudo-differential operator with a real symbol $R_t(\xi)$. The work of Dollard on existence of modified wave operators was extended by various authors to a wider class of long range perturbations (e.g. [5], [3], [2], and [9]). The most general results here are due to Hörmander [9]. Modified wave operators possess properties similar to those of ordinary wave operators and they serve the same purpose. In particular they also intertwine H and H_0 .

The problem of asymptotic completeness of modified wave operators (i.e. the question of the validity of (4) for \tilde{W}_{\pm}) was studied by several authors in case V is a multiplication operator. Results were first obtained for special Coulomb like potentials (e.g. [6,7], [4], [12] and [8]). Recently quite general completeness results were obtained by Kitada [11] and by Ikebe and Isozaki [10]. The conditions imposed in these last mentioned papers are more restrictive than those required by Hörmander in his proof of existence of modified wave operators. In as yet unpublished work the author has established completeness of modified wave operators for the subclass of admissible long range perturbations $V(x, D)$ which satisfy the Hörmander's conditions for existence of modified wave operators.

We consider from now on Schrödinger operators $-\Delta + V(x, D)$ with admissible long range perturbations for which the modified wave operators exist and are complete. Although modified wave operators \tilde{W}_{\pm} are not unique (there is more than one good choice of R_{\pm} in (10)), it is easy to characterize the class of all modified wave operators. Namely, let \tilde{W}_{\pm}^1 be another pair of modified wave operators, one has the relation :
 $\tilde{W}_{\pm}^1 = \tilde{W}_{\pm} F_{\pm}(D)$ where $F_{\pm}(\xi)$ are certain functions with $|F_{\pm}(\xi)| = 1$.

Any pair of asymptotically complete modified wave operators \tilde{W}_{\pm} gives rise to a scattering operator $S = \tilde{W}_{+}^{-1} \tilde{W}_{-}$. Any such S again commutes with H_0 . One defines as before the scattering matrix $k \rightarrow \mathcal{S}(k)$ via restriction of $\hat{S} = \mathfrak{F} S \mathfrak{F}^{-1}$ to the shell $|\xi| = k$. Although we have now a whole family of scattering matrices, the relation between any two scattering matrices $\mathcal{S}(k)$ and $\mathcal{S}_1(k)$ is a simple one, namely we have :

$$(11) \quad \mathcal{S}_1(k) = M_1(k) \mathcal{S}(k) M_2(k)$$

where $M_i(k)$ are multiplication unitary operators on $L^2(S^{n-1})$.

Of course one can consider the whole class of modified wave operators and the corresponding class of scattering matrices also in the case of short range perturbations. In that case we have however a distinguished pair of wave operators and a corresponding distinguished scattering matrix $\mathcal{S}(k)$. Moreover, the corresponding scattering amplitude $T(k) = I - \mathcal{S}(k)$ turns out to be a compact operator for each k . For genuine long range perturbations this does not seem to be case. Namely, it does not seem that $I - \mathcal{S}(k)$ is compact for any choice of $\mathcal{S}(k)$ in the equivalent class of scattering matrices. For this reason for long range perturbations we shall not consider the kernel of $T(k)$ but rather the kernel of $\mathcal{S}(k)$ off the diagonal. If such a kernel is a function $\mathcal{S}(k; \omega, \omega')$ for $\omega \neq \omega'$, then by (11) any other scattering matrix $\mathcal{S}_1(k)$ will have a kernel of the form :

$$\mathcal{S}_1(k; \omega, \omega') = M_1(k; \omega) \mathcal{S}(k; \omega, \omega') M_2(k; \omega')$$

where M_1 and M_2 are functions of modulus 1. Note that when $\mathcal{S}(k)$ is an integral operator, then the scattering differential cross section is uniquely defined for $\omega \neq \omega'$ by the expression : $|\mathcal{S}(k; \omega, \omega')|^2$.

With some modifications one can now formulate the three problems discussed in section 2 in the more general situation of long range

perturbations. Thus the first problem should be restated in the more general case as follows.

Problem I' : Give conditions which ensure that among the equivalent class of scattering matrices there is a scattering matrix $\mathcal{S}(k)$ having a smooth integral kernel $\mathcal{S}(k; \omega, \omega')$ for $\omega \neq \omega'$.

We now state a theorem which extends Theorem 1 to the case of long range perturbations.

Theorem 2 : Suppose that $V(x, D) = V^0(x, D) + V^\infty(x, D)$ where the coefficients of V^0 are C^∞ functions satisfying

$$(12) \quad |D^\beta V_\alpha^0(x)| \leq C_\beta (1 + |x|)^{-\varepsilon - |\beta|}$$

for $\forall \beta$, $|\alpha| \leq 2$, while the coefficients of V^∞ are C^∞ functions which decay more rapidly than any power of $|x|$. Then the following results hold for $H = -\Delta + V$.

(i) There exist two families of generalized eigenfunctions $\Phi_\pm(x, \xi)$ which are C^∞ on $\mathbb{R}^n \times \mathbb{R}^n \setminus \{0\}$. They also verify the estimate (8).

(ii) There exists a representative scattering matrix $\mathcal{S}(k)$ with a kernel $\mathcal{S}(k; \omega, \omega')$ which is a C^∞ function on $S^{n-1} \times S^{n-1}$ for $\omega \neq \omega'$.

(iii) A formula similar to formula (9) relating the generalized eigenfunctions in (i) and the scattering matrix in (ii) holds. Namely, there exists a real phase function $\psi(r; k, \omega)$ ($\psi(r; k, \omega) = kr + o(r)$ as $r \rightarrow \infty$) such that if $\chi(\xi)$ is as in (iii) of Theorem 1, then

$$(13) \quad \lim_{r \rightarrow \infty} (kr)^{(n-1)/2} \exp(-i\psi(r; k, \omega)) [\chi(D_x) \Phi_+(\cdot, k\omega')](r\omega) \\ = -\gamma_n \chi(k\omega) \mathcal{S}(k; \omega, \omega'),$$

where γ_n is a constant.

In this lecture we shall not be able to give the proof of either Theorem 2 or Theorem 1. Both proofs are long. Instead we shall describe some related results which are used in the proofs of these theorems.

§ 4. GENERALIZED EIGENFUNCTIONS AND GREEN'S FUNCTIONS. A REMARKABLE RELATION.

We denote by $B^*(\mathbf{R}^n)$ the Banach space of functions $u \in L^2_{loc}(\mathbf{R}^n)$ such that

$$\|u\|_{B^*}^2 = \sup_{R > 1} \frac{1}{R} \int_{|x| < R} |u|^2 dx < \infty .$$

By $B^{*s}(\mathbf{R}^n)$ we denote the subspace of functions $u \in B^*(\mathbf{R}^n)$ such that

$$\frac{1}{R} \int_{|x| < R} |u|^2 dx \rightarrow 0 \quad \text{as } R \rightarrow \infty .$$

We also set : $L^{2,s}(\mathbf{R}^n) = \{u : (1+|x|)^s u \in L^2(\mathbf{R}^n)\}$. In the framework of these spaces one can prove a strong version of the so called limiting absorption principle .

Theorem 3 : Suppose $\lambda > 0$ is not an eigenvalue of $H = -\Delta + V(x, D)$ where V is an admissible long range perturbation. For any $f \in L^{2,s}(\mathbf{R}^n)$, $s > 1/2$, the following limit exists

$$R(\lambda \pm i0)f = \lim_{\substack{z \rightarrow \lambda \\ \pm \operatorname{Im} z > 0}} R(z)f \quad \text{weakly in } B^*(\mathbf{R}^n) .$$

The boundary values $R(\lambda \pm i0)f \in B^*(\mathbf{R}^n)$ have a certain asymptotic behavior as $|x| \rightarrow \infty$. This can be described as follows.

Theorem 4 : Suppose that the conditions of Theorem 3 hold. Set $\lambda = k^2$ and introduce polar coordinates $x = r\omega$. If

(a) V is short range. Then there exist functions $a_{\pm}(\omega) = a_{\pm}(\omega, k; f)$ which are L^2 functions on S^{n-1} , such that

$$(14) \quad R(k^2 \pm i0)f = r^{-(n-1)/2} e^{\pm ikr} a_{\pm}(\omega, k; f) \pmod{B^*} .$$

(b) If V is an admissible long range potential which satisfies certain conditions (in particular if V satisfies the conditions of Theorem 2), then there exist phase functions $\psi_{\pm}(r; k, \omega) = kr + o(r)$ which depend only on V and an amplitude function $a_{\pm}(\omega) = a_{\pm}(\omega, k; f) \in L^2(S^{n-1})$, such that

$$(15) \quad R(k^2 \pm i0)f = r^{-(n-1)/2} e^{\pm i\psi_{\pm}(r;k,\omega)} a_{\pm}(\omega, k; f) \pmod{B^*}.$$

The amplitude functions $a_{\pm}(\omega, k; f)$ have an interesting connection with the generalized Fourier maps $\mathfrak{F}_{\pm}: L^2 \rightarrow L^2$ which diagonalize H . Indeed, for the unperturbed operator H_0 one finds by a computation (see [1]) that the amplitude $a_{\pm}^0(\omega, k; f)$ in the corresponding formula (14) is given by

$$a_{\pm}^0(\omega, k; f) = c_n^{\pm} k^{(n-3)/2} (\mathfrak{F}f)(\pm k\omega)$$

where \mathfrak{F} is the usual Fourier transform and $c_n^{\pm} = (\pi/2)^{1/2} \exp(\mp \pi i(n-3)/4)$. For general short range perturbations one obtains a similar result

$$(16) \quad a_{\pm}(\omega, k; f) = c_n^{\pm} k^{(n-3)/2} (\mathfrak{F}_{\pm}f)(\pm k\omega),$$

where \mathfrak{F}_{\pm} are distinguished Fourier maps related to the wave operators (3) by the formula :

$$(17) \quad \mathfrak{F}_{\pm} = \mathfrak{F}W_{\pm}^*.$$

It turns out that formulas (16) and (17) are also valid in the long range case for a general class of perturbations for which Theorem 4 holds. Only in this case \mathfrak{F}_{\pm} is some pair of generalized Fourier maps and W_{\pm} is a corresponding pair of modified wave operators.

One expects that the generalized Fourier maps are given by the formula

$$(18) \quad (\mathfrak{F}_{\pm}f)(\xi) = (2\pi)^{-n/2} \int f(x) \overline{\phi_{\pm}(x, \xi)} dx$$

where ϕ_{\pm} are the generalized eigenfunctions. Hence it follows by a formal application of (16) and (18) to $f = \delta_y$, where δ_y is the Dirac function centered at y , that

$$(19) \quad \begin{aligned} a_{\pm}(\omega, k; \delta_y) &= c_n^{\pm} k^{(n-3)/2} (\mathfrak{F}_{\pm}\delta_y)(\pm k\omega) \\ &= (2\pi)^{n/2} c_n^{\pm} k^{(n-3)/2} \overline{\phi_{\pm}(y, \pm k\omega)}. \end{aligned}$$

Combining (19) with (14) or with (15) we obtain formally that if $R(k^2 \pm i0; x, y)$ denote the kernels of $R(k^2 \pm i0)$ (i.e. the Green's functions),

then one can extract the generalized eigenfunctions $\bar{\phi}_{\pm}$ from the kernels by means of the following formulas :

$$(20) \quad \lim_{r \rightarrow \infty} r^{(n-1)/2} e^{+ikr} R(k^2 \pm i0; r\omega, y) = \gamma_n^{\pm} k^{(n-3)/2} \overline{\bar{\phi}_{\pm}(y, \pm k\omega)}$$

for short range perturbations, and

$$(21) \quad \lim_{r \rightarrow \infty} r^{(n-1)/2} e^{\mp i\psi_{\pm}(r; k, \omega)} R(k^2 \pm i0; r\omega, y) = \gamma_n^{\pm} k^{(n-3)/2} \overline{\bar{\phi}_{\pm}(y, \pm k\omega)}$$

for long range perturbations, where γ_n^{\pm} are certain non-zero constants.

The derivation of (20)-(21) which was completely formal can be justified for a large class of perturbations. (In particular (21) holds for perturbations satisfying the conditions of Theorem 2). Formulas (20)-(21) could also be used to define the generalized eigenfunctions. This approach is particularly useful in the case of long range perturbations where as far as we know it is the only available approach to establish the existence of the generalized eigenfunctions.

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