

AFCRC-TN-56-298



NEW YORK UNIVERSITY

Institute of Mathematical Sciences

Division of Electromagnetic Research

RESEARCH REPORT NO. CX-25

On the Eigenfunctions of Many-Particle Systems in Quantum Mechanics

TOSIO KATO

CONTRACT NO. AF 19(122)-463

APRIL 1956

*CX-25
c.1*

5 New York University
Institute of Mathematical Sciences
Division of Electromagnetic Research

Research Report No. CX-25

710
ON THE EIGENFUNCTIONS OF MANY-PARTICLE SYSTEMS
IN QUANTUM MECHANICS

710
Tosio Kato

Tosio Kato
Tosio Kato

Morris Kline
Morris Kline
Project Director

126#3 2/15/56

The research reported in this document has been made possible through the support and sponsorship extended by the Geophysics Research Directorate of the Air Force Cambridge Research Center, under Contract No. AF 19 (122)-463. It is published for technical information only, and does not necessarily represent recommendations or conclusions of the sponsoring agency.

30 New York, 1956

Abstract

The continuity properties or singularities of the eigenfunctions of a many-particle system in non-relativistic quantum mechanics are investigated. It is shown that all eigenfunctions of such a many-particle system are continuous throughout the configuration space, and that the eigenfunctions have partial derivatives of first order (except at the Coulomb-type singular points of the potential) which are bounded functions. The nature of the singularities of the eigenfunctions are described in greater detail.

Table of Contents

	page
1. Introduction	1
2. Assumptions and results	4
3. The Hamiltonian. Integral representation	16
4. Lemmas on the integral operators	21
5. Proof of Theorems I and Ia	35
6. Proof of Theorems II, IIa, IIb	38
References	42

1. Introduction

This paper is concerned with the continuity properties or singularities of eigenfunctions of a many-particle system in non-relativistic quantum mechanics. It may be regarded as a continuation of a previous paper [1] of the writer, in which the fundamental properties, in particular the self-adjointness, of the Hamiltonian operator of such a system has been investigated*.

The main results to be proved in the present paper are: 1) that all eigenfunctions of such a many-particle system are continuous throughout the configuration space**, and 2) that they have partial derivatives of first order (except at the Coulomb-type singular points of the potential) which are bounded functions (see Theorems I, II, Section 2). Actually we are able to give a more detailed description of the nature of the singularities of the eigenfunctions (Theorems Ia, IIa, IIb).

Here and in what follows the word 'eigenfunction' is used in a generalized sense; it denotes not only 'genuine eigenfunctions' belonging to 'point eigenvalues' but also 'wave packets.'[†] A precise definition is given in Section 2. The eigenfunctions belonging to the so-called 'continuous eigenvalues' are not included in this concept; in fact, these 'continuous eigenfunctions' for a many-particle system are not as yet sufficiently well understood mathematically to be useful in the present investigation. In any case, the definition of generalized eigenfunctions shows that they form a dense linear set in the basic Hilbert space.

*Some of the results given below are mentioned in [1], but without a complete description and proof.

**The configuration space is the $3s$ -dimensional space of which the coordinates are the aggregate of all s particles.

[†]For similar use of the word see e.g. Friedrichs [2].

There have been some previous investigations concerning the nature of the singularities of the genuine eigenfunctions of the helium atom (Kemble^[3], Gronwall^[4], Bartlett^[5]). Gronwall discovered a transformation of the helium wave equation into a simple form, and Bartlett continued work along these lines. However, this attack seems not to have led to any positive mathematical results, except to show that the helium wave equation does not possess any solution which admits of a certain simple series expansion.

However, our results stated above show that the eigenfunctions are in general well-behaved, or at least better than previously believed, even though they are not expressible as a simple series.

Our approach to the problem is rather different from the one used by Gronwall and Bartlett. One advantage of our method is that the problem of the existence of the eigenfunctions is separated from the study of their properties. In fact, the existence of generalized eigenfunctions has been proved in [1] for any number of particles. (The existence of genuine eigenfunctions has been proved so far only for the two-electron problem, which is, however, a problem on the nature of the spectrum of a self-adjoint operator in a Hilbert space, and has little to do with the local properties of solutions of the wave equation.) Thus we have only to study the local properties of eigenfunctions which are known to exist (or assumed to exist in the case of genuine eigenfunctions) and to satisfy a certain operational equation. This can be done rather easily by utilizing the usual Green's function for the higher-dimensional Laplace operator.

The results 1), 2) given above are well known in the case of one-particle systems (hydrogen-like atoms), in which the eigenvalue problem can be solved explicitly. In particular, the eigenfunction for the ground state

has the simple form (see e.g. [3])

$$(1.1) \quad \phi = e^{-r}, \quad r = (x^2 + y^2 + z^2)^{1/2}, \quad \left. \frac{\partial \phi}{\partial r} \right|_{r=0} = -\phi(r=0)$$

in a suitable system of units. Thus ϕ is continuous everywhere, whereas its first-order derivatives are bounded but discontinuous at $r = 0$. This discontinuity may be characterized by $(\partial\phi/\partial r)_{r=0} = -\phi(0,0,0)$. In view of this example, the above general results are not likely to admit of much improvement. Rather, we show that the above form of singularity is typical even for the general many-particle problem, in a sense to be described below (see in particular Theorem IIb).

In proving the result 2) regarding the derivatives of eigenfunctions, we had to make some use of certain special properties of the usual Coulomb potential. However, the result 1) on the continuity of eigenfunctions themselves can be proved more generally; it is sufficient to assume that the potential between any pair of particles is a function of their relative positions which is locally quadratically integrable and bounded at infinity.

The present work suggested itself in connection with a recently renewed interest in the precise calculation of non-relativistic eigenvalues and eigenfunctions of the helium atom (see e.g. Chandrasekhar [6] and Kinoshita [7]); this problem seems to be related to the problem of relativistic correction to these eigenvalues. For such a calculation, the variational method initiated by Hylleraas [8] still appears to be the most effective tool. However, some information, at least qualitative, on the singularities of the eigenfunctions is desirable in choosing good trial functions in such a variational calculation. The exact eigenfunctions are of course quite regular (even analytic) at all

points of the configuration space except at the singular points of the potential, but they may well have some sort of singularity at these singular points. It is quite natural to expect that trial functions with the same type of singularity would give a better approximation than functions with different types of singularities.

According to our results summarized above, the singularity is rather mild and seems to justify the use of trial functions of Hylleraas type (cf. Chandrasekhar^[6] and Kinoshita^[7]), but it is hoped that the more detailed description of the singularity given in Theorems IIa, IIb may be of some use in selecting good trial functions.

2. Assumptions and results

We now proceed to state our assumptions and results in more precise form.

The Hamiltonian operator of our system, which consists of s particles, is assumed to have the form (cf. [1])

$$(2.1) \quad H = - \sum_{i=1}^s \mu_i \text{grad}_i^2 - \mu_0 \left(\sum_{i=1}^s \text{grad}_i \right)^2 + W(\underline{r}_1, \dots, \underline{r}_s).$$

Here $\underline{r}_i = (x_i, y_i, z_i)$ is the three-dimensional position vector of the i -th particle, and grad_i is the vector operator $(\partial/\partial x_i, \partial/\partial y_i, \partial/\partial z_i)$; μ_i are constants with $\mu_i > 0$ for $i = 1, 2, \dots, s$ and $\mu_0 \geq 0$. The term with μ_0 comes from the separation of the motion of the center of gravity, and may be interpreted as representing the effect of the finiteness of the mass of atomic nuclei. But (2.1) may also represent the Hamiltonian before this separation of the motion of the system as a whole; then we have simply to put $\mu_0 = 0$.

For an ordinary atomic or molecular system in a free space, the potential

energy $W(\underline{x}_1, \dots, \underline{x}_s)$ is the Coulomb potential; that is, W is the sum of such terms as e_i/r_i and e_{ij}/r_{ij} , where e_i, e_{ij} are constants and $r_i = |\underline{x}_i|$, $r_{ij} = |\underline{x}_i - \underline{x}_j|$. In the greater part of our investigation, however, we need not assume such a specific form of the potential. It is sufficient, at least for the moment, to assume that W can be written as

$$(2.2) \quad W(\underline{x}_1, \dots, \underline{x}_s) = W_0(\underline{x}_1, \dots, \underline{x}_s) + \sum_{i=1}^s V_{oi}(\underline{x}_i) + \sum_{i < j} V_{ij}(\underline{x}_i - \underline{x}_j).$$

where

i) W_0 is a real-valued, measurable function bounded in the whole 3s-dimensional configuration space;

ii) for each i, j with $0 \leq i < j \leq s$, the $V_{ij}(\underline{r})$ are real-valued, measurable functions, defined in the three-dimensional space (\underline{r}), which vanish identically outside of some sphere and satisfy

$$(2.3) \quad \int |V_{ij}(\underline{r})|^\sigma d\underline{r} < \infty,$$

where σ is a fixed constant such that $\sigma \geq 2$.

These assumptions are satisfied by the Coulomb potential. In fact, although the function $1/r$ itself does not satisfy the condition ii) above, it can be written as

$$(2.4) \quad \frac{1}{r} = \frac{\eta(r)}{r} + \frac{1-\eta(r)}{r},$$

where $\eta(r)$ is a function equal to 1 for $r \leq \rho$, $\rho > 0$, and equal to zero otherwise. Then the first term on the right-hand side of (2.4) satisfies the condition ii) with any σ such that $2 \leq \sigma < 3$, while the second term may be absorbed in a

common term W_0 which is bounded.

We note also that the above assumptions with $\sigma = 2$ are exactly those made in the previous paper^[1] except for some change in notation. The apparent difference (there we assumed that the $V_{ij}(\underline{x})$ are locally square integrable and bounded at infinity) disappears if we decompose each $V_{ij}(\underline{x})$ of [1] into two parts in the same way as we have just done for the Coulomb potential.

If (2.3) is true for some σ , it is a fortiori true for smaller $\sigma > 0$, since the $V_{ij}(\underline{x})$ are assumed to vanish outside of a sphere. Thus the assumption (2.3) is stronger for larger σ , and we expect to obtain sharper results when σ is larger. This is the reason why we have left σ unspecified.

Before we state our results sketched in the introduction in more precise theorems, we must make clear what is meant by an eigenfunction. In fact, the operator H as given by (2.1) is only a formal differential operator, and an eigenfunction of H is not determined unless we impose some kind of boundary or continuity conditions at the singular points of the potential; but these continuity conditions are exactly what we shall determine in this paper.

This vicious circle can be avoided by an operator-theoretical consideration based on the fundamental principle of quantum mechanics that every physical quantity should be represented by a self-adjoint operator in a Hilbert space (cf. von Neumann^[9]). It has been proved in [1] that there is a self-adjoint operator \tilde{H} (in the Hilbert space of quadratically integrable functions defined in the configuration space) which is uniquely determined by the formal differential operator H in quite a natural way. In this proof the potential W has been assumed to satisfy the above conditions with the special constant $\sigma = 2$; since (2.3) with $\sigma \geq 2$ implies that the same condition holds for $\sigma = 2$, the result is true a fortiori in the present case for any $\sigma \geq 2$. As explained in [1] in detail,

there is no doubt that this operator \tilde{H} is the correct Hamiltonian of the physical system under consideration. In the next section we shall give the exact definition of \tilde{H} together with its main properties in so far as these are necessary for our purposes.

By a genuine eigenfunction of the system we mean an eigenfunction ϕ of this operator \tilde{H} belonging to a point eigenvalue λ ; thus ϕ should be a solution of $\tilde{H}\phi = \lambda\phi$, $\phi \neq 0$. We shall also consider as eigenfunctions wave packets belonging to this operator. A wave packet is a function belonging to a subspace of the Hilbert space corresponding to a spectral measure for a finite interval in the spectral representation of the operator \tilde{H} , that is, a function ϕ such that $\phi = (E_b - E_a)\phi$ with some $-\infty < a < b < \infty$, where E_λ is the resolution of the identity corresponding to the self-adjoint operator \tilde{H} . Genuine eigenfunctions and wave packets have the common property that the operator \tilde{H} can be applied to them any number of times, that is, they belong to the domain of \tilde{H}^n for any positive integer n . By a generalization, any function possessing this property will hereafter be called an eigenfunction. Actually the concept could further be generalized to include functions belonging to the domain of \tilde{H}^n for sufficiently large but finite n , but we shall not do so for the sake of simplicity.

It should be noted that \tilde{H} is not a differential operator in the naive sense, so that it is not immediately clear that even a genuine eigenfunction is differentiable and satisfies the differential equation $H\phi = \lambda\phi$, although this is true in any region of the configuration space where the potential is regular. But what concerns us here is the behavior of ϕ (or of any eigenfunction in the generalized sense) at the singular points of the potential, and these singular points may well cover the whole space under the general assumptions stated above.

We can now state our results in a precise form. In doing this, it is convenient to use the following abbreviation. We shall say that a function ϕ is (C_θ) if it is uniformly Hölder continuous with exponent θ , that is, if there is

a constant C and θ ($0 < \theta < 1$) such that $|\phi(P) - \phi(Q)| \leq C(\overline{PQ})^\theta$, where P, Q are any two points in the configuration space and \overline{PQ} is the $3s$ -dimensional distance between them. Similarly, ϕ is said to be (C'_θ) if all first-order partial derivatives of ϕ exist and are (C_θ) . It should be noted that we consider only the values $0 < \theta < 1$, so that when we say e.g. that ϕ is (C_θ) with any θ such that $\alpha < \theta < \beta$, this actually implies that ϕ is (C_θ) with any θ such that $\text{Max}(0, \alpha) < \theta < \text{Min}(1, \beta)$.

Now we state

Theorem I. Let the potential W be given by (2.2) with conditions i), ii). Then all eigenfunctions are bounded and are (C_θ) with any $\theta < 2 - \frac{3}{\sigma}$. If $\sigma > 3$, they are (C'_θ) with any $\theta < 1 - \frac{3}{\sigma}$.

The Coulomb potential corresponds to the case in which σ is smaller than, but may be arbitrarily close to, 3. In this case Theorem I shows that the eigenfunctions are (C_θ) with any $\theta < 1$, but it tells us nothing about their derivatives. However, we can obtain more specific results here.

Let us call W a generalized Coulomb potential if it can be expressed in the form (2.2), where W_0 satisfies i) and the V_{ij} satisfy the following condition:

ii') for each $0 \leq i < j \leq s$, $V_{ij}(\underline{r})$ has the form

$$(2.5) \quad V_{ij}(\underline{r}) = e_{ij} \frac{\eta(\underline{r})}{r} + V'_{ij}(\underline{r}),$$

where $r = |\underline{r}|$, e_{ij} are constants, $\eta(\underline{r})$ is the function introduced above, (see (2.4)), and the $V'_{ij}(\underline{r})$ satisfy the condition ii) with some $\sigma > 3$.

Any point where at least one of r_i or r_{ij} vanishes will be called a Coulomb singular point. Thus Coulomb singular points form $(3s-3)$ -dimensional

hyperplanes, of which there are $s(s+1)/2$. Now we can state

Theorem II. Let W be a generalized Coulomb potential. Then all eigenfunctions are continuous and have derivatives of first order except at the Coulomb singular points defined above; these derivatives are bounded.

We can give somewhat more detailed description of the nature of the singularities of the eigenfunctions. To do this, we have to introduce a linear transformation of the $3s$ coordinates (r_1, \dots, r_s) .

This linear transformation is aimed at transforming the purely differential part of (2.1) into the $3s$ -dimensional negative Laplace operator $-\Delta$. This is possible since, by assumption, $\mu_i > 0$ ($i = 1, \dots, s$) and $\mu_0 \geq 0$. It is important, for later use, to note that this purpose is achieved by a linear transformation of the special form

$$(2.6) \quad r'_i = \sum_{k=1}^s a_{ik} r_k$$

$$\left. \begin{aligned} r'_1 &= a_{11} r_1 + a_{12} r_2 \\ r'_i &= a_{i1} r_1 + a_{i2} r_2 \end{aligned} \right\} \begin{aligned} x'_1 &= a_{11} x_1 + a_{12} x_2 \\ y'_1 &= a_{11} y_1 + a_{12} y_2 \end{aligned}$$

which transforms each of three sets of coordinates $(x_i), (y_i), (z_i)$ into themselves and in the same way. This is obvious from (2.1) where these three sets are separated and appear in the same form*. We note also that such a linear transformation does not change the property of a function being quadratically integrable, $(C_0), (C'_0)$, etc.

After such a transformation we denote the new coordinates by $x = (x_1, \dots, x_m)$, $m = 3s$. This new configuration space will be denoted by E_m , and the Hilbert space $L^2(E_m)$ of all quadratically integrable functions will be denoted by \mathcal{H}_m . The

*An example of such a transformation is given in Kemble [3], pp. 64 and 209.

operator (2.1) can now be written as

$$(2.7) \quad H = -\Delta + W(\mathbf{x}),$$

where

$$\Delta = \sum_{i=1}^m \frac{\partial^2}{\partial x_i^2},$$

(2.8)

$$W(\mathbf{x}) = W_0(\mathbf{x}) + \sum_{i=1}^M V_i(\mathbf{x});$$

the $V_i(\mathbf{x})$, $i = 1, \dots, M$, $M = s(s+1)/2$, correspond to $V_{oi}(\mathbf{r}_i)$ and $V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$ of (2.2) in some definite order.

After this linear transformation it is no longer true that each of $V_i(\mathbf{x})$ depends only on three coordinates. But obviously these functions retain their original simple structure: for each i , there is a three-dimensional subspace of E_m such that $V_i(\mathbf{x})$ is a function of the projection of \mathbf{x} into this subspace. In other words, there is an orthogonal transformation of $\mathbf{x} = (x_1, \dots, x_m)$, depending on i , such that $V_i(\mathbf{x})$ takes on the form, in the new coordinate system $\bar{\mathbf{x}} = (\bar{x}_1, \dots, \bar{x}_m)$,

$$(2.9) \quad V_i(\mathbf{x}) = \bar{V}_i(\bar{x}_1, \bar{x}_2, \bar{x}_3). \quad \leftarrow \text{just depends on 3 coordinates}$$

The Laplacian Δ in (2.7) is unchanged by such an orthogonal transformation.

Furthermore, it is clear that the function \bar{V}_i has the same property as the corresponding V_{ij} of (2.2), namely that if the $V_{ij}(\mathbf{r})$ satisfy the condition ii), then the $\bar{V}_i(x_1, x_2, x_3)$ vanish outside of a (three-dimensional) sphere and

$$(2.10) \quad \int |\bar{V}_i(x_1, x_2, x_3)|^\sigma dx_1 dx_2 dx_3 < \infty.$$

Of course (2.10) is still true if σ is replaced by a smaller positive number.

Similarly if the V_{ij} satisfy the condition ii'), we can express \bar{V} in the form

$$(2.11) \quad \bar{V}_i(x_1, x_2, x_3) = \bar{e}_i \frac{\bar{\eta}(r)}{r} + \bar{V}'_i(x_1, x_2, x_3),$$

by denoting by the same letter r the new quantity $r = (x_1^2 + x_2^2 + x_3^2)^{1/2}$; in (2.11) \bar{e}_{ij} is a constant, $\bar{\eta}(r)$ is a function similar to $\eta(r)$ of (2.4), and the \bar{V}'_i satisfy (2.10) with some $\sigma > 3$. It is important here that the original linear transformation have the special form (2.6), for only then, as is seen without difficulty, will the new $r = (x_1^2 + x_2^2 + x_3^2)^{1/2}$ in the first term $\bar{e}_i \bar{\eta}_i(r)/r$ of (2.11) be symmetrical with respect to x_1, x_2, x_3 .

The expression on the right-hand side of (2.9) will be called a canonical form of V_i , and the coordinate system in which V_i has a canonical form will be called a canonical system with respect to V_i . Since the notion of a canonical system depends on V_i , it is in general impossible to give all V_i canonical forms simultaneously. When $\bar{x} = (\bar{x}_1, \dots, \bar{x}_m)$ is a canonical coordinate system for V_i , the first three coordinates $\bar{x}_1, \bar{x}_2, \bar{x}_3$ will be called internal coordinates with respect to V_i , and the rest, $\bar{x}_4, \dots, \bar{x}_m$, external coordinates. The derivatives $\partial f / \partial \bar{x}_i$ of a function f will be similarly classified into internal and external derivatives with respect to V_i . The distinction between internal and external derivatives is not always definite; a derivative may be internal and external at the same time, as is shown by a trivial example $V_i = 0$. But in most cases the distinction is quite definite.

We can now supplement Theorems I, II as follows.

Theorem Ia. Let $\sigma > 2$ in Theorem I. Then any eigenfunction ϕ is the sum of $M = s(s+1)/2$ terms ϕ_1, \dots, ϕ_M such that, for each i, ϕ_i is (C_θ) with any $\theta < 2 - \frac{3}{\sigma}$, and all external derivatives of ϕ_i with respect to V_i exist and are (C_θ) with any $\theta < 3 - \frac{6}{\sigma}$.

This theorem gives us somewhat more detailed information on eigenfunctions, though it is not very useful unless we also know something about the internal derivatives of each ϕ_i . Such is the case if we assume that W is a generalized Coulomb potential; then we have

Theorem IIa. Let W be a generalized Coulomb potential. Then any eigenfunction ϕ is the sum of $M+1$ functions $\phi_0, \phi_1, \dots, \phi_M$ with the following properties:

- 1) ϕ_0 is (C'_θ) for any $\theta < 1 - \frac{2}{\sigma}$. *← has 1st order derivatives*
- 2) If $x = (x_1, \dots, x_m)$ is a canonical coordinate system for V_i , then ψ_i is a function of only $m - 2$ variables $r = (x_1^2 + x_2^2 + x_3^2)^{1/2}, x_4, \dots, x_m$, and ϕ_i is (C'_θ) in these variables for any $\theta < 1$.

Can have discontinuity with respect to x_1, x_2, x_3
 That ϕ_i is (C'_θ) as a function of r, x_4, \dots, x_m does not imply that it is (C'_θ) as a function of x_1, \dots, x_m . Since $\partial\phi_i/\partial x_k = (\partial\phi_i/\partial r)(x_k/r)$ for $k = 1, 2, 3$, the internal derivatives $\partial\phi_i/\partial x_k$ are continuous for $r > 0$ but in general discontinuous for $r = 0$. This discontinuity carries over to the internal derivatives of ϕ with respect to V_i , since the other terms $\phi_0, \dots, \phi_{i-1}, \phi_{i+1}, \dots, \phi_M$ are continuously differentiable at the point $(0, 0, 0, x_4, \dots, x_m)$, unless this point happens to be a Coulomb singular point also for one of the other terms V_j of the potential. This occurs only when (x_4, \dots, x_m) belongs to a subset of lower dimension. Except in this case, then, the internal derivatives of ϕ itself behave for $r \rightarrow 0$ as

$$(2.12) \quad \frac{\partial\phi}{\partial x_k} = a_{ik}(x_4, \dots, x_m) + \left(\frac{\partial\phi_i}{\partial r} \right)_{r=0} \frac{x_k}{r} + o(r^\theta)$$

for each fixed (x_4, \dots, x_m) . This gives $(\partial\phi_i/\partial r)_{r=0}$ a meaning independent of the decomposition $\phi = \phi_0 + \phi_1 + \dots + \phi_M$, which was by no means uniquely determined by the properties stated in Theorem IIa. Thus $(\partial\phi_i/\partial r)_{r=0}$ is an important quantity

giving the measure of the discontinuity of $\partial\phi/\partial x_k$. As is easily seen from (2.12) it is equal to $(\partial\hat{\phi}/\partial r)_{r=0}$, where $\hat{\phi}$ is the average value of ϕ taken over the sphere $r = \text{const.}$ for fixed values of x_1, \dots, x_m (except, of course, for the unimportant case mentioned above).

Now it is interesting to note that this quantity $(\partial\hat{\phi}/\partial r)_{r=0} = (\partial\phi_i/\partial r)_{r=0}$ is proportional to $\phi(0,0,0,x_1,\dots,x_m)$. We have

Theorem IIb. Let W be a generalized Coulomb potential and let

(x_1, \dots, x_m) be a canonical system for V_i . Then

$$(2.13) \quad \left(\frac{\partial\hat{\phi}}{\partial r}\right)_{r=0} = \frac{1}{2} \bar{e}_i \phi(0,0,0,x_1,\dots,x_m)$$

except at some points x_1, \dots, x_m of a set of lower dimension. Here $\hat{\phi}$ is defined above and \bar{e}_i is the constant appearing in the expression (2.11) for V_i .

Theorems IIa and IIb give some information on the characteristic singularity of the eigenfunctions, and this singularity might be said to be a simple generalization of the one encountered in the one-particle system (see (1.1)). In fact, for $s = 1$, the right-hand side of (2.13) reduces to $\frac{1}{2} \bar{e}_1 \phi(0,0,0)$. Thus $\partial\phi/\partial x_k$ are discontinuous if and only if $\phi(0,0,0) \neq 0$, and the degree of discontinuity is proportional to $\phi(0,0,0)$ with coefficient $e/2$, if the operator is written as

$$H = -\Delta + \frac{e}{r} + \dots$$

This result is not quite trivial even for the hydrogen atom, since ϕ may be any wave packet. Of course it could be verified directly for each eigenfunction*.

We shall apply the above results to the case $s = 2$. For simplicity we

*This result follows also from the ordinary differential equation satisfied by the radial part of the eigenfunction of hydrogen atom.

take the Hamiltonian without the μ_0 -term:

$$H = -\Delta_1 - \Delta_2 + \frac{e_1}{r_1} + \frac{e_2}{r_2} + \frac{e_{12}}{r_{12}}.$$

Then we should take $V_1 = e_1 \eta(r_1)/r_1$ etc., according to (2.4). Thus the terms V_1 and V_2 are already in canonical form and we have by (2.13)

$$(2.14) \quad \begin{aligned} \left(\frac{\partial \hat{\phi}^1}{\partial r_1} \right)_{r_1=0} &= \frac{1}{2} e_1 \phi(0, \underline{r}_2), \quad \underline{r}_1 \neq 0, \quad \text{for } \underline{r}_2 \neq 0 \\ \left(\frac{\partial \hat{\phi}^2}{\partial r_2} \right)_{r_2=0} &= \frac{1}{2} e_2 \phi(\underline{r}_1, 0), \quad \underline{r}_2 \neq 0, \quad \text{for } \underline{r}_1 \neq 0 \end{aligned}$$

where $\hat{\phi}^1$ is the average of ϕ for $r_1 = \text{const.}$ and similarly for $\hat{\phi}^2$. To examine the discontinuities at the singular points $r_{12} = 0$, we introduce the orthogonal transformation

$$\bar{r}_1 = 2^{-1/2}(r_1 - r_2), \quad \bar{r}_2 = 2^{-1/2}(r_1 + r_2)$$

so that V_{12} is in the canonical form

$$V_{12} = e_{12} \eta(r_{12})/r_{12} = 2^{-1/2} e_{12} \eta(2^{1/2} \bar{r}_1) / \bar{r}_1.$$

Hence if we write $\phi(\underline{r}_1, \underline{r}_2) = \Psi(\bar{r}_1, \bar{r}_2)$, we have

$$\left(\frac{\partial \hat{\Psi}}{\partial \bar{r}_1} \right)_{\bar{r}_1=0} = 2^{-3/2} e_{12} \Psi(0, \bar{r}_2).$$

But

$$\Psi(0, \bar{r}_2) = \phi(2^{-1/2} \bar{r}_2, 2^{-1/2} \bar{r}_2) = \phi\left(\frac{1}{2}(\bar{r}_1 + \bar{r}_2), \frac{1}{2}(\bar{r}_1 + \bar{r}_2)\right),$$

and

$$\partial/\partial \bar{r}_1 = 2^{1/2} \partial/\partial r_{12},$$

so that we get

$$(2.15) \quad \left(\frac{\partial \hat{\phi}^{12}}{\partial r_{12}} \right)_{r_{12}=0} = \frac{1}{4} e_{12} \phi \left(\frac{1}{2} (r_1 + r_2), \frac{1}{2} (r_1 + r_2) \right), \quad (r_1 + r_2 \neq 0).$$

Not good near origin

Of course here $\hat{\phi}^{12}$ means the average of ϕ taken over the sphere $r_{12} = \text{const.}$ with a fixed value of $r_1 + r_2$. The equalities (2.14) and (2.15) give some quantitative information on the singularity of the eigenfunctions of a two-particle system.

As a simple example, consider the case $e_1 = e_2 = -2$, $e_{12} = 0$. Then the eigenvalue problem can be solved by separation of variables. The ground state solution is

Helium problem no interaction

$$(2.16) \quad \phi = e^{-r_1 - r_2}; \quad e^{-r_i}$$

then (2.14) is immediately verified.

A remark is in order here. By Theorem IIa, ϕ should be written as the sum $\phi = \phi_0 + \phi_1 + \phi_2$, where ϕ_0 is fairly regular and ϕ_1 and ϕ_2 have singularities with respect to r_1 and r_2 respectively. But (2.16) shows that ϕ is the product of two factors e^{-r_1} and e^{-r_2} , each with its characteristic singularity, and it is by no means obvious that ϕ can be expressed as the sum of the above form. Nevertheless this should be possible according to the general result. In fact, we can write for example

when taking derivatives

$$e^{-r_1 - r_2} = \left(e^{-r_1 + r_1} \right) \left(e^{-r_2 + r_2} \right) + r_1 \left(-e^{-r_2 - r_2 + \frac{r_2^2}{r_1 + r_2}} \right) + r_2 \left(-e^{-r_1 - r_1 + \frac{r_1^2}{r_1 + r_2}} \right),$$

and it can easily be shown that this decomposition of $e^{-r_1 - r_2}$ into the sum of three terms satisfies the above requirements.

this has a singularity in $\frac{r_1^2}{r_1 + r_2}$ and we let $r_2 \rightarrow 0$

3. The Hamiltonian. Integral representation

In this section we deduce an integral representation valid for any eigenfunction. Before doing this, however, it is necessary to recall some of the results of the previous paper [1] regarding the definition and basic properties of the correct Hamiltonian operator of our system. First we note that the linear transformation of the coordinates, introduced in the preceding section to bring H into the form (2.7), does not affect the validity of the results of [1]. Also we note that our operator written in the form (2.7) has a meaning even when m is not equal to $3s$, with s an integer. In what follows we shall therefore admit any positive integer $m \geq 3$.

It has been shown in [1] that the formal differential operator (2.7) leads in a natural way to a unique self-adjoint operator \tilde{H} in the Hilbert space $\mathcal{H}_m = L^2(E_m)$, which is to be taken as the correct Hamiltonian of our system.

To define \tilde{H} , it is convenient to begin with the 'kinetic energy' part $-\Delta$ of (2.7). This operator can be dealt with most conveniently in the 'momentum representation.' We introduce the Fourier-Plancherel transforms $F(p)$ of functions $f(x)$ of \mathcal{H}_m :

$$(3.1) \quad F(p) = (2\pi)^{-m/2} \int \exp(-ipx) f(x) dx,$$
$$p = (p_1, \dots, p_m), \quad px = p_1 x_1 + \dots + p_m x_m,$$
$$dx = dx_1 \dots dx_m.$$

Here and in what follows the integral without any specified region of integration is understood to be taken over the whole space. Actually, however, the integral on the right-hand side of (3.1) is to be taken in the sense of mean convergence in L_2 . The set of $F(p)$ are exactly L_2 over the p -space, and the correspondence

$f(x) \longleftrightarrow F(p)$ is unitary. $f(x)$ and $F(p)$ may be regarded as different representations of one and the same vector of the abstract Hilbert space. The m -dimensional space with coordinates $p = (p_1, \dots, p_m)$ is called the momentum space and $F(p)$ is the momentum representation of $f(x)$.

We now define an operator T_0 by

$$(3.2) \quad T_0 f = f^*,$$

where

$$(3.3) \quad \begin{aligned} f(x) \longleftrightarrow F(p), \quad f^*(x) \longleftrightarrow F^*(p), \\ p^2 F(p) = F^*(p), \quad p^2 = p_1^2 + \dots + p_m^2. \end{aligned}$$

In other words, T_0 is a multiplication operator by p^2 in the momentum representation. The domain \mathcal{D}_0 of T_0 is by definition the set of all functions $f(x) \in \mathcal{H}_y$ whose momentum representation $F(p)$ is such that $p^2 F(p)$ is quadratically integrable, or, what is equivalent,

$$(3.4) \quad \int |F(p)|^2 dp < \infty, \quad \int p_i^4 |F(p)|^2 dp < \infty, \quad i = 1, 2, \dots, m.$$

It is clear that T_0 thus defined is a self-adjoint operator. Its domain \mathcal{D}_0 can also be characterized directly in terms of the configuration representation $f(x)$ with the aid of the notion of the class \mathcal{P}_2^* , but we do not need it here.

T_0 is equal to the negative Laplacian $-\Delta$ in the following sense. If $f(x)$ is a function sufficiently smooth and rapidly vanishing at infinity, the expression $-\Delta f$ has a clear meaning; $T_0 f$ is also defined for such f and we

*See Calkin^[10] and Morrey^[11].

have $T_0 f = -\Delta f$. In general, $T_0 f$ can be defined as a limit of such an expression. More precisely, for any given function $f \in \mathcal{D}_0$, there is a sequence $\left\{ f_n \right\}$ of smooth functions of the above kind* such that

$$f_n \rightarrow f, \quad -\Delta f_n \rightarrow T_0 f \quad (n \rightarrow \infty).$$

Here the convergence \rightarrow means strong convergence in the Hilbert space \mathcal{H}_0 .

We next consider the 'potential energy' operator W . Since W is a function of x and is a multiplication operator in the configuration representation, its meaning as an operator in \mathcal{H}_0 is clear: Wf is defined if and only if f and Wf are quadratically integrable.

It is remarkable that Wf is defined for all $f \in \mathcal{D}_0$. This makes the definition of the correct Hamiltonian \tilde{H} quite simple; \tilde{H} is to be defined by

$$(3.5) \quad \tilde{H} = T_0 + W.$$

This implies that \tilde{H} has the same domain \mathcal{D}_0 as T_0 and $\tilde{H}f = T_0 f + Wf$ for $f \in \mathcal{D}_0$. It has been proved that \tilde{H} thus defined is self-adjoint and hence admits of a spectral representation.

We now derive an integral representation for a function u belonging to \mathcal{D}_0 , which is to be the basis for all further results.

First we introduce the necessary integral operators.

Let $\zeta(t)$ be a real-valued function defined for a real variable $t \geq 0$, such that

*It has been proved in [1] that f_n may be assumed to have the form $P(\mathbf{x}) \exp(-\frac{1}{2} \mathbf{x}^2)$, where $P(\mathbf{x})$ is a polynomial of x_1, \dots, x_m .

$$(3.6) \quad \zeta(t) = \begin{cases} 1 & (0 \leq t \leq 1), \\ 0 & (t \geq 2). \end{cases}$$

It is also assumed that $\zeta(t)$ is sufficiently smooth for $t \geq 0$ and non-increasing.

Fixing such a function $\zeta(t)$, we define

$$(3.7) \quad g(x) = g(x_1, \dots, x_m) = (m-2)^{-1} \omega_m^{-1} |x|^{-m+2} \zeta(|x|),$$

where $|x| = (x_1^2 + \dots + x_m^2)^{1/2}$ and where $\omega_m = 2\pi^{m/2} / \Gamma(m/2)$ is the surface area of the unit sphere in E_m .

$g(x)$ is equal to an elementary solution of the Laplace equation $\Delta u = 0$, at least for $|x| \leq 1$. This could be expressed conveniently by the symbolic equation

$$(3.8) \quad \Delta g(x) = -\delta(x) + k(x)$$

where the delta function $\delta(x)$ is the m -dimensional. Here $k(x) = \Delta g(x)$ for $|x| \neq 0$, so that $k(x)$ is a smooth function vanishing identically for $|x| \leq 1$ as well as for $|x| \geq 2$.

By virtue of Green's formula, the symbolic relation (3.8) gives

$$(3.9) \quad u(x) = - \int g(x-y) \Delta u(y) dy + \int k(x-y) u(y) dy.$$

This formula is valid for any smooth function $u(x)$. It is to be noted that the integrals of (3.9) are taken only in the finite sphere $|y-x| \leq 2$, since $g(y-x)$

and $k(y-x)$ vanish for $|y-x| \geq 2$.

If in addition $u(x)$ vanishes rapidly for $|x| \rightarrow \infty$, then we have $-\Delta u = T_0 u$, so that (3.9) may be written in the form

$$(3.10) \quad u = GT_0 u + Ku,$$

where G and K are integral operators with the kernels $g(x-y)$ and $k(x-y)$ respectively.

We shall now show that (3.10) is true not only for such smooth functions but for all u belonging to \mathcal{D}_0 .

To do this we note that G and K are bounded linear operators defined everywhere in \mathcal{H}_y . This follows from the fact that the functions $g(x)$ and $k(x)$ are integrable in the whole space*.

Now let $u \in \mathcal{D}_0$ be arbitrary. Then there is a sequence $\{u_n\}$ of smooth functions such that $u_n \rightarrow u$, $T_0 u_n = -\Delta u_n \rightarrow T_0 u$ ($n \rightarrow \infty$). From (3.10) we know that these smooth functions satisfy

$$u_n = GT_0 u_n + Ku_n.$$

Since G and K are bounded operators, $u_n \rightarrow u$ and $T_0 u_n \rightarrow T_0 u$ imply $Ku_n \rightarrow Ku$ and $GT_0 u_n \rightarrow GT_0 u$. Thus the limit $n \rightarrow \infty$ gives the desired result (3.10) for any $u \in \mathcal{D}_0$.

For any $u \in \mathcal{D}_0$ we know that $\tilde{H}u$ is defined and $\tilde{H}u = T_0 u + Wu$, that is,

*For completeness we sketch a proof here. We have for any $u \in \mathcal{H}_y$

$$\begin{aligned} \left[\int |g(x-y)| |u(y)| dy \right]^2 &\leq \int |g(x-y)| dy \int |g(x-y)| |u(y)|^2 dy \\ &= C \int |g(x-y)| |u(y)|^2 dy, \text{ where we set } C = \int |g(x)| dx. \text{ Hence} \\ \int dx \left[\int |g(x-y)| |u(y)|^2 dy \right] &\leq C \int |u(y)|^2 dy \int |g(x-y)| dx = C^2 \|u\|^2. \end{aligned}$$

It follows from Fubini's theorem that $v(x) = \int g(x-y) u(y) dy$ exists almost everywhere and $v \in \mathcal{H}_y$, $\|v\| \leq C \|u\|$. Thus $v = Ku$ is defined for every $u \in \mathcal{H}_y$ and K is a bounded operator.

$T_0 u = \tilde{H}u - Wu$. Putting this into (3.10), we obtain

$$u = G\tilde{H}u + Ku - GW_0 u,$$

and then, substituting for W from (2.8), we have

$$(3.11) \quad u = G\tilde{H}u + Ku - GW_0 u - \sum_{i=1}^M G V_i u,$$

since we know that each V_i may be applied to u separately (see [1]). (3.11) gives an integral representation of u in terms of Hu and u itself, and serves as a basis for further investigation.

4. Lemmas on the integral operators

We proceed to investigate the integral operators G , K , GW_0 and GV_i appearing in (3.11). G and K are rather simple; they are bounded operators in L^2_γ , as shown in the preceding section. In particular, since the kernel $k(x-y)$ of K is a smooth function, K transforms every function $u \in L^2_\gamma$ into a smooth function. The kernel $g(x-y)$ of G has a singularity given by (3.7), but this singularity is familiar in potential theory; and it is well known that, e.g., if u is Hölder continuous, then Gu has continuous derivatives of second order. The operator GW_0 is bounded and defined everywhere since both the operators G and W_0 are bounded and defined everywhere. Moreover, it is clear that GW_0 is a single integral operator with kernel $g(x-y)W_0(y)$.

The operators GV_i are somewhat more complicated. According to the definition of the product of two operators in a Hilbert space, GV_i is defined

only for functions u such that $V_i u$ and $G(V_i u)$ are both defined. But the V_i are in general unbounded and not defined everywhere, and hence the GV_i are also not defined everywhere. It can be shown, however, that the GV_i are nevertheless bounded.

In what follows let V stand for any one of the V_i for simplicity. Then the operator GV is obviously a restriction of the integral operator A defined by

$$(4.1) \quad (Au)(x) = \int g(x-y) V(y) u(y) dy,$$

and, as we shall show, A is a bounded linear operator defined everywhere in \mathcal{H}_p .

More generally, we can regard A as a linear operator which transforms an element from a Banach space $L^p = L^p(E_m)$ into another Banach space L^q . Here L^p is, as usual, the space of all (equivalent classes of) complex-valued functions $u(x)$ with the finite p -norm

$$(4.2) \quad \|u\|_p = \left[\int |u(x)|^p dx \right]^{1/p}.$$

We shall consider the values $2 \leq p \leq \infty$ and define as usual $\|u\|_\infty = \sup |u(x)|$. As a linear operator on L^p to L^q , Au is defined for $u \in L^p$ if and only if the right-hand side of (4.1) exists as a Lebesgue integral for almost all x and if the function Au thus defined belongs to L^q . When we use A in this sense, we write it A_p^q .

Similarly we shall consider the operator $B = GW_0$:

$$(4.3) \quad (Bu)(x) = \int g(x-y) W_0(y) u(y) dy$$

in these Banach spaces, and we use the notation B_p^q in the same way.

For these operators in Banach spaces, we now prove several lemmas.

In this section $V(x) = V_1(x)$ is assumed to be of the general form (2.9) satisfying (2.10). We begin with an auxiliary lemma.

Lemma 1. Let $g_\mu(x) = |x|^{-m+\mu} \zeta_1(|x|)$, where $0 \leq \mu < m$ and $\zeta_1(t)$ is a smooth function with the property (3.6). If α, β are real numbers such that

$$(4.4) \quad \alpha \geq 0, \quad 0 \leq \beta \leq \sigma, \quad 0 < (m-\mu)\alpha + \frac{3}{\sigma}\beta < m,$$

then there is a finite constant C , independent of x , such that*

$$(4.5) \quad \int |g_\mu(x-y)|^\alpha |V(y)|^\beta dy \leq C.$$

Proof. First we note the following simple formula:

$$(4.6) \quad \int |x|^{-\nu} \zeta_1(|x|) dx_1 \dots dx_m = \frac{\pi^{(m-3)/2} \Gamma(\frac{\nu-m+3}{2})}{\Gamma(\frac{\nu}{2})} r^{-\nu+m-3} + f(r^2),$$

where $m \geq 4$, $\nu > m-3$, $r = (x_1^2 + x_2^2 + x_3^2)^{1/2}$ and $f(r^2)$ is a bounded function smooth at least for $r^2 < 1$. As is seen from the proof below, (4.6) holds even if the factor $\zeta_1(|x|)$ is omitted.

To prove this formula, we introduce the variable $\lambda = (x_1^2 + \dots + x_m^2)^{1/2}$ and transform the integral into

$$\omega_{m-3} \int_0^\infty (r^2 + \lambda^2)^{-\nu/2} \zeta_1\left((r^2 + \lambda^2)^{1/2}\right) \lambda^{m-4} d\lambda = \omega_{m-3} \int_r^\infty \zeta_1(t) (t^2 - r^2)^{(m-5)/2} t^{-\nu+1} dt.$$

*If $\alpha = 0$, $|g_\mu(x-y)|^\alpha$ in (4.5) is to be put equal to zero whenever $g_\mu(x-y) = 0$.

In other words, the integral of (4.5) is a finite integral taken over $|y-x| \leq 2$ whether or not $\alpha > 0$.

We then split the integral into two parts by writing $\zeta_1(t) = 1 + (\zeta_1(t)-1)$. The first part gives the first term on the right-hand side of (4.6). Since $\zeta_1(t)-1$ vanishes for $0 \leq t \leq 1$, the second part is easily seen to represent a smooth function of r^2 for $r^2 < 1$.

Now (4.5) is obvious if $\beta = 0$, since then $0 < (m-\mu) \alpha < m$ by hypothesis. So we shall assume $\beta > 0$ in the remainder of the proof.

To prove (4.5) in the general case, we assume that V (which is one of the V_i , $i=1, \dots, M$) is already in the canonical form $V = \nabla(x_1, x_2, x_3)$ (see (2.9)); this does not affect the generality, for an orthogonal transformation of the coordinates x_1, \dots, x_m does not change the form of g_μ . Then, denoting the integral (4.5) by $I(x)$, we have

$$\begin{aligned} I(x) &= \int |g_\mu(x-y)|^\alpha |V(y)|^\beta dy = \int |V(x-y)|^\beta |g_\mu(y)|^\alpha dy \\ (4.7) \quad &= \int_{E_3} |\nabla(x_1-y_1, x_2-y_2, x_3-y_3)|^\beta dy_1 dy_2 dy_3 \int_{E_{m-3}} |g_\mu(y)|^\alpha dy_4 \dots dy_m. \end{aligned}$$

Here $|g_\mu(y)|^\alpha = |y|^{-\alpha(m-\mu)} |\zeta_1(|y|)|^\alpha$ and $|\zeta_1(t)|^\alpha$ has the same property (3.6) as $\zeta_1(t)$ itself if $\alpha > 0$. Hence we can apply the formula (4.6) to the last $(m-3)$ -dimensional integral of the above expression, provided

$$(4.8) \quad \nu = \alpha(m-\mu) > m-3,$$

which we assume for the moment. Noting that this integral is zero if $s = (y_1^2 + y_2^2 + y_3^2)^{1/2} \geq 2$, we see that it is majorized by an expression $Cs^{-\alpha(m-\mu)+m-3}$ with some constant C . Thus we have

$$(4.9) \quad I(x) \leq C \int_{s \leq 2} |\nabla(x_1-y_1, x_2-y_2, x_3-y_3)|^\beta s^{-\alpha(m-\mu)+m-3} dy_1 dy_2 dy_3.$$

The assumption (4.4) implies that

$$\frac{1}{3} [\alpha(m-\mu)-(m-3)] + \frac{\beta}{\sigma} < 1,$$

where both terms on the left-hand side are positive by (4.8) and our assumption $\beta > 0$. Hence we can take two positive numbers a, b such that

$$(4.10) \quad \frac{1}{a} + \frac{1}{b} = 1, \quad \frac{1}{a} > \frac{1}{3} [\alpha(m-\mu)-(m-3)], \quad \frac{1}{b} = \frac{\beta}{\sigma}.$$

On applying the Hölder inequality to the integral on the right-hand side of (4.9), we obtain

$$I(x) \leq C \left[\int_{s \leq 2} |V(x_1-y_1, x_2-y_2, x_3-y_3)|^{\beta b} dy_1 dy_2 dy_3 \right]^{1/b} \\ \cdot \left[\int_{s \leq 2} s^{-[\alpha(m-\mu)-(m-3)]a} dy_1 dy_2 dy_3 \right]^{1/a}.$$

The second factor on the right-hand side is finite and independent of x , because $[\alpha(m-\mu)-(m-3)]a < 3$ by (4.10). The first factor is not decreased by replacing the region of integration by the whole space E_3 ; then the integral is obviously independent of x and yet finite because $b\beta = \sigma$ by (4.10). This proves (4.5) under the assumption (4.8).

To deal with the case $\alpha(m-\mu) \leq m-3$, suppose for the moment that $\beta < \sigma$, and set

$$\varepsilon = 1 - \frac{\beta}{\sigma} > 0, \quad \alpha' = \frac{m-3+\varepsilon}{m-\mu}.$$

Then

$$(m-\mu) \alpha' + \frac{3}{\sigma} \beta = m-2\varepsilon < m,$$

so that the assumption (4.4) is satisfied by the pair α', β instead of α, β . Furthermore $\alpha'(m-\mu) > m-3$, and so (4.8) is also satisfied by α' . Therefore, (4.5) is seen to hold if α is replaced by α' . Also* (4.5) is true for $\alpha = 0$, for $0 < \beta < \sigma$. Thus (4.5) must be true for any α between 0 and α' , and this proves (4.5) for our α , since $0 \leq \alpha \leq (m-3)(m-\mu)^{-1} < \alpha'$.

In the only remaining case, $\beta = \sigma$, we have $(m-\mu)\alpha < m-3$, by (4.4). Thus the last integral $\int |g_\mu(y)|^\alpha dy_4 \dots dy_m$ of (4.7) has an upper bound independent of (y_1, y_2, y_3) .* Thus the desired result follows immediately, by (2.10). This completes the proof of Lemma 1.

Now we state

Lemma 2. Let $m \geq 4$, $2 \leq p \leq q \leq \infty$. If $\frac{1}{q} > \frac{1}{p} - \frac{2}{m}$, then B_p^q is a bounded linear operator defined everywhere in L^p . If

$$(4.11) \quad \frac{1}{q} > \frac{1}{p} - (2 - \frac{3}{\sigma}) \frac{1}{m},$$

then the same is true for Λ_p^q .

Proof. We first give the proof for Λ_p^q . Let $m_0 = \text{Min} \left[m, (2 - \frac{3}{\sigma})p \right]$ and let ϵ be such that $0 < \epsilon < \frac{m_0}{2}$. Further, set

$$\gamma = \frac{m-\epsilon}{m-2}, \quad \delta = \frac{m_0-2\epsilon}{m-2}, \quad \alpha = \frac{p-\gamma+\delta}{p-1},$$

$$\beta = \frac{p}{p-1}, \quad q = \frac{p}{\gamma-\delta}.$$

Since $m \geq m_0$ and $0 < \epsilon < m_0/2$, we see that $\gamma > \delta > 0$ and hence $q > p$. Also $\beta > 0$ and $\gamma < \frac{m}{m-2} \leq 2 \leq p$, so that $\alpha > 0$. Furthermore, it is easily seen that

$$(4.12) \quad (m-2)\alpha + \frac{3}{\sigma}\beta - m = \frac{1}{p-1} \left[m_0 - (2 - \frac{3}{\sigma})p - \epsilon \right] < 0.$$

*See footnote following (4.4).

With these preliminaries, we consider the expression (4.1). Proceeding rather formally for the moment, we have

$$(4.13) \quad |(Au)(x)| \leq \int (|g(x-y)|^{\frac{\gamma}{q}} |u(y)|^{\frac{p}{q}} (|g(x-y)|^{1-\frac{\gamma}{q}} |v(y)|) |u(y)|^{1-\frac{p}{q}} dy.$$

Note that $\gamma/q, p/q, 1-(\gamma/q) \geq 1-(\gamma/p), 1-(p/q)$ are all non-negative.

If we set $s = pq(q-p)^{-1}$, we have

$$\frac{1}{q} + \frac{1}{\beta} + \frac{1}{s} = 1$$

and we can apply the Hölder inequality with three factors in the integrand, obtaining

$$\begin{aligned} |(Au)(x)| &\leq \left[\int (|g(x-y)|^{\frac{\gamma}{q}} |u(y)|^{\frac{p}{q}} dy \right]^{\frac{1}{q}} \cdot \\ &\cdot \left[\int (|g(x-y)|^{1-\frac{\gamma}{q}} |v(y)|)^{\beta} dy \right]^{\frac{1}{\beta}} \cdot \left[\int |u(y)|^{(1-\frac{p}{q})s} dy \right]^{\frac{1}{s}}. \end{aligned}$$

Since

$$(1-\frac{\gamma}{q})\beta = \alpha, \quad (1-\frac{p}{q})s = p,$$

as is easily verified, it follows that

$$|(Au)(x)| \leq \left[\int |g(x-y)|^{\gamma} |u(y)|^p dy \right]^{\frac{1}{q}} \cdot \left[\int |g(x-y)|^{\alpha} |v(y)|^{\beta} dy \right]^{\frac{1}{\beta}} \cdot \|u\|_{\frac{p}{s}}.$$

The second factor on the right-hand side is finite and bounded by a constant independent of x , because Lemma 1 is applicable with $\mu = 2$, by (4.12), and $\beta = p(p-1)^{-1} \leq 2 \leq \sigma$. Hence

$$|(Au)(x)|^q \leq C \|u\|_p^{pq/s} \int |g(x-y)|^\gamma |u(y)|^p dy.$$

We integrate this inequality with respect to x and change the order of integration on the right-hand side. Since $\gamma < m(m-2)^{-1}$, we have

$$\int |g(x-y)|^\gamma dx = \int |g(x)|^\gamma dx < \infty$$

and thus we arrive at the inequality*

$$\begin{aligned} \int |(Au)(x)|^q dx &\leq C \|u\|_p^{pq/s} \int |u(y)|^p dy \\ &= C \|u\|_p^{(pq/s)+p} = C \|u\|_p^q \end{aligned}$$

or

$$\|Au\|_q \leq C \|u\|_p.$$

It is now clear that these rather formal calculations show, by a standard reasoning based on Fubini's theorem, that the integral (4.1) defining $(Au)(x)$ exists almost everywhere, that $Au \in L^q$ if $u \in L^p$, and that $A = A_p^q$ is a bounded operator. But it is easily seen that

$$q = \frac{m-\varepsilon}{m-m_0+\varepsilon} p.$$

Thus q can be made to take any value such that $p < q < mp(m-m_0)^{-1}$ by giving ε a suitable value such that $0 < \varepsilon < m_0/2$. In other words, q may be arbitrary if

*Here and in what follows we use the letter C to denote an indefinite constant.

$$\frac{m-m_0}{m} \frac{1}{p} < \frac{1}{q} < \frac{1}{p}.$$

Recalling the definition of m_0 , we see that this is identical with the condition for q in Lemma 2, unless $q = p$ or $q = \infty$. But the case $q = p < \infty$ is obtained if we put $\epsilon = m_0/2$ in the above proof. Then we have $q = p$, $s = \infty$, and everything carries through if we interpret each expression accordingly; here we actually need not introduce the number s . The other case $q = \infty$ can be dealt with similarly, with minor changes, so we may omit the details. This completes the proof of the part of Lemma 2 concerning A_p^q .

The result for B_p^q can be proved in exactly the same way. This time we have only to set $m_0 = \text{Min}(m, 2p)$ and note that $W_0(y)$ is a bounded function.

Now we state

Lemma 3. If $u \in L^p$ with $p > m(2 - \frac{3}{\theta})^{-1}$, then the function Au is bounded and (C_θ) for any $\theta < 2 - \frac{3}{\theta} - \frac{m}{p}$. If $u \in L^p$ with $p > \frac{m}{2}$, then Bu is bounded and (C_θ) for any $\theta < 2 - \frac{m}{p}$ ($p \geq 2$ is always assumed).

Proof. First we prove the following inequality:

$$(4.14) \quad |x-y|^{-\theta} |g(x) - g(y)| \leq C(g_{2-\theta}(x) + g_{2-\theta}(y)),$$

where $0 < \theta < 1$ and where $g_{2-\theta}(x)$ is a function of the form considered in Lemma 1.

To prove this, we may obviously assume that $|x| \leq |y|$. Since $g(x) = C|x|^{-(m-2)}\zeta(|x|)$, we have, writing $\nu = m-2$ for simplicity,

$$|g(x)-g(y)| \leq C \left[(|x|^{-\nu} - |y|^{-\nu})\zeta(|x|) + |y|^{-\nu} \left\{ \zeta(|x|) - \zeta(|y|) \right\} \right].$$

But

$$\begin{aligned} |x|^{-\nu} - |y|^{-\nu} &= |x|^{-\nu} |y|^{-\nu} (|y|^{\nu} - |x|^{\nu}) \leq |x|^{-\nu} |y|^{-\nu} (|y| - |x|) \nu |y|^{\nu-1} \\ &\leq \nu |x|^{-\nu} |y|^{-1} |y-x| \leq \nu |y-x|^{\theta} |x|^{-\nu} |y|^{-1} (2|y|)^{1-\theta} \\ &\leq 2^{1-\theta} \nu |y-x|^{\theta} |x|^{-\nu} |y|^{-\theta} \leq 2^{1-\theta} \nu |y-x|^{\theta} |x|^{-\nu-\theta} \end{aligned}$$

and

$$\begin{aligned} |\zeta(|x|) - \zeta(|y|)| &\leq (|y| - |x|) \max_{|x| \leq t \leq |y|} |\zeta'(t)| \\ &\leq |y-x| \max_{t \geq |x|} |\zeta'(t)| \leq C |y-x|^{\theta} (2|y|)^{1-\theta} \zeta_2(|x|), \end{aligned}$$

where $\max_{\tau \geq t} |\zeta'(\tau)|$ is a function equal to a constant for $t \leq 1$ and vanishing

for $t \geq 2$. We can therefore write $\max_{\tau \geq t} |\zeta'(\tau)|$ as $C\zeta_2(t)$, where the function $\zeta_2(t)$ has the property (3.6).

Collecting the above results, we obtain

$$|y-x|^{-\theta} |g(x) - g(y)| \leq C |x|^{-\nu-\theta} \zeta_1(|x|) + C |y|^{1-\nu-\theta} \zeta_2(|x|).$$

Here $1-\nu-\theta = -m + 3 - \theta < 0$, so that we can replace $|y|^{1-\nu-\theta}$ by $|x|^{1-\nu-\theta}$, which in turn can be replaced by $2|x|^{-\nu-\theta}$, since we need to consider only the case $|x| \leq 2$ on account of the factor $\zeta_2(|x|)$. Thus we have

$$\begin{aligned} (4.15) \quad |y-x|^{-\theta} |g(x) - g(y)| &\leq |x|^{-\nu-\theta} (C\zeta_1(|x|) + C\zeta_2|x|) = C|x|^{-\nu-\theta} \zeta_1(|x|) \\ &= C\zeta_{2-\theta}(|x|), \quad (|x| \leq |y|), \end{aligned}$$

where $\zeta_1(t)$ again satisfies (3.6). This proves (4.14).

We now turn to the proof of Lemma 3. By hypothesis the right-hand side of (4.11) is negative, so that Lemma 2 shows that A_p^∞ is a bounded operator. In fact, the integral (4.1) for $(Au)(x)$ exists for all x (actually this corresponds to the case of Lemma 2 for which a detailed proof was omitted).

Furthermore

$$|(Au)(x') - (Au)(x)| \leq \int |g(x'-y) - g(x-y)| |V(y)u(y)| dy.$$

It follows from (4.14) that

$$|(Au)(x') - (Au)(x)| \leq C|x'-x|^\theta \int |g_\mu(x'-y) + g_\mu(x-y)| |V(y)u(y)| dy$$

with $\mu = 2 - \theta$. But

$$(4.16) \quad \int |g_\mu(x-y)| |V(y)| |u(y)| dy \leq \left[\int |g_\mu(x-y)|^\beta |V(y)|^\beta dy \right]^{\frac{1}{\beta}} \left[\int |u(y)|^p dy \right]^{\frac{1}{p}}$$

with $\beta = \frac{p}{p-1} \leq \sigma$. Here

$$(m-\mu)\beta + \frac{3}{\sigma}\beta = (m-2+\theta + \frac{3}{\sigma}) \frac{p}{p-1} < m$$

if $\theta < 2 - \frac{3}{\sigma} - \frac{m}{p}$. Hence Lemma 1 applied with $\alpha = \beta$ shows that the first factor on the right-hand side of (4.16) has a finite bound independent of x . Since a similar result holds for the term involving x' , we get

$$|(Au)(x') - (Au)(x)| \leq C|x'-x|^\theta \|u\|_p.$$

This proves Lemma 3 for Au .

The proof for Bu is again similar but simpler. Since $W_0(y)$ is bounded, the constant β above has only to satisfy $\beta < m(m-\mu)^{-1}$, and this is the case if $\theta < 2 - \frac{m}{p}$.

Lemma 4. If $u \in L^p$ with $p > m$, then Bu is (C'_θ) with any $\theta < 1 - \frac{m}{p}$.
If $\sigma > 3$ and $u \in L^p$ with $p > m(1 - \frac{3}{\sigma})^{-1}$, then Au is (C'_θ) with any $\theta < 1 - \frac{3}{\sigma} - \frac{m}{p}$.

Proof. Formal differentiation of (4.1) gives

$$(4.17) \quad (Au)_{x_i}(x) = \frac{\partial}{\partial x_i} (Au)(x) = - \int g_0(x-y)(x_i - y_i) V(y) u(y) dy,$$

where

$$(4.18) \quad g_0(x) = \omega_m^{-1} |x|^{-m} \left[\zeta(|x|) - \frac{|x|}{m-2} \zeta'(|x|) \right] = \omega_m^{-1} |x|^{-m} \zeta_0(|x|);$$

$\zeta_0(t)$ is again a function satisfying (3.6). Thus $g_0(x)$ has, apart from a constant factor, the form $g_\mu(x)$ with $\mu = 0$ which is discussed in Lemma 1.

If we show that the right-hand side of (4.17) exists for all x and is a function (C_θ) , the formal differentiation is easily justified and the lemma is proved. But the continuity of (4.17) can be proved quite in the same way as in Lemma 3. We need only to establish the following inequality, corresponding to (4.14):

$$(4.19) \quad |x-y|^{-\theta} |x_i g_0(x) - y_i g_0(y)| \leq C(g_{1-\theta}(x) + g_{1-\theta}(y)), \quad 0 < \theta < 1,$$

where $g_{1-\theta}(x)$ is again a function of the form $g_\mu(x)$ with $\mu = 1 - \theta$ but with some new $\zeta_3(t)$ instead of $\zeta_1(t)$. This inequality can be proved easily by using (4.15).

The detailed proof of this and of Lemma 4 may be omitted.

Lemma 5. Let u be (C_δ) with some $\delta > \frac{3}{\sigma} - 1$. Then Au has external partial derivatives with respect to V , which are (C_θ) for any $\theta < \delta + 1 - \frac{3}{\sigma}$.

Proof. Without loss of generality we may assume that V is in a canonical form $V = \bar{V}(x_1, x_2, x_3)$. We construct the formal derivative (4.17) of Au with respect to one of external coordinates x_i , $i = 4, \dots, m$. We can write it in the following form:

$$(4.20) \quad (Au)_{x_i}(x) = - \int g_0(x-y)(x_i-y_i) \bar{V}(y_1, y_2, y_3) [u(y) - u(x)] dy, \quad i = 4, \dots, m,$$

since the integral involving $u(x)$ vanishes, because of symmetry. Since

$$|u(y) - u(x)| \leq C|y-x|^\delta \text{ by hypothesis, the integrand in (4.20) is majorized by } C|g_0(x-y)| |x-y|^{1+\delta} |\bar{V}(y_1, y_2, y_3)|, \text{ which is of the form } C|g_{1+\delta}(x-y)| |V(y)|$$

in the notation of Lemma 1. Applying Lemma 1 with $\alpha = \beta = 1$, we see that this integral has a finite upper bound independent of x . Thus the integral (4.20) is absolutely convergent.

If we show the Hölder continuity of the function thus defined by the right-hand side of (4.20), which we denote by $v(x)$ for the moment, the formal differentiation (4.17) is justified and the lemma is proved.

To prove the Hölder continuity of $v(x)$, we consider the expression $v(x') - v(x)$. Following a familiar procedure, we consider a sphere Σ with center x and radius $2|x' - x| = \rho$, and write

$$\begin{aligned}
 |v(x') - v(x)| \leq & \left| \int_{\Sigma} g_0(x-y)(x_i-y_i) v(y) [u(y) - u(x)] dy \right| \\
 & + \left| \int_{\Sigma} g_0(x'-y)(x'_i-y_i) v(y) [u(y) - u(x')] dy \right| \\
 & + \left| \int_{E_m - \Sigma} [g_0(x'-y)(x'_i-y_i) - g_0(x-y)(x_i-y_i)] v(y) [u(y) - u(x')] dy \right| \\
 & + \left| u(x') - u(x) \right| \left| \int_{E_m - \Sigma} g_0(x-y)(x_i-y_i) v(y) dy \right|.
 \end{aligned}$$

The four integrals on the right-hand side will be denoted by I_1, I_2, I_3, I_4 .

$|I_1|$ and $|I_2|$ can be estimated by the same method used above in showing that $v(x)$ exists, the only difference being in the region of integration. By inspecting the proof of Lemma 1, it is easily seen that

$$|I_1| \leq C \left[\int_{s \leq \rho} s^{-(2-\delta)a} \cdot 4\pi s^2 ds \right]^{\frac{1}{a}} \leq C \rho^{\frac{3}{a} - (2-\delta)}$$

where, by (4.10),

$$\frac{1}{a} = 1 - \frac{1}{b} = 1 - \frac{1}{\sigma},$$

since we are setting $\alpha = \beta = 1$. Thus we obtain $|I_1| \leq C \rho^{1+\delta - \frac{3}{\sigma}}$. $|I_2|$ satisfies an inequality of the same form, because we can estimate it by enlarging Σ to a sphere with center x' and radius 2ρ .

In I_3 we use (4.19) to obtain

$$|I_3| \leq C |x' - x|^\theta \int_{E_m - \Sigma} |g_{1-\theta}(x' - y) + g_{1-\theta}(x - y)| |v(y)| |u(y) - u(x')| dy.$$

Noting that $|u(y) - u(x')| \leq C|x' - y|^\delta$ and $|x' - y| \leq 2|x - y|$ for $y \in E_m - \Sigma$, we get

$$|I_3| \leq \rho^\theta \left[C \int_{E_m - \Sigma} |g_{1-\theta+\delta}(x'-y)| |v(y)| dy + C \int_{E_m - \Sigma} |g_{1-\theta+\delta}(x-y)| |v(y)| dy \right].$$

In particular, let θ be such that $\theta < \delta + 1 - \frac{3}{\sigma}$. Then $1 - \theta + \delta > \frac{3}{\sigma}$ and Lemma 1 applied with $\alpha = \beta = 1$ shows that the integrals on the right-hand side of the above expression are bounded functions of x or x' (even if the integrals are taken over the whole space).

Noting finally that $I_4 = 0$, because of symmetry, and summing up the above results, we see that $|v(x') - v(x)| \leq C \rho^\theta = C |x' - x|^\theta$ if $\theta < 1$, $\theta < \delta + 1 - \frac{3}{\sigma}$ and $|x' - x|$ is bounded. But the last restriction for $|x' - x|$ is not necessary, for $v(x)$ is bounded. This completes the proof of Lemma 5.

5. Proof of Theorems I and Ia

We first prove the following lemma.

Lemma 6. Let $u \in \mathcal{O}_0$ and $\tilde{H} u \in L^p$ for some $p \geq 2$. Then $u \in L^q$ for any $q \geq 0$ such that $\frac{1}{2} \geq \frac{1}{q} > \frac{1}{p} - \frac{2}{m}$. If $p > m/2$, then u is bounded and (C $_{\theta}$) for any $\theta < \text{Min} (2 - \frac{m}{p}, 2 - \frac{3}{\sigma})$. Further, if $p > m$ and $\sigma > 3$, u is (C $'_{\theta}$) for any $\theta < \text{Min} (1 - \frac{m}{p}, 1 - \frac{3}{\sigma})$.

Proof. Let J be the set of positive numbers q (including ∞) such that $u \in L^q$. Since $u \in \mathcal{H}_\gamma = L^2$, J contains at least one point $q = 2$. As is well known, J is an interval. Let b be the upper end of this interval. Then, for any $\epsilon > 0$, there is a number $q' \in J$ such that $\frac{1}{q'} < \frac{1}{b} + \epsilon$.

Consider the integral expression (3.11). This can be written as

$$(5.1) \quad u = G \tilde{H} u + K u - B u - \sum_{i=1}^M A_i u,$$

where A_i is the integral operator defined by (4.1) with $V = V_i$ and B is given by (4.3) (see the beginning of Section 4). We note that all terms of (5.1) belong to $\mathcal{H} = L^2$.

Since the operator G is a special case of $B = GW_0$ with $W_0 = 1$, the first term of (5.1), $G\tilde{H}u$, belongs to L^q with any q such that $\frac{1}{p} \geq \frac{1}{q} > \frac{1}{p} - \frac{2}{m}$, as seen from Lemma 2*. But since $G\tilde{H}u \in L^2$, this is true with any q such that $\frac{1}{2} \geq \frac{1}{q} > \frac{1}{p} - \frac{2}{m}$. For the same reason, the third term of (5.1), $-Bu$, belongs to L^q with any q such that $\frac{1}{2} \geq \frac{1}{q} > \frac{1}{q'} - \frac{2}{m}$, for $u \in L^{q'}$. Similarly by Lemma 2, it follows that each $A_i u \in L^q$ with any q such that $\frac{1}{2} \geq \frac{1}{q} > \frac{1}{q'} - (2 - \frac{3}{\sigma}) \frac{1}{m}$. Finally Ku is a smooth function belonging to L^2 so that $Ku \in L^q$ for any $q \geq 2$. Collecting these results, we see that $u \in L^q$ with any $q \geq 2$ such that $\frac{1}{q}$ is larger than the largest number among $0, \frac{1}{p} - \frac{2}{m}, \frac{1}{q'} - \frac{2}{m}, \frac{1}{q'} - (2 - \frac{3}{\sigma}) \frac{1}{m}$. Noting that the fourth of these is larger than the third, we conclude that

$$\begin{aligned} \frac{1}{\sigma} &\leq \text{Max} \left[\frac{1}{p} - \frac{2}{m}, \frac{1}{q'} - (2 - \frac{3}{\sigma}) \frac{1}{m}, 0 \right] \\ &\leq \text{Max} \left[\frac{1}{p} - \frac{2}{m}, \frac{1}{\sigma} + \varepsilon - (2 - \frac{3}{\sigma}) \frac{1}{m}, 0 \right]. \end{aligned}$$

Since $\varepsilon > 0$ is arbitrary and $2 - \frac{3}{\sigma} \geq \frac{1}{2} > 0$, it is impossible for the second number in the square brackets to be the maximum. Thus we conclude that

$$\frac{1}{\sigma} \leq \text{Max} \left[\frac{1}{p} - \frac{2}{m}, 0 \right].$$

This proves the first part of Lemma 6.

* In Lemma 2 we assumed $m \geq 4$, so the argument here is not applicable to the case $m = 3$. However, we know (see [1]) that every $u \in \mathcal{O}_0$ is continuous and bounded if $m = 3$. Thus Lemma 6 holds for all $m \geq 3$.

Next suppose that $p > m/2$. Then the above result shows that $u \in L^q$ with any $q \geq 2$. It follows from Lemma 3 that all $A_i u$ are (C_θ) for any $\theta < 2 - \frac{3}{\sigma}$ and that Bu is (C_θ) for any $\theta < 2$ (in fact, for $\theta < 1$). Since $\tilde{H} u \in L^p$, Lemma 3 with $G = B$ also shows that $G \tilde{H} u$ is (C_θ) for any $\theta < 2 - \frac{m}{p}$. Finally Ku is a smooth function and hence is (C_θ) for any $\theta < 1$. Summing up, we conclude that u is (C_θ) with any $\theta < \text{Min} (2 - \frac{3}{\sigma}, 2 - \frac{m}{p})$. This proves the second part of Lemma 6.

The last part can be proved in the same way by making use of Lemma 4.

Theorem I can now be proved easily. Suppose that u belongs to the domain of \tilde{H}^n , where n is a positive integer to be determined later, and set $\tilde{H}^{n-k} u = f_k$, $k = 0, 1, \dots, n$. Since $f_1 \in \mathcal{D}_0$ and $\tilde{H} f_1 = f_0 \in \mathcal{H} = L^2$, it follows from Lemma 6 that $f_1 \in L^q$ for any $\frac{1}{q} > \frac{1}{2} - \frac{2}{m}$. Since in turn $\tilde{H} f_2 = f_1$, it follows from Lemma 6 that $f_2 \in L^q$ for any $\frac{1}{q} > \frac{1}{2} - 2 \frac{2}{m}$. Repeating this argument, we see that $f_k \in L^q$ for any $\frac{1}{q} > \frac{1}{2} - \frac{2k}{m}$. If we take k equal to the first integer larger than $\frac{m}{4} - \frac{1}{2}$, we have $f_k \in L^q$ with some $q > m$. Then by Lemma 6, f_{k+1} must be (C_θ) for any $\theta < 2 - \frac{3}{\sigma}$. If we choose $n = k+1$, we see that $u = f_{k+1}$ has such a property. Thus every function u belonging to the domain of \tilde{H}^{k+1} with the above k is (C_θ) with any $\theta < 2 - \frac{3}{\sigma}$. Since an eigenfunction belongs to the domain of \tilde{H}^n for all n , the first part of Theorem I has been proved.

Next suppose that $\sigma > 3$. We see that, in the above argument, $f_k \in L^q$ for any $q \geq 2$ if k is the first integer not smaller than $m/4$. Then Lemma 6 shows that $f_{k+1} \in (C'_\theta)$ with any $\theta < 1 - \frac{3}{\sigma}$, and the second part of Theorem I follows as above.

Theorem Ia can be proved by making use of Lemma 5. Let ϕ be an eigenfunction. Then we have by (5.1)

$$(5.2) \quad \phi = G \tilde{H} \phi + K\phi - B\phi - \sum A_i \phi.$$

Since $\tilde{H} \phi$ is also an eigenfunction, it is (C_θ) with some θ , by Theorem I, and hence $G \tilde{H} \phi$ has continuous derivatives of second order. The same is true for $K \phi$. Since $\phi \in L^p$ for any $p \geq 2$, $B \phi$ is (C'_θ) for any $\theta < 1$, by Lemma 4. Thus the sum of first three terms of (5.2) is (C'_θ) for any $\theta < 1$.

Let $\phi_i = -A_i \phi$. We know by Theorem I that $\phi \in (C_\delta)$ for any $\delta < 2 - \frac{3}{\sigma}$. Noting that $2 - \frac{3}{\sigma} > \frac{3}{\sigma} - 1$ by the assumption $\sigma > 2$, we see from Lemma 5 that ϕ_i has external derivatives which are (C_θ) with any $\theta < 2 - \frac{3}{\sigma} + 1 - \frac{3}{\sigma} = 3 - \frac{6}{\sigma}$. This proves Theorem Ia, since the first three terms of (5.2) may be added to any of the ϕ_i without changing the properties of the latter.

6. Proof of Theorems II, IIa, IIb

We now assume that the potential W is a generalized Coulomb potential given by (2.8), (2.9) and (2.11). We denote by V any one of the V_i ($i = 1, \dots, M$) and consider again the integral operator A given by (4.1). We assume that V is already in its canonical form, that is,

$$(6.1) \quad V = \bar{e} \frac{\bar{q}(r)}{r} + \bar{V}'(x_1, x_2, x_3), \quad r = (x_1^2 + x_2^2 + x_3^2)^{1/2},$$

where

$$(6.2) \quad \int |\bar{V}'(x_1, x_2, x_3)|^\sigma dx_1 dx_2 dx_3 < \infty$$

with some $\sigma > 3$.

We first prove

Lemma 7. Let $u \in L^2$ be bounded and (C_δ) for some $\delta > 1 - \frac{3}{m}$. Then Au can be written as $Au = v + w$, where v and w have the following properties: v is (C'_θ) for any $\theta < \text{Min} \left[1 - \frac{3}{\sigma}, 1 - (1-\delta) \frac{m}{3} \right]$; w is a function of r and external coordinates x_1, \dots, x_m only; $w \in (C'_\theta)$ for any $\theta < \delta$ in the variables r, x_1, \dots, x_m ; and

$$(6.3) \quad \left(\frac{\partial w}{\partial r} \right)_{r=0} = -\frac{1}{2} \bar{e} u(0, 0, 0, x_1, \dots, x_m).$$

Proof: Consider (4.1) for $(Au)(x)$. If we substitute (6.1) for $V(y)$, the contribution from the second term of (6.1) is a function which is (C'_θ) for any $\theta < 1 - \frac{3}{\sigma}$; this follows from Lemma 4, where we may put $p \rightarrow \infty$. Thus this contribution satisfies the condition on v stated in Lemma 7. Hence we may assume

$$(6.4) \quad v = \bar{e} \frac{\bar{\eta}(r)}{r}$$

in what follows. Here $\bar{\eta}(r) = 1$ for $r \leq \rho$ and $\bar{\eta}(r) = 0$ for $r > \rho$ with some constant $\rho > 0$, which may be assumed to be smaller than 1.

We now write in (4.1)

$$(6.5) \quad u(y) = u_0(y) + [u(y) - u_0(y)]$$

with

$$(6.6) \quad u_0(x) = u(0,0,0,x_1,\dots,x_m) \cdot$$

Then the contribution to Au from the second term of (6.5) is seen to be Hölder continuous. In fact, since $|u(x) - u_0(x)| \leq C r^\delta$ by hypothesis, and (6.4) is true, the function $z(x) = V(x) [u(x) - u_0(x)]$ belongs to L^p at least locally (and uniformly)*, with any p such that $(1-\delta)p < 3$. It follows from Lemma 4** applied to Bz with $B = G$ that this contribution Gz is (C'_θ) for any $\theta < 1 - \frac{m}{p}$ and hence any $\theta < 1 - (1-\delta)\frac{m}{3}$. Thus this part also satisfies the condition on v .

Thus our problem is reduced to showing that

$$(6.7) \quad w(x) = \int g(x-y) V(y) u_0(y) dy,$$

where V is given by (6.4), has the properties stated in Lemma 7. By symmetry it

* Here a function u is said to belong to L^p locally and uniformly if the integral $\int |u|^p dx$ extended over a sphere of a fixed radius has a finite upper bound independent of the position of the sphere.

** Lemma 4 holds if $u \in L^p$ locally and uniformly instead of $u \in L^p(E_m)$; this follows easily from the fact that $(Au)(x)$ and $(Au)_{x_i}(x)$ depend only on the values of $u(y)$ for $|y-x| \leq 2$.

is obvious that $w(x)$ is a function of r, x_4, \dots, x_m only. Also it follows from Lemma 5 that all external derivatives $w_{x_1}(x)$, ($i \geq 4$) are (C_θ) with any $\theta < \delta$, because we may take σ arbitrarily close to 3 for the Coulomb potential (6.4).

We must still examine the properties of $w_r = \partial w / \partial r$. For this we may assume $x_2 = x_3 = 0$ and consider w_{x_1} . We have, using the notation of (4.18),

$$w_{x_1} = - \int g_0(x-y) (x_1 - y_1) V(y) u_0(y) dy;$$

in any case this is true if $x_1 > 0$, and represents a function which is smooth for $x_1 > 0$. So we have only to consider small values of $|x_1|$. Now we write again

$$u_0(y) = u_0(x) + [u_0(y) - u_0(x)] .$$

The contribution to Au from the second term in the above expression can be dealt with exactly in the same way as in the proof of Lemma 5 and gives a function (C_θ) with $\theta < \delta$ as above. The remaining part

$$(6.8) \quad - u_0(x) \int g_0(x-y) (x_1 - y_1) V(y) dy$$

can be reduced to a 3-dimensional integral by (4.6), for the only factor involving y_4, \dots, y_m is $g_0(x-y)$. Using (4.18), (6.4) and the fact that $\omega_m = 2\pi^{m/2} / \Gamma(m/2)$, we thus obtain for the integral of (6.8) the following expression:

$$(6.9) \quad \frac{\bar{e}}{4\pi} \int_{s \leq \rho} \frac{x_1 - y_1}{t^3} \frac{dy_1 dy_2 dy_3}{s} + c \int_{s \leq \rho} f(t^2)(x_1 - y_1) \frac{dy_1 dy_2 dy_3}{s}$$

where $s = (y_1^2 + y_2^2 + y_3^2)^{1/2}$ and $t = [(x_1 - y_1)^2 + y_2^2 + y_3^2]^{1/2}$, and $f(t^2)$ is a smooth function of t^2 at least for $t^2 < 1$. The second integral of (6.9) is thus a smooth function of x_1 for small x_1 and need not be considered in detail, whereas the first integral can be explicitly evaluated without difficulty, yielding

the value $2\pi \operatorname{sign} x_1$ (this value is independent of ρ). In this way we arrive at the result

$$w_{x_1}(x_1, 0, 0, x_4, \dots, x_m) = -\frac{\bar{e}}{2} (\operatorname{sign} x_1) u_0(x) + \dots$$

where ... is a function at least (C_θ) for any $\theta < 1$. This completes the proof of Lemma 7.

Theorems II, IIa and IIb now follow easily. Obviously Theorem II is a consequence of Theorem IIa. To prove Theorem IIa we note that, since the generalized Coulomb potential W now satisfies the conditions i), ii) for any $\sigma < 3$, all eigenfunctions ϕ are bounded and (C_θ) for any $\theta < 1$. Then we consider the integral expression (5.2). Since $\tilde{H}\phi$ as well as ϕ is an eigenfunction, the first three terms on the right-hand side of (5.2) are seen to be smooth functions, as before. From Lemma 7 with δ as close to 1 as we like, we see that each $-A_i\phi$ of the remaining sum is the sum of two parts $\Psi_i + \phi_i$, where Ψ_i is (C_θ^i) for any $\theta < 1 - \frac{3}{\sigma}$ and ϕ_i is a function (C_θ^i) for any $\theta < 1$ of $(m-2)$ variables, which are r, x_4, \dots, x_m in the canonical coordinate system for V_i . If we combine all the Ψ_i together with the smooth function given by the first three terms of (5.2) into one function ϕ_0 , the assertion of Theorem IIa follows. Theorem IIb then follows from (6.3) and the discussion given after the statement of Theorem IIa.

References

- [1] T. Kato - Fundamental properties of Hamiltonian operators of Schrödinger type; Transactions of Amer. Math. Soc., 70, 195-211 (1951).
- [2] K. Friedrichs - On differential operators in Hilbert spaces; Amer. J. Math., 61, 523-514 (1939).
- [3] E.C. Kemble - The fundamental principles of quantum mechanics; International series in physics, New York and London, McGraw-Hill, 1937.
- [4] T.H. Gronwall - Helium wave equation; Phys. Rev., 51, 655-660 (1937).
- [5] J.H. Bartlett, Jr. - Helium wave equation; Phys. Rev., 51, 661-669 (1937).
- [6] S. ChandraSekhar and G. Herzberg - Energies of the ground states of He, Li^+ and O^{6+} ; Phys. Rev., 98, 1050-1054 (1955).
- [7] T. Kinoshita - To be published.
- [8] E.A. Hylleraas - Neue Berechnung der Energie des Heliums im Grundzustandes, sowie des tiefsten Terms von Ortho-Helium; Zeitschrift für Physik 54, 347-366 (1929); Ueber den Grundterm der Zweielektronenprobleme von H^- , He, Li^+ , Be^{++} usw., ibid. 65, 209-225 (1930).
- [9] J. von Neumann - Mathematische Grundlagen der Quantenmechanik; Berlin, 1932
- [10] J.W. Calkin - Functions of several variables and absolute continuity, I; Duke Mathematical Journal, 6, 170-186 (1940).
- [11] C.B. Morrey, Jr. - Functions of several variables and absolute continuity, II; Duke Mathematical Journal, 6, 187-215 (1940).

NYU
CX-
25

Kato

On the eigenfunctions of
many-particle systems in
quantum mechanics.

